



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:41 PM GMT

PDB ID : 4V82
Title : Crystal structure of cyanobacterial Photosystem II in complex with terbutryn
Authors : Gabdulkhakov, A.; Broser, M.; Guskov, A.; Kern, J.; Glockner, C.; Muh, F.;
Saenger, W.; Zouni, A.
Deposited on : 2010-11-30
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

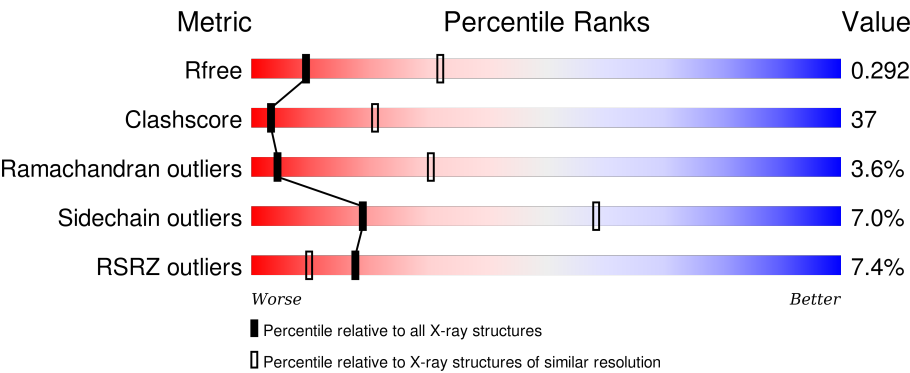
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	344	
1	BA	344	
2	AB	510	
2	BB	510	
3	AC	461	

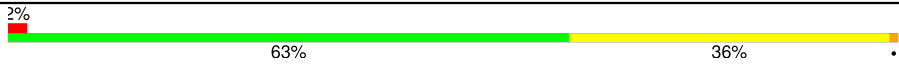
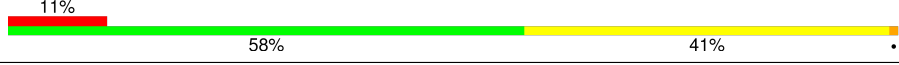
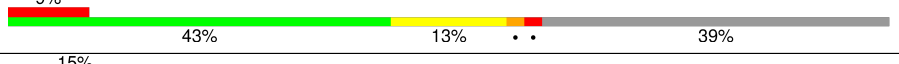
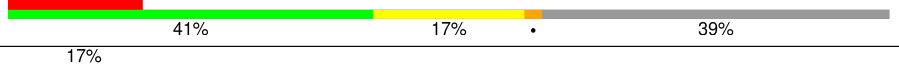
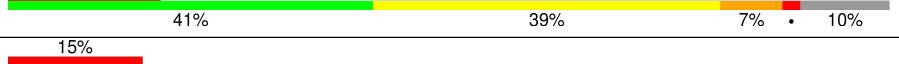

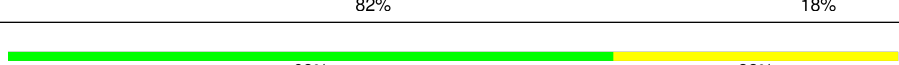
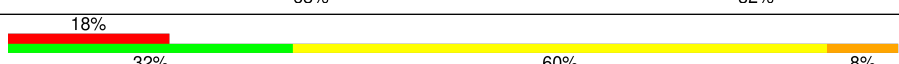
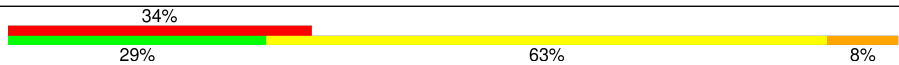

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	BC	461	
4	AD	352	
4	BD	352	
5	AE	84	
5	BE	84	
6	AF	45	
6	BF	45	
7	AH	66	
7	BH	66	
8	AI	38	
8	BI	38	
9	AJ	40	
9	BJ	40	
10	AK	37	
10	BK	37	
11	AL	37	
11	BL	37	
12	AM	36	
12	BM	36	
13	AO	247	
13	BO	247	
14	AT	32	
14	BT	32	
15	AU	104	
15	BU	104	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	AV	137	
16	BV	137	
17	Ay	46	
17	By	46	
18	AX	41	
18	BX	41	
19	AY	28	
19	BY	28	
20	AZ	62	
20	BZ	62	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CL	BA	5404[A]	-	-	-	X
24	CLA	AA	404	X	-	-	-
24	CLA	AA	405	X	-	-	-
24	CLA	AA	406	X	-	-	X
24	CLA	AA	407	X	-	-	X
24	CLA	AB	601	X	-	-	X
24	CLA	AB	602	X	-	-	-
24	CLA	AB	603	X	-	-	-
24	CLA	AB	604	X	-	-	-
24	CLA	AB	605	X	-	-	X
24	CLA	AB	606	X	-	-	-
24	CLA	AB	607	X	-	-	-
24	CLA	AB	608	X	-	-	X
24	CLA	AB	609	X	-	-	X
24	CLA	AB	610	X	-	-	-
24	CLA	AB	611	X	-	-	-
24	CLA	AB	612	X	-	-	-
24	CLA	AB	613	X	-	-	-
24	CLA	AB	614	X	-	-	-
24	CLA	AB	615	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	AB	616	X	-	-	X
24	CLA	AC	501	X	-	-	-
24	CLA	AC	502	X	-	-	X
24	CLA	AC	503	X	-	-	X
24	CLA	AC	504	X	-	-	X
24	CLA	AC	505	X	-	-	X
24	CLA	AC	506	X	-	-	-
24	CLA	AC	507	X	-	-	-
24	CLA	AC	508	X	-	-	X
24	CLA	AC	509	X	-	-	-
24	CLA	AC	510	X	-	-	-
24	CLA	AC	511	X	-	X	-
24	CLA	AC	512	X	-	-	X
24	CLA	AC	513	X	-	-	X
24	CLA	AD	401	X	-	-	-
24	CLA	AD	404	X	-	-	X
24	CLA	BA	5405	X	-	-	-
24	CLA	BA	5406	X	-	X	-
24	CLA	BA	5407	X	-	-	-
24	CLA	BA	5408	X	-	-	-
24	CLA	BB	5605	X	-	-	X
24	CLA	BB	5606	X	-	-	-
24	CLA	BB	5607	X	-	-	-
24	CLA	BB	5608	X	-	-	-
24	CLA	BB	5609	X	-	-	X
24	CLA	BB	5610	X	-	-	-
24	CLA	BB	5611	X	-	-	-
24	CLA	BB	5612	X	-	-	X
24	CLA	BB	5613	X	-	-	-
24	CLA	BB	5614	X	-	-	-
24	CLA	BB	5615	X	-	-	-
24	CLA	BB	5616	X	-	-	-
24	CLA	BB	5617	X	-	-	X
24	CLA	BB	5618	X	-	-	-
24	CLA	BB	5619	X	-	-	-
24	CLA	BB	5620	X	-	-	-
24	CLA	BC	5501	X	-	-	-
24	CLA	BC	5502	X	-	-	-
24	CLA	BC	5503	X	-	-	-
24	CLA	BC	5504	X	-	-	X
24	CLA	BC	5505	X	-	-	-
24	CLA	BC	5506	X	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	BC	5507	X	-	-	-
24	CLA	BC	5508	X	-	-	-
24	CLA	BC	5509	X	-	-	-
24	CLA	BC	5510	X	-	-	-
24	CLA	BC	5511	X	-	X	X
24	CLA	BC	5512	X	-	-	-
24	CLA	BC	5513	X	-	-	X
24	CLA	BD	5402	X	-	-	-
24	CLA	BD	5405	X	-	-	-
25	MST	AA	408	-	-	X	-
25	MST	BA	5409	-	-	X	-
27	BCR	AB	617	-	-	-	X
27	BCR	AC	515	-	-	-	X
27	BCR	AC	516	-	-	-	X
27	BCR	AJ	101	-	-	-	X
27	BCR	AK	102	-	-	-	X
27	BCR	AT	101	-	-	-	X
27	BCR	AX	101	-	-	-	X
27	BCR	BB	5621	-	-	-	X
27	BCR	BB	5622	-	-	-	X
27	BCR	BC	5514	-	-	-	X
27	BCR	BC	5515	-	-	-	X
27	BCR	BC	5516	-	-	-	X
27	BCR	BD	5407	-	-	-	X
27	BCR	BJ	5101	-	-	-	X
27	BCR	BT	5101	-	-	-	X
27	BCR	BX	5101	-	-	-	X
28	DGD	AA	411	-	-	-	X
28	DGD	AB	628	-	-	-	X
28	DGD	AC	517	-	-	-	X
28	DGD	AC	518	X	-	-	X
28	DGD	AC	519	X	-	X	X
28	DGD	AE	101	-	-	-	X
28	DGD	BA	5412	-	-	-	X
28	DGD	BB	5602	-	-	-	X
28	DGD	BC	5518	X	-	-	X
28	DGD	BC	5519	X	-	X	X
28	DGD	BE	5102	-	-	-	X
28	DGD	BH	5101	-	-	-	X
29	LHG	BA	5415	-	-	-	X
30	SQD	AB	622	-	-	-	X
30	SQD	AF	102	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	SQD	BA	5401	-	-	-	X
30	SQD	BB	5625	-	-	-	X
30	SQD	BF	5102	-	-	-	X
31	LMG	AA	414	-	-	-	X
31	LMG	AA	417	-	-	-	X
31	LMG	AB	620	-	-	-	X
31	LMG	AB	621	-	-	-	X
31	LMG	AC	520	-	-	-	X
31	LMG	AC	521	-	-	-	X
31	LMG	AD	407	-	-	-	X
31	LMG	AD	408	-	-	-	X
31	LMG	AJ	102	-	-	-	X
31	LMG	AM	101	-	-	-	X
31	LMG	BA	5402	-	-	-	X
31	LMG	BB	5624	-	-	-	X
31	LMG	BC	5520	-	-	-	X
31	LMG	BC	5521	-	-	-	X
31	LMG	BD	5408	-	-	-	X
31	LMG	BD	5409	-	-	-	X
31	LMG	BD	5410	-	-	-	X
31	LMG	BE	5101	-	-	-	X
31	LMG	BL	5101	-	-	-	X
31	LMG	BM	5102	-	-	-	X
32	LMT	AB	624	-	-	-	X
32	LMT	AB	629	-	-	-	X
32	LMT	AB	630	-	-	-	X
32	LMT	AD	409	-	-	-	X
32	LMT	AI	102	-	-	-	X
32	LMT	AI	103	-	-	-	X
32	LMT	AM	102	-	-	-	X
32	LMT	BB	5603	-	-	-	X
32	LMT	BB	5604	-	-	-	X
32	LMT	BB	5627	-	-	-	X
32	LMT	BC	5522	-	-	-	X
32	LMT	BD	5411	-	-	-	X
32	LMT	BI	5102	-	-	-	X
32	LMT	BM	5101	-	-	-	X
33	DMS	AB	625	-	-	-	X
33	DMS	AU	201	-	-	-	X
33	DMS	AV	202	-	-	-	X
33	DMS	BB	5628	-	-	-	X
33	DMS	BB	5629	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	DMS	BV	5203	-	-	-	X
34	PHO	AD	402	X	-	-	-
34	PHO	AD	403	X	-	-	-
34	PHO	BD	5403	X	-	-	-
34	PHO	BD	5404	X	-	-	-
35	PL9	AD	405	-	-	-	X
36	HEM	BF	5101	-	-	-	X

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 50266 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem Q(B) protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			
1	BA	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			
2	BB	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			

- Molecule 3 is a protein called Photosystem II CP43 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			
3	BC	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	341	Total	C	N	O	S	0	0	0
			2711	1797	441	461	12			
4	BD	341	Total	C	N	O	S	0	0	0
			2711	1797	441	461	12			

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	AE	82	Total	C	N	O	0	0	0
			666	434	108	124			
5	BE	82	Total	C	N	O	0	0	0
			666	434	108	124			

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			
6	BF	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			
7	BH	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AI	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			
8	BI	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AJ	38	Total	C	N	O	S	0	0	0
			271	182	42	46	1			
9	BJ	38	Total	C	N	O	S	0	0	0
			271	182	42	46	1			

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	AK	37	Total	C	N	O	0	0	0
			293	204	43	46			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	BK	37	Total	C	N	O	0	0	0
			293	204	43	46			

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AL	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	BL	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AM	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			
12	BM	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AO	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			
13	BO	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AT	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			
14	BT	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	AU	97	Total	C	N	O	0	0	0
			774	491	129	154			
15	BU	97	Total	C	N	O	0	0	0
			774	491	129	154			

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AV	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			
16	BV	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			

- Molecule 17 is a protein called Photosystem II reaction center protein ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Ay	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			
17	By	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			

- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AX	37	Total	C	N	O		0	0	0
			270	182	41	47				
18	BX	37	Total	C	N	O		0	0	0
			270	182	41	47				

- Molecule 19 is a protein called PHOTOSYSTEM II PSBX PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AY	28	Total	C	N	O		0	0	0
			140	84	28	28				
19	BY	28	Total	C	N	O		0	0	0
			140	84	28	28				

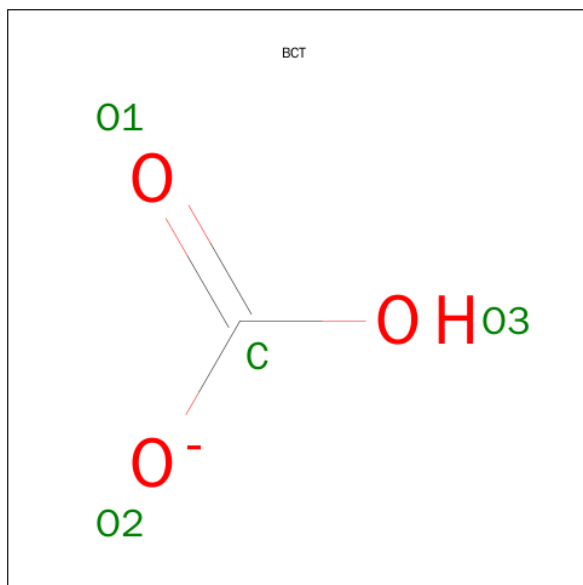
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AZ	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
20	BZ	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	AA	1	Total	Fe	0	0
			1	1		
21	BD	1	Total	Fe	0	0
			1	1		

- Molecule 22 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).

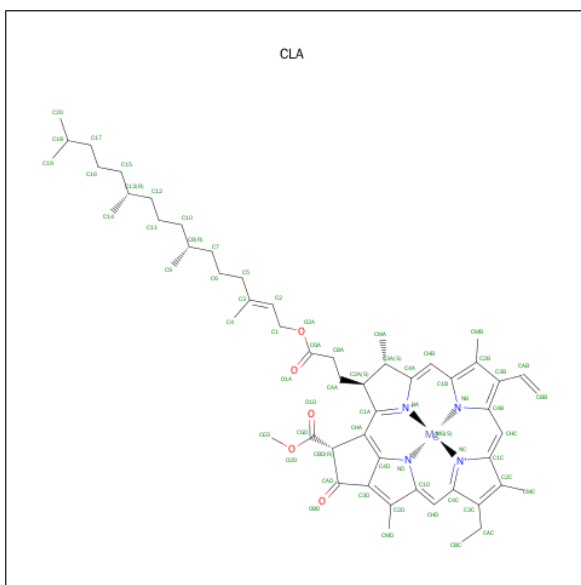


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	AA	1	Total	C	O	0	0
			4	1	3		
22	BA	1	Total	C	O	0	0
			4	1	3		

- Molecule 23 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	AA	1	Total	Cl	0	1
			2	2		
23	BA	1	Total	Cl	0	1
			2	2		

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).

[illegible]

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AD	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	AD	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

Continued on next page...

Continued from previous page...

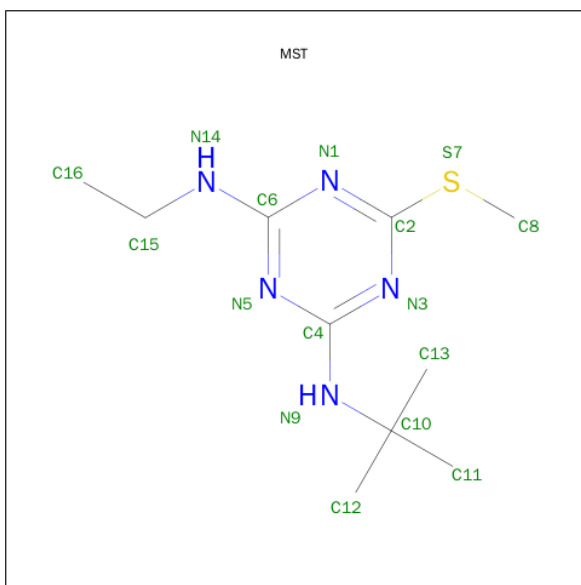
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

Continued on next page...

Continued from previous page...

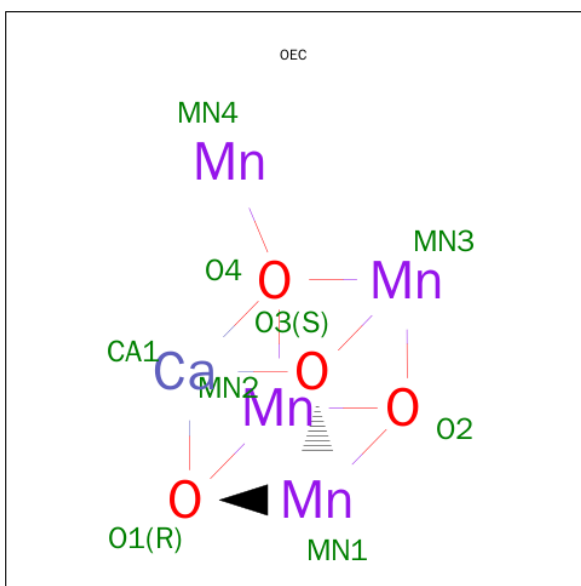
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BD	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BD	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 25 is 2-T-BUTYLAMINO-4-ETHYLAMINO-6-METHYLTHIO-S-TRIAZINE (three-letter code: MST) (formula: C₁₀H₁₉N₅S).



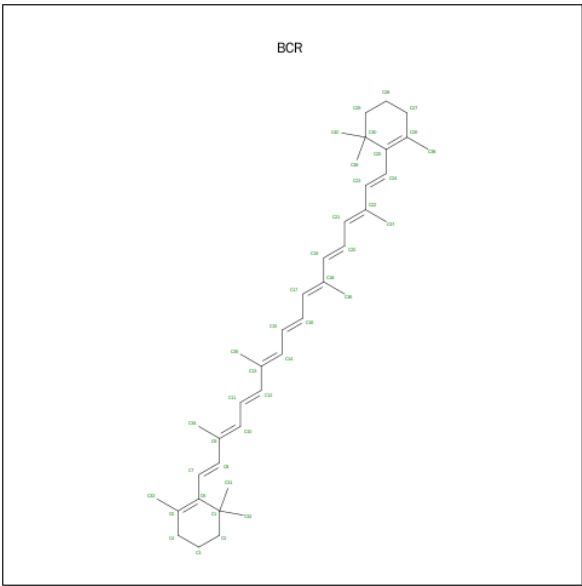
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	AA	1	Total	C	N	S	0	0
			16	10	5	1		
25	BA	1	Total	C	N	S	0	0
			16	10	5	1		

- Molecule 26 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn_4O_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	AA	1	Total	Ca	Mn	0	0
			5	1	4		
26	BA	1	Total	Ca	Mn	0	0
			5	1	4		

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



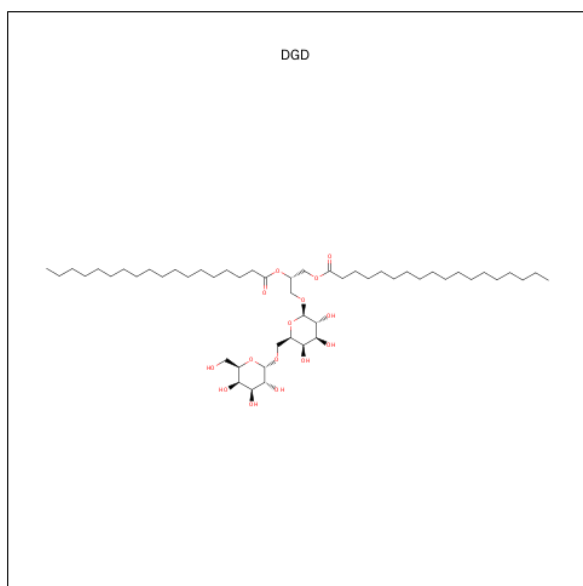
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	AA	1	Total C 40 40	0	0
27	AB	1	Total C 40 40	0	0
27	AB	1	Total C 40 40	0	0
27	AB	1	Total C 40 40	0	0
27	AC	1	Total C 40 40	0	0
27	AC	1	Total C 40 40	0	0
27	AC	1	Total C 40 40	0	0
27	AD	1	Total C 40 40	0	0
27	AJ	1	Total C 40 40	0	0
27	AK	1	Total C 40 40	0	0
27	AT	1	Total C 40 40	0	0
27	AX	1	Total C 40 40	0	0
27	BA	1	Total C 40 40	0	0

Continued on next page...

Continued from previous page...

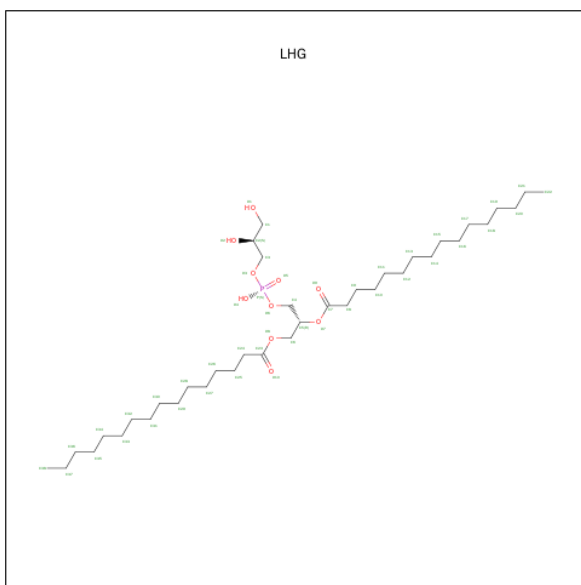
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	BB	1	Total C 40 40	0	0
27	BB	1	Total C 40 40	0	0
27	BB	1	Total C 40 40	0	0
27	BC	1	Total C 40 40	0	0
27	BC	1	Total C 40 40	0	0
27	BC	1	Total C 40 40	0	0
27	BD	1	Total C 40 40	0	0
27	BJ	1	Total C 40 40	0	0
27	BK	1	Total C 40 40	0	0
27	BT	1	Total C 40 40	0	0
27	BX	1	Total C 40 40	0	0

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



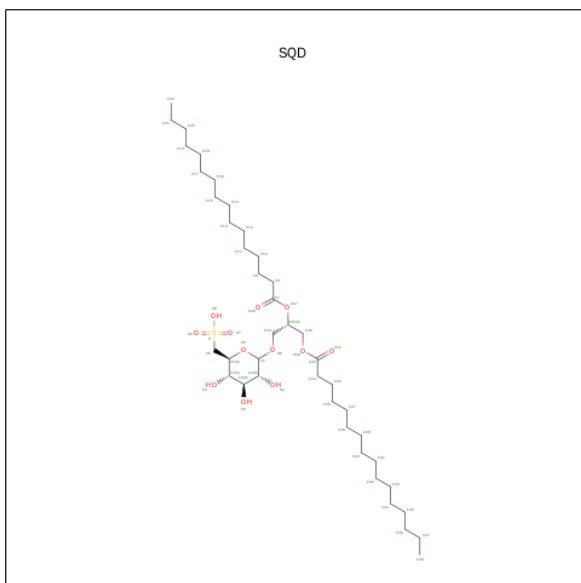
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	AA	1	Total	C	O	0	0
			56	41	15		
28	AB	1	Total	C	O	0	0
			52	37	15		
28	AC	1	Total	C	O	0	0
			53	38	15		
28	AC	1	Total	C	O	0	0
			62	47	15		
28	AC	1	Total	C	O	0	0
			66	51	15		
28	AE	1	Total	C	O	0	0
			63	48	15		
28	AH	1	Total	C	O	0	0
			58	43	15		
28	BA	1	Total	C	O	0	0
			56	41	15		
28	BB	1	Total	C	O	0	0
			52	37	15		
28	BC	1	Total	C	O	0	0
			53	38	15		
28	BC	1	Total	C	O	0	0
			62	47	15		
28	BC	1	Total	C	O	0	0
			66	51	15		
28	BE	1	Total	C	O	0	0
			63	48	15		
28	BH	1	Total	C	O	0	0
			58	43	15		

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



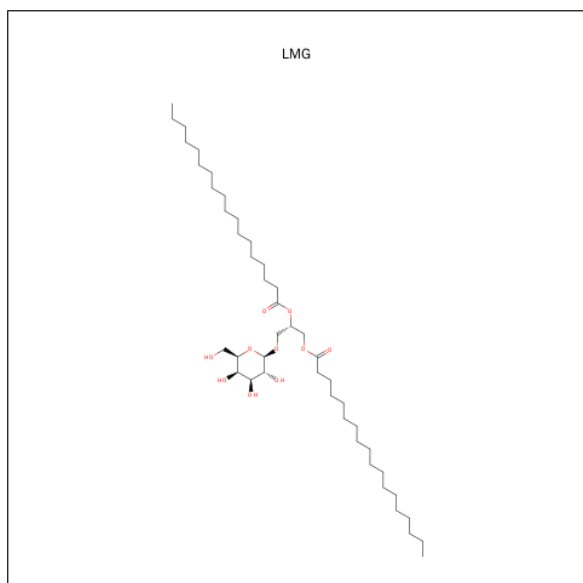
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	AA	1	Total	C	O	P	0	0
			39	28	10	1		
29	AA	1	Total	C	O	P	0	0
			37	26	10	1		
29	BA	1	Total	C	O	P	0	0
			39	28	10	1		
29	BA	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	AA	1	Total	C	O	S	0	0
			51	38	12	1		
30	AA	1	Total	C	O	S	0	0
			54	41	12	1		
30	AB	1	Total	C	O	S	0	0
			43	30	12	1		
30	AB	1	Total	C	O	S	0	0
			47	34	12	1		
30	AF	1	Total	C	O	S	0	0
			45	32	12	1		
30	BA	1	Total	C	O	S	0	0
			54	41	12	1		
30	BA	1	Total	C	O	S	0	0
			51	38	12	1		
30	BB	1	Total	C	O	S	0	0
			47	34	12	1		
30	BB	1	Total	C	O	S	0	0
			43	30	12	1		
30	BF	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



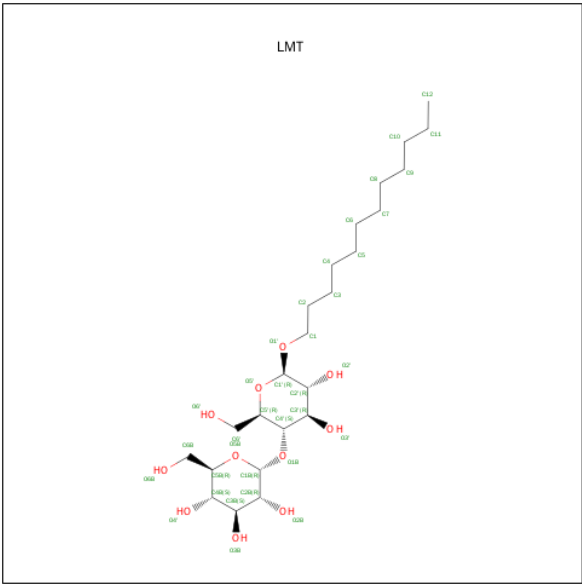
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	AA	1	Total	C	O	0	0
			44	34	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	AA	1	Total	C	O	0	0
			42	32	10		
31	AB	1	Total	C	O	0	0
			51	41	10		
31	AB	1	Total	C	O	0	0
			49	39	10		
31	AC	1	Total	C	O	0	0
			48	38	10		
31	AC	1	Total	C	O	0	0
			45	35	10		
31	AD	1	Total	C	O	0	0
			49	39	10		
31	AD	1	Total	C	O	0	0
			48	38	10		
31	AI	1	Total	C	O	0	0
			43	33	10		
31	AJ	1	Total	C	O	0	0
			46	36	10		
31	AM	1	Total	C	O	0	0
			42	32	10		
31	BA	1	Total	C	O	0	0
			42	32	10		
31	BB	1	Total	C	O	0	0
			49	39	10		
31	BC	1	Total	C	O	0	0
			48	38	10		
31	BC	1	Total	C	O	0	0
			45	35	10		
31	BD	1	Total	C	O	0	0
			46	36	10		
31	BD	1	Total	C	O	0	0
			49	39	10		
31	BD	1	Total	C	O	0	0
			48	38	10		
31	BE	1	Total	C	O	0	0
			44	34	10		
31	BI	1	Total	C	O	0	0
			43	33	10		
31	BL	1	Total	C	O	0	0
			51	41	10		
31	BM	1	Total	C	O	0	0
			42	32	10		

- Molecule 32 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



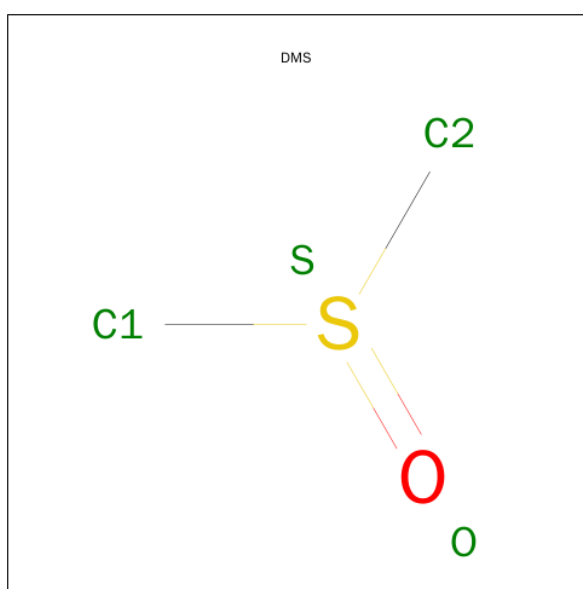
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AD	1	Total	C	O	0	0
			31	20	11		
32	AI	1	Total	C	O	0	0
			35	24	11		
32	AI	1	Total	C	O	0	0
			35	24	11		
32	AM	1	Total	C	O	0	0
			35	24	11		
32	BB	1	Total	C	O	0	0
			35	24	11		
32	BB	1	Total	C	O	0	0
			35	24	11		
32	BB	1	Total	C	O	0	0
			35	24	11		
32	BB	1	Total	C	O	0	0
			35	24	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	BC	1	Total	C	O	0	0
			35	24	11		
32	BD	1	Total	C	O	0	0
			31	20	11		
32	BI	1	Total	C	O	0	0
			35	24	11		
32	BM	1	Total	C	O	0	0
			35	24	11		

- Molecule 33 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



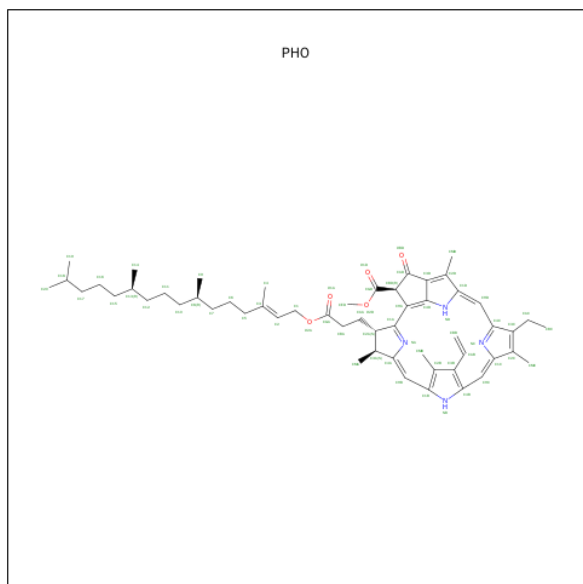
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	AB	1	Total	C	O	S	0	0
			4	2	1	1		
33	AB	1	Total	C	O	S	0	0
			4	2	1	1		
33	AU	1	Total	C	O	S	0	0
			4	2	1	1		
33	AV	1	Total	C	O	S	0	0
			4	2	1	1		
33	BB	1	Total	C	O	S	0	0
			4	2	1	1		
33	BB	1	Total	C	O	S	0	0
			4	2	1	1		
33	BV	1	Total	C	O	S	0	0
			4	2	1	1		

Continued on next page...

Continued from previous page...

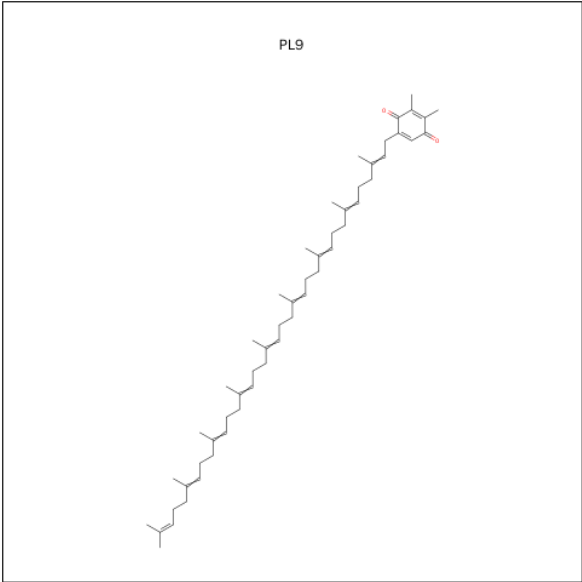
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	BV	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 34 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



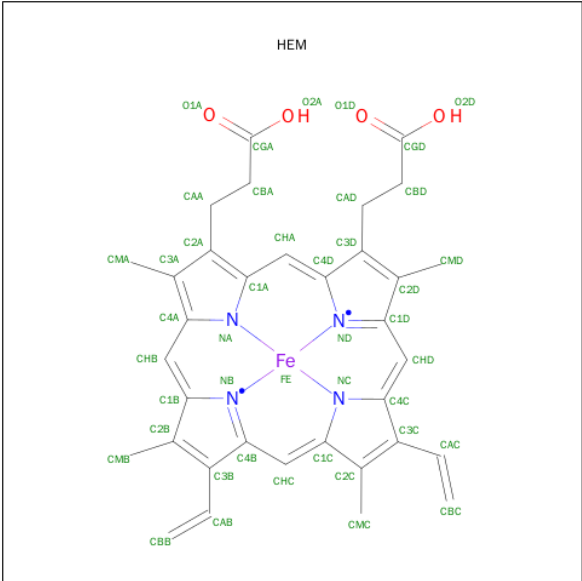
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	AD	1	Total	C	N	O	0	0
			64	55	4	5		
34	AD	1	Total	C	N	O	0	0
			64	55	4	5		
34	BD	1	Total	C	N	O	0	0
			64	55	4	5		
34	BD	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 35 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	AD	1	Total	C	O	0	0
			55	53	2		
35	BD	1	Total	C	O	0	0
			55	53	2		

- Molecule 36 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
36	AF	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
36	AV	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
36	BF	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
36	BV	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

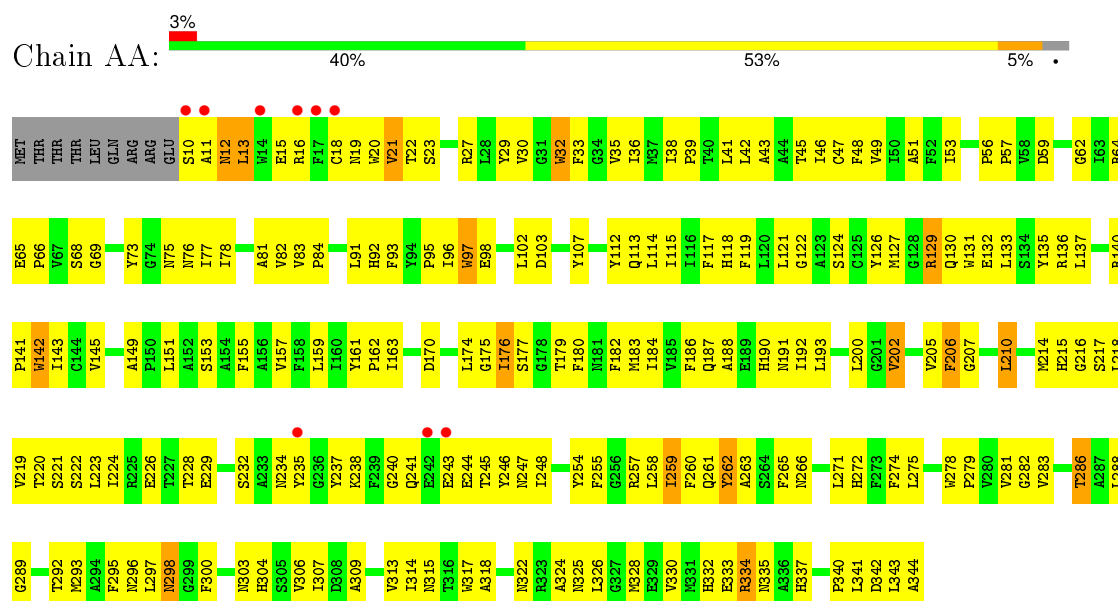
- Molecule 37 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	BO	1	Total 1	Ca 1	0	0
37	AK	1	Total 1	Ca 1	0	0
37	BF	1	Total 1	Ca 1	0	0
37	BK	1	Total 1	Ca 1	0	0
37	AO	1	Total 1	Ca 1	0	0
37	AF	1	Total 1	Ca 1	0	0

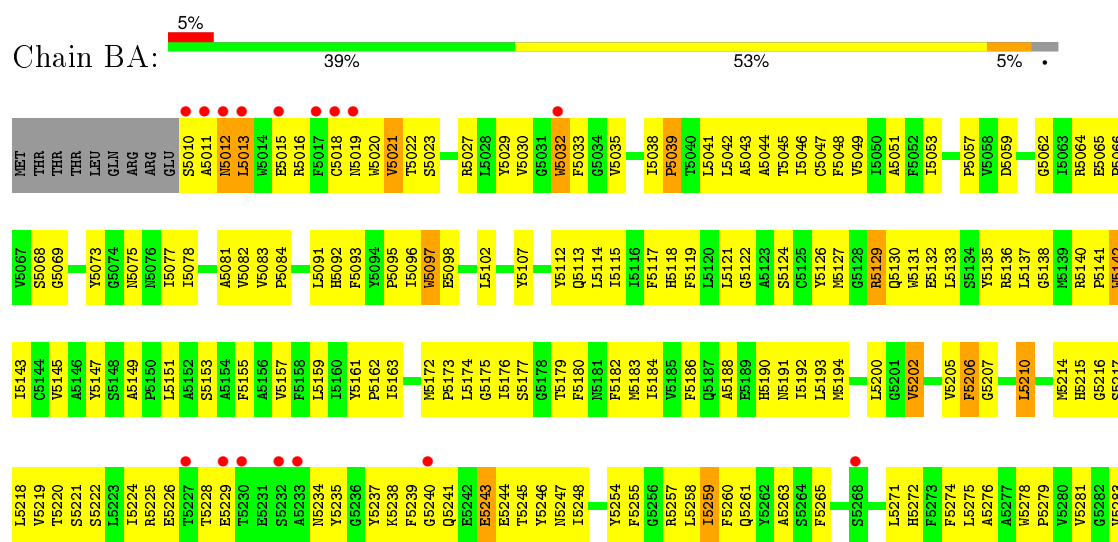
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Photosystem Q(B) protein 1

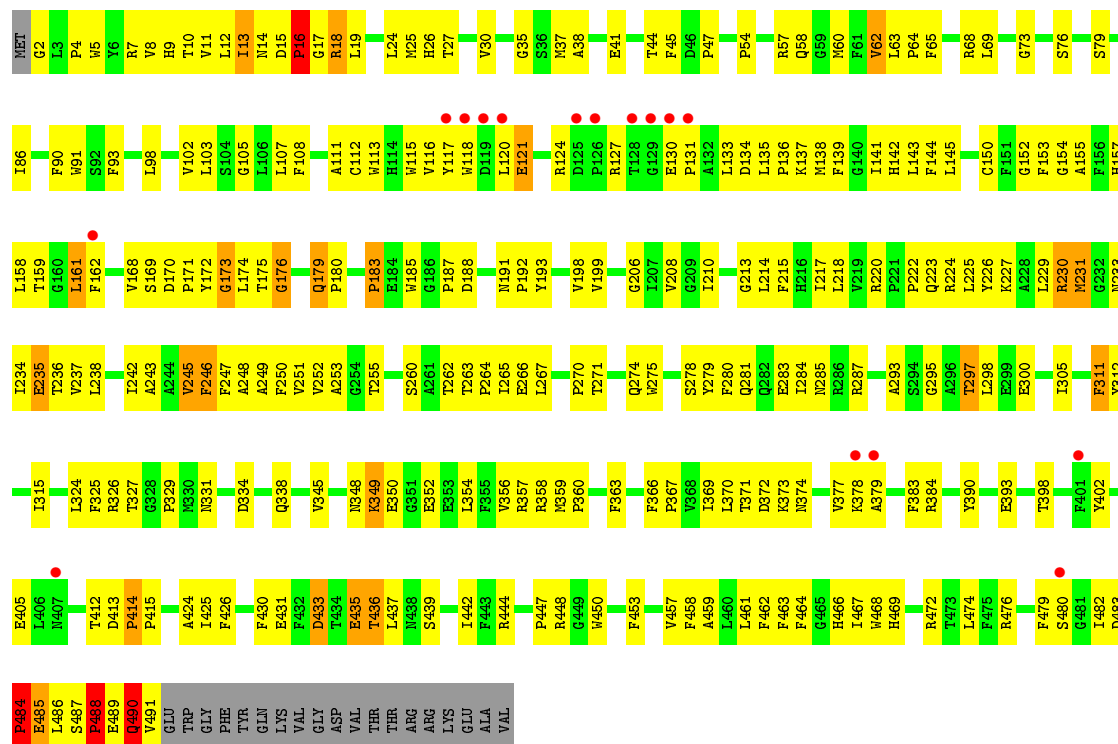


• Molecule 1: Photosystem Q(B) protein 1

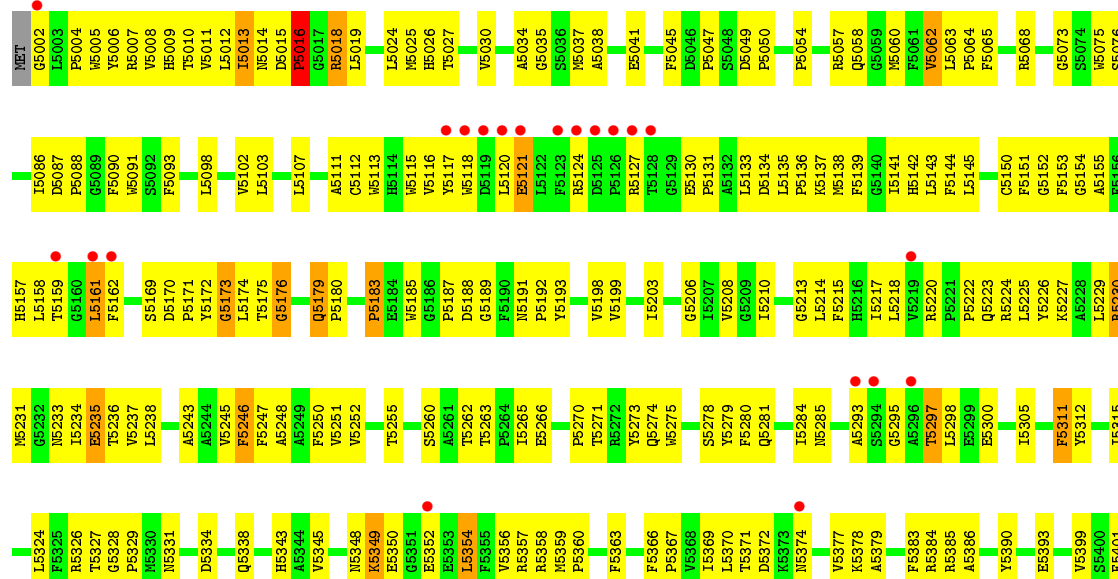


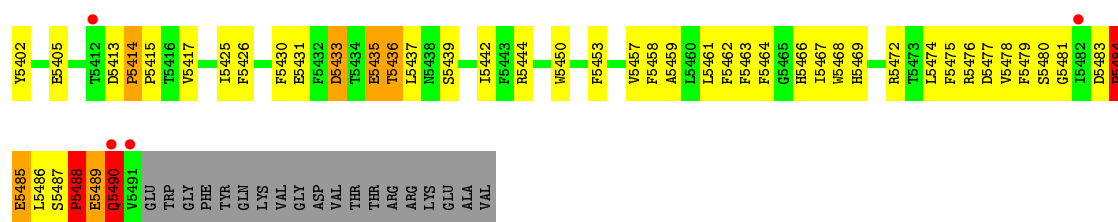


• Molecule 2: Photosystem II core light harvesting protein

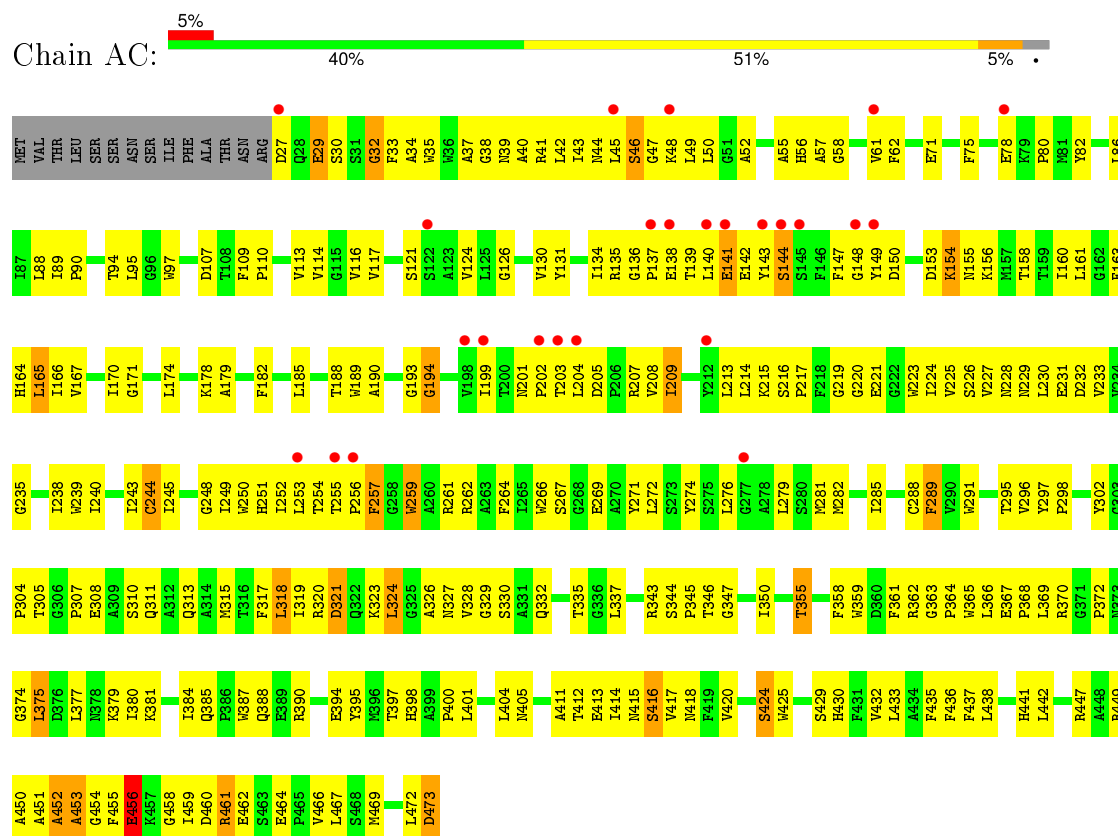


• Molecule 2: Photosystem II core light harvesting protein

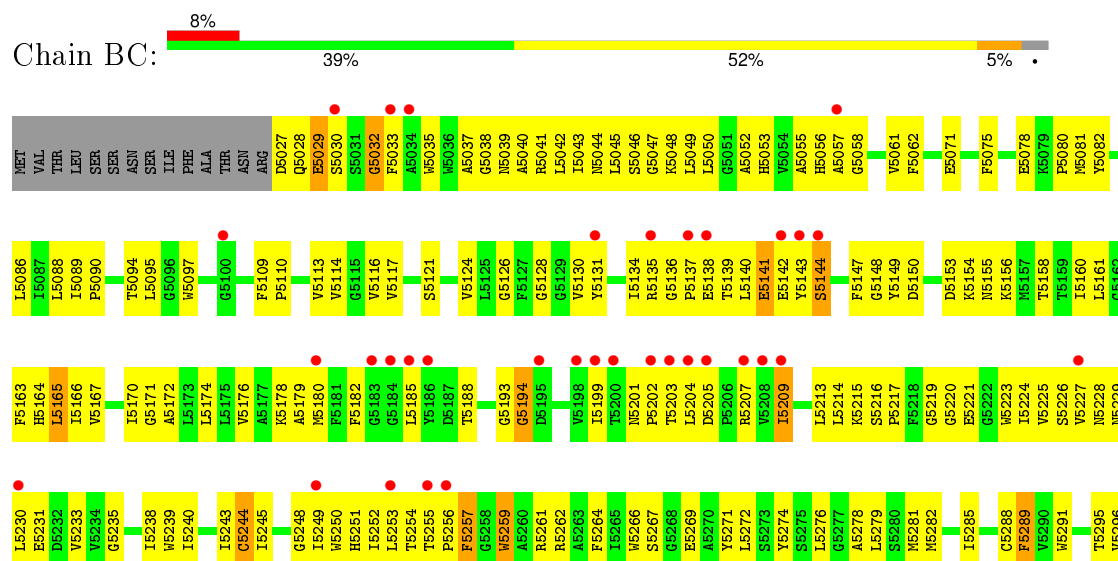


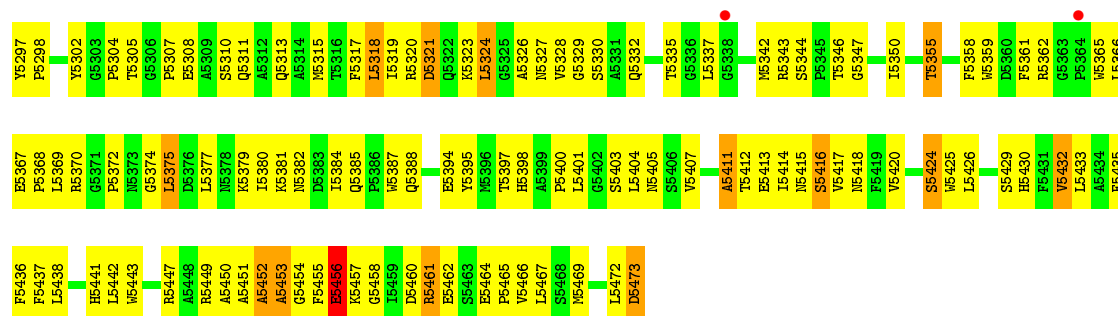


• Molecule 3: Photosystem II CP43 protein

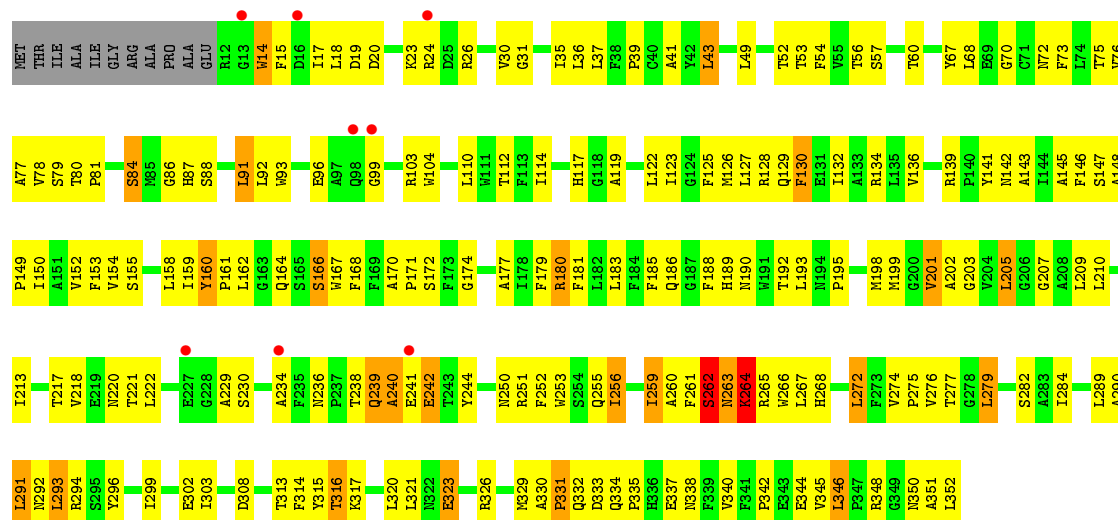
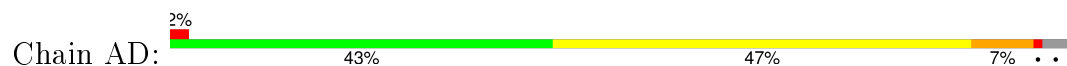


• Molecule 3: Photosystem II CP43 protein

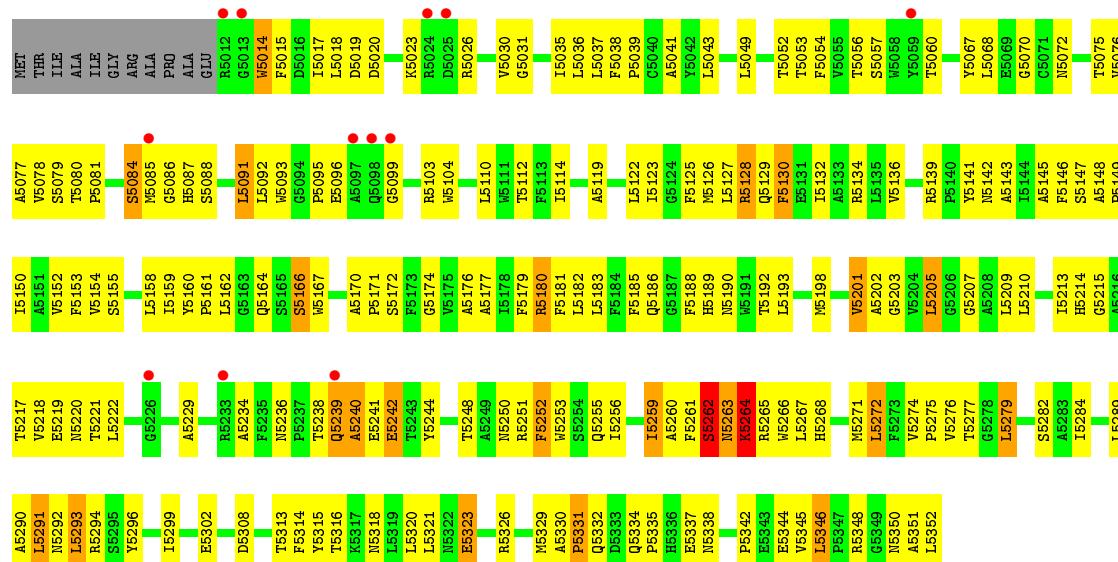
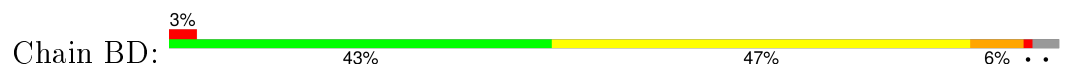




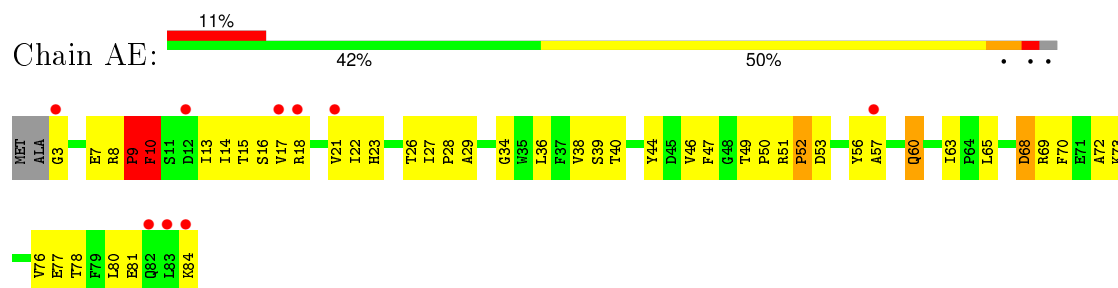
• Molecule 4: Photosystem II D2 protein



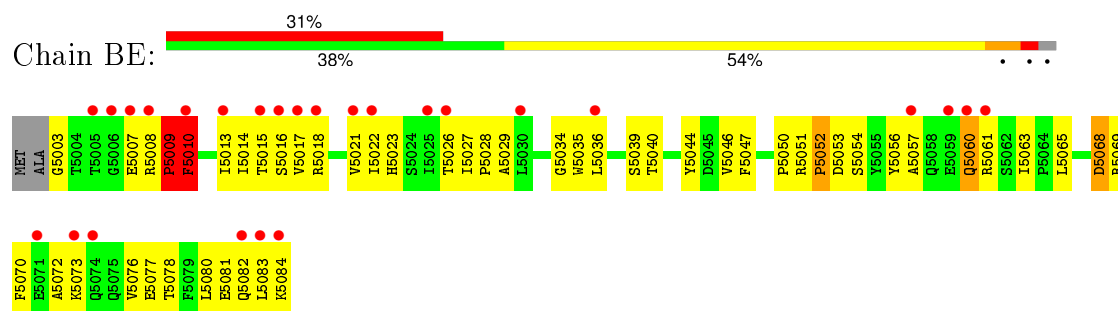
• Molecule 4: Photosystem II D2 protein



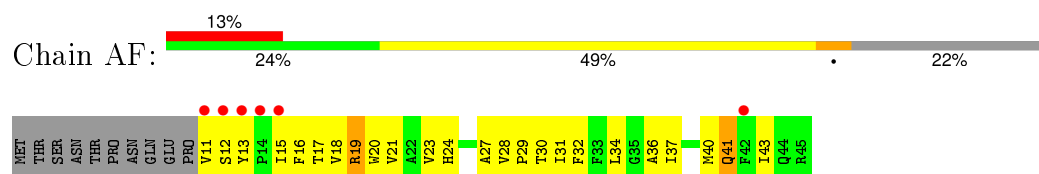
- Molecule 5: Cytochrome b559 subunit alpha



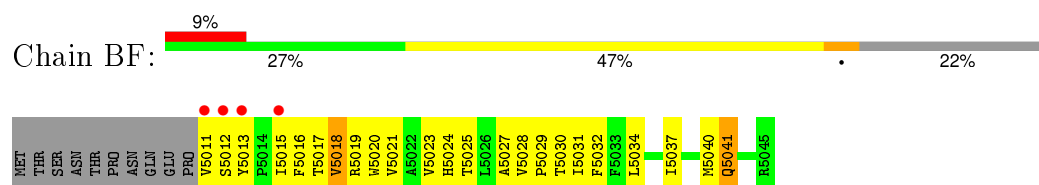
- Molecule 5: Cytochrome b559 subunit alpha



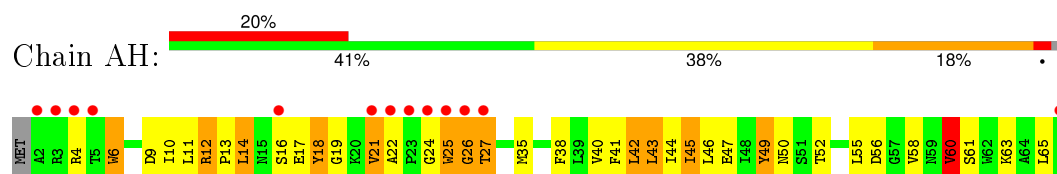
- Molecule 6: Cytochrome b559 subunit beta



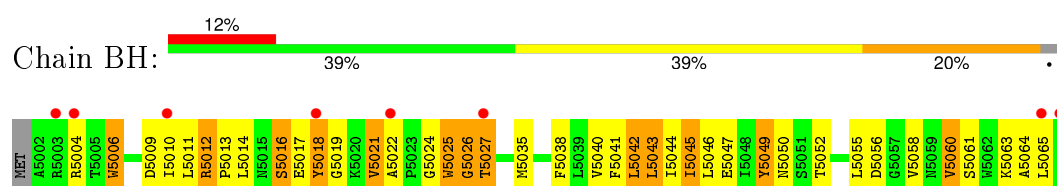
- Molecule 6: Cytochrome b559 subunit beta



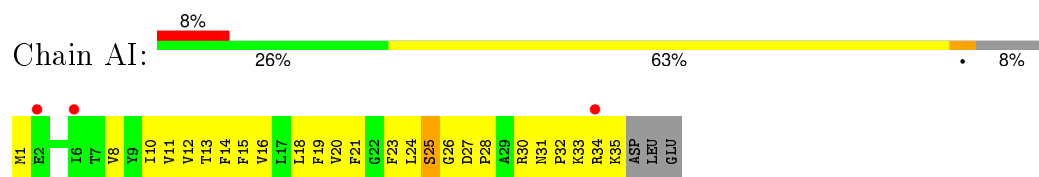
- Molecule 7: Photosystem II reaction center protein H



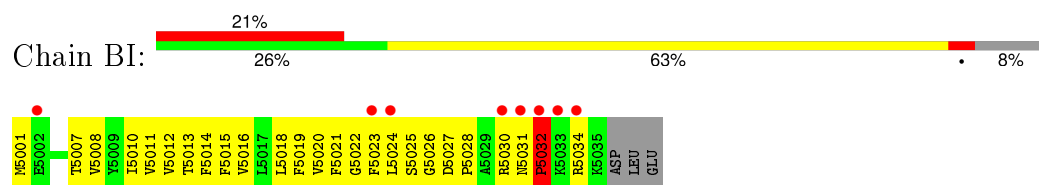
- Molecule 7: Photosystem II reaction center protein H



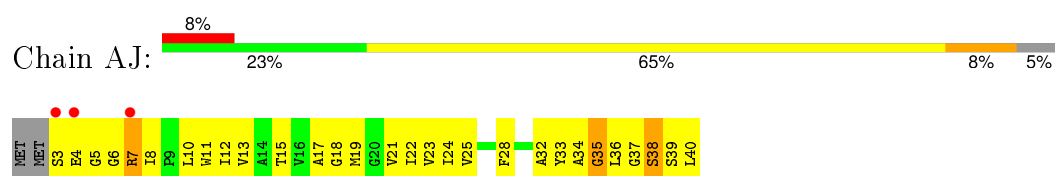
- Molecule 8: Photosystem II reaction center protein I



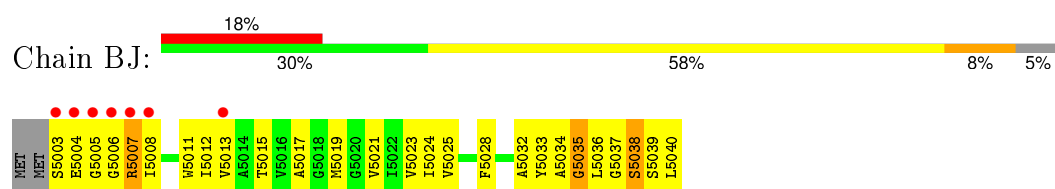
- Molecule 8: Photosystem II reaction center protein I



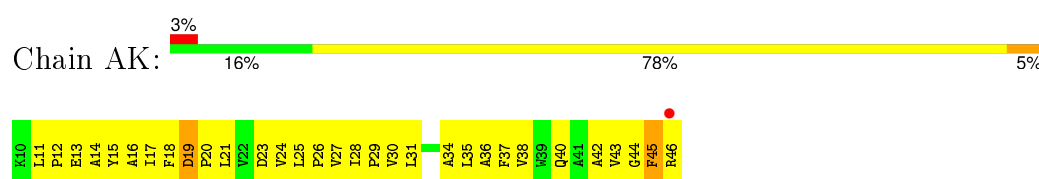
- Molecule 9: Photosystem II reaction center protein J



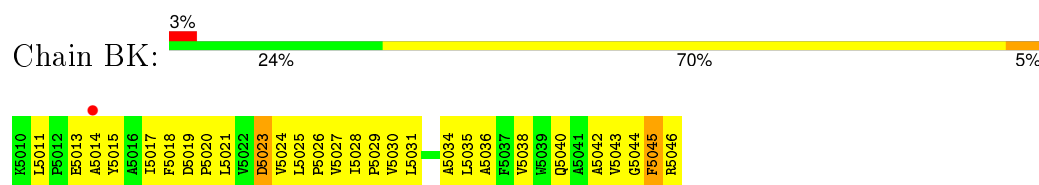
- Molecule 9: Photosystem II reaction center protein J



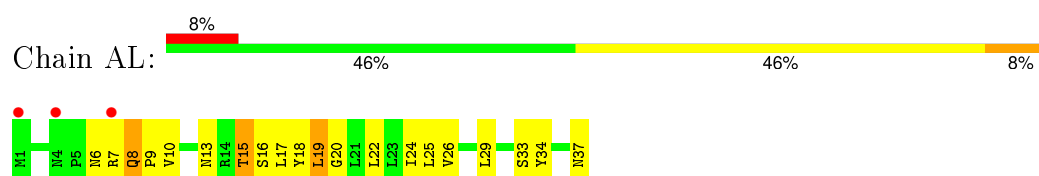
- Molecule 10: Photosystem II reaction center protein K



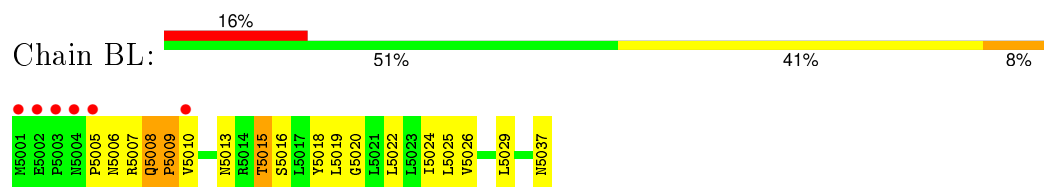
- Molecule 10: Photosystem II reaction center protein K



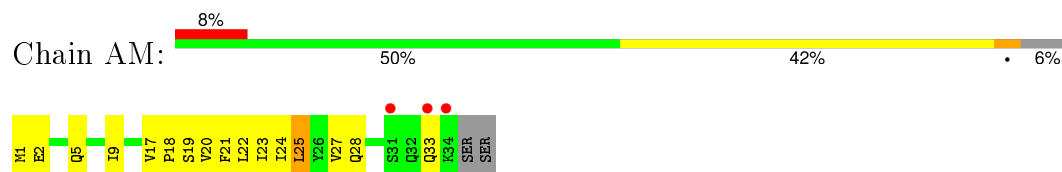
- Molecule 11: Photosystem II reaction center protein L



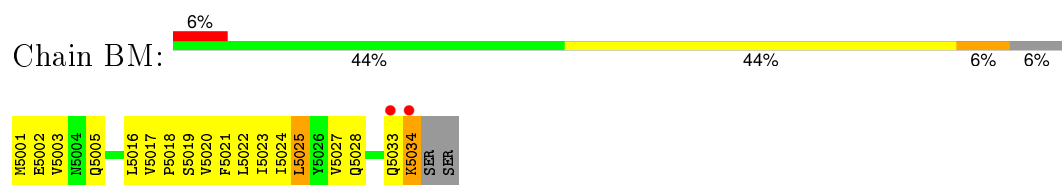
- Molecule 11: Photosystem II reaction center protein L



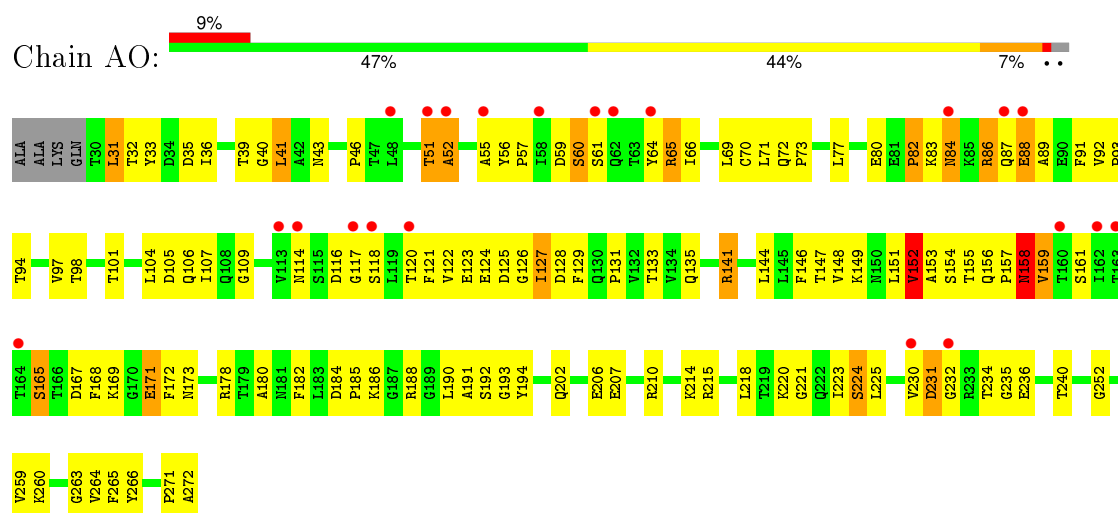
- Molecule 12: Photosystem II reaction center protein M



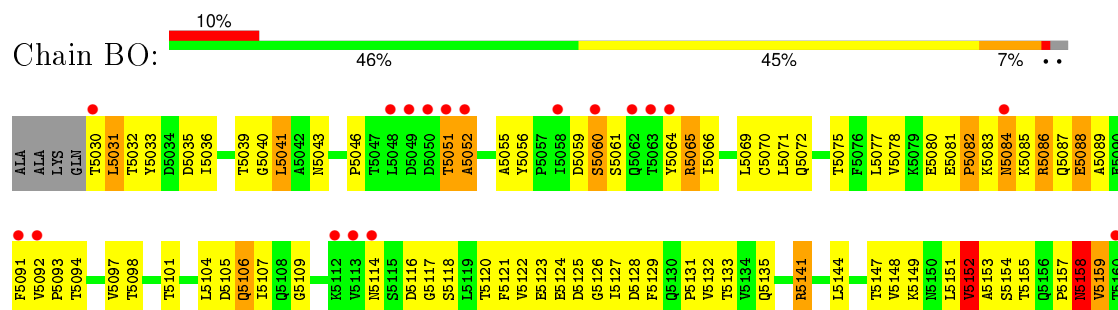
- Molecule 12: Photosystem II reaction center protein M

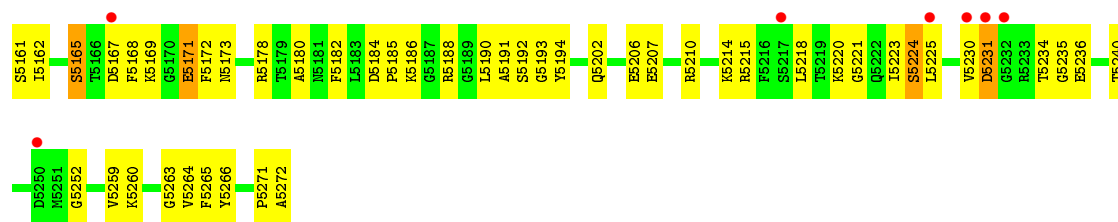


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

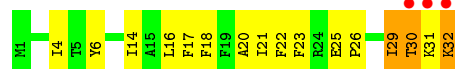


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

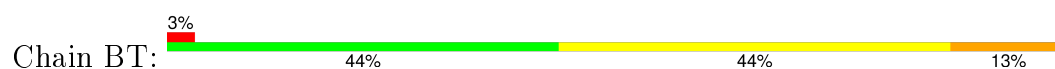




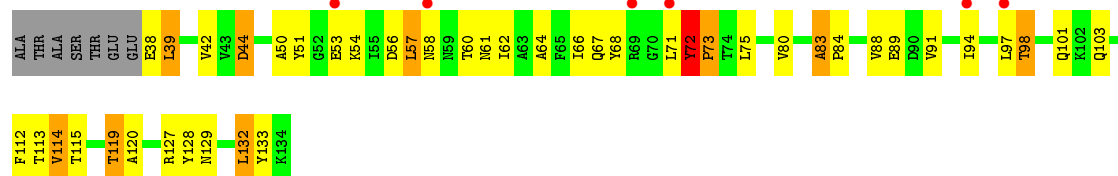
• Molecule 14: Photosystem II reaction center protein T



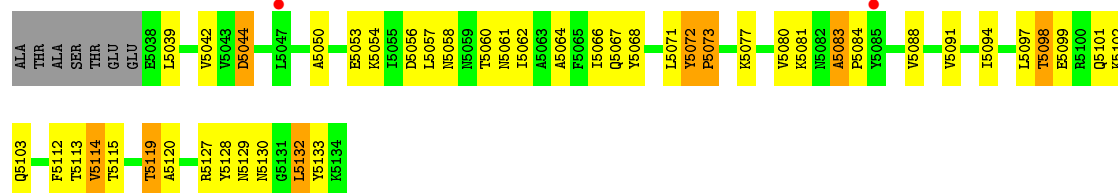
• Molecule 14: Photosystem II reaction center protein T



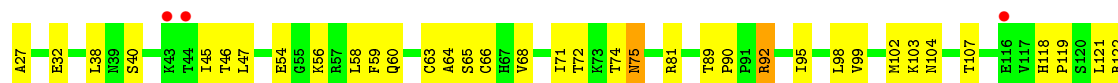
• Molecule 15: Photosystem II 12 kDa extrinsic protein



• Molecule 15: Photosystem II 12 kDa extrinsic protein

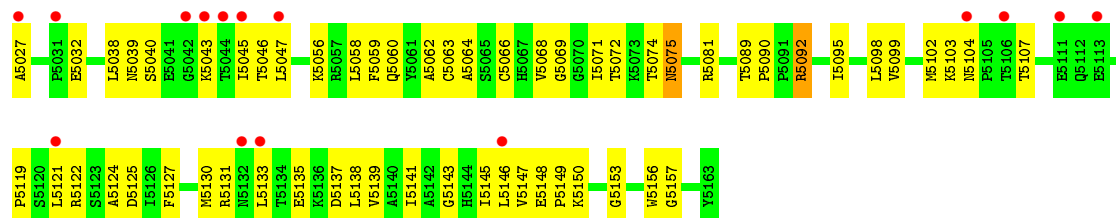


• Molecule 16: Cytochrome c-550

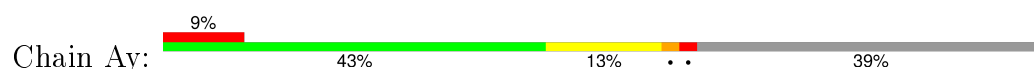




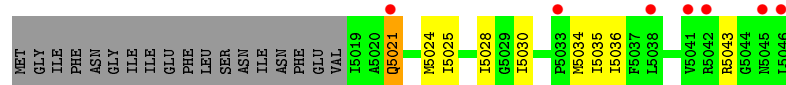
• Molecule 16: Cytochrome c-550



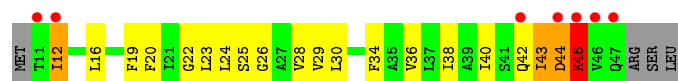
• Molecule 17: Photosystem II reaction center protein ycf12



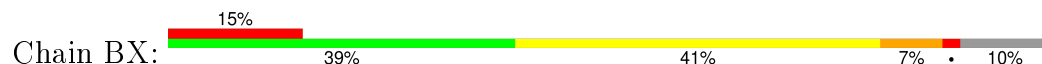
• Molecule 17: Photosystem II reaction center protein ycf12



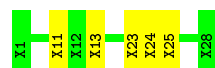
• Molecule 18: Photosystem II reaction center X protein



• Molecule 18: Photosystem II reaction center X protein

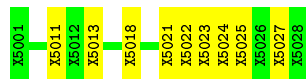


• Molecule 19: PHOTOSYSTEM II PSBX PROTEIN



- Molecule 19: PHOTOSYSTEM II PSBX PROTEIN

Chain BY:  68% 32%



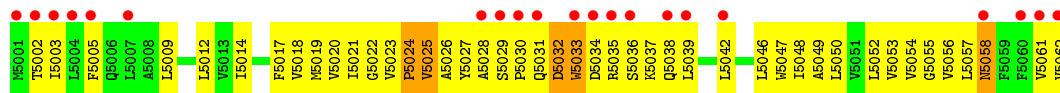
- Molecule 20: Photosystem II reaction center protein Z

Chain AZ:  18% 32% 60% 8%



- Molecule 20: Photosystem II reaction center protein Z

Chain BZ:  34% 29% 63% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	128.08Å 225.37Å 305.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 39.38 – 3.10	Depositor EDS
% Data completeness (in resolution range)	94.1 (20.00-3.20) 99.1 (39.38-3.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.12Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.269 , 0.299 0.270 , 0.292	Depositor DCC
R_{free} test set	2899 reflections (2.04%)	DCC
Wilson B-factor (Å ²)	95.5	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 78.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 159033 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	50266	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, PHO, DGD, CL, CA, MST, LMT, CLA, PL9, BCT, DMS, FE2, OEC, HEM, SQD, BCR, LMG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.50	0/2713	0.72	0/3700
1	BA	0.52	0/2713	0.72	0/3700
2	AB	0.51	0/3986	0.73	0/5433
2	BB	0.52	0/3986	0.73	3/5433 (0.1%)
3	AC	0.46	0/3556	0.71	1/4842 (0.0%)
3	BC	0.47	0/3556	0.71	1/4842 (0.0%)
4	AD	0.53	0/2806	0.73	0/3825
4	BD	0.55	0/2806	0.73	0/3825
5	AE	0.51	0/685	0.76	0/933
5	BE	0.54	0/685	0.77	0/933
6	AF	0.75	0/291	0.78	0/397
6	BF	0.71	0/291	0.74	0/397
7	AH	0.47	0/520	0.78	0/709
7	BH	0.49	0/520	0.79	0/709
8	AI	0.58	0/293	0.77	0/395
8	BI	0.64	0/293	0.81	0/395
9	AJ	0.55	0/277	0.86	0/375
9	BJ	0.67	0/277	0.88	0/375
10	AK	0.54	0/303	0.73	0/416
10	BK	0.62	0/303	0.73	0/416
11	AL	0.58	0/311	0.78	1/422 (0.2%)
11	BL	0.57	0/311	0.81	0/422
12	AM	0.65	0/270	0.87	0/367
12	BM	0.66	0/270	0.85	0/367
13	AO	0.49	0/1876	0.76	0/2548
13	BO	0.48	0/1876	0.76	1/2548 (0.0%)
14	AT	0.80	1/284 (0.4%)	0.82	0/381
14	BT	0.81	1/284 (0.4%)	0.87	2/381 (0.5%)
15	AU	0.54	0/785	0.84	2/1064 (0.2%)
15	BU	0.52	0/785	0.83	0/1064
16	AV	0.46	0/1081	0.70	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	BV	0.46	0/1081	0.70	0/1468
17	Ay	1.12	1/202 (0.5%)	1.24	1/272 (0.4%)
17	By	1.03	1/202 (0.5%)	1.22	1/272 (0.4%)
18	AX	0.57	0/273	0.76	0/370
18	BX	0.63	0/273	0.69	0/370
20	AZ	0.53	0/490	0.75	1/669 (0.1%)
20	BZ	0.60	0/490	0.80	0/669
All	All	0.53	4/42004 (0.0%)	0.75	14/57172 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	1
2	BB	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	By	5030	ILE	CA-CB	-5.67	1.41	1.54
14	BT	5032	LYS	C-OXT	5.50	1.33	1.23
17	Ay	35	ILE	CA-CB	-5.35	1.42	1.54
14	AT	32	LYS	CA-CB	5.19	1.65	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	BO	5030	THR	N-CA-CB	-5.76	99.35	110.30
2	BB	5488	PRO	N-CA-C	5.72	126.97	112.10
2	BB	5489	GLU	N-CA-C	5.65	126.27	111.00
14	BT	5004	ILE	CB-CA-C	-5.65	100.31	111.60
3	AC	32	GLY	N-CA-C	-5.56	99.19	113.10
17	By	5021	GLN	N-CA-CB	-5.41	100.87	110.60
14	BT	5032	LYS	CB-CA-C	-5.38	99.64	110.40
17	Ay	25	ILE	CB-CA-C	-5.38	100.84	111.60
11	AL	19	LEU	CA-CB-CG	5.35	127.61	115.30
15	AU	57	LEU	CA-CB-CG	-5.30	103.11	115.30
3	BC	5032	GLY	N-CA-C	-5.08	100.39	113.10
15	AU	72	TYR	N-CA-C	5.08	124.71	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BB	5354	LEU	CA-CB-CG	-5.07	103.64	115.30
20	AZ	7	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	262	TYR	Sidechain
2	BB	5273	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	2628	0	2524	300	0
1	BA	2628	0	2524	309	0
2	AB	3850	0	3718	344	0
2	BB	3850	0	3718	351	0
3	AC	3444	0	3365	350	0
3	BC	3444	0	3365	358	0
4	AD	2711	0	2610	245	0
4	BD	2711	0	2610	255	0
5	AE	666	0	651	68	0
5	BE	666	0	651	76	0
6	AF	282	0	291	36	0
6	BF	282	0	291	32	0
7	AH	507	0	521	65	0
7	BH	507	0	521	69	0
8	AI	286	0	308	34	0
8	BI	286	0	305	37	0
9	AJ	271	0	276	36	0
9	BJ	271	0	276	38	0
10	AK	293	0	305	48	0
10	BK	293	0	305	45	0
11	AL	304	0	316	34	0
11	BL	304	0	313	35	0
12	AM	267	0	289	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	BM	267	0	286	26	0
13	AO	1845	0	1801	137	0
13	BO	1845	0	1801	142	0
14	AT	275	0	288	28	0
14	BT	275	0	285	27	0
15	AU	774	0	773	52	0
15	BU	774	0	773	51	0
16	AV	1060	0	1068	48	0
16	BV	1060	0	1068	48	0
17	Ay	201	0	226	0	0
17	By	201	0	226	0	0
18	AX	270	0	299	33	0
18	BX	270	0	299	27	0
19	AY	140	0	32	3	0
19	BY	140	0	32	7	0
20	AZ	479	0	516	53	0
20	BZ	479	0	513	55	0
21	AA	1	0	0	0	0
21	BD	1	0	0	0	0
22	AA	4	0	0	0	0
22	BA	4	0	0	0	0
23	AA	2	0	0	1	0
23	BA	2	0	0	0	0
24	AA	260	0	288	41	0
24	AB	1040	0	1152	133	0
24	AC	845	0	936	91	0
24	AD	130	0	144	17	0
24	BA	260	0	288	44	0
24	BB	1040	0	1152	142	0
24	BC	845	0	936	94	0
24	BD	130	0	144	18	0
25	AA	16	0	19	9	0
25	BA	16	0	19	9	0
26	AA	5	0	0	0	0
26	BA	5	0	0	0	0
27	AA	40	0	56	4	0
27	AB	120	0	168	8	0
27	AC	120	0	168	24	0
27	AD	40	0	56	2	0
27	AJ	40	0	56	4	0
27	AK	40	0	56	5	0
27	AT	40	0	56	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	AX	40	0	56	8	0
27	BA	40	0	56	3	0
27	BB	120	0	168	8	0
27	BC	120	0	168	25	0
27	BD	40	0	56	2	0
27	BJ	40	0	56	3	0
27	BK	40	0	56	5	0
27	BT	40	0	56	6	0
27	BX	40	0	56	4	0
28	AA	56	0	70	9	0
28	AB	52	0	62	0	0
28	AC	181	0	243	63	0
28	AE	63	0	87	1	0
28	AH	58	0	74	9	0
28	BA	56	0	70	9	0
28	BB	52	0	62	5	0
28	BC	181	0	243	64	0
28	BE	63	0	87	1	0
28	BH	58	0	74	8	0
29	AA	76	0	95	7	0
29	BA	76	0	95	9	0
30	AA	105	0	145	2	0
30	AB	90	0	109	9	0
30	AF	45	0	53	1	0
30	BA	105	0	145	3	0
30	BB	90	0	109	11	0
30	BF	45	0	53	1	0
31	AA	86	0	111	17	0
31	AB	100	0	139	21	0
31	AC	93	0	125	11	0
31	AD	97	0	134	15	0
31	AI	43	0	56	3	0
31	AJ	46	0	61	2	0
31	AM	42	0	54	6	0
31	BA	42	0	53	3	0
31	BB	49	0	68	4	0
31	BC	93	0	125	10	0
31	BD	143	0	195	15	0
31	BE	44	0	58	4	0
31	BI	43	0	56	4	0
31	BL	51	0	71	18	0
31	BM	42	0	54	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	AB	140	0	184	15	0
32	AD	31	0	35	0	0
32	AI	70	0	92	9	0
32	AM	35	0	46	1	0
32	BB	140	0	184	16	0
32	BC	35	0	46	3	0
32	BD	31	0	35	1	0
32	BI	35	0	46	5	0
32	BM	35	0	46	2	0
33	AB	8	0	12	0	0
33	AU	4	0	6	0	0
33	AV	4	0	6	0	0
33	BB	8	0	12	0	0
33	BV	8	0	12	0	0
34	AD	128	0	148	14	0
34	BD	128	0	148	15	0
35	AD	55	0	80	15	0
35	BD	55	0	80	16	0
36	AF	43	0	30	8	0
36	AV	43	0	30	4	0
36	BF	43	0	30	7	0
36	BV	43	0	30	6	0
37	AF	1	0	0	0	0
37	AK	1	0	0	0	0
37	AO	1	0	0	0	0
37	BF	1	0	0	0	0
37	BK	1	0	0	0	0
37	BO	1	0	0	0	0
All	All	50266	0	51335	3700	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

All (3700) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:278:TRP:CE3	28:AC:519:DGD:HAG2	1.69	1.27
1:BA:5278:TRP:CE3	28:BC:5519:DGD:HAG2	1.78	1.17
15:AU:83:ALA:HB1	15:AU:84:PRO:HD2	1.25	1.15
24:AB:608:CLA:H42	4:AD:127:LEU:HD11	1.29	1.14
24:BB:5612:CLA:H42	4:BD:5127:LEU:HD11	1.29	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:BU:5083:ALA:HB1	15:BU:5084:PRO:HD2	1.29	1.09
10:AK:28:ILE:HA	10:AK:31:LEU:HD12	1.35	1.09
1:BA:5325:ASN:HA	1:BA:5328:MET:HE3	1.34	1.08
1:AA:102:LEU:HB2	31:AA:417:LMG:H351	1.10	1.08
10:BK:5028:ILE:HA	10:BK:5031:LEU:HD12	1.35	1.08
2:BB:5027:THR:HG22	2:BB:5107:LEU:HD13	1.36	1.08
1:AA:278:TRP:CE3	28:AC:519:DGD:CIA	2.38	1.07
13:BO:5087:GLN:O	13:BO:5088:GLU:HG3	1.54	1.07
9:AJ:15:THR:HG21	10:AK:38:VAL:HG13	1.33	1.06
16:AV:63:CYS:SG	36:AV:201:HEM:HAB	1.96	1.06
1:BA:5200:LEU:HD11	28:BC:5519:DGD:HAW2	1.38	1.05
28:BA:5412:DGD:O2D	3:BC:5216:SER:HB2	1.57	1.04
13:AO:82:PRO:HG3	13:AO:89:ALA:HB2	1.35	1.04
9:BJ:5015:THR:HG21	10:BK:5038:VAL:HG13	1.35	1.04
13:BO:5082:PRO:HG3	13:BO:5089:ALA:HB2	1.34	1.04
14:AT:29:ILE:HD12	14:AT:29:ILE:H	1.22	1.04
1:AA:200:LEU:CD1	28:AC:519:DGD:HAW2	1.88	1.03
13:AO:87:GLN:O	13:AO:88:GLU:HG3	1.56	1.03
3:AC:52:ALA:HA	24:AC:511:CLA:HMB3	1.42	1.02
1:BA:5200:LEU:CD1	28:BC:5519:DGD:HAW2	1.89	1.01
2:BB:5260:SER:OG	2:BB:5262:THR:HG22	1.61	1.00
3:BC:5254:THR:HG22	3:BC:5255:THR:H	1.26	1.00
2:AB:27:THR:HG22	2:AB:107:LEU:HD13	1.40	1.00
28:AA:411:DGD:O2D	3:AC:216:SER:HB2	1.61	1.00
1:AA:200:LEU:HD11	28:AC:519:DGD:HAW2	1.42	0.99
2:AB:260:SER:OG	2:AB:262:THR:HG22	1.60	0.99
1:AA:325:ASN:HA	1:AA:328:MET:HE3	1.41	0.99
3:BC:5052:ALA:HA	24:BC:5511:CLA:HMB3	1.43	0.98
4:AD:14:TRP:HE1	7:AH:25:TRP:HH2	1.12	0.97
3:AC:254:THR:HG22	3:AC:255:THR:H	1.26	0.97
3:AC:305:THR:HG22	3:AC:308:GLU:HB2	1.47	0.97
5:BE:5056:TYR:O	16:BV:5027:ALA:HB2	1.64	0.96
1:BA:5278:TRP:CE3	28:BC:5519:DGD:CIA	2.48	0.96
2:BB:5476:ARG:HB3	2:BB:5476:ARG:HH11	1.31	0.95
24:BC:5501:CLA:HMB3	27:BC:5516:BCR:H403	1.48	0.95
4:BD:5014:TRP:HE1	7:BH:5025:TRP:HH2	1.14	0.95
16:BV:5063:CYS:SG	36:BV:5201:HEM:HAB	2.07	0.94
13:BO:5069:LEU:HB3	13:BO:5107:ILE:HB	1.48	0.94
2:AB:476:ARG:HH11	2:AB:476:ARG:HB3	1.32	0.94
3:AC:305:THR:HG22	3:AC:308:GLU:CB	1.97	0.94
2:BB:5476:ARG:NH1	2:BB:5476:ARG:HB3	1.82	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:248:ALA:HA	24:AB:603:CLA:H42	1.49	0.93
3:AC:29:GLU:HB3	10:AK:46:ARG:HH11	1.31	0.93
2:AB:16:PRO:HG3	2:AB:133:LEU:HD11	1.48	0.93
3:AC:461:ARG:HG3	3:AC:461:ARG:HH11	1.31	0.93
4:BD:5274:VAL:HA	35:BD:5406:PL9:H253	1.51	0.93
3:BC:5461:ARG:HG3	3:BC:5461:ARG:HH11	1.33	0.93
1:BA:5341:LEU:HB2	3:BC:5313:GLN:HE22	1.30	0.92
13:AO:230:VAL:HG12	13:AO:231:ASP:H	1.35	0.92
5:AE:15:THR:HG22	9:AJ:7:ARG:H	1.34	0.92
2:AB:476:ARG:NH1	2:AB:476:ARG:HB3	1.84	0.92
18:BX:5026:GLY:O	18:BX:5029:VAL:HG12	1.70	0.92
3:BC:5305:THR:HG22	3:BC:5308:GLU:CB	2.00	0.92
3:BC:5239:TRP:HE3	3:BC:5243:ILE:HD11	1.34	0.91
2:BB:5248:ALA:HA	24:BB:5607:CLA:H42	1.52	0.91
3:BC:5305:THR:HG22	3:BC:5308:GLU:HB2	1.50	0.91
1:BA:5102:LEU:HB2	31:BA:5402:LMG:H351	1.51	0.91
5:BE:5015:THR:HG22	9:BJ:5007:ARG:H	1.35	0.91
4:BD:5103:ARG:HG3	5:BE:5073:LYS:HG3	1.52	0.91
24:BB:5607:CLA:HBB1	24:BB:5609:CLA:H171	1.52	0.91
24:AA:405:CLA:HED1	35:AD:405:PL9:H372	1.53	0.90
24:AC:501:CLA:HMB3	27:AC:516:BCR:H403	1.54	0.90
2:BB:5016:PRO:HG3	2:BB:5133:LEU:HD11	1.49	0.90
15:BU:5088:VAL:O	15:BU:5091:VAL:HG12	1.72	0.90
24:AB:603:CLA:HBB1	24:AB:605:CLA:H171	1.52	0.90
13:AO:69:LEU:HB3	13:AO:107:ILE:HB	1.51	0.90
1:AA:102:LEU:CB	31:AA:417:LMG:H351	2.00	0.90
2:AB:12:LEU:HD13	2:AB:19:LEU:HA	1.53	0.89
2:BB:5004:PRO:HG2	2:BB:5007:ARG:HD2	1.55	0.89
15:AU:83:ALA:HB1	15:AU:84:PRO:CD	2.02	0.89
18:AX:26:GLY:O	18:AX:29:VAL:HG12	1.72	0.89
4:AD:87:HIS:CD2	4:AD:166:SER:HA	2.07	0.89
14:AT:18:PHE:HB2	27:AT:101:BCR:H10C	1.54	0.89
4:BD:5087:HIS:CD2	4:BD:5166:SER:HA	2.07	0.88
1:BA:5278:TRP:HH2	28:BC:5519:DGD:HGB1	1.38	0.88
24:BA:5406:CLA:HED1	35:BD:5406:PL9:H372	1.55	0.88
5:AE:46:VAL:HG13	28:AE:101:DGD:HG31	1.53	0.88
2:BB:5012:LEU:HD13	2:BB:5019:LEU:HA	1.56	0.88
3:AC:239:TRP:HE3	3:AC:243:ILE:HD11	1.35	0.88
3:BC:5451:ALA:HA	3:BC:5456:GLU:OE2	1.73	0.88
4:AD:103:ARG:HG3	5:AE:73:LYS:HG3	1.56	0.88
4:AD:88:SER:HB2	5:AE:69:ARG:NH2	1.88	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BH:5061:SER:HA	28:BH:5101:DGD:HE4	1.54	0.87
13:BO:5230:VAL:HG12	13:BO:5231:ASP:H	1.39	0.87
3:AC:451:ALA:HA	3:AC:456:GLU:OE2	1.74	0.87
15:AU:88:VAL:O	15:AU:91:VAL:HG12	1.74	0.87
2:AB:414:PRO:HB2	2:AB:415:PRO:HD3	1.56	0.86
3:AC:29:GLU:HB3	10:AK:46:ARG:NH1	1.90	0.86
5:BE:5046:VAL:HG13	28:BE:5102:DGD:HG31	1.56	0.86
15:BU:5083:ALA:HB1	15:BU:5084:PRO:CD	2.04	0.86
5:AE:15:THR:HG23	9:AJ:8:ILE:O	1.75	0.85
2:BB:5179:GLN:HA	2:BB:5179:GLN:HE21	1.41	0.85
3:BC:5380:ILE:HA	3:BC:5384:ILE:HD11	1.55	0.85
3:BC:5117:VAL:HG11	31:BC:5521:LMG:H192	1.58	0.85
4:BD:5122:LEU:HD21	24:BD:5402:CLA:H92	1.58	0.85
3:AC:130:VAL:HG13	24:AC:511:CLA:H92	1.59	0.85
4:AD:148:ALA:HB2	4:AD:276:VAL:HG13	1.58	0.85
3:BC:5113:VAL:O	3:BC:5117:VAL:HG23	1.75	0.85
1:AA:341:LEU:HB2	3:AC:313:GLN:HE22	1.40	0.85
3:AC:113:VAL:O	3:AC:117:VAL:HG23	1.75	0.85
4:BD:5148:ALA:HB3	4:BD:5149:PRO:HD3	1.59	0.84
7:AH:61:SER:HA	28:AH:101:DGD:HE4	1.59	0.84
2:AB:179:GLN:HE21	2:AB:179:GLN:HA	1.43	0.84
4:AD:274:VAL:HA	35:AD:405:PL9:H253	1.57	0.84
1:BA:5033:PHE:HE1	24:BC:5505:CLA:H92	1.41	0.84
3:AC:380:ILE:HA	3:AC:384:ILE:HD11	1.58	0.84
1:AA:177:SER:HA	1:AA:180:PHE:HD2	1.42	0.84
5:BE:5015:THR:HG22	9:BJ:5007:ARG:N	1.93	0.84
5:BE:5015:THR:HG23	9:BJ:5008:ILE:O	1.77	0.84
2:BB:5383:PHE:O	13:BO:5192:SER:HA	1.78	0.84
2:AB:223:GLN:HG3	2:AB:227:LYS:HE3	1.60	0.84
16:BV:5066:CYS:SG	36:BV:5201:HEM:HAC	2.18	0.84
24:BA:5406:CLA:H93	34:BD:5403:PHO:HMA1	1.60	0.83
5:AE:56:TYR:O	16:AV:27:ALA:HB2	1.78	0.83
1:AA:278:TRP:CZ3	28:AC:519:DGD:HAG2	2.12	0.83
1:BA:5289:GLY:O	1:BA:5292:THR:HG22	1.77	0.83
24:AA:405:CLA:H93	34:AD:402:PHO:HMA1	1.60	0.83
2:BB:5464:PHE:HD2	24:BB:5615:CLA:HAC2	1.43	0.83
13:AO:32:THR:O	13:AO:36:ILE:HD12	1.79	0.83
13:BO:5032:THR:O	13:BO:5036:ILE:HD12	1.77	0.83
3:BC:5130:VAL:HG13	24:BC:5511:CLA:H92	1.60	0.83
5:AE:15:THR:HG22	9:AJ:7:ARG:N	1.93	0.83
4:BD:5148:ALA:HB2	4:BD:5276:VAL:HG13	1.58	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BO:5031:LEU:HD12	13:BO:5031:LEU:H	1.44	0.83
31:AD:408:LMG:HC8	11:AL:19:LEU:HD23	1.60	0.83
3:AC:307:PRO:HB3	3:AC:358:PHE:CD1	2.14	0.83
24:BC:5504:CLA:C15	28:BC:5519:DGD:HA91	2.08	0.82
1:BA:5278:TRP:CH2	28:BC:5519:DGD:HBG1	2.13	0.82
7:AH:55:LEU:HD21	18:AX:16:LEU:HD23	1.59	0.82
4:BD:5088:SER:HB2	5:BE:5069:ARG:NH2	1.94	0.82
16:AV:66:CYS:SG	36:AV:201:HEM:HAC	2.20	0.82
2:AB:464:PHE:HD2	24:AB:611:CLA:HAC2	1.45	0.82
32:AB:629:LMT:H51	14:BT:5004:ILE:HG13	1.60	0.82
35:BD:5406:PL9:H201	31:BL:5101:LMG:H182	1.61	0.82
1:AA:278:TRP:HH2	28:AC:519:DGD:HBG1	1.42	0.82
3:BC:5116:VAL:HG21	27:BC:5515:BCR:H323	1.62	0.82
2:AB:155:ALA:O	2:AB:161:LEU:HD22	1.79	0.82
1:AA:192:ILE:HA	1:AA:293:MET:HE3	1.62	0.81
2:AB:121:GLU:HG3	7:AH:4:ARG:HA	1.60	0.81
2:BB:5357:ARG:HH11	2:BB:5357:ARG:HG3	1.45	0.81
3:AC:385:GLN:H	3:AC:388:GLN:NE2	1.79	0.81
2:BB:5155:ALA:O	2:BB:5161:LEU:HD22	1.80	0.81
1:BA:5214:MET:HA	1:BA:5214:MET:CE	2.10	0.81
10:AK:19:ASP:N	10:AK:20:PRO:HD2	1.96	0.81
2:BB:5354:LEU:HD23	2:BB:5378:LYS:HB2	1.62	0.81
4:AD:17:ILE:HG21	18:AX:42:GLN:HG2	1.63	0.81
2:BB:5354:LEU:CD2	2:BB:5378:LYS:HB2	2.11	0.81
5:AE:36:LEU:O	5:AE:40:THR:HG23	1.80	0.81
1:BA:5084:PRO:HA	1:BA:5112:TYR:CD2	2.15	0.81
1:AA:214:MET:HA	1:AA:214:MET:CE	2.11	0.81
3:BC:5029:GLU:HB3	10:BK:5046:ARG:HH11	1.46	0.81
31:BD:5410:LMG:HC8	11:BL:5019:LEU:HD23	1.61	0.81
3:BC:5307:PRO:HB3	3:BC:5358:PHE:CD1	2.15	0.80
1:BA:5214:MET:HA	1:BA:5214:MET:HE3	1.63	0.80
3:BC:5310:SER:OG	3:BC:5355:THR:HG23	1.82	0.80
5:BE:5036:LEU:O	5:BE:5040:THR:HG23	1.82	0.80
24:AB:603:CLA:HAC2	24:AB:606:CLA:HBB2	1.64	0.80
31:AB:620:LMG:H182	35:AD:405:PL9:H201	1.63	0.80
31:BI:5101:LMG:H152	32:BI:5102:LMT:H52	1.62	0.80
1:BA:5281:VAL:CG1	28:BC:5519:DGD:HAG3	2.11	0.80
1:AA:33:PHE:HE1	24:AC:505:CLA:H92	1.45	0.80
2:AB:354:LEU:CD2	2:AB:378:LYS:HB2	2.12	0.80
18:AX:34:PHE:O	18:AX:38:ILE:HG12	1.82	0.80
14:AT:4:ILE:HG13	32:BB:5603:LMT:H51	1.64	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:5464:GLU:HB3	3:BC:5467:LEU:HD12	1.64	0.80
4:AD:122:LEU:HD21	24:AD:401:CLA:H92	1.64	0.80
31:AA:414:LMG:O3	5:AE:9:PRO:HB3	1.81	0.80
4:BD:5221:THR:HG23	4:BD:5244:TYR:HB2	1.63	0.80
2:AB:357:ARG:HH11	2:AB:357:ARG:HG3	1.46	0.80
2:AB:297:THR:HG23	2:AB:300:GLU:H	1.47	0.80
18:BX:5034:PHE:O	18:BX:5038:ILE:HG12	1.82	0.79
2:BB:5135:LEU:HB2	2:BB:5136:PRO:HD3	1.62	0.79
2:AB:135:LEU:HB2	2:AB:136:PRO:HD3	1.63	0.79
24:BB:5607:CLA:HAC2	24:BB:5610:CLA:HBB2	1.65	0.79
3:BC:5155:ASN:HA	3:BC:5158:THR:HG22	1.65	0.79
2:AB:383:PHE:O	13:AO:192:SER:HA	1.82	0.79
31:AI:101:LMG:H152	32:AI:102:LMT:H52	1.64	0.79
4:BD:5152:VAL:HG21	4:BD:5279:LEU:HD13	1.64	0.79
24:BD:5405:CLA:H41	18:BX:5023:LEU:HD12	1.64	0.79
3:AC:116:VAL:HG21	27:AC:515:BCR:H323	1.63	0.79
1:BA:5143:ILE:HD11	4:BD:5217:THR:HA	1.64	0.79
5:BE:5009:PRO:HB3	31:BE:5101:LMG:O3	1.81	0.79
1:BA:5177:SER:HA	1:BA:5180:PHE:HD2	1.47	0.79
3:AC:372:PRO:O	13:AO:36:ILE:HD13	1.82	0.79
1:AA:84:PRO:HA	1:AA:112:TYR:CD2	2.16	0.79
1:AA:278:TRP:CH2	28:AC:519:DGD:HBG1	2.18	0.79
24:AA:407:CLA:H43	24:AC:505:CLA:H201	1.64	0.79
16:AV:63:CYS:SG	36:AV:201:HEM:CAB	2.71	0.79
2:BB:5173:GLY:HA3	2:BB:5265:ILE:HD11	1.64	0.79
7:AH:21:VAL:HG23	7:AH:22:ALA:O	1.83	0.78
1:BA:5258:LEU:HB3	1:BA:5259:ILE:HD13	1.65	0.78
1:AA:258:LEU:HB3	1:AA:259:ILE:HD13	1.63	0.78
2:BB:5224:ARG:HG3	7:BH:5025:TRP:HD1	1.46	0.78
20:AZ:19:MET:O	20:AZ:23:VAL:HG23	1.83	0.78
2:AB:354:LEU:HD23	2:AB:378:LYS:HB2	1.63	0.78
20:BZ:5036:SER:HA	20:BZ:5039:LEU:HG	1.65	0.78
24:BC:5504:CLA:H151	28:BC:5519:DGD:HA91	1.64	0.78
1:BA:5192:ILE:HA	1:BA:5293:MET:HE3	1.66	0.78
4:BD:5017:ILE:HG21	18:BX:5042:GLN:HG2	1.63	0.78
31:BC:5520:LMG:O9	31:BC:5520:LMG:O8	2.01	0.78
15:BU:5072:TYR:HB3	15:BU:5073:PRO:HD3	1.66	0.78
1:BA:5278:TRP:HB3	1:BA:5279:PRO:HD3	1.64	0.78
7:BH:5042:LEU:HD12	7:BH:5045:ILE:HD11	1.64	0.78
1:AA:289:GLY:O	1:AA:292:THR:HG22	1.82	0.78
31:AC:520:LMG:O8	31:AC:520:LMG:O9	2.01	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BA:5408:CLA:H43	24:BC:5505:CLA:H201	1.66	0.78
3:AC:461:ARG:CG	3:AC:461:ARG:HH11	1.96	0.78
1:BA:5083:VAL:HG22	4:BD:5314:PHE:HE2	1.49	0.78
13:BO:5032:THR:HG22	13:BO:5035:ASP:OD2	1.83	0.77
4:AD:148:ALA:HB3	4:AD:149:PRO:HD3	1.65	0.77
1:BA:5133:LEU:HD23	4:BD:5252:PHE:CD1	2.18	0.77
2:BB:5489:GLU:HB2	5:BE:5003:GLY:N	1.98	0.77
20:BZ:5032:ASP:CG	20:BZ:5033:TRP:H	1.87	0.77
28:BA:5412:DGD:O2D	3:BC:5216:SER:CB	2.32	0.77
7:BH:5055:LEU:HD21	18:BX:5016:LEU:HD23	1.64	0.77
10:AK:27:VAL:O	10:AK:30:VAL:HG12	1.82	0.77
1:AA:127:MET:HE3	3:AC:442:LEU:HD21	1.67	0.77
3:AC:48:LYS:HE2	3:AC:138:GLU:HG3	1.67	0.77
20:AZ:36:SER:HA	20:AZ:39:LEU:HG	1.65	0.77
3:AC:415:ASN:O	3:AC:416:SER:HB3	1.85	0.77
3:BC:5219:GLY:HA2	28:BC:5517:DGD:O3D	1.85	0.77
4:AD:129:GLN:NE2	4:AD:143:ALA:HA	2.00	0.77
3:AC:464:GLU:HB3	3:AC:467:LEU:HD12	1.65	0.77
24:AC:511:CLA:H202	20:AZ:20:VAL:HA	1.66	0.77
3:AC:117:VAL:HG11	31:AC:521:LMG:H192	1.67	0.77
2:AB:483:ASP:CB	2:AB:484:PRO:HD2	2.14	0.77
2:BB:5068:ARG:HH22	24:BB:5608:CLA:HED1	1.49	0.77
2:BB:5223:GLN:HG3	2:BB:5227:LYS:HE3	1.66	0.76
3:AC:62:PHE:HE2	10:AK:29:PRO:HD3	1.51	0.76
13:AO:32:THR:HG22	13:AO:35:ASP:OD2	1.83	0.76
2:BB:5297:THR:HG23	2:BB:5300:GLU:H	1.50	0.76
15:AU:72:TYR:HB3	15:AU:73:PRO:HD3	1.67	0.76
24:AC:504:CLA:C15	28:AC:519:DGD:HA91	2.14	0.76
24:BA:5405:CLA:H13	24:BA:5406:CLA:H91	1.67	0.76
3:BC:5062:PHE:HE2	10:BK:5029:PRO:HD3	1.50	0.76
4:AD:221:THR:HG23	4:AD:244:TYR:HB2	1.67	0.76
28:AA:411:DGD:O2D	3:AC:216:SER:CB	2.33	0.76
24:AD:404:CLA:H41	18:AX:23:LEU:HD12	1.65	0.76
2:BB:5461:LEU:HD11	31:BB:5624:LMG:H412	1.68	0.76
12:AM:33:GLN:HB3	12:BM:5033:GLN:HB3	1.65	0.76
3:AC:155:ASN:HA	3:AC:158:THR:HG22	1.66	0.76
1:AA:262:TYR:CE1	31:AA:414:LMG:HC5	2.21	0.76
1:BA:5259:ILE:N	1:BA:5259:ILE:HD13	2.01	0.76
6:AF:11:VAL:HG12	6:AF:12:SER:H	1.49	0.76
2:AB:121:GLU:CG	7:AH:4:ARG:HA	2.16	0.76
2:AB:4:PRO:HG2	2:AB:7:ARG:HD2	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BC:5514:BCR:H353	27:BK:5102:BCR:H321	1.68	0.76
3:BC:5461:ARG:CG	3:BC:5461:ARG:HH11	1.97	0.76
5:BE:5078:THR:HA	5:BE:5081:GLU:HG2	1.68	0.76
12:BM:5001:MET:HG2	12:BM:5002:GLU:H	1.51	0.76
13:AO:128:ASP:OD2	13:AO:149:LYS:HG2	1.86	0.75
7:AH:42:LEU:HD12	7:AH:45:ILE:HD11	1.67	0.75
2:BB:5016:PRO:CG	2:BB:5133:LEU:HD11	2.16	0.75
1:BA:5255:PHE:CE1	1:BA:5259:ILE:HD11	2.21	0.75
2:AB:468:TRP:HD1	2:AB:469:HIS:HD1	1.31	0.75
24:AB:604:CLA:H11	24:AB:612:CLA:H152	1.68	0.75
3:BC:5372:PRO:O	13:BO:5036:ILE:HD13	1.86	0.75
2:BB:5121:GLU:HG3	7:BH:5004:ARG:HA	1.67	0.75
24:AC:503:CLA:H191	24:AC:503:CLA:HMD2	1.67	0.75
27:AC:514:BCR:H353	27:AK:102:BCR:H321	1.68	0.75
4:AD:88:SER:HB2	5:AE:69:ARG:CZ	2.17	0.75
2:BB:5414:PRO:HB2	2:BB:5415:PRO:HD3	1.68	0.75
1:BA:5049:VAL:O	1:BA:5053:ILE:HG13	1.87	0.75
3:BC:5048:LYS:HE2	3:BC:5138:GLU:HG3	1.66	0.75
4:BD:5091:LEU:HD22	7:BH:5052:THR:HG21	1.69	0.75
2:BB:5462:PHE:HA	24:BB:5615:CLA:HMC1	1.69	0.74
10:BK:5027:VAL:O	10:BK:5030:VAL:HG12	1.86	0.74
4:BD:5103:ARG:NH1	5:BE:5077:GLU:HG3	2.02	0.74
3:BC:5385:GLN:H	3:BC:5388:GLN:NE2	1.85	0.74
31:AA:417:LMG:H201	2:BB:5098:LEU:HD13	1.69	0.74
1:BA:5315:ASN:HD21	4:BD:5332:GLN:HE22	1.35	0.74
1:AA:330:VAL:HG11	4:AD:348:ARG:HG2	1.69	0.74
1:BA:5064:ARG:O	13:BO:5178:ARG:NH2	2.21	0.74
4:AD:152:VAL:HG21	4:AD:279:LEU:HD13	1.67	0.74
2:BB:5121:GLU:CG	7:BH:5004:ARG:HA	2.18	0.74
3:AC:219:GLY:HA2	28:AC:517:DGD:O3D	1.86	0.74
13:BO:5171:GLU:HG2	13:BO:5172:PHE:N	2.02	0.74
13:AO:230:VAL:HG12	13:AO:231:ASP:N	2.03	0.74
1:AA:13:LEU:HA	1:AA:16:ARG:HD3	1.69	0.74
10:AK:18:PHE:HE1	20:AZ:9:LEU:HG	1.51	0.74
13:BO:5178:ARG:HH11	13:BO:5178:ARG:HG3	1.53	0.74
13:AO:31:LEU:HD12	13:AO:31:LEU:H	1.51	0.74
13:AO:178:ARG:HH11	13:AO:178:ARG:HG3	1.53	0.74
2:AB:474:LEU:HD13	30:AB:622:SQD:H81	1.69	0.74
1:BA:5272:HIS:CD2	4:BD:5218:VAL:HG21	2.23	0.74
3:BC:5453:ALA:O	8:BI:5034:ARG:HB2	1.87	0.74
24:AB:608:CLA:H52	24:AB:609:CLA:H8	1.70	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:222:PRO:HG3	7:AH:27:THR:H	1.53	0.73
3:BC:5209:ILE:HG23	27:BC:5516:BCR:H382	1.70	0.73
13:BO:5031:LEU:HD12	13:BO:5031:LEU:N	2.03	0.73
2:AB:16:PRO:CG	2:AB:133:LEU:HD11	2.17	0.73
1:AA:64:ARG:O	13:AO:178:ARG:NH2	2.21	0.73
2:BB:5483:ASP:CB	2:BB:5484:PRO:HD2	2.16	0.73
13:AO:171:GLU:HG2	13:AO:172:PHE:N	2.02	0.73
2:AB:371:THR:HG22	2:AB:377:VAL:HA	1.70	0.73
5:AE:34:GLY:HA2	6:AF:32:PHE:CE1	2.22	0.73
2:AB:224:ARG:HG3	7:AH:25:TRP:HD1	1.51	0.73
24:BB:5608:CLA:H11	24:BB:5616:CLA:H152	1.71	0.73
4:AD:189:HIS:HA	4:AD:294:ARG:HD2	1.69	0.73
10:BK:5018:PHE:HE1	20:BZ:5009:LEU:HG	1.53	0.73
2:BB:5474:LEU:HD13	30:BB:5625:SQD:H81	1.68	0.73
3:AC:397:THR:HG21	16:AV:66:CYS:SG	2.27	0.73
24:AC:513:CLA:HMC2	27:AC:515:BCR:H372	1.70	0.73
2:BB:5324:LEU:HA	4:BD:5293:LEU:CD2	2.18	0.73
2:AB:248:ALA:HA	24:AB:603:CLA:C4	2.19	0.73
24:BB:5612:CLA:H52	24:BB:5613:CLA:H8	1.71	0.73
3:AC:55:ALA:HB1	27:AC:514:BCR:H373	1.69	0.73
3:AC:248:GLY:O	3:AC:252:ILE:HG12	1.89	0.73
1:AA:300:PHE:HE2	28:AC:519:DGD:O1A	1.71	0.73
1:AA:18:CYS:O	1:AA:22:THR:HG22	1.89	0.73
4:AD:103:ARG:NH1	5:AE:77:GLU:HG3	2.04	0.73
1:BA:5127:MET:HE3	3:BC:5442:LEU:HD21	1.71	0.73
5:BE:5018:ARG:O	5:BE:5022:ILE:HG13	1.89	0.73
8:AI:16:VAL:O	8:AI:20:VAL:HG23	1.87	0.72
14:AT:21:ILE:HD12	27:AT:101:BCR:H332	1.71	0.72
24:BC:5509:CLA:H121	24:BC:5509:CLA:HBD	1.71	0.72
1:AA:259:ILE:HD13	1:AA:259:ILE:N	2.03	0.72
3:BC:5055:ALA:HB1	27:BC:5514:BCR:H373	1.68	0.72
1:AA:278:TRP:HB3	1:AA:279:PRO:HD3	1.70	0.72
3:BC:5029:GLU:HB3	10:BK:5046:ARG:NH1	2.04	0.72
3:AC:429:SER:O	3:AC:432:VAL:HG12	1.89	0.72
1:AA:260:PHE:CE1	1:AA:263:ALA:HB2	2.25	0.72
1:AA:315:ASN:HD21	4:AD:332:GLN:HE22	1.37	0.72
2:BB:5371:THR:HG22	2:BB:5377:VAL:HA	1.71	0.72
2:BB:5086:ILE:HD12	2:BB:5086:ILE:O	1.89	0.72
3:BC:5117:VAL:CG1	31:BC:5521:LMG:H192	2.20	0.72
35:BD:5406:PL9:H23	35:BD:5406:PL9:H303	1.71	0.72
4:BD:5018:LEU:HD22	18:BX:5038:ILE:HD13	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:5214:LEU:O	2:BB:5218:LEU:HG	1.89	0.72
8:BI:5016:VAL:O	8:BI:5020:VAL:HG23	1.90	0.72
7:BH:5021:VAL:HG23	7:BH:5022:ALA:O	1.88	0.72
13:AO:120:THR:HG22	13:AO:154:SER:OG	1.90	0.72
3:BC:5254:THR:HG22	3:BC:5255:THR:N	2.04	0.72
2:BB:5324:LEU:HA	4:BD:5293:LEU:HD23	1.72	0.72
1:BA:5334:ARG:HD3	4:BD:5320:LEU:CD1	2.20	0.72
1:BA:5013:LEU:HA	1:BA:5016:ARG:HD3	1.69	0.72
2:AB:86:ILE:HD12	2:AB:86:ILE:O	1.90	0.72
13:BO:5120:THR:HG22	13:BO:5154:SER:OG	1.90	0.72
24:AC:504:CLA:H151	28:AC:519:DGD:HA91	1.69	0.72
1:AA:83:VAL:HG22	4:AD:314:PHE:HE2	1.53	0.72
3:BC:5318:LEU:HG	3:BC:5328:VAL:HG11	1.69	0.71
3:BC:5418:ASN:CB	28:BC:5519:DGD:HE2	2.19	0.71
20:BZ:5002:THR:HG23	20:BZ:5003:ILE:N	2.06	0.71
4:AD:91:LEU:HD22	7:AH:52:THR:HG21	1.70	0.71
35:AD:405:PL9:H303	35:AD:405:PL9:H23	1.70	0.71
4:BD:5053:THR:HG22	4:BD:5067:TYR:CE2	2.25	0.71
2:BB:5425:ILE:HG22	2:BB:5426:PHE:CD2	2.25	0.71
2:AB:137:LYS:O	2:AB:141:ILE:HG13	1.90	0.71
3:BC:5397:THR:HG21	16:BV:5066:CYS:SG	2.30	0.71
13:AO:83:LYS:HG2	13:AO:84:ASN:H	1.55	0.71
1:AA:57:PRO:HG3	1:AA:68:SER:HB3	1.72	0.71
1:AA:133:LEU:HD23	4:AD:252:PHE:CD1	2.26	0.71
1:AA:234:ASN:HD21	4:AD:266:TRP:HB2	1.56	0.71
3:AC:254:THR:HG22	3:AC:255:THR:N	2.04	0.71
20:BZ:5019:MET:O	20:BZ:5023:VAL:HG23	1.90	0.71
1:AA:255:PHE:CE1	1:AA:259:ILE:HD11	2.25	0.71
3:AC:344:SER:O	13:AO:101:THR:HG22	1.90	0.71
12:AM:20:VAL:HG21	12:BM:5020:VAL:HG21	1.72	0.71
4:AD:134:ARG:HA	4:AD:134:ARG:HE	1.56	0.71
4:AD:274:VAL:HB	4:AD:275:PRO:HD3	1.73	0.71
6:AF:28:VAL:HB	6:AF:29:PRO:HD3	1.73	0.71
2:AB:425:ILE:HG22	2:AB:426:PHE:CD2	2.26	0.71
15:AU:94:ILE:O	15:AU:97:LEU:HG	1.91	0.71
24:AC:509:CLA:HBD	24:AC:509:CLA:H121	1.71	0.71
7:AH:58:VAL:HG13	7:AH:58:VAL:O	1.91	0.71
11:BL:5013:ASN:HD21	11:BL:5015:THR:HG22	1.56	0.71
20:AZ:52:LEU:O	20:AZ:56:VAL:HG23	1.91	0.71
20:AZ:2:THR:HG23	20:AZ:3:ILE:N	2.06	0.71
3:BC:5344:SER:O	13:BO:5101:THR:HG22	1.91	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:5004:PRO:HD2	2:BB:5007:ARG:HB2	1.71	0.70
3:AC:310:SER:OG	3:AC:355:THR:HG23	1.91	0.70
5:BE:5034:GLY:HA2	6:BF:5032:PHE:CE1	2.26	0.70
2:AB:235:GLU:HG2	2:AB:235:GLU:O	1.91	0.70
5:AE:18:ARG:O	5:AE:22:ILE:HG13	1.90	0.70
24:AA:404:CLA:H13	24:AA:405:CLA:H91	1.73	0.70
2:BB:5235:GLU:HG2	2:BB:5235:GLU:O	1.91	0.70
3:BC:5337:LEU:HD12	13:BO:5131:PRO:HG3	1.73	0.70
10:BK:5028:ILE:HA	10:BK:5031:LEU:CD1	2.18	0.70
3:AC:305:THR:HG23	3:AC:308:GLU:H	1.55	0.70
2:BB:5130:GLU:HB2	2:BB:5131:PRO:HD2	1.73	0.70
2:AB:461:LEU:HD11	31:AB:621:LMG:H412	1.71	0.70
2:BB:5121:GLU:HG2	7:BH:5004:ARG:HD2	1.73	0.70
1:AA:39:PRO:HB2	24:AA:407:CLA:HBB1	1.74	0.70
24:AB:610:CLA:H111	24:AB:615:CLA:HAA1	1.74	0.70
2:AB:116:VAL:HG21	27:AB:619:BCR:H271	1.73	0.70
24:BB:5618:CLA:OBD	11:BL:5010:VAL:HG21	1.90	0.70
2:AB:98:LEU:HD13	31:BA:5402:LMG:H201	1.73	0.70
2:BB:5116:VAL:HG21	27:BB:5623:BCR:H271	1.71	0.70
3:BC:5429:SER:O	3:BC:5432:VAL:HG12	1.90	0.70
1:AA:49:VAL:O	1:AA:53:ILE:HG13	1.92	0.70
3:AC:305:THR:CG2	3:AC:308:GLU:H	2.04	0.70
16:BV:5066:CYS:SG	36:BV:5201:HEM:CAC	2.79	0.70
2:AB:183:PRO:HG3	2:AB:199:VAL:CG1	2.21	0.70
15:AU:58:ASN:OD1	15:AU:84:PRO:HA	1.92	0.70
2:BB:5068:ARG:HH12	24:BB:5608:CLA:HED1	1.56	0.70
1:AA:288:LEU:HD13	3:AC:432:VAL:HG23	1.74	0.70
1:BA:5260:PHE:CE1	1:BA:5263:ALA:HB2	2.27	0.70
4:BD:5189:HIS:HA	4:BD:5294:ARG:HD2	1.74	0.70
2:BB:5191:ASN:HB2	7:BH:5058:VAL:CG2	2.20	0.70
24:BC:5511:CLA:H202	20:BZ:5020:VAL:HA	1.74	0.70
24:BC:5503:CLA:H191	24:BC:5503:CLA:HMD2	1.72	0.69
4:BD:5088:SER:HB2	5:BE:5069:ARG:CZ	2.22	0.69
16:BV:5135:GLU:O	16:BV:5139:VAL:HG23	1.91	0.69
2:BB:5137:LYS:O	2:BB:5141:ILE:HG13	1.92	0.69
1:BA:5032:TRP:HA	1:BA:5032:TRP:CE3	2.27	0.69
7:BH:5058:VAL:O	7:BH:5058:VAL:HG13	1.92	0.69
2:BB:5297:THR:HG22	2:BB:5300:GLU:OE1	1.92	0.69
20:BZ:5052:LEU:O	20:BZ:5056:VAL:HG23	1.93	0.69
3:AC:224:ILE:O	3:AC:227:VAL:HG23	1.93	0.69
11:AL:13:ASN:HD21	11:AL:15:THR:HG22	1.56	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AM:33:GLN:CB	12:BM:5033:GLN:HB3	2.21	0.69
15:BU:5094:ILE:O	15:BU:5097:LEU:HG	1.92	0.69
2:AB:298:LEU:HD23	2:AB:402:TYR:CZ	2.28	0.69
4:BD:5018:LEU:HD22	18:BX:5038:ILE:CD1	2.22	0.69
1:AA:143:ILE:HD11	4:AD:217:THR:HA	1.75	0.69
1:AA:334:ARG:HD3	4:AD:320:LEU:CD1	2.23	0.69
2:BB:5120:LEU:HD13	24:BB:5620:CLA:HMD2	1.75	0.69
24:BB:5614:CLA:H111	24:BB:5619:CLA:HAA1	1.75	0.69
5:AE:17:VAL:O	5:AE:21:VAL:HG23	1.93	0.69
1:BA:5261:GLN:NE2	2:BB:5489:GLU:HG3	2.07	0.69
3:BC:5154:LYS:HE2	3:BC:5261:ARG:HD2	1.74	0.69
7:AH:55:LEU:O	7:AH:58:VAL:HG12	1.92	0.69
4:BD:5274:VAL:HB	4:BD:5275:PRO:HD3	1.74	0.69
3:BC:5158:THR:O	3:BC:5251:HIS:HB3	1.92	0.69
6:AF:27:ALA:HB1	36:AF:101:HEM:HBC2	1.74	0.69
4:AD:54:PHE:HB3	5:AE:47:PHE:CD2	2.27	0.69
4:AD:122:LEU:HB3	4:AD:150:ILE:CD1	2.22	0.69
3:BC:5113:VAL:HG11	31:BC:5521:LMG:H132	1.74	0.69
4:BD:5103:ARG:HH12	5:BE:5077:GLU:HG3	1.58	0.69
1:BA:5271:LEU:HD12	25:BA:5409:MST:H162	1.73	0.69
20:AZ:49:ALA:O	20:AZ:53:VAL:HG23	1.93	0.69
13:AO:92:VAL:CG1	13:AO:93:PRO:HD2	2.23	0.69
1:AA:278:TRP:CD2	28:AC:519:DGD:HAG2	2.25	0.69
1:BA:5300:PHE:HE2	28:BC:5519:DGD:O1A	1.75	0.69
1:AA:177:SER:HA	1:AA:180:PHE:CD2	2.28	0.69
24:BC:5502:CLA:HBB2	24:BC:5510:CLA:H152	1.74	0.69
3:AC:318:LEU:HG	3:AC:328:VAL:HG11	1.75	0.69
4:BD:5054:PHE:HB3	5:BE:5047:PHE:CD2	2.28	0.69
30:BB:5625:SQD:H172	32:BB:5627:LMT:H101	1.74	0.69
13:BO:5230:VAL:HG12	13:BO:5231:ASP:N	2.08	0.69
3:BC:5415:ASN:O	3:BC:5416:SER:HB3	1.93	0.68
1:AA:234:ASN:ND2	4:AD:266:TRP:HB2	2.08	0.68
2:AB:462:PHE:HA	24:AB:611:CLA:HMC1	1.74	0.68
20:AZ:32:ASP:CG	20:AZ:33:TRP:H	1.96	0.68
6:BF:5027:ALA:HB1	36:BF:5101:HEM:HBC2	1.73	0.68
1:BA:5018:CYS:O	1:BA:5022:THR:HG22	1.93	0.68
2:BB:5248:ALA:HA	24:BB:5607:CLA:C4	2.22	0.68
3:AC:347:GLY:HA3	13:AO:43:ASN:HB2	1.74	0.68
4:AD:192:THR:HG23	24:AD:401:CLA:HBC2	1.74	0.68
3:BC:5472:LEU:HG	4:BD:5251:ARG:NH1	2.08	0.68
1:BA:5278:TRP:CZ3	28:BC:5519:DGD:HAG2	2.27	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5038:ILE:HG23	30:BA:5401:SQD:H131	1.76	0.68
4:BD:5250:ASN:HD22	4:BD:5262:SER:HB3	1.57	0.68
1:BA:5234:ASN:HD21	4:BD:5266:TRP:HB2	1.57	0.68
27:AC:515:BCR:H312	20:AZ:55:GLY:HA2	1.74	0.68
4:AD:18:LEU:HD22	18:AX:38:ILE:HD13	1.75	0.68
2:AB:250:PHE:CD2	2:AB:459:ALA:HB1	2.29	0.68
3:AC:215:LYS:HB3	3:AC:223:TRP:HA	1.76	0.68
3:AC:240:ILE:O	3:AC:244:CYS:HB2	1.93	0.68
8:AI:11:VAL:HG22	32:AI:102:LMT:H101	1.76	0.68
1:BA:5234:ASN:ND2	4:BD:5266:TRP:HB2	2.09	0.68
24:BC:5513:CLA:HMC2	27:BC:5515:BCR:H372	1.76	0.68
4:BD:5192:THR:HG23	24:BD:5402:CLA:HBC2	1.75	0.68
4:BD:5129:GLN:NE2	4:BD:5143:ALA:HA	2.08	0.68
1:BA:5288:LEU:HD13	3:BC:5432:VAL:HG23	1.76	0.68
5:AE:23:HIS:HA	5:AE:26:THR:OG1	1.93	0.68
2:AB:4:PRO:HD2	2:AB:7:ARG:HB2	1.76	0.68
3:AC:209:ILE:HG23	27:AC:516:BCR:H382	1.76	0.68
18:AX:12:ILE:HG13	18:AX:12:ILE:O	1.94	0.68
3:AC:385:GLN:H	3:AC:388:GLN:HE21	1.41	0.68
4:AD:53:THR:HG22	4:AD:67:TYR:CE2	2.29	0.68
2:BB:5005:TRP:O	2:BB:5008:VAL:HG13	1.93	0.68
3:AC:158:THR:O	3:AC:251:HIS:HB3	1.93	0.68
30:AB:622:SQD:H172	32:AB:624:LMT:H101	1.75	0.68
2:BB:5357:ARG:NH1	2:BB:5357:ARG:HG3	2.06	0.68
15:AU:58:ASN:ND2	15:AU:114:VAL:HG13	2.08	0.68
1:BA:5039:PRO:HB2	24:BA:5408:CLA:HBB1	1.74	0.68
3:BC:5062:PHE:HE2	10:BK:5028:ILE:HB	1.58	0.68
16:AV:66:CYS:SG	36:AV:201:HEM:CAC	2.81	0.68
6:AF:17:THR:HG23	6:AF:20:TRP:H	1.59	0.68
2:AB:188:ASP:OD1	7:AH:58:VAL:HA	1.94	0.67
12:AM:33:GLN:HB3	12:BM:5033:GLN:CB	2.23	0.67
3:AC:62:PHE:HE2	10:AK:28:ILE:HB	1.59	0.67
3:BC:5150:ASP:HB3	3:BC:5153:ASP:HB2	1.75	0.67
3:AC:262:ARG:HH21	32:AI:103:LMT:H5'	1.59	0.67
2:BB:5065:PHE:O	24:BB:5609:CLA:HBA1	1.94	0.67
2:AB:121:GLU:HG2	7:AH:4:ARG:HD2	1.74	0.67
10:BK:5040:GLN:HA	10:BK:5043:VAL:HG12	1.74	0.67
2:BB:5010:THR:O	2:BB:5013:ILE:HG13	1.94	0.67
3:BC:5305:THR:CG2	3:BC:5308:GLU:H	2.08	0.67
4:AD:103:ARG:HH12	5:AE:77:GLU:HG3	1.60	0.67
3:AC:473:ASP:HB2	14:AT:26:PRO:HB3	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5239:PHE:O	14:BT:5029:ILE:HA	1.95	0.67
12:BM:5025:LEU:O	12:BM:5028:GLN:HG3	1.95	0.67
2:BB:5068:ARG:HH12	24:BB:5608:CLA:CED	2.07	0.67
27:AC:515:BCR:C31	20:AZ:55:GLY:HA2	2.24	0.67
2:AB:297:THR:HG22	2:AB:300:GLU:OE1	1.94	0.67
13:AO:114:ASN:HD21	13:AO:120:THR:HG23	1.59	0.67
13:BO:5092:VAL:CG1	13:BO:5093:PRO:HD2	2.24	0.67
2:BB:5250:PHE:CD2	2:BB:5459:ALA:HB1	2.30	0.67
3:AC:52:ALA:HA	24:AC:511:CLA:CMB	2.23	0.67
1:AA:272:HIS:CD2	4:AD:218:VAL:HG21	2.30	0.67
2:AB:324:LEU:HA	4:AD:293:LEU:HD23	1.76	0.67
1:AA:214:MET:HE3	1:AA:214:MET:HA	1.74	0.67
2:AB:103:LEU:HD21	24:AB:605:CLA:HMC3	1.76	0.67
24:AC:502:CLA:HBB2	24:AC:510:CLA:H152	1.76	0.67
14:BT:5029:ILE:HD12	14:BT:5029:ILE:H	1.58	0.67
2:AB:324:LEU:HA	4:AD:293:LEU:CD2	2.24	0.67
2:BB:5379:ALA:HA	2:BB:5390:TYR:HB3	1.76	0.67
7:AH:9:ASP:O	7:AH:12:ARG:HB2	1.95	0.67
2:AB:130:GLU:HB2	2:AB:131:PRO:HD2	1.76	0.67
2:AB:8:VAL:HB	24:AB:614:CLA:O1D	1.95	0.67
2:BB:5233:ASN:O	2:BB:5236:THR:HG22	1.95	0.67
1:BA:5136:ARG:NH2	8:BI:5027:ASP:OD1	2.27	0.67
1:BA:5190:HIS:HB3	1:BA:5293:MET:HE2	1.76	0.67
2:AB:234:ILE:HD12	2:AB:237:VAL:HG21	1.77	0.67
3:BC:5215:LYS:HB3	3:BC:5223:TRP:HA	1.75	0.67
3:BC:5240:ILE:O	3:BC:5244:CYS:HB2	1.95	0.67
31:AA:414:LMG:HO2	5:AE:10:PHE:HD2	1.43	0.67
3:BC:5347:GLY:HA3	13:BO:5043:ASN:HB2	1.75	0.67
4:AD:56:THR:HG21	5:AE:50:PRO:HD3	1.77	0.67
4:BD:5134:ARG:HA	4:BD:5134:ARG:HE	1.60	0.67
3:AC:150:ASP:HB3	3:AC:153:ASP:HB2	1.77	0.67
3:BC:5089:ILE:N	3:BC:5090:PRO:HD2	2.10	0.67
13:BO:5128:ASP:OD2	13:BO:5149:LYS:HG2	1.93	0.67
1:AA:93:PHE:CD2	1:AA:95:PRO:HD3	2.30	0.67
16:BV:5063:CYS:SG	36:BV:5201:HEM:CAB	2.81	0.67
3:BC:5308:GLU:HB2	3:BC:5361:PHE:CE1	2.29	0.67
3:BC:5199:ILE:H	3:BC:5199:ILE:HD12	1.60	0.67
4:BD:5171:PRO:HG3	4:BD:5181:PHE:CZ	2.29	0.67
1:AA:33:PHE:CE1	24:AC:505:CLA:H92	2.29	0.66
2:AB:62:VAL:HG13	24:AB:605:CLA:HED3	1.77	0.66
13:BO:5169:LYS:HG2	13:BO:5224:SER:HB3	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:199:ILE:HD12	3:AC:199:ILE:H	1.60	0.66
1:BA:5297:LEU:HD11	3:BC:5404:LEU:HD12	1.77	0.66
2:BB:5224:ARG:HG3	7:BH:5025:TRP:CD1	2.30	0.66
2:BB:5222:PRO:HG3	7:BH:5027:THR:H	1.58	0.66
3:AC:134:ILE:HD11	24:AC:511:CLA:H93	1.77	0.66
15:AU:66:ILE:HG22	15:AU:66:ILE:O	1.95	0.66
3:BC:5040:ALA:O	3:BC:5043:ILE:HG13	1.95	0.66
1:AA:161:TYR:HB3	1:AA:162:PRO:HD3	1.77	0.66
24:AB:613:CLA:HED3	24:AB:613:CLA:H2	1.76	0.66
24:BB:5612:CLA:H18	24:BB:5613:CLA:H192	1.77	0.66
3:BC:5062:PHE:CE2	10:BK:5029:PRO:HD3	2.29	0.66
3:BC:5254:THR:CG2	3:BC:5255:THR:H	2.06	0.66
10:AK:40:GLN:HA	10:AK:43:VAL:HG12	1.76	0.66
16:BV:5133:LEU:H	16:BV:5133:LEU:HD12	1.59	0.66
3:BC:5248:GLY:O	3:BC:5252:ILE:HG12	1.94	0.66
2:AB:233:ASN:O	2:AB:236:THR:HG22	1.95	0.66
24:AB:608:CLA:H18	24:AB:609:CLA:H192	1.77	0.66
4:AD:250:ASN:HD22	4:AD:262:SER:HB3	1.60	0.66
4:BD:5261:PHE:HA	31:BD:5410:LMG:O2	1.96	0.66
10:AK:28:ILE:HA	10:AK:31:LEU:CD1	2.17	0.66
10:AK:17:ILE:H	10:AK:17:ILE:HD12	1.59	0.66
2:AB:173:GLY:HA3	2:AB:265:ILE:HD11	1.76	0.66
5:BE:5027:ILE:HB	5:BE:5028:PRO:HD3	1.78	0.66
18:AX:36:VAL:O	18:AX:40:ILE:HG22	1.96	0.66
2:AB:222:PRO:HG3	7:AH:26:GLY:HA3	1.76	0.66
2:AB:5:TRP:O	2:AB:8:VAL:HG13	1.95	0.66
1:BA:5033:PHE:CE1	24:BC:5505:CLA:H92	2.27	0.66
2:AB:357:ARG:HG3	2:AB:357:ARG:NH1	2.06	0.66
20:AZ:32:ASP:HA	20:AZ:34:ASP:OD2	1.95	0.66
1:AA:81:ALA:HB2	1:AA:175:GLY:HA3	1.77	0.66
24:BC:5504:CLA:H172	28:BC:5519:DGD:HAE1	1.76	0.66
2:AB:120:LEU:HD13	24:AB:616:CLA:HMD2	1.78	0.66
3:AC:62:PHE:CE2	10:AK:29:PRO:HD3	2.29	0.66
10:BK:5019:ASP:N	10:BK:5020:PRO:HD2	2.10	0.66
13:AO:39:THR:OG1	13:AO:41:LEU:HB2	1.96	0.66
13:AO:31:LEU:N	13:AO:31:LEU:HD12	2.11	0.66
3:AC:337:LEU:HD12	13:AO:131:PRO:HG3	1.77	0.66
1:BA:5330:VAL:HG11	4:BD:5348:ARG:HG2	1.77	0.66
30:BB:5601:SQD:H81	30:BB:5601:SQD:H242	1.78	0.66
2:BB:5208:VAL:HG21	24:BB:5606:CLA:HMC1	1.78	0.66
4:AD:129:GLN:HE22	4:AD:143:ALA:HA	1.61	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:5453:ALA:HA	8:BI:5034:ARG:O	1.95	0.66
15:BU:5057:LEU:HD11	15:BU:5112:PHE:HB3	1.76	0.66
1:AA:102:LEU:HB2	31:AA:417:LMG:C35	2.06	0.66
3:BC:5224:ILE:O	3:BC:5227:VAL:HG23	1.94	0.66
1:BA:5221:SER:HB2	4:BD:5139:ARG:O	1.96	0.66
3:BC:5305:THR:HG23	3:BC:5308:GLU:H	1.59	0.66
2:BB:5008:VAL:HB	24:BB:5618:CLA:O1D	1.95	0.66
13:AO:87:GLN:O	13:AO:88:GLU:CG	2.41	0.66
3:AC:44:ASN:C	3:AC:45:LEU:HD12	2.17	0.66
1:AA:39:PRO:HB2	24:AA:407:CLA:CBB	2.25	0.66
1:BA:5176:ILE:HG22	1:BA:5180:PHE:CE2	2.30	0.66
24:BB:5617:CLA:H2	24:BB:5617:CLA:HED3	1.77	0.66
3:AC:254:THR:CG2	3:AC:255:THR:H	2.07	0.66
4:BD:5103:ARG:HG3	5:BE:5073:LYS:CG	2.26	0.66
13:BO:5114:ASN:HD21	13:BO:5120:THR:HG23	1.60	0.66
16:AV:133:LEU:HD12	16:AV:133:LEU:H	1.61	0.66
1:BA:5081:ALA:HB2	1:BA:5175:GLY:HA3	1.77	0.66
30:AB:627:SQD:H242	30:AB:627:SQD:H81	1.76	0.66
3:AC:405:ASN:HB2	28:AC:519:DGD:HG32	1.77	0.65
1:BA:5278:TRP:CD2	28:BC:5519:DGD:HAG2	2.29	0.65
2:AB:191:ASN:HB2	7:AH:58:VAL:CG2	2.25	0.65
1:BA:5180:PHE:CD1	4:BD:5192:THR:HB	2.31	0.65
4:BD:5122:LEU:HB3	4:BD:5150:ILE:CD1	2.26	0.65
15:BU:5068:TYR:HB2	15:BU:5071:LEU:HD12	1.77	0.65
24:AB:614:CLA:OBD	11:AL:10:VAL:HG21	1.95	0.65
2:AB:65:PHE:O	24:AB:605:CLA:HBA1	1.96	0.65
31:AI:101:LMG:O9	31:AI:101:LMG:O8	2.14	0.65
3:BC:5282:MET:HG2	24:BC:5501:CLA:H71	1.78	0.65
1:AA:238:LYS:HD2	14:AT:32:LYS:HB3	1.79	0.65
15:BU:5066:ILE:O	15:BU:5066:ILE:HG22	1.95	0.65
3:BC:5262:ARG:HH21	32:BC:5522:LMT:H5'	1.61	0.65
2:AB:489:GLU:HB2	5:AE:3:GLY:N	2.11	0.65
4:AD:261:PHE:HA	31:AD:408:LMG:O2	1.96	0.65
11:AL:16:SER:HA	11:AL:19:LEU:HG	1.75	0.65
11:BL:5026:VAL:HG21	31:BL:5101:LMG:H202	1.78	0.65
2:AB:468:TRP:HD1	2:AB:469:HIS:ND1	1.94	0.65
8:AI:19:PHE:CE1	8:AI:23:PHE:HE2	2.14	0.65
1:BA:5039:PRO:HB2	24:BA:5408:CLA:CBB	2.27	0.65
2:BB:5183:PRO:HG3	2:BB:5199:VAL:CG1	2.27	0.65
13:BO:5087:GLN:O	13:BO:5088:GLU:CG	2.41	0.65
5:BE:5017:VAL:O	5:BE:5021:VAL:HG23	1.95	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:5103:ARG:CG	5:BE:5073:LYS:HG3	2.26	0.65
6:AF:11:VAL:HG12	6:AF:12:SER:N	2.10	0.65
20:AZ:2:THR:HG23	20:AZ:3:ILE:H	1.60	0.65
1:AA:228:THR:HG22	1:AA:229:GLU:H	1.60	0.65
3:BC:5416:SER:C	28:BC:5519:DGD:O3E	2.35	0.65
1:BA:5093:PHE:CD2	1:BA:5095:PRO:HD3	2.31	0.65
3:BC:5134:ILE:HD11	24:BC:5511:CLA:H93	1.79	0.65
2:AB:134:ASP:OD2	2:AB:137:LYS:HB2	1.97	0.65
2:AB:183:PRO:HG3	2:AB:199:VAL:HG11	1.78	0.65
1:BA:5057:PRO:HG3	1:BA:5068:SER:HB3	1.77	0.65
1:AA:278:TRP:CE3	28:AC:519:DGD:HAG1	2.30	0.65
3:AC:416:SER:N	28:AC:519:DGD:O3E	2.30	0.65
3:BC:5405:ASN:HB2	28:BC:5519:DGD:HG32	1.77	0.65
31:BI:5101:LMG:O8	31:BI:5101:LMG:O9	2.15	0.65
5:BE:5010:PHE:HD2	31:BE:5101:LMG:HO2	1.45	0.65
5:BE:5023:HIS:HA	5:BE:5026:THR:OG1	1.96	0.65
16:AV:71:ILE:HD12	16:AV:72:THR:N	2.11	0.65
2:AB:187:PRO:HB3	24:AB:601:CLA:HMB2	1.78	0.65
2:AB:68:ARG:HH12	24:AB:604:CLA:CED	2.09	0.65
2:BB:5062:VAL:HG13	24:BB:5609:CLA:HED3	1.78	0.65
31:BD:5410:LMG:O6	11:BL:5015:THR:HG21	1.97	0.65
3:BC:5062:PHE:CE2	10:BK:5028:ILE:HB	2.32	0.65
3:AC:110:PRO:O	3:AC:114:VAL:HG23	1.97	0.65
3:AC:89:ILE:N	3:AC:90:PRO:HD2	2.12	0.65
1:AA:271:LEU:HD12	25:AA:408:MST:H162	1.78	0.65
1:BA:5097:TRP:HA	8:BI:5001:MET:SD	2.36	0.65
2:AB:213:GLY:O	2:AB:217:ILE:HG13	1.97	0.65
1:AA:32:TRP:CE3	1:AA:32:TRP:HA	2.32	0.65
2:AB:10:THR:O	2:AB:13:ILE:HG13	1.95	0.65
16:BV:5071:ILE:HD12	16:BV:5072:THR:N	2.12	0.65
3:BC:5320:ARG:O	3:BC:5324:LEU:HD23	1.96	0.65
3:AC:282:MET:HG2	24:AC:501:CLA:H71	1.79	0.65
2:BB:5009:HIS:HB2	24:BB:5615:CLA:HBA2	1.79	0.65
2:BB:5234:ILE:HD12	2:BB:5237:VAL:HG21	1.78	0.65
3:BC:5223:TRP:CD2	3:BC:5224:ILE:HG13	2.32	0.65
4:BD:5153:PHE:HB2	24:BD:5402:CLA:H41	1.79	0.65
2:BB:5222:PRO:HG3	7:BH:5026:GLY:HA3	1.78	0.65
3:AC:179:ALA:HB1	3:AC:199:ILE:HD13	1.79	0.65
5:AE:51:ARG:HG3	5:AE:51:ARG:HH11	1.62	0.65
4:AD:153:PHE:HB2	24:AD:401:CLA:H41	1.79	0.65
2:AB:224:ARG:HG2	7:AH:24:GLY:O	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:78:THR:HA	5:AE:81:GLU:HG2	1.78	0.65
2:BB:5150:CYS:HB2	24:BB:5607:CLA:HMC3	1.78	0.64
15:BU:5058:ASN:ND2	15:BU:5114:VAL:HG13	2.11	0.64
3:AC:308:GLU:HB2	3:AC:361:PHE:CE1	2.32	0.64
1:AA:257:ARG:HG3	1:AA:257:ARG:HH11	1.62	0.64
3:AC:362:ARG:HE	3:AC:370:ARG:HH11	1.45	0.64
2:BB:5393:GLU:HG2	15:BU:5044:ASP:O	1.97	0.64
1:AA:300:PHE:CE2	28:AC:519:DGD:O1A	2.50	0.64
3:BC:5416:SER:C	28:BC:5519:DGD:HO3E	2.01	0.64
1:AA:288:LEU:HD22	3:AC:432:VAL:HG23	1.80	0.64
5:AE:27:ILE:HB	5:AE:28:PRO:HD3	1.79	0.64
3:BC:5437:PHE:HA	24:BC:5508:CLA:CMC	2.27	0.64
20:BZ:5002:THR:HG23	20:BZ:5003:ILE:H	1.60	0.64
3:AC:320:ARG:O	3:AC:324:LEU:HD23	1.97	0.64
3:BC:5052:ALA:HA	24:BC:5511:CLA:CMB	2.24	0.64
16:AV:135:GLU:O	16:AV:139:VAL:HG23	1.97	0.64
3:BC:5149:TYR:HA	3:BC:5156:LYS:HD3	1.77	0.64
1:BA:5048:PHE:HB2	1:BA:5115:ILE:HD13	1.79	0.64
24:AC:503:CLA:H171	24:AC:510:CLA:HBB2	1.79	0.64
10:AK:24:VAL:O	10:AK:27:VAL:HG12	1.98	0.64
13:AO:234:THR:OG1	13:AO:236:GLU:HG2	1.98	0.64
2:AB:384:ARG:HD3	15:AU:132:LEU:CD1	2.28	0.64
2:BB:5213:GLY:O	2:BB:5217:ILE:HG13	1.96	0.64
10:BK:5017:ILE:H	10:BK:5017:ILE:HD12	1.62	0.64
3:AC:413:GLU:HG3	3:AC:414:ILE:H	1.62	0.64
31:AD:408:LMG:O6	11:AL:15:THR:HG21	1.98	0.64
3:BC:5179:ALA:HB1	3:BC:5199:ILE:HD13	1.77	0.64
1:BA:5228:THR:HG22	1:BA:5229:GLU:H	1.61	0.64
1:BA:5010:SER:HB3	1:BA:5016:ARG:NH1	2.13	0.64
1:AA:228:THR:HG22	1:AA:229:GLU:N	2.12	0.64
2:BB:5246:PHE:CD1	2:BB:5246:PHE:C	2.71	0.64
1:AA:136:ARG:NH2	8:AI:27:ASP:OD1	2.31	0.64
3:BC:5418:ASN:CA	28:BC:5519:DGD:HE2	2.27	0.64
2:AB:9:HIS:HB2	24:AB:611:CLA:HBA2	1.79	0.64
3:BC:5030:SER:HB3	10:BK:5046:ARG:O	1.98	0.64
2:AB:278:SER:HB3	2:AB:281:GLN:HE21	1.63	0.64
1:AA:281:VAL:CG1	28:AC:519:DGD:HAG3	2.27	0.64
2:AB:247:PHE:HB2	24:AB:608:CLA:HBC1	1.80	0.64
2:AB:68:ARG:HH22	24:AB:604:CLA:HED1	1.62	0.64
7:AH:38:PHE:HB2	27:AX:101:BCR:H10C	1.78	0.64
2:BB:5103:LEU:HD21	24:BB:5609:CLA:HMC3	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:42:LEU:HD23	24:AC:511:CLA:HED3	1.79	0.64
20:AZ:35:ARG:O	20:AZ:38:GLN:HB3	1.98	0.64
2:AB:214:LEU:O	2:AB:218:LEU:HG	1.97	0.64
1:BA:5077:ILE:HD11	14:BT:5006:TYR:HB3	1.79	0.64
4:BD:5261:PHE:CD2	4:BD:5267:LEU:HD12	2.33	0.63
31:BB:5624:LMG:H411	4:BD:5284:ILE:HG12	1.80	0.63
13:BO:5039:THR:OG1	13:BO:5041:LEU:HB2	1.98	0.63
2:AB:208:VAL:HG21	24:AB:602:CLA:HMC1	1.79	0.63
31:AB:620:LMG:H202	11:AL:26:VAL:HG21	1.79	0.63
3:AC:437:PHE:HA	24:AC:508:CLA:CMC	2.28	0.63
28:AH:101:DGD:O1B	28:AH:101:DGD:C1G	2.46	0.63
3:BC:5449:ARG:HG2	24:BC:5505:CLA:HED1	1.80	0.63
3:AC:154:LYS:HE2	3:AC:261:ARG:HD2	1.81	0.63
8:BI:5014:PHE:CZ	8:BI:5018:LEU:HD11	2.33	0.63
28:BC:5518:DGD:HG11	31:BC:5520:LMG:H301	1.81	0.63
2:BB:5187:PRO:HB3	24:BB:5605:CLA:HMB2	1.79	0.63
2:BB:5191:ASN:HB2	7:BH:5058:VAL:HG23	1.79	0.63
24:BC:5501:CLA:HMB3	27:BC:5516:BCR:C40	2.26	0.63
8:BI:5011:VAL:HG22	32:BI:5102:LMT:H101	1.80	0.63
4:BD:5236:ASN:ND2	4:BD:5239:GLN:O	2.29	0.63
13:BO:5144:LEU:CD1	13:BO:5259:VAL:HG11	2.29	0.63
13:BO:5218:LEU:HD22	15:BU:5119:THR:HG21	1.80	0.63
1:AA:176:ILE:HG22	1:AA:180:PHE:CE2	2.34	0.63
4:BD:5041:ALA:HB1	34:BD:5404:PHO:H42	1.81	0.63
4:AD:103:ARG:CG	5:AE:73:LYS:HG3	2.28	0.63
8:AI:8:VAL:O	8:AI:12:VAL:HG23	1.97	0.63
16:AV:95:ILE:O	16:AV:99:VAL:HG23	1.99	0.63
3:AC:304:PRO:HB3	3:AC:395:TYR:CD1	2.33	0.63
28:AC:518:DGD:HG11	31:AC:520:LMG:H301	1.81	0.63
2:AB:68:ARG:HH12	24:AB:604:CLA:HED1	1.64	0.63
3:AC:288:CYS:SG	28:AC:517:DGD:HA21	2.39	0.63
28:BH:5101:DGD:O1B	28:BH:5101:DGD:C1G	2.45	0.63
15:BU:5058:ASN:OD1	15:BU:5084:PRO:HA	1.98	0.63
3:AC:117:VAL:CG1	31:AC:521:LMG:H192	2.28	0.63
3:BC:5385:GLN:H	3:BC:5388:GLN:HE21	1.46	0.63
4:BD:5080:THR:HG23	4:BD:5172:SER:OG	1.99	0.63
2:AB:191:ASN:HB2	7:AH:58:VAL:HG23	1.80	0.63
3:BC:5437:PHE:CZ	24:BC:5502:CLA:HMC1	2.34	0.63
3:AC:461:ARG:CG	3:AC:461:ARG:NH1	2.60	0.63
5:BE:5076:VAL:O	5:BE:5080:LEU:HD22	1.98	0.63
5:AE:26:THR:O	5:AE:29:ALA:HB3	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:124:ARG:HH11	2:AB:124:ARG:HG3	1.63	0.63
1:AA:274:PHE:CE2	25:AA:408:MST:H133	2.33	0.63
20:AZ:14:ILE:O	20:AZ:18:VAL:HG23	1.99	0.63
1:AA:221:SER:HB2	4:AD:139:ARG:O	1.99	0.63
11:BL:5016:SER:HA	11:BL:5019:LEU:HG	1.80	0.63
1:BA:5343:LEU:O	1:BA:5344:ALA:HB2	1.99	0.63
13:BO:5206:GLU:CD	13:BO:5206:GLU:H	2.01	0.63
1:BA:5304:HIS:CE1	3:BC:5414:ILE:HD12	2.33	0.63
6:BF:5028:VAL:HB	6:BF:5029:PRO:HD3	1.81	0.63
13:BO:5234:THR:OG1	13:BO:5236:GLU:HG2	1.99	0.63
11:BL:5008:GLN:HE21	11:BL:5008:GLN:N	1.97	0.62
1:BA:5177:SER:HA	1:BA:5180:PHE:CD2	2.32	0.62
2:BB:5118:TRP:CH2	11:BL:5005:PRO:HD2	2.34	0.62
13:BO:5069:LEU:HD12	13:BO:5070:CYS:H	1.63	0.62
16:BV:5095:ILE:O	16:BV:5099:VAL:HG23	1.98	0.62
7:BH:5038:PHE:HB2	27:BX:5101:BCR:H10C	1.81	0.62
4:BD:5053:THR:HG22	4:BD:5067:TYR:CD2	2.34	0.62
13:AO:144:LEU:CD1	13:AO:259:VAL:HG11	2.29	0.62
3:BC:5413:GLU:HG3	3:BC:5414:ILE:H	1.64	0.62
2:AB:150:CYS:HB2	24:AB:603:CLA:HMC3	1.82	0.62
2:BB:5224:ARG:HG2	7:BH:5024:GLY:O	1.99	0.62
8:BI:5019:PHE:CE1	8:BI:5023:PHE:HE2	2.17	0.62
1:AA:45:THR:HG23	1:AA:46:ILE:N	2.14	0.62
4:AD:207:GLY:HA3	4:AD:275:PRO:HG3	1.80	0.62
35:AD:405:PL9:C23	35:AD:405:PL9:H303	2.30	0.62
2:BB:5008:VAL:HG23	2:BB:5009:HIS:CD2	2.34	0.62
1:AA:265:PHE:CD1	1:AA:271:LEU:HA	2.34	0.62
1:BA:5228:THR:HG22	1:BA:5229:GLU:N	2.15	0.62
16:BV:5047:LEU:HD11	16:BV:5143:GLY:HA3	1.81	0.62
2:AB:379:ALA:HA	2:AB:390:TYR:HB3	1.80	0.62
11:BL:5018:TYR:CE2	14:BT:5020:ALA:HA	2.35	0.62
4:BD:5241:GLU:H	4:BD:5241:GLU:CD	2.01	0.62
4:AD:103:ARG:HG3	5:AE:73:LYS:CG	2.28	0.62
4:AD:80:THR:HB	4:AD:81:PRO:HD2	1.80	0.62
4:AD:185:PHE:CE2	4:AD:289:LEU:HD12	2.34	0.62
5:BE:5008:ARG:HH22	5:BE:5016:SER:HB3	1.64	0.62
4:AD:261:PHE:CD2	4:AD:267:LEU:HD12	2.35	0.62
2:BB:5298:LEU:HD23	2:BB:5402:TYR:CZ	2.35	0.62
5:AE:34:GLY:CA	6:AF:32:PHE:CE1	2.83	0.62
3:AC:432:VAL:CG1	3:AC:433:LEU:N	2.63	0.62
1:BA:5193:LEU:HD13	4:BD:5179:PHE:HB3	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BV:5092:ARG:HG3	16:BV:5092:ARG:HH11	1.65	0.62
2:AB:133:LEU:HB3	2:AB:138:MET:CE	2.30	0.62
11:AL:13:ASN:ND2	11:AL:15:THR:HG22	2.15	0.62
3:BC:5039:ASN:HB3	24:BC:5509:CLA:CBB	2.30	0.62
3:BC:5062:PHE:HD2	10:BK:5029:PRO:HG3	1.65	0.62
1:AA:48:PHE:HB2	1:AA:115:ILE:HD13	1.81	0.62
15:AU:58:ASN:HD22	15:AU:114:VAL:HG13	1.64	0.62
4:AD:14:TRP:CD1	4:AD:15:PHE:N	2.68	0.62
2:AB:179:GLN:HE21	2:AB:180:PRO:HD2	1.64	0.62
18:BX:5036:VAL:O	18:BX:5040:ILE:HG22	1.99	0.62
1:BA:5296:ASN:HB2	3:BC:5400:PRO:O	2.00	0.62
2:BB:5284:ILE:HG23	2:BB:5305:ILE:HD12	1.82	0.62
1:BA:5306:VAL:HG13	1:BA:5314:ILE:O	2.00	0.62
3:AC:416:SER:C	28:AC:519:DGD:O3E	2.38	0.62
1:AA:200:LEU:HD13	28:AC:519:DGD:HAW2	1.76	0.62
2:AB:329:PRO:HD3	24:AB:607:CLA:HED1	1.82	0.62
2:AB:8:VAL:HG23	2:AB:9:HIS:CD2	2.34	0.62
1:BA:5161:TYR:HB3	1:BA:5162:PRO:HD3	1.82	0.62
3:BC:5288:CYS:SG	28:BC:5517:DGD:HA21	2.39	0.62
3:AC:62:PHE:HD2	10:AK:29:PRO:HG3	1.65	0.62
6:BF:5017:THR:HG23	6:BF:5020:TRP:H	1.65	0.62
4:BD:5080:THR:HB	4:BD:5081:PRO:HD2	1.81	0.62
3:AC:40:ALA:O	3:AC:43:ILE:HG13	2.00	0.62
2:AB:206:GLY:O	2:AB:210:ILE:HG13	2.00	0.62
24:AB:608:CLA:H143	24:AD:404:CLA:HMB2	1.82	0.61
2:AB:224:ARG:HG3	7:AH:25:TRP:CD1	2.34	0.61
3:BC:5041:ARG:NH1	24:BC:5511:CLA:OBD	2.33	0.61
5:AE:26:THR:HB	36:AF:101:HEM:HAB	1.81	0.61
13:AO:123:GLU:HG2	13:AO:124:GLU:N	2.15	0.61
3:BC:5047:GLY:O	3:BC:5050:LEU:HB3	2.00	0.61
13:AO:69:LEU:HD12	13:AO:70:CYS:H	1.65	0.61
1:BA:5012:ASN:HD22	1:BA:5015:GLU:HB2	1.66	0.61
4:BD:5239:GLN:O	4:BD:5240:ALA:HB3	2.00	0.61
16:AV:99:VAL:O	16:AV:103:LYS:HG3	2.00	0.61
2:BB:5284:ILE:HG23	2:BB:5305:ILE:CD1	2.30	0.61
31:AB:621:LMG:H411	4:AD:284:ILE:HG12	1.82	0.61
2:BB:5068:ARG:HH22	24:BB:5608:CLA:CED	2.12	0.61
2:BB:5027:THR:CG2	2:BB:5107:LEU:HD13	2.21	0.61
2:BB:5134:ASP:OD2	2:BB:5137:LYS:HB2	2.00	0.61
2:AB:453:PHE:HB2	4:AD:291:LEU:HD23	1.82	0.61
11:BL:5007:ARG:O	11:BL:5007:ARG:HD2	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:62:PHE:CE2	10:AK:28:ILE:HB	2.34	0.61
1:BA:5064:ARG:HD3	1:BA:5064:ARG:N	2.14	0.61
2:AB:142:HIS:HA	2:AB:145:LEU:HD12	1.83	0.61
13:BO:5151:LEU:HD12	13:BO:5152:VAL:H	1.65	0.61
5:BE:5051:ARG:HG3	5:BE:5051:ARG:HH11	1.65	0.61
2:BB:5247:PHE:HB2	24:BB:5612:CLA:HBC1	1.81	0.61
1:BA:5200:LEU:HD13	28:BC:5519:DGD:HAW2	1.78	0.61
24:AB:611:CLA:H201	24:AB:613:CLA:H92	1.82	0.61
29:AA:412:LHG:HC11	3:AC:447:ARG:NH2	2.16	0.61
2:BB:5468:TRP:HD1	2:BB:5469:HIS:ND1	1.98	0.61
28:BA:5412:DGD:HO2D	3:BC:5216:SER:HB2	1.64	0.61
3:BC:5114:VAL:HG22	31:BC:5521:LMG:H141	1.81	0.61
4:BD:5207:GLY:HA3	4:BD:5275:PRO:HG3	1.83	0.61
3:BC:5324:LEU:N	3:BC:5324:LEU:HD22	2.15	0.61
3:BC:5033:PHE:CE1	4:BD:5229:ALA:CB	2.84	0.61
24:BB:5612:CLA:H143	24:BD:5405:CLA:HMB2	1.83	0.61
3:BC:5264:PHE:HE1	27:BC:5516:BCR:H321	1.66	0.61
2:AB:179:GLN:NE2	2:AB:180:PRO:HD2	2.15	0.61
1:AA:10:SER:HB3	1:AA:16:ARG:NH1	2.14	0.61
3:AC:324:LEU:HD22	3:AC:324:LEU:N	2.16	0.61
1:BA:5131:TRP:CE3	1:BA:5132:GLU:N	2.69	0.61
24:BC:5511:CLA:H151	20:BZ:5024:PRO:HG3	1.83	0.61
2:BB:5383:PHE:CZ	13:BO:5193:GLY:HA2	2.35	0.61
27:AC:514:BCR:H391	10:AK:36:ALA:HB2	1.81	0.61
1:AA:133:LEU:O	1:AA:137:LEU:HG	2.00	0.61
3:AC:472:LEU:HG	4:AD:251:ARG:NH1	2.16	0.61
3:AC:223:TRP:CD2	3:AC:224:ILE:HG13	2.36	0.61
9:AJ:11:TRP:CE2	9:AJ:12:ILE:HG13	2.36	0.61
4:AD:18:LEU:HD22	18:AX:38:ILE:CD1	2.29	0.61
7:BH:5009:ASP:O	7:BH:5012:ARG:HB2	2.01	0.61
2:BB:5278:SER:HB3	2:BB:5281:GLN:HE21	1.65	0.61
3:AC:30:SER:HB3	10:AK:46:ARG:O	2.00	0.61
2:BB:5173:GLY:CA	2:BB:5265:ILE:HD11	2.31	0.61
13:AO:169:LYS:HG2	13:AO:224:SER:HB3	1.82	0.61
2:AB:246:PHE:C	2:AB:246:PHE:CD1	2.72	0.61
13:AO:151:LEU:HD12	13:AO:152:VAL:H	1.64	0.61
1:AA:343:LEU:O	1:AA:344:ALA:HB2	2.01	0.61
2:BB:5183:PRO:HG3	2:BB:5199:VAL:HG11	1.83	0.60
1:AA:262:TYR:CZ	31:AA:414:LMG:HC5	2.36	0.60
6:BF:5017:THR:O	6:BF:5021:VAL:HG23	2.00	0.60
8:BI:5008:VAL:O	8:BI:5012:VAL:HG23	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:222:PRO:HD2	2:AB:225:LEU:HD12	1.83	0.60
2:BB:5133:LEU:HB3	2:BB:5138:MET:CE	2.30	0.60
3:AC:113:VAL:HG11	31:AC:521:LMG:H132	1.83	0.60
1:BA:5300:PHE:CE2	28:BC:5519:DGD:O1A	2.54	0.60
2:AB:153:PHE:N	24:AB:606:CLA:HMC3	2.16	0.60
1:AA:262:TYR:OH	31:AA:414:LMG:HC5	2.00	0.60
16:AV:92:ARG:HH11	16:AV:92:ARG:HG3	1.66	0.60
7:BH:5006:TRP:CE2	7:BH:5010:ILE:HD11	2.36	0.60
35:BD:5406:PL9:C23	35:BD:5406:PL9:H303	2.31	0.60
16:BV:5038:LEU:HD12	16:BV:5095:ILE:HB	1.83	0.60
4:BD:5253:TRP:HA	4:BD:5256:ILE:HG22	1.84	0.60
1:AA:131:TRP:CE3	1:AA:132:GLU:N	2.70	0.60
2:AB:479:PHE:O	2:AB:480:SER:HB2	2.01	0.60
24:BC:5504:CLA:H152	28:BC:5519:DGD:HA91	1.84	0.60
24:AB:610:CLA:H121	24:AB:610:CLA:O1D	2.01	0.60
28:AA:411:DGD:HO2D	3:AC:216:SER:HB2	1.65	0.60
12:AM:19:SER:O	12:AM:23:ILE:HD13	2.01	0.60
15:BU:5113:THR:O	15:BU:5114:VAL:HG23	2.01	0.60
10:BK:5018:PHE:CE1	20:BZ:5009:LEU:HG	2.36	0.60
9:AJ:17:ALA:O	9:AJ:21:VAL:HG23	2.01	0.60
1:AA:324:ALA:HB2	4:AD:329:MET:SD	2.42	0.60
1:AA:306:VAL:HG13	1:AA:314:ILE:O	2.02	0.60
2:BB:5068:ARG:NH2	24:BB:5608:CLA:HED1	2.17	0.60
4:AD:80:THR:HG23	4:AD:172:SER:OG	2.01	0.60
3:AC:437:PHE:CZ	24:AC:502:CLA:HMC1	2.36	0.60
24:BC:5503:CLA:H171	24:BC:5510:CLA:HBB2	1.83	0.60
10:AK:18:PHE:CE1	20:AZ:9:LEU:HG	2.36	0.60
29:AA:415:LHG:HC41	29:AA:415:LHG:O9	2.02	0.60
12:BM:5001:MET:CG	12:BM:5002:GLU:H	2.13	0.60
16:AV:104:ASN:HA	16:AV:122:ARG:HD3	1.83	0.60
3:BC:5044:ASN:C	3:BC:5045:LEU:HD12	2.21	0.60
1:AA:297:LEU:HD11	3:AC:404:LEU:HD12	1.84	0.60
2:AB:284:ILE:HG23	2:AB:305:ILE:CD1	2.31	0.60
2:AB:284:ILE:HG23	2:AB:305:ILE:HD12	1.82	0.60
2:BB:5384:ARG:HD3	15:BU:5132:LEU:CD1	2.32	0.60
1:BA:5289:GLY:O	1:BA:5292:THR:CG2	2.49	0.60
24:AB:603:CLA:H161	7:AH:38:PHE:HE2	1.65	0.60
24:BB:5608:CLA:HMD2	24:BB:5616:CLA:H193	1.83	0.60
3:AC:41:ARG:NH1	24:AC:511:CLA:OBD	2.34	0.60
1:AA:188:ALA:HB2	1:AA:328:MET:HB2	1.84	0.60
3:AC:149:TYR:HA	3:AC:156:LYS:HD3	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:5145:ALA:HB2	4:BD:5272:LEU:HD21	1.83	0.60
2:BB:5124:ARG:HH11	2:BB:5124:ARG:HG3	1.67	0.60
13:BO:5118:SER:HB3	13:BO:5157:PRO:HA	1.84	0.60
2:AB:113:TRP:CE2	2:AB:117:TYR:HD1	2.20	0.60
30:AB:622:SQD:H442	4:AD:23:LYS:HE2	1.82	0.60
3:BC:5156:LYS:O	3:BC:5160:ILE:HG13	2.02	0.60
2:BB:5142:HIS:HA	2:BB:5145:LEU:HD12	1.83	0.60
13:AO:64:TYR:HD1	13:AO:271:PRO:HA	1.67	0.60
1:AA:326:LEU:HD21	3:AC:412:THR:HB	1.84	0.60
3:BC:5216:SER:HB3	3:BC:5221:GLU:HB2	1.84	0.60
27:BC:5516:BCR:HC41	8:BI:5020:VAL:HG13	1.82	0.60
27:BC:5514:BCR:H391	10:BK:5036:ALA:HB2	1.83	0.60
7:AH:6:TRP:CE2	7:AH:10:ILE:HD11	2.37	0.60
29:BA:5413:LHG:HC11	3:BC:5447:ARG:NH2	2.17	0.60
3:BC:5143:TYR:O	3:BC:5144:SER:HB2	2.02	0.60
3:BC:5413:GLU:HG3	3:BC:5414:ILE:N	2.17	0.59
3:AC:216:SER:HB3	3:AC:221:GLU:HB2	1.84	0.59
3:AC:233:VAL:HA	27:AC:516:BCR:H281	1.84	0.59
3:AC:52:ALA:CA	24:AC:511:CLA:HMB3	2.27	0.59
3:BC:5042:LEU:HD23	24:BC:5511:CLA:HED3	1.82	0.59
3:AC:167:VAL:HG11	24:AC:512:CLA:H3A	1.84	0.59
9:BJ:5017:ALA:O	9:BJ:5021:VAL:HG23	2.01	0.59
2:AB:27:THR:CG2	2:AB:107:LEU:HD13	2.25	0.59
24:AA:405:CLA:HBA2	31:AB:620:LMG:C25	2.32	0.59
10:BK:5024:VAL:O	10:BK:5027:VAL:HG12	2.02	0.59
5:AE:8:ARG:HH22	5:AE:16:SER:HB3	1.67	0.59
2:BB:5265:ILE:HG13	2:BB:5266:GLU:N	2.17	0.59
2:AB:359:MET:HB2	2:AB:425:ILE:HG23	1.84	0.59
1:BA:5288:LEU:HD22	3:BC:5432:VAL:HG23	1.82	0.59
1:BA:5265:PHE:CD1	1:BA:5271:LEU:HA	2.36	0.59
2:AB:280:PHE:CE2	2:AB:312:TYR:HB3	2.36	0.59
2:AB:349:LYS:HG3	2:AB:350:GLU:OE1	2.02	0.59
16:AV:47:LEU:HD11	16:AV:143:GLY:HA3	1.83	0.59
8:AI:1:MET:HE1	32:BB:5604:LMT:H41	1.84	0.59
3:BC:5178:LYS:HA	3:BC:5182:PHE:HB2	1.83	0.59
2:BB:5188:ASP:OD1	7:BH:5058:VAL:HA	2.03	0.59
13:BO:5083:LYS:HG2	13:BO:5084:ASN:H	1.66	0.59
13:AO:230:VAL:CG1	13:AO:231:ASP:H	2.13	0.59
4:AD:53:THR:HG22	4:AD:67:TYR:CD2	2.38	0.59
3:BC:5415:ASN:HB3	9:BJ:5039:SER:OG	2.03	0.59
4:BD:5014:TRP:CD1	4:BD:5015:PHE:N	2.70	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AF:19:ARG:HH11	6:AF:19:ARG:HG3	1.67	0.59
3:AC:324:LEU:CD2	3:AC:324:LEU:N	2.66	0.59
10:BK:5017:ILE:N	10:BK:5017:ILE:HD12	2.17	0.59
1:BA:5257:ARG:HH11	1:BA:5257:ARG:HG3	1.66	0.59
13:AO:206:GLU:CD	13:AO:206:GLU:H	2.05	0.59
24:AB:604:CLA:H121	24:AB:615:CLA:HBA1	1.83	0.59
1:BA:5220:THR:HG23	4:BD:5141:TYR:HD1	1.68	0.59
3:AC:362:ARG:HE	3:AC:370:ARG:NH1	1.99	0.59
2:BB:5487:SER:N	2:BB:5488:PRO:HD2	2.17	0.59
35:BD:5406:PL9:H262	35:BD:5406:PL9:C30	2.32	0.59
11:BL:5013:ASN:ND2	11:BL:5015:THR:HG22	2.18	0.59
3:AC:305:THR:HG22	3:AC:308:GLU:HB3	1.81	0.59
1:BA:5083:VAL:HG22	4:BD:5314:PHE:CE2	2.36	0.59
16:BV:5099:VAL:O	16:BV:5103:LYS:HG3	2.02	0.59
13:AO:218:LEU:HD22	15:AU:119:THR:HG21	1.84	0.59
24:BC:5504:CLA:H151	28:BC:5519:DGD:C9A	2.31	0.59
24:BB:5607:CLA:H161	7:BH:5038:PHE:HE2	1.68	0.59
3:BC:5037:ALA:C	24:BC:5508:CLA:HBA1	2.23	0.59
24:AC:511:CLA:H151	20:AZ:24:PRO:HG3	1.84	0.59
5:BE:5026:THR:HB	36:BF:5101:HEM:HAB	1.85	0.59
5:AE:51:ARG:NH1	5:AE:51:ARG:HG3	2.15	0.59
1:AA:97:TRP:HA	8:AI:1:MET:SD	2.43	0.59
6:BF:5037:ILE:HA	6:BF:5040:MET:SD	2.43	0.59
8:AI:14:PHE:CZ	8:AI:18:LEU:HD11	2.38	0.59
3:AC:178:LYS:HA	3:AC:182:PHE:HB2	1.84	0.59
1:AA:296:ASN:HB2	3:AC:400:PRO:O	2.02	0.59
4:AD:299:ILE:HG13	11:AL:37:ASN:HD21	1.67	0.59
1:BA:5032:TRP:HA	1:BA:5032:TRP:HE3	1.67	0.59
2:AB:483:ASP:HB3	2:AB:484:PRO:HD2	1.85	0.59
3:BC:5033:PHE:CE1	4:BD:5229:ALA:HB3	2.38	0.59
3:BC:5170:ILE:HG22	3:BC:5174:LEU:CD2	2.33	0.59
3:BC:5405:ASN:HB2	28:BC:5519:DGD:C3G	2.32	0.59
35:AD:405:PL9:H262	35:AD:405:PL9:C30	2.33	0.59
7:BH:5055:LEU:O	7:BH:5058:VAL:HG12	2.02	0.59
1:BA:5188:ALA:HB2	1:BA:5328:MET:HB2	1.85	0.59
10:BK:5031:LEU:O	10:BK:5034:ALA:HB3	2.03	0.59
2:AB:384:ARG:HD3	15:AU:132:LEU:HD11	1.85	0.59
15:AU:68:TYR:HB2	15:AU:71:LEU:HD12	1.84	0.59
3:AC:413:GLU:HG3	3:AC:414:ILE:N	2.18	0.59
3:AC:418:ASN:CB	28:AC:519:DGD:HE2	2.32	0.59
24:AA:405:CLA:H92	34:AD:402:PHO:HMB3	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:150:ILE:O	4:AD:154:VAL:HG23	2.03	0.59
24:BB:5612:CLA:H202	7:BH:5043:LEU:HD11	1.83	0.59
1:AA:64:ARG:HD3	1:AA:64:ARG:N	2.17	0.59
6:AF:15:ILE:HG22	6:AF:16:PHE:HD1	1.68	0.59
2:AB:356:VAL:HG22	2:AB:370:LEU:HD21	1.85	0.59
15:AU:98:THR:HG23	15:AU:101:GLN:OE1	2.03	0.59
1:AA:180:PHE:CD1	4:AD:192:THR:HB	2.38	0.58
2:BB:5458:PHE:HB3	24:BB:5608:CLA:HBC2	1.84	0.58
3:AC:156:LYS:O	3:AC:160:ILE:HG13	2.03	0.58
1:BA:5013:LEU:CA	1:BA:5016:ARG:HD3	2.33	0.58
4:AD:49:LEU:O	4:AD:53:THR:HG23	2.03	0.58
3:BC:5324:LEU:CD2	3:BC:5324:LEU:N	2.65	0.58
3:AC:33:PHE:CE1	4:AD:229:ALA:CB	2.85	0.58
12:AM:25:LEU:O	12:AM:28:GLN:HG3	2.03	0.58
24:AC:501:CLA:HMB3	27:AC:516:BCR:C40	2.31	0.58
3:AC:264:PHE:HE1	27:AC:516:BCR:H321	1.67	0.58
10:BK:5026:PRO:O	10:BK:5029:PRO:HD2	2.02	0.58
20:AZ:31:GLN:O	20:AZ:32:ASP:HB3	2.02	0.58
7:BH:5012:ARG:N	7:BH:5013:PRO:HD2	2.18	0.58
6:BF:5015:ILE:HG22	6:BF:5016:PHE:HD1	1.68	0.58
4:BD:5299:ILE:HG13	11:BL:5037:ASN:HD21	1.68	0.58
28:BC:5519:DGD:HG2	9:BJ:5033:TYR:OH	2.03	0.58
1:BA:5020:TRP:CD1	1:BA:5020:TRP:C	2.75	0.58
9:BJ:5011:TRP:CE3	10:BK:5042:ALA:HB2	2.39	0.58
15:AU:54:LYS:HD2	15:AU:113:THR:HG23	1.86	0.58
24:BB:5615:CLA:H201	24:BB:5617:CLA:H92	1.84	0.58
3:BC:5167:VAL:HG11	24:BC:5512:CLA:H3A	1.83	0.58
1:BA:5163:ILE:HG12	28:BC:5517:DGD:HB31	1.85	0.58
35:BD:5406:PL9:H301	35:BD:5406:PL9:C33	2.34	0.58
5:BE:5026:THR:O	5:BE:5029:ALA:HB3	2.02	0.58
2:AB:490:GLN:OE1	2:AB:490:GLN:O	2.21	0.58
2:AB:144:PHE:CE1	2:AB:210:ILE:HG23	2.39	0.58
1:AA:333:GLU:HB2	1:AA:337:HIS:HE1	1.68	0.58
3:AC:453:ALA:O	8:AI:34:ARG:HB2	2.03	0.58
3:BC:5110:PRO:O	3:BC:5114:VAL:HG23	2.02	0.58
3:BC:5116:VAL:HG23	3:BC:5117:VAL:N	2.19	0.58
2:BB:5359:MET:HB2	2:BB:5425:ILE:HG23	1.85	0.58
1:AA:271:LEU:C	1:AA:271:LEU:HD23	2.24	0.58
2:BB:5246:PHE:C	2:BB:5246:PHE:HD1	2.07	0.58
16:BV:5056:LYS:O	16:BV:5060:GLN:HG3	2.03	0.58
4:AD:41:ALA:HB1	34:AD:403:PHO:H42	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BT:5018:PHE:HB2	27:BT:5101:BCR:HC8	1.84	0.58
20:BZ:5033:TRP:HD1	20:BZ:5033:TRP:O	1.87	0.58
3:BC:5432:VAL:CG1	3:BC:5433:LEU:N	2.65	0.58
2:BB:5349:LYS:HG3	2:BB:5350:GLU:OE1	2.03	0.58
6:BF:5011:VAL:HG12	6:BF:5012:SER:H	1.69	0.58
2:AB:230:ARG:O	2:AB:233:ASN:HB3	2.04	0.58
3:AC:279:LEU:HD23	3:AC:282:MET:HE3	1.85	0.58
3:AC:39:ASN:HB3	24:AC:509:CLA:CBB	2.33	0.58
14:AT:18:PHE:HB2	27:AT:101:BCR:HC8	1.84	0.58
1:BA:5274:PHE:CE2	25:BA:5409:MST:H133	2.37	0.58
3:AC:257:PHE:O	3:AC:261:ARG:HG3	2.03	0.58
2:BB:5170:ASP:HB2	2:BB:5171:PRO:CD	2.32	0.58
3:AC:39:ASN:HB2	24:AC:508:CLA:HBA2	1.84	0.58
24:BB:5608:CLA:H121	24:BB:5619:CLA:HBA1	1.85	0.58
3:BC:5279:LEU:HD12	3:BC:5437:PHE:HE1	1.69	0.58
4:BD:5086:GLY:CA	4:BD:5166:SER:HB2	2.34	0.58
4:BD:5267:LEU:HD23	4:BD:5267:LEU:C	2.24	0.58
1:BA:5272:HIS:HD2	4:BD:5218:VAL:HG21	1.68	0.58
4:AD:244:TYR:OH	4:AD:264:LYS:HD2	2.03	0.58
16:BV:5133:LEU:H	16:BV:5133:LEU:CD1	2.16	0.58
1:AA:332:HIS:CD2	1:AA:333:GLU:HG3	2.38	0.58
16:AV:74:THR:O	16:AV:75:ASN:HB2	2.03	0.58
2:BB:5479:PHE:O	2:BB:5480:SER:HB2	2.03	0.58
6:BF:5018:VAL:HG12	6:BF:5019:ARG:N	2.19	0.58
8:BI:5027:ASP:N	8:BI:5028:PRO:CD	2.66	0.58
24:BB:5618:CLA:H202	31:BL:5101:LMG:H422	1.86	0.58
2:BB:5179:GLN:NE2	2:BB:5180:PRO:HD2	2.18	0.58
4:BD:5244:TYR:OH	4:BD:5264:LYS:HD2	2.04	0.58
4:AD:171:PRO:HG3	4:AD:181:PHE:CZ	2.39	0.58
3:BC:5367:GLU:HB2	3:BC:5368:PRO:HD3	1.86	0.58
3:AC:47:GLY:O	3:AC:50:LEU:HB3	2.03	0.58
1:AA:219:VAL:HG11	4:AD:268:HIS:CD2	2.38	0.58
1:BA:5307:ILE:HG22	1:BA:5313:VAL:HA	1.86	0.58
24:BA:5406:CLA:HBA2	31:BL:5101:LMG:C25	2.33	0.58
2:AB:383:PHE:CZ	13:AO:193:GLY:HA2	2.39	0.58
1:BA:5190:HIS:HB3	1:BA:5293:MET:CE	2.34	0.58
1:BA:5219:VAL:HG11	4:BD:5268:HIS:CD2	2.38	0.58
2:BB:5113:TRP:CE2	2:BB:5117:TYR:HD1	2.22	0.58
2:AB:135:LEU:HD23	2:AB:138:MET:HE1	1.86	0.57
3:AC:37:ALA:C	24:AC:508:CLA:HBA1	2.25	0.57
18:AX:16:LEU:O	18:AX:16:LEU:HD13	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:5226:SER:O	28:BC:5517:DGD:HE62	2.04	0.57
1:BA:5341:LEU:HB2	3:BC:5313:GLN:NE2	2.10	0.57
1:AA:330:VAL:CG1	4:AD:348:ARG:HG2	2.34	0.57
3:BC:5377:LEU:O	3:BC:5381:LYS:HB2	2.04	0.57
14:BT:5022:PHE:C	14:BT:5023:PHE:HD2	2.06	0.57
6:BF:5037:ILE:HG22	9:BJ:5028:PHE:CE1	2.38	0.57
13:BO:5123:GLU:HG2	13:BO:5124:GLU:N	2.17	0.57
24:AB:604:CLA:HMD2	24:AB:612:CLA:H193	1.86	0.57
1:BA:5283:VAL:HG21	34:BD:5403:PHO:HBC3	1.86	0.57
2:BB:5153:PHE:N	24:BB:5610:CLA:HMC3	2.19	0.57
24:BC:5505:CLA:O1A	8:BI:5023:PHE:CE1	2.57	0.57
1:AA:260:PHE:CZ	1:AA:263:ALA:HB2	2.39	0.57
3:AC:449:ARG:HG2	24:AC:505:CLA:HED1	1.86	0.57
8:AI:13:THR:HA	8:AI:16:VAL:HG12	1.86	0.57
30:BB:5625:SQD:H442	4:BD:5023:LYS:HE2	1.85	0.57
24:BB:5606:CLA:H11	7:BH:5049:TYR:HD2	1.69	0.57
3:BC:5297:TYR:HA	3:BC:5302:TYR:HE2	1.69	0.57
6:AF:37:ILE:HA	6:AF:40:MET:SD	2.44	0.57
24:AB:602:CLA:HBD	24:AB:602:CLA:H43	1.86	0.57
3:AC:279:LEU:HA	3:AC:282:MET:HE3	1.86	0.57
1:BA:5045:THR:HG23	1:BA:5046:ILE:N	2.18	0.57
24:BC:5512:CLA:H203	31:BC:5521:LMG:H381	1.86	0.57
11:BL:5008:GLN:N	11:BL:5008:GLN:NE2	2.52	0.57
20:AZ:23:VAL:O	20:AZ:26:ALA:HB3	2.05	0.57
13:AO:32:THR:O	13:AO:36:ILE:CD1	2.52	0.57
2:AB:458:PHE:HB3	24:AB:604:CLA:HBC2	1.86	0.57
3:AC:226:SER:O	28:AC:517:DGD:HE62	2.04	0.57
7:AH:58:VAL:O	7:AH:58:VAL:CG1	2.52	0.57
2:BB:5135:LEU:HD23	2:BB:5138:MET:HE1	1.86	0.57
32:BB:5627:LMT:H112	7:BH:5035:MET:HE2	1.87	0.57
2:BB:5262:THR:HG23	2:BB:5263:THR:HG23	1.86	0.57
2:AB:270:PRO:HG3	2:AB:312:TYR:HD2	1.69	0.57
3:BC:5220:GLY:N	28:BC:5517:DGD:O3D	2.35	0.57
2:AB:483:ASP:CG	2:AB:484:PRO:HD2	2.24	0.57
1:AA:13:LEU:CA	1:AA:16:ARG:HD3	2.34	0.57
1:AA:57:PRO:HD3	1:AA:73:TYR:CD2	2.40	0.57
1:BA:5317:TRP:CD1	4:BD:5177:ALA:HB2	2.38	0.57
3:BC:5039:ASN:HB2	24:BC:5508:CLA:HBA2	1.85	0.57
20:AZ:33:TRP:O	20:AZ:37:LYS:HB2	2.05	0.57
1:BA:5315:ASN:HD21	4:BD:5332:GLN:NE2	2.02	0.57
2:BB:5483:ASP:HB3	2:BB:5484:PRO:HD2	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AO:92:VAL:HG13	13:AO:93:PRO:HD2	1.87	0.57
3:AC:199:ILE:HD12	3:AC:199:ILE:N	2.18	0.57
4:BD:5056:THR:HG21	5:BE:5050:PRO:HD3	1.87	0.57
4:AD:335:PRO:HB2	5:AE:65:LEU:HD21	1.86	0.57
1:BA:5289:GLY:HA2	1:BA:5292:THR:HG22	1.86	0.57
2:BB:5237:VAL:HG22	24:BB:5614:CLA:HBC2	1.86	0.57
5:BE:5015:THR:HB	9:BJ:5006:GLY:HA2	1.87	0.57
24:AC:504:CLA:H2	28:AC:518:DGD:HA21	1.87	0.57
3:BC:5405:ASN:HA	28:BC:5519:DGD:HG11	1.87	0.57
28:BC:5519:DGD:O3D	9:BJ:5037:GLY:O	2.20	0.57
24:BB:5614:CLA:O1D	24:BB:5614:CLA:H121	2.04	0.57
1:AA:190:HIS:HB3	1:AA:293:MET:HE2	1.87	0.57
13:BO:5114:ASN:ND2	13:BO:5120:THR:HG23	2.20	0.57
2:AB:246:PHE:C	2:AB:246:PHE:HD1	2.08	0.57
3:AC:33:PHE:CE1	4:AD:229:ALA:HB3	2.38	0.57
24:AC:504:CLA:H172	28:AC:519:DGD:HAE1	1.85	0.57
24:BB:5613:CLA:HMC2	27:BX:5101:BCR:H343	1.85	0.57
3:BC:5233:VAL:HA	27:BC:5516:BCR:H281	1.87	0.57
5:BE:5017:VAL:HG22	9:BJ:5008:ILE:HD11	1.87	0.57
13:BO:5218:LEU:CD2	15:BU:5119:THR:HG21	2.35	0.57
3:AC:143:TYR:O	3:AC:144:SER:HB2	2.05	0.57
2:AB:327:THR:O	2:AB:444:ARG:NE	2.36	0.57
18:BX:5045:LYS:N	18:BX:5045:LYS:HD3	2.19	0.57
1:BA:5191:ASN:HB2	3:BC:5411:ALA:HB1	1.85	0.57
1:BA:5278:TRP:O	1:BA:5281:VAL:HG12	2.05	0.56
32:AB:624:LMT:H92	7:AH:35:MET:CE	2.35	0.56
24:BB:5606:CLA:HBD	24:BB:5606:CLA:H43	1.86	0.56
3:BC:5057:ALA:HB1	24:BC:5512:CLA:HED2	1.85	0.56
4:BD:5150:ILE:O	4:BD:5154:VAL:HG23	2.06	0.56
32:BB:5627:LMT:H92	7:BH:5035:MET:CE	2.35	0.56
3:BC:5062:PHE:HZ	10:BK:5028:ILE:HD12	1.69	0.56
5:BE:5077:GLU:HA	5:BE:5080:LEU:HD23	1.87	0.56
13:BO:5098:THR:HG23	13:BO:5133:THR:HB	1.87	0.56
25:AA:408:MST:N3	25:AA:408:MST:H122	2.20	0.56
2:AB:280:PHE:O	2:AB:284:ILE:HG13	2.05	0.56
4:AD:239:GLN:O	4:AD:240:ALA:HB3	2.04	0.56
2:AB:170:ASP:HB2	2:AB:171:PRO:CD	2.35	0.56
3:AC:367:GLU:HB2	3:AC:368:PRO:HD3	1.87	0.56
28:AA:411:DGD:O1B	28:AA:411:DGD:C1G	2.53	0.56
1:BA:5180:PHE:CE1	4:BD:5192:THR:HB	2.40	0.56
7:BH:5058:VAL:O	7:BH:5058:VAL:CG1	2.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AO:114:ASN:ND2	13:AO:120:THR:HG23	2.19	0.56
27:AC:516:BCR:HC41	8:AI:20:VAL:HG13	1.86	0.56
2:AB:462:PHE:CZ	24:AB:613:CLA:HMB3	2.40	0.56
24:AB:609:CLA:HMC2	27:AX:101:BCR:H343	1.87	0.56
2:BB:5462:PHE:HA	24:BB:5615:CLA:CMC	2.35	0.56
4:BD:5086:GLY:C	4:BD:5166:SER:HB2	2.25	0.56
4:BD:5158:LEU:O	4:BD:5162:LEU:HG	2.06	0.56
10:AK:26:PRO:O	10:AK:29:PRO:HD2	2.06	0.56
13:AO:80:GLU:O	13:AO:89:ALA:HB1	2.06	0.56
3:BC:5375:LEU:HB3	3:BC:5380:ILE:HD11	1.87	0.56
3:AC:116:VAL:HG23	3:AC:117:VAL:N	2.20	0.56
5:AE:56:TYR:HE1	5:AE:63:ILE:HD12	1.69	0.56
1:AA:262:TYR:CE1	31:AA:414:LMG:C5	2.89	0.56
4:BD:5221:THR:CG2	4:BD:5244:TYR:HB2	2.35	0.56
2:BB:5271:THR:OG1	2:BB:5274:GLN:HG3	2.05	0.56
1:AA:15:GLU:O	1:AA:19:ASN:OD1	2.23	0.56
3:AC:343:ARG:NH1	3:AC:347:GLY:O	2.38	0.56
3:BC:5199:ILE:N	3:BC:5199:ILE:HD12	2.20	0.56
8:AI:27:ASP:N	8:AI:28:PRO:CD	2.68	0.56
2:BB:5453:PHE:HB2	4:BD:5291:LEU:HD23	1.87	0.56
3:BC:5304:PRO:HB3	3:BC:5395:TYR:CD1	2.40	0.56
20:BZ:5014:ILE:O	20:BZ:5018:VAL:HG23	2.05	0.56
3:BC:5362:ARG:HE	3:BC:5370:ARG:HH11	1.52	0.56
1:AA:278:TRP:O	1:AA:281:VAL:HG12	2.04	0.56
5:AE:69:ARG:HG3	5:AE:70:PHE:N	2.21	0.56
2:BB:5027:THR:HG22	2:BB:5107:LEU:CD1	2.24	0.56
8:BI:5013:THR:HA	8:BI:5016:VAL:HG12	1.85	0.56
10:AK:31:LEU:O	10:AK:34:ALA:HB3	2.05	0.56
13:BO:5154:SER:O	13:BO:5168:PHE:HA	2.05	0.56
5:BE:5051:ARG:HG3	5:BE:5051:ARG:NH1	2.19	0.56
3:BC:5297:TYR:HA	3:BC:5302:TYR:CE2	2.40	0.56
1:AA:126:TYR:O	1:AA:130:GLN:HG3	2.06	0.56
1:BA:5326:LEU:HD21	3:BC:5412:THR:HB	1.87	0.56
5:BE:5014:ILE:CG2	9:BJ:5013:VAL:HG11	2.35	0.56
24:AB:611:CLA:C5	24:AB:614:CLA:HBC2	2.36	0.56
3:BC:5149:TYR:HA	3:BC:5156:LYS:CD	2.35	0.56
2:AB:262:THR:HG23	2:AB:263:THR:HG23	1.88	0.56
16:AV:133:LEU:CD1	16:AV:133:LEU:H	2.18	0.56
2:AB:271:THR:OG1	2:AB:274:GLN:HG3	2.05	0.56
13:BO:5173:ASN:ND2	13:BO:5220:LYS:HD3	2.20	0.56
24:AC:505:CLA:O1A	8:AI:23:PHE:CE1	2.59	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AI:13:THR:O	8:AI:16:VAL:HG12	2.06	0.56
1:BA:5221:SER:HB3	4:BD:5141:TYR:HB2	1.86	0.56
15:BU:5083:ALA:CB	15:BU:5084:PRO:CD	2.82	0.56
3:BC:5158:THR:HG21	3:BC:5254:THR:O	2.06	0.56
3:BC:5461:ARG:NH2	4:BD:5242:GLU:O	2.38	0.56
4:AD:145:ALA:HB2	4:AD:272:LEU:HD21	1.86	0.56
3:AC:114:VAL:HG22	31:AC:521:LMG:H141	1.87	0.56
13:AO:148:VAL:HA	13:AO:172:PHE:CD2	2.40	0.56
2:AB:235:GLU:OE1	2:AB:472:ARG:NH1	2.39	0.56
2:BB:5206:GLY:O	2:BB:5210:ILE:HG13	2.05	0.56
2:BB:5280:PHE:CE2	2:BB:5312:TYR:HB3	2.40	0.56
2:BB:5270:PRO:HG3	2:BB:5312:TYR:HD2	1.70	0.56
1:AA:142:TRP:HB2	4:AD:220:ASN:OD1	2.05	0.56
13:BO:5215:ARG:NH1	13:BO:5252:GLY:O	2.38	0.56
1:AA:221:SER:HB3	4:AD:141:TYR:HB2	1.88	0.56
2:AB:250:PHE:CE2	2:AB:459:ALA:HB1	2.41	0.56
2:BB:5329:PRO:HD3	24:BB:5611:CLA:HED1	1.86	0.56
1:BA:5092:HIS:HD2	3:BC:5219:GLY:HA3	1.71	0.56
10:BK:5035:LEU:HA	10:BK:5038:VAL:HG23	1.88	0.56
13:BO:5080:GLU:O	13:BO:5089:ALA:HB1	2.05	0.56
3:AC:42:LEU:CD2	24:AC:511:CLA:HED3	2.36	0.56
5:BE:5056:TYR:HE1	5:BE:5063:ILE:HD12	1.71	0.56
2:BB:5179:GLN:HE21	2:BB:5180:PRO:HD2	1.71	0.56
4:BD:5129:GLN:HE22	4:BD:5143:ALA:HA	1.70	0.56
1:BA:5133:LEU:O	1:BA:5137:LEU:HG	2.06	0.56
1:BA:5124:SER:O	1:BA:5127:MET:HB3	2.06	0.56
3:AC:44:ASN:O	3:AC:45:LEU:HD12	2.05	0.56
4:AD:330:ALA:HB3	4:AD:331:PRO:HD3	1.88	0.56
3:AC:170:ILE:HG22	3:AC:174:LEU:CD2	2.36	0.56
5:AE:57:ALA:H	5:AE:60:GLN:NE2	2.04	0.56
4:AD:241:GLU:H	4:AD:241:GLU:CD	2.08	0.56
1:AA:157:VAL:HG21	24:AA:405:CLA:CMC	2.36	0.56
1:AA:180:PHE:CE1	4:AD:192:THR:HB	2.41	0.56
2:BB:5462:PHE:CZ	24:BB:5617:CLA:HMB3	2.41	0.56
5:BE:5069:ARG:HG3	5:BE:5070:PHE:N	2.20	0.56
5:AE:15:THR:HB	9:AJ:6:GLY:HA2	1.87	0.56
3:BC:5305:THR:HG22	3:BC:5308:GLU:HB3	1.83	0.56
3:AC:57:ALA:HB1	24:AC:512:CLA:HED2	1.88	0.56
15:AU:66:ILE:HG12	15:AU:72:TYR:CG	2.41	0.56
2:BB:5369:ILE:O	2:BB:5370:LEU:HD23	2.04	0.56
3:AC:374:GLY:O	3:AC:375:LEU:C	2.44	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:5343:ARG:NH1	3:BC:5347:GLY:O	2.39	0.56
1:BA:5057:PRO:HD3	1:BA:5073:TYR:CD2	2.41	0.56
4:BD:5092:LEU:HA	4:BD:5104:TRP:CD1	2.41	0.56
24:AB:608:CLA:H203	24:AD:404:CLA:HBA2	1.89	0.56
32:AB:624:LMT:H112	7:AH:35:MET:HE2	1.89	0.56
24:BA:5406:CLA:H93	34:BD:5403:PHO:HHB	1.88	0.56
15:BU:5058:ASN:HD22	15:BU:5114:VAL:HG13	1.69	0.56
3:BC:5374:GLY:O	3:BC:5375:LEU:C	2.44	0.56
4:BD:5346:LEU:O	4:BD:5348:ARG:HG3	2.06	0.56
1:AA:77:ILE:HD11	14:AT:6:TYR:HB3	1.87	0.56
3:AC:405:ASN:HA	28:AC:519:DGD:HG11	1.88	0.55
28:BC:5518:DGD:HB22	28:BC:5519:DGD:HA21	1.88	0.55
2:AB:133:LEU:HB3	2:AB:138:MET:HE2	1.88	0.55
3:AC:233:VAL:HA	27:AC:516:BCR:C28	2.36	0.55
3:AC:95:LEU:HD13	24:AC:502:CLA:H143	1.89	0.55
35:AD:405:PL9:H301	35:AD:405:PL9:C33	2.34	0.55
18:AX:12:ILE:HA	27:AX:101:BCR:H401	1.88	0.55
3:BC:5124:VAL:HB	27:BC:5515:BCR:H362	1.88	0.55
14:AT:29:ILE:N	14:AT:29:ILE:HD12	2.06	0.55
24:AC:513:CLA:H42	24:AC:513:CLA:HAA1	1.88	0.55
1:BA:5048:PHE:HA	1:BA:5115:ILE:HD11	1.88	0.55
3:BC:5416:SER:N	28:BC:5519:DGD:O3E	2.37	0.55
24:BA:5406:CLA:H92	34:BD:5403:PHO:HMB3	1.87	0.55
24:BB:5605:CLA:HMB1	27:BX:5101:BCR:H393	1.88	0.55
5:BE:5076:VAL:O	5:BE:5080:LEU:CD2	2.54	0.55
2:BB:5483:ASP:CG	2:BB:5484:PRO:HD2	2.26	0.55
2:BB:5144:PHE:CE1	2:BB:5210:ILE:HG23	2.41	0.55
3:BC:5033:PHE:HE1	4:BD:5229:ALA:CB	2.19	0.55
16:AV:81:ARG:HH11	16:AV:81:ARG:HG2	1.70	0.55
1:AA:304:HIS:CE1	3:AC:414:ILE:HD12	2.41	0.55
1:BA:5281:VAL:HG11	28:BC:5519:DGD:CIA	2.36	0.55
24:AB:601:CLA:HMB1	27:AX:101:BCR:H393	1.88	0.55
8:BI:5013:THR:O	8:BI:5016:VAL:HG12	2.06	0.55
1:AA:330:VAL:HG12	4:AD:348:ARG:HA	1.89	0.55
25:BA:5409:MST:N3	25:BA:5409:MST:H131	2.20	0.55
1:AA:217:SER:HA	1:AA:220:THR:HG22	1.88	0.55
4:AD:86:GLY:C	4:AD:166:SER:HB2	2.26	0.55
24:AA:405:CLA:H201	14:AT:14:ILE:HD11	1.86	0.55
3:BC:5225:VAL:HG22	3:BC:5289:PHE:CD1	2.42	0.55
4:BD:5014:TRP:NE1	7:BH:5025:TRP:HH2	1.95	0.55
2:BB:5154:GLY:O	2:BB:5159:THR:HG23	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BO:5092:VAL:HG13	13:BO:5093:PRO:HD2	1.87	0.55
4:BD:5239:GLN:O	4:BD:5240:ALA:CB	2.54	0.55
2:BB:5384:ARG:HD3	15:BU:5132:LEU:HD11	1.89	0.55
3:BC:5170:ILE:HG22	3:BC:5174:LEU:HD23	1.88	0.55
9:BJ:5011:TRP:CG	10:BK:5042:ALA:HA	2.41	0.55
15:BU:5098:THR:HG23	15:BU:5101:GLN:OE1	2.07	0.55
12:BM:5005:GLN:HE22	32:BM:5101:LMT:H3'	1.71	0.55
2:AB:231:MET:HG2	24:AB:610:CLA:HMC1	1.89	0.55
4:BD:5266:TRP:CD1	31:BD:5410:LMG:HC1	2.42	0.55
3:BC:5155:ASN:O	3:BC:5158:THR:HG22	2.07	0.55
20:BZ:5033:TRP:CD1	20:BZ:5033:TRP:O	2.60	0.55
15:BU:5066:ILE:HG12	15:BU:5072:TYR:CG	2.42	0.55
4:AD:253:TRP:HA	4:AD:256:ILE:HG22	1.89	0.55
1:AA:205:VAL:HG21	24:AA:404:CLA:CMA	2.37	0.55
24:AB:602:CLA:H11	7:AH:49:TYR:HD2	1.71	0.55
1:BA:5176:ILE:HG22	1:BA:5180:PHE:HE2	1.71	0.55
27:BC:5515:BCR:H312	20:BZ:5055:GLY:HA2	1.88	0.55
3:BC:5461:ARG:CG	3:BC:5461:ARG:NH1	2.61	0.55
5:AE:76:VAL:O	5:AE:80:LEU:HD22	2.06	0.55
2:AB:121:GLU:HG3	7:AH:4:ARG:CA	2.36	0.55
2:BB:5176:GLY:HA3	2:BB:5266:GLU:OE1	2.06	0.55
1:AA:124:SER:O	1:AA:127:MET:HB3	2.07	0.55
4:AD:221:THR:CG2	4:AD:244:TYR:HB2	2.36	0.55
4:BD:5049:LEU:O	4:BD:5053:THR:HG23	2.06	0.55
1:BA:5271:LEU:HD21	25:BA:5409:MST:H83	1.89	0.55
2:BB:5275:TRP:CH2	2:BB:5358:ARG:HD3	2.41	0.55
1:AA:191:ASN:HB2	3:AC:411:ALA:HB1	1.89	0.55
4:AD:201:VAL:O	4:AD:205:LEU:HB2	2.07	0.55
1:AA:340:PRO:HG2	3:AC:317:PHE:CZ	2.42	0.55
1:AA:20:TRP:C	1:AA:20:TRP:CD1	2.80	0.55
31:AB:620:LMG:H191	11:AL:22:LEU:HG	1.88	0.55
7:BH:5055:LEU:HB2	7:BH:5058:VAL:HG12	1.89	0.55
29:BA:5415:LHG:HC41	29:BA:5415:LHG:O9	2.05	0.55
12:AM:20:VAL:HG22	12:BM:5020:VAL:HG11	1.89	0.55
3:BC:5257:PHE:O	3:BC:5261:ARG:HG3	2.06	0.55
32:AB:630:LMT:H41	8:BI:5001:MET:CE	2.36	0.55
2:BB:5348:ASN:OD1	2:BB:5352:GLU:HB2	2.06	0.55
1:BA:5289:GLY:C	1:BA:5292:THR:HG22	2.27	0.55
2:AB:90:PHE:CE2	2:AB:91:TRP:CZ3	2.94	0.55
4:AD:259:ILE:HG12	31:AD:408:LMG:H301	1.89	0.55
12:AM:23:ILE:HG12	31:AM:101:LMG:H212	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5217:SER:HA	1:BA:5220:THR:HG22	1.89	0.55
1:BA:5157:VAL:HG21	24:BA:5406:CLA:CMC	2.36	0.55
24:BC:5513:CLA:H42	24:BC:5513:CLA:HAA1	1.88	0.55
3:AC:35:TRP:O	24:AC:511:CLA:HMD3	2.07	0.55
1:AA:341:LEU:HB2	3:AC:313:GLN:NE2	2.17	0.55
2:BB:5354:LEU:HD21	2:BB:5378:LYS:HB2	1.89	0.55
20:BZ:5032:ASP:CG	20:BZ:5033:TRP:N	2.57	0.55
32:AB:630:LMT:H41	8:BI:5001:MET:HE1	1.89	0.55
13:AO:64:TYR:CD1	13:AO:271:PRO:HA	2.41	0.55
3:BC:5281:MET:O	3:BC:5285:ILE:HG13	2.06	0.55
13:BO:5064:TYR:HD1	13:BO:5271:PRO:HA	1.72	0.55
4:BD:5313:THR:OG1	4:BD:5315:TYR:HB3	2.07	0.55
2:BB:5230:ARG:O	2:BB:5233:ASN:HB3	2.07	0.55
30:BB:5625:SQD:H152	32:BB:5627:LMT:H81	1.89	0.55
3:AC:62:PHE:HZ	10:AK:28:ILE:HD12	1.71	0.55
3:BC:5453:ALA:C	8:BI:5034:ARG:HB2	2.27	0.55
7:BH:5011:LEU:C	7:BH:5013:PRO:HD2	2.28	0.55
25:AA:408:MST:N3	25:AA:408:MST:H131	2.21	0.55
13:AO:173:ASN:ND2	13:AO:220:LYS:HD3	2.22	0.55
1:BA:5281:VAL:CG1	28:BC:5519:DGD:CIA	2.84	0.55
24:AB:613:CLA:H203	31:AD:407:LMG:H401	1.89	0.55
28:BA:5412:DGD:C1G	28:BA:5412:DGD:O1B	2.55	0.55
27:BC:5515:BCR:C31	20:BZ:5055:GLY:HA2	2.37	0.55
2:AB:76:SER:HB3	31:BA:5402:LMG:H301	1.88	0.55
24:AC:512:CLA:H203	31:AC:521:LMG:H381	1.88	0.55
1:BA:5064:ARG:HD3	1:BA:5064:ARG:H	1.72	0.55
1:AA:288:LEU:HD13	3:AC:432:VAL:CG2	2.37	0.55
4:BD:5053:THR:HG22	4:BD:5067:TYR:HE2	1.72	0.55
4:BD:5077:ALA:HB2	4:BD:5174:GLY:HA3	1.88	0.55
13:AO:92:VAL:HG12	13:AO:93:PRO:HD2	1.88	0.55
1:BA:5330:VAL:HG12	4:BD:5348:ARG:HA	1.87	0.55
2:AB:487:SER:N	2:AB:488:PRO:HD2	2.22	0.55
3:BC:5326:ALA:HB2	15:BU:5128:TYR:CG	2.42	0.55
28:AC:519:DGD:HE62	9:AJ:40:LEU:HD11	1.89	0.54
1:AA:38:ILE:HB	1:AA:39:PRO:HD3	1.89	0.54
2:AB:18:ARG:HD3	2:AB:118:TRP:HB3	1.87	0.54
1:BA:5234:ASN:HB2	31:BL:5101:LMG:O3	2.05	0.54
30:AA:416:SQD:H302	24:BB:5620:CLA:H51	1.88	0.54
3:BC:5095:LEU:HD13	24:BC:5502:CLA:H143	1.87	0.54
4:BD:5086:GLY:HA2	4:BD:5166:SER:HB2	1.88	0.54
15:AU:57:LEU:HD11	15:AU:112:PHE:HB3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AO:116:ASP:C	13:AO:116:ASP:OD2	2.46	0.54
3:BC:5259:TRP:HD1	3:BC:5259:TRP:H	1.55	0.54
13:BO:5086:ARG:O	13:BO:5086:ARG:NE	2.40	0.54
1:AA:289:GLY:HA2	1:AA:292:THR:HG22	1.90	0.54
1:AA:32:TRP:HE3	1:AA:32:TRP:HA	1.72	0.54
3:AC:279:LEU:HD12	3:AC:437:PHE:HE1	1.73	0.54
2:AB:222:PRO:CG	7:AH:27:THR:H	2.20	0.54
2:BB:5068:ARG:NH1	24:BB:5608:CLA:HED1	2.22	0.54
2:BB:5222:PRO:HD2	2:BB:5225:LEU:HD12	1.88	0.54
24:BB:5617:CLA:H203	31:BD:5409:LMG:H401	1.88	0.54
3:BC:5279:LEU:HD23	3:BC:5282:MET:HE3	1.89	0.54
3:BC:5279:LEU:HA	3:BC:5282:MET:HE3	1.89	0.54
8:BI:5010:ILE:HG21	32:BI:5102:LMT:H82	1.88	0.54
3:BC:5035:TRP:O	24:BC:5511:CLA:HMD3	2.07	0.54
7:BH:5017:GLU:CD	7:BH:5017:GLU:H	2.10	0.54
20:BZ:5012:LEU:HD12	20:BZ:5012:LEU:O	2.08	0.54
24:AB:609:CLA:OBD	7:AH:27:THR:HB	2.06	0.54
24:BB:5615:CLA:C5	24:BB:5618:CLA:HBC2	2.38	0.54
3:BC:5279:LEU:HD22	24:BC:5503:CLA:H143	1.89	0.54
20:BZ:5023:VAL:O	20:BZ:5026:ALA:HB3	2.08	0.54
3:AC:466:VAL:HA	3:AC:469:MET:HE1	1.89	0.54
15:BU:5064:ALA:O	15:BU:5067:GLN:HG2	2.06	0.54
4:BD:5330:ALA:HB3	4:BD:5331:PRO:HD3	1.89	0.54
24:AB:610:CLA:HBB1	24:AB:610:CLA:HHC	1.89	0.54
4:AD:14:TRP:NE1	7:AH:25:TRP:HH2	1.93	0.54
7:AH:55:LEU:HB2	7:AH:58:VAL:HG12	1.88	0.54
2:BB:5183:PRO:HB2	2:BB:5185:TRP:CH2	2.42	0.54
13:AO:154:SER:O	13:AO:168:PHE:HA	2.07	0.54
5:BE:5034:GLY:CA	6:BF:5032:PHE:CE1	2.90	0.54
1:BA:5069:GLY:HA2	1:BA:5075:ASN:ND2	2.22	0.54
13:AO:117:GLY:O	13:AO:159:VAL:HG12	2.07	0.54
1:AA:214:MET:HE2	1:AA:214:MET:HA	1.90	0.54
2:AB:27:THR:HG22	2:AB:107:LEU:CD1	2.28	0.54
24:AB:603:CLA:H161	7:AH:38:PHE:CE2	2.43	0.54
4:AD:152:VAL:HG11	24:AD:401:CLA:H11	1.88	0.54
2:BB:5018:ARG:HD3	2:BB:5118:TRP:HB3	1.89	0.54
31:BD:5410:LMG:H192	31:BL:5101:LMG:H201	1.89	0.54
3:AC:126:GLY:O	3:AC:130:VAL:HG23	2.07	0.54
20:BZ:5032:ASP:C	20:BZ:5034:ASP:N	2.60	0.54
4:AD:128:ARG:HG2	4:AD:129:GLN:N	2.22	0.54
1:AA:261:GLN:NE2	2:AB:489:GLU:HG3	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AV:71:ILE:C	16:AV:71:ILE:HD12	2.28	0.54
27:BD:5407:BCR:H343	27:BD:5407:BCR:H321	1.89	0.54
3:AC:281:MET:O	3:AC:285:ILE:HG13	2.07	0.54
13:BO:5180:ALA:HB1	13:BO:5191:ALA:HB2	1.90	0.54
28:AA:411:DGD:O1B	28:AA:411:DGD:HG12	2.07	0.54
24:AB:614:CLA:H202	31:AB:620:LMG:H422	1.90	0.54
12:AM:33:GLN:HA	31:AM:101:LMG:HC62	1.90	0.54
2:BB:5058:GLN:O	24:BB:5611:CLA:HED3	2.07	0.54
20:AZ:33:TRP:O	20:AZ:33:TRP:HD1	1.90	0.54
4:BD:5185:PHE:CE2	4:BD:5289:LEU:HD12	2.42	0.54
2:AB:12:LEU:CD1	2:AB:19:LEU:HD12	2.38	0.54
2:BB:5133:LEU:HB3	2:BB:5138:MET:HE2	1.89	0.54
35:BD:5406:PL9:H401	11:BL:5029:LEU:HD23	1.90	0.54
3:BC:5042:LEU:CD2	24:BC:5511:CLA:HED3	2.37	0.54
1:BA:5315:ASN:ND2	4:BD:5332:GLN:NE2	2.56	0.54
1:BA:5064:ARG:HG3	1:BA:5064:ARG:HH11	1.71	0.54
1:BA:5240:GLY:HA3	14:BT:5029:ILE:HG22	1.88	0.54
24:AA:405:CLA:H93	34:AD:402:PHO:HHB	1.89	0.54
2:AB:237:VAL:HG22	24:AB:610:CLA:HBC2	1.88	0.54
35:AD:405:PL9:H401	11:AL:29:LEU:HD23	1.90	0.54
24:BA:5405:CLA:H202	34:BD:5403:PHO:HMA2	1.89	0.54
24:BA:5406:CLA:C9	34:BD:5403:PHO:HHB	2.37	0.54
4:BD:5259:ILE:HG12	31:BD:5410:LMG:H301	1.89	0.54
3:BC:5155:ASN:CA	3:BC:5158:THR:HG22	2.36	0.54
3:BC:5311:GLN:OE1	3:BC:5355:THR:HG22	2.08	0.54
3:AC:166:ILE:HG23	3:AC:245:ILE:HG23	1.90	0.54
1:BA:5013:LEU:N	1:BA:5016:ARG:HH11	2.06	0.54
1:BA:5081:ALA:CB	1:BA:5175:GLY:HA3	2.37	0.54
2:BB:5011:VAL:HG23	11:BL:5006:ASN:O	2.07	0.54
6:BF:5011:VAL:HG12	6:BF:5012:SER:N	2.23	0.54
4:BD:5335:PRO:HB2	5:BE:5065:LEU:HD21	1.89	0.54
11:AL:18:TYR:CE2	14:AT:20:ALA:HA	2.43	0.54
1:BA:5278:TRP:CE3	28:BC:5519:DGD:HAG1	2.41	0.54
1:BA:5119:PHE:HZ	24:BA:5405:CLA:H101	1.72	0.54
3:BC:5223:TRP:CE3	3:BC:5224:ILE:HG13	2.43	0.54
5:AE:76:VAL:O	5:AE:80:LEU:CD2	2.56	0.54
1:AA:12:ASN:HD22	1:AA:15:GLU:HB2	1.73	0.54
1:BA:5012:ASN:ND2	1:BA:5015:GLU:HB2	2.22	0.54
2:BB:5246:PHE:CE2	2:BB:5463:PHE:HA	2.43	0.54
2:AB:393:GLU:HG2	15:AU:44:ASP:O	2.08	0.54
10:AK:43:VAL:HG21	10:AK:46:ARG:HE	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:64:ARG:HH11	1:AA:64:ARG:HG3	1.73	0.54
12:BM:5023:ILE:HG12	31:BM:5102:LMG:H212	1.90	0.54
1:BA:5260:PHE:CZ	1:BA:5263:ALA:HB2	2.43	0.54
3:BC:5472:LEU:HG	4:BD:5251:ARG:HH12	1.72	0.54
2:AB:265:ILE:HG13	2:AB:266:GLU:N	2.21	0.54
4:BD:5238:THR:O	4:BD:5239:GLN:O	2.26	0.54
2:BB:5356:VAL:HA	2:BB:5370:LEU:HD22	1.90	0.54
2:BB:5331:ASN:HB3	2:BB:5437:LEU:HD22	1.88	0.54
18:BX:5022:GLY:HA2	18:BX:5025:SER:OG	2.08	0.54
16:BV:5104:ASN:HA	16:BV:5122:ARG:HD3	1.90	0.54
1:BA:5340:PRO:HG2	3:BC:5317:PHE:CZ	2.43	0.54
3:BC:5250:TRP:C	3:BC:5250:TRP:CD1	2.81	0.54
3:AC:259:TRP:HD1	3:AC:259:TRP:H	1.56	0.54
15:AU:113:THR:O	15:AU:114:VAL:HG23	2.08	0.53
15:AU:50:ALA:HB1	15:AU:113:THR:HG21	1.90	0.53
1:BA:5244:GLU:OE2	4:BD:5264:LYS:NZ	2.41	0.53
1:BA:5271:LEU:HD23	1:BA:5271:LEU:C	2.28	0.53
1:AA:81:ALA:CB	1:AA:175:GLY:HA3	2.37	0.53
16:AV:38:LEU:HD12	16:AV:95:ILE:HB	1.89	0.53
2:AB:192:PRO:HD2	7:AH:60:VAL:HG12	1.91	0.53
1:BA:5126:TYR:O	1:BA:5130:GLN:HG3	2.07	0.53
2:AB:157:HIS:HD2	2:AB:158:LEU:HD23	1.73	0.53
24:AA:404:CLA:H202	34:AD:402:PHO:HMA2	1.89	0.53
2:BB:5250:PHE:CE2	2:BB:5459:ALA:HB1	2.43	0.53
24:BB:5609:CLA:H141	24:BB:5614:CLA:HED2	1.88	0.53
24:BB:5612:CLA:H203	24:BD:5405:CLA:HBA2	1.89	0.53
10:AK:19:ASP:N	10:AK:20:PRO:CD	2.70	0.53
3:AC:163:PHE:O	3:AC:167:VAL:HG23	2.09	0.53
1:AA:262:TYR:HE1	31:AA:414:LMG:HC5	1.72	0.53
3:AC:170:ILE:HG22	3:AC:174:LEU:HD23	1.91	0.53
16:BV:5146:LEU:O	16:BV:5150:LYS:HG3	2.08	0.53
1:AA:119:PHE:HZ	24:AA:404:CLA:H101	1.74	0.53
9:AJ:19:MET:O	9:AJ:23:VAL:HG23	2.07	0.53
3:BC:5155:ASN:HA	3:BC:5158:THR:CG2	2.34	0.53
3:AC:432:VAL:HG13	3:AC:433:LEU:N	2.23	0.53
1:AA:315:ASN:HD21	4:AD:332:GLN:NE2	2.05	0.53
3:BC:5044:ASN:O	3:BC:5045:LEU:HD12	2.08	0.53
9:BJ:5011:TRP:CE2	9:BJ:5012:ILE:HG13	2.42	0.53
1:BA:5332:HIS:HB3	4:BD:5321:LEU:HD21	1.90	0.53
4:BD:5068:LEU:HD11	5:BE:5044:TYR:CE1	2.43	0.53
2:AB:215:PHE:C	2:AB:215:PHE:CD2	2.82	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:415:ASN:O	3:AC:416:SER:CB	2.55	0.53
1:AA:92:HIS:HD2	3:AC:219:GLY:HA3	1.72	0.53
4:AD:86:GLY:CA	4:AD:166:SER:HB2	2.38	0.53
24:BA:5406:CLA:H201	14:BT:5014:ILE:HD11	1.90	0.53
3:AC:311:GLN:OE1	3:AC:355:THR:HG22	2.08	0.53
20:BZ:5049:ALA:O	20:BZ:5053:VAL:HG23	2.07	0.53
4:AD:26:ARG:HH11	4:AD:26:ARG:HG3	1.72	0.53
24:BC:5504:CLA:H2	28:BC:5518:DGD:HA21	1.89	0.53
2:AB:462:PHE:CE1	24:AB:613:CLA:HMB3	2.44	0.53
24:AB:608:CLA:H202	7:AH:43:LEU:HD11	1.90	0.53
31:AD:408:LMG:H392	27:AT:101:BCR:HC32	1.91	0.53
18:AX:12:ILE:HG23	18:AX:12:ILE:O	2.09	0.53
4:BD:5088:SER:CB	5:BE:5069:ARG:NH2	2.69	0.53
3:AC:124:VAL:HB	27:AC:515:BCR:H362	1.89	0.53
5:BE:5010:PHE:HD2	31:BE:5101:LMG:O2	1.92	0.53
1:BA:5190:HIS:O	1:BA:5298:ASN:HB3	2.09	0.53
13:AO:98:THR:HG23	13:AO:133:THR:HB	1.89	0.53
2:AB:348:ASN:OD1	2:AB:352:GLU:HB2	2.08	0.53
1:BA:5324:ALA:HB2	4:BD:5329:MET:SD	2.49	0.53
2:BB:5327:THR:O	2:BB:5444:ARG:NE	2.39	0.53
15:AU:64:ALA:O	15:AU:67:GLN:HG2	2.08	0.53
3:AC:437:PHE:CZ	24:AC:510:CLA:HMB3	2.44	0.53
2:BB:5231:MET:HG2	24:BB:5614:CLA:HMC1	1.90	0.53
11:BL:5022:LEU:HG	31:BL:5101:LMG:H191	1.89	0.53
11:BL:5022:LEU:O	11:BL:5026:VAL:HG22	2.08	0.53
3:AC:33:PHE:CD1	4:AD:229:ALA:HB3	2.43	0.53
3:AC:405:ASN:HB2	28:AC:519:DGD:C3G	2.38	0.53
3:AC:279:LEU:HD22	24:AC:503:CLA:H143	1.90	0.53
1:BA:5155:PHE:CE1	28:BA:5412:DGD:HBE1	2.44	0.53
2:BB:5030:VAL:HG12	24:BB:5609:CLA:HHH	1.91	0.53
3:BC:5149:TYR:CA	3:BC:5156:LYS:HD3	2.38	0.53
1:BA:5254:TYR:CD1	4:BD:5132:ILE:HG22	2.43	0.53
13:AO:144:LEU:HD13	13:AO:259:VAL:HG11	1.90	0.53
8:AI:1:MET:CE	32:BB:5604:LMT:H41	2.39	0.53
3:BC:5368:PRO:O	3:BC:5379:LYS:HE2	2.08	0.53
2:BB:5087:ASP:OD1	28:BB:5602:DGD:HD62	2.08	0.53
27:AD:406:BCR:H321	27:AD:406:BCR:H343	1.91	0.53
2:BB:5363:PHE:HD1	4:BD:5326:ARG:HD2	1.74	0.53
4:AD:160:TYR:HB3	4:AD:161:PRO:CD	2.39	0.53
16:BV:5074:THR:O	16:BV:5075:ASN:HB2	2.08	0.53
4:BD:5037:LEU:HD13	4:BD:5125:PHE:N	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:462:PHE:HA	24:AB:611:CLA:CMC	2.37	0.53
24:AB:616:CLA:H51	30:BA:5401:SQD:H302	1.90	0.53
2:BB:5062:VAL:CG1	24:BB:5609:CLA:HED3	2.39	0.53
3:BC:5387:TRP:CE2	3:BC:5388:GLN:HG3	2.44	0.53
2:AB:183:PRO:HB2	2:AB:185:TRP:CH2	2.44	0.53
2:AB:183:PRO:HG3	2:AB:199:VAL:HG12	1.90	0.53
13:AO:218:LEU:CD2	15:AU:119:THR:HG21	2.39	0.53
1:AA:332:HIS:HB3	4:AD:321:LEU:HD21	1.91	0.53
2:AB:154:GLY:O	2:AB:159:THR:HG23	2.08	0.53
1:BA:5333:GLU:HB2	1:BA:5337:HIS:HE1	1.74	0.53
13:AO:118:SER:HB3	13:AO:157:PRO:HA	1.91	0.53
1:AA:307:ILE:HG22	1:AA:313:VAL:HA	1.89	0.53
20:AZ:12:LEU:O	20:AZ:12:LEU:HD12	2.08	0.53
1:AA:289:GLY:O	1:AA:292:THR:CG2	2.53	0.53
24:AC:504:CLA:H151	28:AC:519:DGD:C9A	2.36	0.53
1:AA:234:ASN:HB2	31:AB:620:LMG:O3	2.09	0.53
2:AB:68:ARG:HH22	24:AB:604:CLA:CED	2.21	0.53
1:AA:220:THR:HG23	4:AD:141:TYR:HD1	1.73	0.53
10:AK:35:LEU:HA	10:AK:38:VAL:HG23	1.89	0.53
4:BD:5076:VAL:O	4:BD:5077:ALA:HB2	2.09	0.53
4:AD:313:THR:OG1	4:AD:315:TYR:HB3	2.09	0.53
2:AB:135:LEU:HD13	2:AB:237:VAL:CG2	2.39	0.53
2:AB:91:TRP:CD1	24:AB:606:CLA:HBD	2.43	0.53
2:AB:225:LEU:HD23	32:AB:624:LMT:H42	1.91	0.53
24:BA:5406:CLA:H152	24:BA:5406:CLA:H102	1.91	0.53
3:BC:5233:VAL:HA	27:BC:5516:BCR:C28	2.38	0.53
20:AZ:21:ILE:O	20:AZ:25:VAL:HG22	2.09	0.53
5:BE:5017:VAL:HG22	9:BJ:5008:ILE:CD1	2.38	0.53
12:AM:20:VAL:O	12:AM:24:ILE:HG13	2.07	0.53
4:BD:5134:ARG:HE	4:BD:5134:ARG:CA	2.21	0.53
3:BC:5166:ILE:HG23	3:BC:5245:ILE:HG23	1.91	0.53
5:BE:5008:ARG:HD3	5:BE:5013:ILE:HG12	1.91	0.53
20:AZ:47:TRP:O	20:AZ:50:LEU:HB2	2.09	0.53
1:BA:5142:TRP:HB2	4:BD:5220:ASN:OD1	2.09	0.53
24:AA:405:CLA:C9	34:AD:402:PHO:HHB	2.39	0.52
2:BB:5005:TRP:CH2	31:BL:5101:LMG:H291	2.44	0.52
24:BB:5614:CLA:HHC	24:BB:5614:CLA:HBB1	1.89	0.52
20:BZ:5030:PRO:C	20:BZ:5032:ASP:H	2.12	0.52
20:BZ:5035:ARG:O	20:BZ:5038:GLN:HB3	2.09	0.52
4:AD:239:GLN:O	4:AD:240:ALA:CB	2.56	0.52
3:BC:5137:PRO:HB2	3:BC:5139:THR:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BF:5041:GLN:HE21	6:BF:5041:GLN:N	2.07	0.52
1:AA:234:ASN:HD21	4:AD:266:TRP:CB	2.21	0.52
24:AA:405:CLA:H102	24:AA:405:CLA:H152	1.91	0.52
30:AB:622:SQD:H152	32:AB:624:LMT:H81	1.90	0.52
4:AD:267:LEU:C	4:AD:267:LEU:HD23	2.30	0.52
3:BC:5113:VAL:CG1	31:BC:5521:LMG:H132	2.40	0.52
3:BC:5279:LEU:HD23	3:BC:5282:MET:CE	2.39	0.52
3:BC:5042:LEU:HD13	24:BC:5511:CLA:HMA3	1.90	0.52
3:BC:5126:GLY:O	3:BC:5130:VAL:HG23	2.09	0.52
1:BA:5254:TYR:OH	4:BD:5129:GLN:HB3	2.09	0.52
20:AZ:30:PRO:C	20:AZ:32:ASP:H	2.12	0.52
20:AZ:34:ASP:OD1	20:AZ:35:ARG:N	2.42	0.52
13:BO:5223:ILE:HG12	13:BO:5224:SER:N	2.25	0.52
20:BZ:5002:THR:CG2	20:BZ:5003:ILE:N	2.72	0.52
3:BC:5337:LEU:HD12	13:BO:5131:PRO:CG	2.39	0.52
2:AB:246:PHE:CE2	2:AB:463:PHE:HA	2.44	0.52
4:AD:238:THR:O	4:AD:239:GLN:O	2.28	0.52
1:BA:5202:VAL:HG11	24:BA:5407:CLA:OBD	2.10	0.52
24:AC:504:CLA:H152	28:AC:519:DGD:HA91	1.90	0.52
24:AC:504:CLA:H61	28:AC:518:DGD:HA61	1.89	0.52
24:AB:611:CLA:H51	24:AB:614:CLA:HBC2	1.92	0.52
24:BB:5613:CLA:OBD	7:BH:5027:THR:HB	2.10	0.52
2:BB:5030:VAL:HG22	24:BB:5617:CLA:C3C	2.39	0.52
3:AC:38:GLY:HA3	24:AC:511:CLA:HMD3	1.92	0.52
3:AC:149:TYR:HA	3:AC:156:LYS:CD	2.40	0.52
2:BB:5324:LEU:HA	4:BD:5293:LEU:HD21	1.91	0.52
14:BT:5022:PHE:C	14:BT:5023:PHE:CD2	2.83	0.52
13:BO:5144:LEU:HD13	13:BO:5259:VAL:HG11	1.90	0.52
16:AV:90:PRO:O	16:AV:92:ARG:HD3	2.10	0.52
3:AC:33:PHE:HE1	4:AD:229:ALA:CB	2.21	0.52
3:AC:259:TRP:N	3:AC:259:TRP:CD1	2.78	0.52
1:BA:5035:VAL:HA	27:BA:5411:BCR:H333	1.90	0.52
16:AV:56:LYS:O	16:AV:60:GLN:HG3	2.09	0.52
2:BB:5143:LEU:HD12	2:BB:5143:LEU:O	2.10	0.52
4:BD:5302:GLU:OE2	4:BD:5302:GLU:HA	2.10	0.52
2:AB:62:VAL:CG1	24:AB:605:CLA:HED3	2.39	0.52
2:BB:5238:LEU:HB2	24:BB:5616:CLA:HMD3	1.91	0.52
15:BU:5054:LYS:HD2	15:BU:5113:THR:HG23	1.90	0.52
31:AA:414:LMG:O2	5:AE:10:PHE:HD2	1.92	0.52
16:AV:133:LEU:N	16:AV:133:LEU:HD12	2.24	0.52
4:AD:334:GLN:N	4:AD:335:PRO:HD3	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BO:5210:ARG:HA	15:BU:5039:LEU:CD1	2.40	0.52
16:BV:5081:ARG:HH11	16:BV:5081:ARG:HG2	1.73	0.52
1:AA:155:PHE:CE1	28:AA:411:DGD:HBE1	2.44	0.52
24:AB:615:CLA:H142	24:AB:616:CLA:H151	1.91	0.52
3:AC:220:GLY:N	28:AC:517:DGD:O3D	2.42	0.52
1:BA:5220:THR:CG2	4:BD:5141:TYR:HD1	2.23	0.52
1:BA:5157:VAL:HG11	24:BA:5406:CLA:HMC3	1.92	0.52
2:BB:5010:THR:HG22	2:BB:5013:ILE:HD11	1.92	0.52
2:BB:5090:PHE:CE2	2:BB:5091:TRP:CZ3	2.97	0.52
2:BB:5157:HIS:HD2	2:BB:5158:LEU:HD23	1.75	0.52
24:BB:5612:CLA:C4	4:BD:5127:LEU:HD11	2.20	0.52
1:AA:29:TYR:CD2	1:AA:133:LEU:HD13	2.45	0.52
12:AM:27:VAL:HG12	12:BM:5028:GLN:HB3	1.90	0.52
10:AK:17:ILE:N	10:AK:17:ILE:HD12	2.23	0.52
3:AC:452:ALA:O	3:AC:454:GLY:N	2.42	0.52
16:AV:119:PRO:HA	16:AV:127:PHE:CD2	2.44	0.52
4:AD:308:ASP:OD1	4:AD:308:ASP:C	2.47	0.52
2:AB:10:THR:C	2:AB:12:LEU:H	2.11	0.52
31:AB:620:LMG:H201	31:AD:408:LMG:H192	1.90	0.52
11:AL:22:LEU:O	11:AL:26:VAL:HG22	2.10	0.52
2:BB:5139:PHE:CZ	24:BB:5613:CLA:HMB3	2.45	0.52
2:AB:260:SER:HG	2:AB:262:THR:HG22	1.70	0.52
20:BZ:5002:THR:CG2	20:BZ:5003:ILE:H	2.22	0.52
2:AB:331:ASN:HB3	2:AB:437:LEU:HD22	1.92	0.52
13:AO:215:ARG:NH1	13:AO:252:GLY:O	2.43	0.52
3:BC:5141:GLU:CD	3:BC:5141:GLU:H	2.13	0.52
3:BC:5140:LEU:HB2	3:BC:5148:GLY:HA2	1.91	0.52
1:BA:5289:GLY:CA	1:BA:5292:THR:HG22	2.38	0.52
3:BC:5418:ASN:HA	28:BC:5519:DGD:HE2	1.91	0.52
2:AB:238:LEU:N	24:AB:612:CLA:HMD3	2.25	0.52
3:AC:279:LEU:HD23	3:AC:282:MET:CE	2.39	0.52
3:AC:437:PHE:HA	24:AC:508:CLA:HMC3	1.91	0.52
2:BB:5010:THR:C	2:BB:5012:LEU:H	2.11	0.52
31:BL:5101:LMG:H302	12:BM:5022:LEU:HD21	1.91	0.52
4:BD:5128:ARG:HG2	4:BD:5129:GLN:N	2.24	0.52
20:AZ:32:ASP:C	20:AZ:34:ASP:N	2.60	0.52
20:AZ:32:ASP:OD1	20:AZ:36:SER:HB2	2.10	0.52
3:AC:140:LEU:HB2	3:AC:148:GLY:HA2	1.92	0.52
3:AC:250:TRP:C	3:AC:250:TRP:CD1	2.82	0.52
24:AB:601:CLA:HBB1	24:AB:601:CLA:HHC	1.91	0.52
2:AB:30:VAL:HG22	24:AB:613:CLA:C3C	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5093:PHE:CZ	24:BA:5408:CLA:HBA1	2.45	0.52
3:BC:5149:TYR:CB	3:BC:5156:LYS:HD3	2.40	0.52
4:BD:5154:VAL:O	4:BD:5158:LEU:HB2	2.10	0.52
2:AB:354:LEU:HD21	2:AB:378:LYS:HB2	1.90	0.52
2:AB:356:VAL:HG22	2:AB:370:LEU:CD2	2.40	0.52
4:AD:236:ASN:ND2	4:AD:239:GLN:O	2.37	0.52
3:BC:5366:LEU:C	3:BC:5366:LEU:HD23	2.30	0.52
1:AA:193:LEU:HD13	4:AD:179:PHE:HB3	1.91	0.52
13:AO:91:PHE:CE1	13:AO:260:LYS:HB2	2.45	0.52
20:BZ:5042:LEU:O	20:BZ:5046:LEU:HB2	2.10	0.52
13:AO:180:ALA:HB1	13:AO:191:ALA:HB2	1.92	0.52
13:AO:46:PRO:HD2	13:AO:266:TYR:HD2	1.74	0.52
3:AC:366:LEU:HD23	3:AC:366:LEU:C	2.29	0.52
1:AA:176:ILE:HG22	1:AA:180:PHE:HE2	1.73	0.52
1:AA:216:GLY:O	1:AA:220:THR:HG22	2.10	0.52
4:AD:158:LEU:O	4:AD:162:LEU:HG	2.09	0.52
4:AD:88:SER:CB	5:AE:69:ARG:NH2	2.69	0.52
3:BC:5037:ALA:O	24:BC:5508:CLA:HBA1	2.10	0.52
3:BC:5052:ALA:CA	24:BC:5511:CLA:HMB3	2.28	0.52
5:AE:8:ARG:HD3	5:AE:13:ILE:HG12	1.92	0.52
5:AE:17:VAL:HG22	9:AJ:8:ILE:HD11	1.92	0.52
3:AC:149:TYR:CB	3:AC:156:LYS:HD3	2.40	0.52
1:BA:5315:ASN:ND2	4:BD:5332:GLN:HE22	2.06	0.52
1:BA:5064:ARG:HG3	1:BA:5064:ARG:NH1	2.25	0.52
3:AC:252:ILE:HG22	3:AC:253:LEU:HD23	1.91	0.52
5:AE:26:THR:HB	36:AF:101:HEM:CAB	2.40	0.52
25:BA:5409:MST:H122	25:BA:5409:MST:N3	2.24	0.52
7:AH:12:ARG:N	7:AH:13:PRO:HD2	2.25	0.52
3:BC:5362:ARG:HE	3:BC:5370:ARG:NH1	2.07	0.52
4:BD:5072:ASN:HA	31:BD:5408:LMG:HC72	1.92	0.52
13:BO:5059:ASP:C	13:BO:5061:SER:H	2.13	0.52
3:AC:193:GLY:O	3:AC:194:GLY:C	2.49	0.52
27:AT:101:BCR:H19C	27:BB:5622:BCR:H363	1.91	0.52
2:BB:5091:TRP:CD1	24:BB:5610:CLA:HBD	2.45	0.52
2:BB:5461:LEU:HD21	31:BB:5624:LMG:C43	2.39	0.52
13:BO:5230:VAL:CG1	13:BO:5231:ASP:H	2.17	0.52
2:AB:369:ILE:O	2:AB:370:LEU:HD23	2.09	0.52
4:BD:5201:VAL:O	4:BD:5205:LEU:HB2	2.09	0.52
1:BA:5027:ARG:NH1	1:BA:5027:ARG:O	2.43	0.52
3:BC:5214:LEU:N	3:BC:5214:LEU:HD22	2.24	0.52
4:BD:5026:ARG:HG3	4:BD:5026:ARG:HH11	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BC:5519:DGD:HE62	9:BJ:5040:LEU:HD11	1.93	0.51
1:BA:5159:LEU:HD11	28:BC:5517:DGD:HB51	1.92	0.51
4:BD:5274:VAL:HA	35:BD:5406:PL9:C25	2.34	0.51
3:BC:5038:GLY:HA3	24:BC:5511:CLA:HMD3	1.92	0.51
10:AK:18:PHE:C	10:AK:20:PRO:HD2	2.29	0.51
20:BZ:5031:GLN:O	20:BZ:5032:ASP:HB3	2.11	0.51
6:AF:11:VAL:CG1	6:AF:12:SER:H	2.20	0.51
2:BB:5121:GLU:HG3	7:BH:5004:ARG:CA	2.39	0.51
1:AA:315:ASN:ND2	4:AD:332:GLN:NE2	2.57	0.51
13:AO:84:ASN:ND2	2:BB:5431:GLU:OE2	2.43	0.51
1:BA:5082:VAL:HB	1:BA:5174:LEU:HB2	1.91	0.51
4:BD:5350:ASN:O	4:BD:5352:LEU:N	2.42	0.51
2:BB:5192:PRO:HD2	7:BH:5060:VAL:HG12	1.93	0.51
4:AD:35:ILE:O	24:AD:404:CLA:HBB2	2.11	0.51
1:AA:283:VAL:HG21	34:AD:402:PHO:HBC3	1.91	0.51
11:BL:5008:GLN:HB3	11:BL:5009:PRO:HD2	1.93	0.51
10:BK:5020:PRO:O	10:BK:5023:ASP:HB2	2.11	0.51
20:AZ:42:LEU:O	20:AZ:46:LEU:HB2	2.09	0.51
27:BK:5102:BCR:H331	27:BK:5102:BCR:HC8	1.92	0.51
1:BA:5011:ALA:O	1:BA:5012:ASN:CB	2.58	0.51
12:BM:5020:VAL:O	12:BM:5024:ILE:HG13	2.11	0.51
1:BA:5288:LEU:HD13	3:BC:5432:VAL:CG2	2.37	0.51
4:AD:77:ALA:HB2	4:AD:174:GLY:HA3	1.91	0.51
4:BD:5171:PRO:HG3	4:BD:5181:PHE:CE2	2.46	0.51
13:BO:5180:ALA:HB2	15:BU:5120:ALA:O	2.09	0.51
4:BD:5188:PHE:CZ	4:BD:5326:ARG:HG2	2.46	0.51
13:BO:5046:PRO:HD2	13:BO:5266:TYR:HD2	1.75	0.51
4:AD:92:LEU:HA	4:AD:104:TRP:CD1	2.45	0.51
1:AA:289:GLY:C	1:AA:292:THR:HG22	2.31	0.51
3:AC:415:ASN:HB3	9:AJ:39:SER:OG	2.08	0.51
24:AA:405:CLA:HMD2	24:AD:401:CLA:CBB	2.40	0.51
1:AA:38:ILE:HG23	30:AA:416:SQD:H131	1.93	0.51
1:AA:93:PHE:CZ	24:AA:407:CLA:HBA1	2.44	0.51
2:AB:10:THR:HG22	2:AB:13:ILE:HD11	1.92	0.51
2:AB:58:GLN:O	24:AB:607:CLA:HED3	2.10	0.51
2:BB:5012:LEU:CD1	2:BB:5019:LEU:HD12	2.40	0.51
2:BB:5027:THR:HG23	24:BB:5609:CLA:HMC1	1.93	0.51
2:BB:5135:LEU:HD13	2:BB:5237:VAL:CG2	2.41	0.51
3:BC:5163:PHE:O	3:BC:5167:VAL:HG23	2.09	0.51
4:BD:5259:ILE:HD13	14:BT:5021:ILE:HG12	1.93	0.51
24:BD:5405:CLA:H42	18:BX:5023:LEU:HA	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AJ:15:THR:O	9:AJ:19:MET:HG3	2.09	0.51
1:BA:5271:LEU:HD21	25:BA:5409:MST:C8	2.40	0.51
3:BC:5259:TRP:N	3:BC:5259:TRP:CD1	2.77	0.51
9:BJ:5019:MET:O	9:BJ:5023:VAL:HG23	2.10	0.51
3:AC:297:TYR:HA	3:AC:302:TYR:CE2	2.46	0.51
24:BC:5504:CLA:H61	28:BC:5518:DGD:HA61	1.92	0.51
14:AT:22:PHE:C	14:AT:23:PHE:HD2	2.14	0.51
1:BA:5020:TRP:O	1:BA:5021:VAL:C	2.49	0.51
24:BB:5607:CLA:H161	7:BH:5038:PHE:CE2	2.45	0.51
15:BU:5050:ALA:HB1	15:BU:5113:THR:HG21	1.93	0.51
3:AC:377:LEU:O	3:AC:381:LYS:HB2	2.10	0.51
4:AD:76:VAL:O	4:AD:77:ALA:HB2	2.10	0.51
4:BD:5334:GLN:N	4:BD:5335:PRO:HD3	2.24	0.51
4:AD:161:PRO:HB3	4:AD:170:ALA:HB2	1.93	0.51
16:BV:5058:LEU:HD13	16:BV:5137:ASP:HB3	1.92	0.51
2:AB:293:ALA:C	2:AB:295:GLY:H	2.14	0.51
2:BB:5433:ASP:OD1	2:BB:5433:ASP:C	2.47	0.51
3:BC:5204:LEU:HD21	3:BC:5238:ILE:HG21	1.92	0.51
2:AB:461:LEU:HD21	31:AB:621:LMG:C43	2.41	0.51
28:BA:5412:DGD:HG12	28:BA:5412:DGD:O1B	2.11	0.51
2:BB:5462:PHE:CE1	24:BB:5617:CLA:HMB3	2.44	0.51
24:BB:5619:CLA:H142	24:BB:5620:CLA:H151	1.92	0.51
4:BD:5266:TRP:HE1	31:BD:5410:LMG:HC72	1.74	0.51
5:AE:8:ARG:HB2	6:AF:13:TYR:CB	2.41	0.51
1:AA:64:ARG:HD3	1:AA:64:ARG:H	1.75	0.51
1:AA:83:VAL:HG22	4:AD:314:PHE:CE2	2.41	0.51
6:AF:23:VAL:O	6:AF:27:ALA:CB	2.59	0.51
7:AH:13:PRO:HG2	7:AH:14:LEU:H	1.75	0.51
1:BA:5129:ARG:NH2	4:BD:5256:ILE:HA	2.26	0.51
3:AC:453:ALA:HA	8:AI:34:ARG:O	2.10	0.51
18:BX:5022:GLY:HA2	18:BX:5025:SER:HG	1.75	0.51
3:BC:5458:GLY:HA2	4:BD:5222:LEU:O	2.11	0.51
2:AB:229:LEU:O	2:AB:231:MET:N	2.43	0.51
3:AC:158:THR:HG21	3:AC:254:THR:O	2.09	0.51
5:BE:5072:ALA:O	5:BE:5076:VAL:HG23	2.10	0.51
1:AA:82:VAL:HB	1:AA:174:LEU:HB2	1.92	0.51
4:AD:302:GLU:OE2	4:AD:302:GLU:HA	2.11	0.51
24:AB:611:CLA:H142	31:AB:620:LMG:H371	1.92	0.51
2:BB:5187:PRO:HB3	24:BB:5605:CLA:CMB	2.41	0.51
2:AB:377:VAL:HG11	4:AD:342:PRO:HG2	1.93	0.51
2:BB:5315:ILE:HG22	2:BB:5426:PHE:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:173:GLY:CA	2:AB:265:ILE:HD11	2.41	0.51
2:BB:5280:PHE:O	2:BB:5284:ILE:HG13	2.10	0.51
3:BC:5297:TYR:HD1	3:BC:5302:TYR:CE2	2.29	0.51
18:BX:5024:LEU:O	18:BX:5028:VAL:HG23	2.10	0.51
15:BU:5080:VAL:HG22	15:BU:5127:ARG:HH21	1.76	0.51
13:BO:5071:LEU:HD23	13:BO:5265:PHE:HB3	1.91	0.51
3:AC:321:ASP:OD2	15:AU:129:ASN:HB2	2.11	0.51
32:AB:624:LMT:H92	7:AH:35:MET:HE2	1.92	0.51
3:AC:37:ALA:O	24:AC:508:CLA:HBA1	2.11	0.51
4:AD:86:GLY:HA2	4:AD:166:SER:HB2	1.93	0.51
7:AH:55:LEU:HB2	7:AH:58:VAL:CG1	2.41	0.51
24:BB:5615:CLA:H142	31:BL:5101:LMG:H371	1.92	0.51
3:AC:42:LEU:HD13	24:AC:511:CLA:HMA3	1.93	0.51
5:AE:8:ARG:HB2	6:AF:13:TYR:HB3	1.93	0.51
2:AB:383:PHE:HE1	13:AO:194:TYR:CE2	2.29	0.51
1:AA:244:GLU:OE2	4:AD:264:LYS:NZ	2.43	0.51
20:AZ:2:THR:CG2	20:AZ:3:ILE:H	2.23	0.51
2:AB:356:VAL:HA	2:AB:370:LEU:HD22	1.93	0.51
3:AC:171:GLY:O	3:AC:174:LEU:HB2	2.11	0.51
3:AC:327:ASN:HB3	13:AO:125:ASP:OD1	2.11	0.51
11:AL:8:GLN:HE21	11:AL:8:GLN:N	2.08	0.51
31:AC:520:LMG:H292	27:AJ:101:BCR:H363	1.93	0.51
3:AC:264:PHE:HE1	27:AC:516:BCR:C32	2.24	0.51
2:BB:5015:ASP:N	2:BB:5016:PRO:HD3	2.26	0.51
2:BB:5091:TRP:CZ3	24:BB:5610:CLA:O1A	2.64	0.51
2:BB:5225:LEU:HD23	32:BB:5627:LMT:H42	1.92	0.51
14:BT:5018:PHE:HB2	27:BT:5101:BCR:H10C	1.93	0.51
3:BC:5028:GLN:HB2	24:BC:5511:CLA:CED	2.41	0.51
2:BB:5383:PHE:HE1	13:BO:5194:TYR:CE2	2.29	0.51
4:BD:5218:VAL:HG22	4:BD:5244:TYR:CE2	2.45	0.51
2:AB:383:PHE:HE1	13:AO:194:TYR:CD2	2.29	0.51
20:BZ:5034:ASP:OD1	20:BZ:5035:ARG:N	2.44	0.51
4:AD:134:ARG:CA	4:AD:134:ARG:HE	2.20	0.51
1:AA:129:ARG:NH2	4:AD:256:ILE:HA	2.26	0.51
2:BB:5251:VAL:O	2:BB:5255:THR:HG23	2.11	0.51
2:BB:5366:PHE:CD1	2:BB:5367:PRO:HD2	2.46	0.51
3:BC:5315:MET:HE1	3:BC:5369:LEU:HD12	1.92	0.51
3:BC:5094:THR:HG22	3:BC:5298:PRO:HD2	1.93	0.51
2:BB:5063:LEU:N	2:BB:5064:PRO:HD2	2.26	0.51
2:AB:243:ALA:HB2	2:AB:466:HIS:CE1	2.46	0.51
2:AB:30:VAL:HG12	24:AB:605:CLA:HHD	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:238:LEU:HB2	24:AB:612:CLA:HMD3	1.93	0.51
3:BC:5288:CYS:HB3	28:BC:5517:DGD:HG2	1.92	0.51
2:AB:414:PRO:HB2	2:AB:415:PRO:CD	2.35	0.51
15:AU:66:ILE:CG1	15:AU:72:TYR:CD1	2.94	0.51
13:AO:223:ILE:HG12	13:AO:224:SER:N	2.25	0.51
6:AF:23:VAL:O	6:AF:27:ALA:HB2	2.10	0.51
4:AD:53:THR:HG22	4:AD:67:TYR:HE2	1.75	0.51
13:BO:5092:VAL:HG12	13:BO:5093:PRO:HD2	1.91	0.51
1:AA:317:TRP:CD1	4:AD:177:ALA:HB2	2.46	0.51
4:AD:87:HIS:HB2	28:AH:101:DGD:O2D	2.11	0.50
31:AB:620:LMG:HC91	11:AL:19:LEU:CD1	2.41	0.50
1:BA:5205:VAL:HG21	24:BA:5405:CLA:CMA	2.41	0.50
3:BC:5264:PHE:HE1	27:BC:5516:BCR:C32	2.25	0.50
18:AX:43:ILE:O	18:AX:43:ILE:HG22	2.10	0.50
1:AA:262:TYR:HE1	31:AA:414:LMG:C5	2.24	0.50
2:AB:2:GLY:HA3	11:AL:9:PRO:HG2	1.93	0.50
2:AB:176:GLY:HA3	2:AB:266:GLU:OE1	2.12	0.50
18:BX:5044:ASP:O	18:BX:5045:LYS:HB3	2.11	0.50
3:AC:458:GLY:HA2	4:AD:222:LEU:O	2.10	0.50
27:AB:618:BCR:H363	27:BT:5101:BCR:H19C	1.92	0.50
31:AM:101:LMG:O2	11:BL:5009:PRO:HB3	2.11	0.50
2:BB:5354:LEU:N	2:BB:5354:LEU:HD12	2.26	0.50
2:BB:5172:TYR:OH	7:BH:5063:LYS:HE2	2.11	0.50
4:BD:5253:TRP:HB2	4:BD:5260:ALA:HB2	1.93	0.50
29:BA:5413:LHG:HC11	3:BC:5447:ARG:CZ	2.41	0.50
5:AE:14:ILE:CG2	9:AJ:13:VAL:HG11	2.41	0.50
13:AO:240:THR:HA	13:AO:264:VAL:HA	1.92	0.50
1:AA:92:HIS:CD2	3:AC:219:GLY:HA3	2.45	0.50
24:BC:5505:CLA:H2	24:BC:5505:CLA:HAA1	1.94	0.50
20:AZ:23:VAL:HG12	20:AZ:27:TYR:CE2	2.46	0.50
1:BA:5275:LEU:HD13	25:BA:5409:MST:H83	1.93	0.50
16:BV:5133:LEU:N	16:BV:5133:LEU:HD12	2.24	0.50
1:BA:5057:PRO:HD3	1:BA:5073:TYR:CE2	2.47	0.50
3:BC:5033:PHE:CD1	4:BD:5229:ALA:HB3	2.45	0.50
3:AC:321:ASP:OD1	3:AC:321:ASP:N	2.42	0.50
4:AD:37:LEU:HD13	4:AD:125:PHE:N	2.26	0.50
1:AA:200:LEU:HD11	28:AC:519:DGD:CCA	2.29	0.50
3:BC:5415:ASN:CB	9:BJ:5039:SER:OG	2.60	0.50
24:AB:612:CLA:H171	24:AB:613:CLA:HBB2	1.92	0.50
24:AC:502:CLA:H122	24:AC:503:CLA:HMB2	1.93	0.50
24:AA:405:CLA:H92	34:AD:402:PHO:CMB	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AH:50:ASN:HD22	28:AH:101:DGD:HA21	1.76	0.50
8:AI:19:PHE:CZ	8:AI:23:PHE:HE2	2.29	0.50
24:BA:5406:CLA:H92	34:BD:5403:PHO:CMB	2.41	0.50
2:BB:5139:PHE:HZ	24:BB:5613:CLA:HMB3	1.77	0.50
3:BC:5437:PHE:CZ	24:BC:5510:CLA:HMB3	2.47	0.50
3:BC:5437:PHE:HA	24:BC:5508:CLA:HMC3	1.92	0.50
11:BL:5019:LEU:CD1	31:BL:5101:LMG:HC91	2.42	0.50
1:AA:11:ALA:O	1:AA:12:ASN:CB	2.60	0.50
3:AC:262:ARG:HH21	32:AI:103:LMT:C5'	2.25	0.50
8:AI:21:PHE:HE1	32:AI:103:LMT:H41	1.75	0.50
10:AK:14:ALA:O	10:AK:17:ILE:HD13	2.10	0.50
1:AA:48:PHE:HA	1:AA:115:ILE:HD11	1.92	0.50
13:AO:46:PRO:HD2	13:AO:266:TYR:CD2	2.45	0.50
13:BO:5046:PRO:HD2	13:BO:5266:TYR:CD2	2.46	0.50
16:BV:5119:PRO:HA	16:BV:5127:PHE:CD2	2.46	0.50
2:BB:5215:PHE:C	2:BB:5215:PHE:CD2	2.85	0.50
2:BB:5405:GLU:HA	2:BB:5405:GLU:OE1	2.10	0.50
24:AC:501:CLA:CAD	24:AC:503:CLA:H12	2.42	0.50
24:AD:401:CLA:H2	34:AD:403:PHO:HBB1	1.92	0.50
24:BB:5616:CLA:H171	24:BB:5617:CLA:HBB2	1.93	0.50
18:BX:5012:ILE:O	18:BX:5012:ILE:HG13	2.11	0.50
13:BO:5032:THR:O	13:BO:5036:ILE:CD1	2.54	0.50
20:BZ:5033:TRP:O	20:BZ:5037:LYS:HB2	2.12	0.50
6:AF:19:ARG:O	6:AF:23:VAL:HG23	2.11	0.50
3:BC:5377:LEU:CD2	13:BO:5126:GLY:HA2	2.41	0.50
3:AC:326:ALA:HB2	15:AU:128:TYR:CG	2.46	0.50
3:AC:350:ILE:HG21	3:AC:359:TRP:HB2	1.93	0.50
3:BC:5193:GLY:O	3:BC:5194:GLY:C	2.48	0.50
3:AC:235:GLY:O	3:AC:238:ILE:HB	2.12	0.50
3:BC:5321:ASP:OD1	3:BC:5321:ASP:N	2.44	0.50
1:BA:5234:ASN:HD21	4:BD:5266:TRP:CB	2.23	0.50
2:BB:5377:VAL:HG11	4:BD:5342:PRO:HG2	1.93	0.50
13:AO:155:THR:HG23	13:AO:168:PHE:CE2	2.47	0.50
1:AA:57:PRO:HG3	1:AA:68:SER:CB	2.39	0.50
14:BT:5022:PHE:O	14:BT:5023:PHE:CD2	2.64	0.50
1:BA:5182:PHE:O	1:BA:5186:PHE:HB2	2.12	0.50
13:BO:5091:PHE:CE1	13:BO:5260:LYS:HB2	2.47	0.50
1:AA:20:TRP:O	1:AA:21:VAL:C	2.50	0.50
2:AB:5:TRP:CH2	31:AB:620:LMG:H291	2.47	0.50
3:AC:225:VAL:CG2	28:AC:517:DGD:HG11	2.41	0.50
4:BD:5279:LEU:HD22	24:BD:5402:CLA:HMA2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AK:43:VAL:CG2	10:AK:46:ARG:HE	2.24	0.50
1:AA:190:HIS:HB3	1:AA:293:MET:CE	2.41	0.50
27:AK:102:BCR:HC8	27:AK:102:BCR:H331	1.93	0.50
3:BC:5335:THR:HA	13:BO:5178:ARG:HD3	1.94	0.50
7:AH:11:LEU:HA	7:AH:14:LEU:HD12	1.93	0.50
13:AO:234:THR:HG1	13:AO:236:GLU:HG2	1.76	0.50
10:BK:5017:ILE:H	10:BK:5017:ILE:CD1	2.25	0.50
3:AC:368:PRO:O	3:AC:379:LYS:HE2	2.12	0.50
4:AD:190:ASN:HB2	4:AD:296:TYR:CE1	2.47	0.50
3:AC:418:ASN:CA	28:AC:519:DGD:HE2	2.42	0.50
2:AB:25:MET:HE2	27:AB:617:BCR:H393	1.93	0.50
4:AD:86:GLY:O	4:AD:166:SER:HB2	2.12	0.50
27:BC:5516:BCR:HC41	8:BI:5020:VAL:CG1	2.41	0.50
24:BA:5406:CLA:HMD2	24:BD:5402:CLA:CBB	2.42	0.50
14:AT:29:ILE:N	14:AT:29:ILE:CD1	2.71	0.50
1:BA:5258:LEU:HB3	1:BA:5259:ILE:CD1	2.40	0.50
3:BC:5055:ALA:CB	27:BC:5514:BCR:H373	2.38	0.50
12:BM:5025:LEU:N	12:BM:5025:LEU:HD23	2.27	0.50
5:BE:5014:ILE:O	5:BE:5014:ILE:HG22	2.12	0.50
13:BO:5225:LEU:N	13:BO:5225:LEU:HD12	2.27	0.50
31:AB:620:LMG:H302	12:AM:22:LEU:HD21	1.93	0.50
24:BB:5615:CLA:H51	24:BB:5618:CLA:HBC2	1.94	0.50
3:BC:5276:LEU:HD21	24:BC:5508:CLA:HBB1	1.93	0.50
11:BL:5022:LEU:HD13	14:BT:5016:LEU:HD23	1.94	0.50
3:AC:109:PHE:O	3:AC:113:VAL:HG23	2.11	0.50
1:BA:5275:LEU:HD13	25:BA:5409:MST:C8	2.42	0.50
10:AK:17:ILE:H	10:AK:17:ILE:CD1	2.23	0.50
3:AC:89:ILE:N	3:AC:90:PRO:CD	2.75	0.50
6:BF:5018:VAL:CG1	6:BF:5019:ARG:N	2.74	0.50
13:BO:5064:TYR:CD1	13:BO:5271:PRO:HA	2.47	0.50
1:AA:235:TYR:C	1:AA:237:TYR:H	2.16	0.50
13:AO:86:ARG:NE	13:AO:86:ARG:O	2.45	0.50
29:AA:412:LHG:HC11	3:AC:447:ARG:CZ	2.41	0.49
3:AC:223:TRP:CE3	3:AC:224:ILE:HG13	2.46	0.49
3:AC:29:GLU:CB	10:AK:46:ARG:NH1	2.71	0.49
1:AA:258:LEU:HB3	1:AA:259:ILE:CD1	2.39	0.49
3:BC:5171:GLY:O	3:BC:5174:LEU:HB2	2.12	0.49
13:BO:5117:GLY:O	13:BO:5159:VAL:HG12	2.11	0.49
1:AA:200:LEU:HD21	28:AC:519:DGD:HAW1	1.94	0.49
1:AA:289:GLY:CA	1:AA:292:THR:HG22	2.42	0.49
28:AC:519:DGD:HG2	9:AJ:33:TYR:OH	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:141:TYR:OH	31:AD:407:LMG:HC2	2.11	0.49
4:AD:154:VAL:O	4:AD:158:LEU:HB2	2.12	0.49
1:BA:5043:ALA:HB3	1:BA:5118:HIS:HD2	1.77	0.49
3:BC:5225:VAL:CG2	28:BC:5517:DGD:HG11	2.42	0.49
4:BD:5141:TYR:OH	31:BD:5409:LMG:HC2	2.13	0.49
9:AJ:18:GLY:HA3	27:AK:102:BCR:H371	1.94	0.49
4:BD:5053:THR:HA	4:BD:5067:TYR:CD2	2.47	0.49
2:BB:5235:GLU:OE1	2:BB:5472:ARG:NH1	2.44	0.49
1:AA:271:LEU:HD21	25:AA:408:MST:C8	2.41	0.49
1:BA:5257:ARG:NH1	1:BA:5257:ARG:HG3	2.26	0.49
15:BU:5080:VAL:HG22	15:BU:5127:ARG:NH2	2.27	0.49
4:AD:350:ASN:O	4:AD:352:LEU:N	2.42	0.49
1:AA:69:GLY:HA2	1:AA:75:ASN:ND2	2.27	0.49
2:BB:5311:PHE:HA	2:BB:5430:PHE:CZ	2.47	0.49
2:AB:311:PHE:HA	2:AB:430:PHE:CZ	2.47	0.49
4:AD:193:LEU:O	4:AD:193:LEU:HG	2.11	0.49
13:BO:5186:LYS:HA	13:BO:5186:LYS:HE2	1.92	0.49
2:AB:91:TRP:CZ3	24:AB:606:CLA:O1A	2.65	0.49
3:AC:225:VAL:HG22	3:AC:289:PHE:CD1	2.47	0.49
24:AB:608:CLA:C4	4:AD:127:LEU:HD11	2.21	0.49
24:BB:5605:CLA:HBC3	7:BH:5041:PHE:CE1	2.47	0.49
3:BC:5109:PHE:O	3:BC:5113:VAL:HG23	2.12	0.49
5:AE:7:GLU:O	5:AE:9:PRO:HD3	2.12	0.49
20:BZ:5029:SER:C	20:BZ:5031:GLN:H	2.16	0.49
15:AU:72:TYR:O	15:AU:73:PRO:C	2.48	0.49
2:AB:371:THR:HG22	2:AB:377:VAL:CA	2.41	0.49
3:AC:137:PRO:HB2	3:AC:139:THR:O	2.12	0.49
31:BC:5520:LMG:H292	27:BJ:5101:BCR:H363	1.93	0.49
15:AU:83:ALA:CB	15:AU:84:PRO:CD	2.80	0.49
2:AB:243:ALA:HB2	2:AB:466:HIS:ND1	2.27	0.49
2:BB:5450:TRP:HB3	24:BB:5611:CLA:HMB2	1.95	0.49
3:BC:5114:VAL:CG2	31:BC:5521:LMG:H141	2.41	0.49
2:BB:5224:ARG:HG3	7:BH:5025:TRP:HA	1.94	0.49
12:BM:5017:VAL:HG12	12:BM:5018:PRO:N	2.26	0.49
3:AC:55:ALA:CB	27:AC:514:BCR:H373	2.40	0.49
13:AO:225:LEU:N	13:AO:225:LEU:HD12	2.28	0.49
20:AZ:2:THR:CG2	20:AZ:3:ILE:N	2.73	0.49
14:BT:5025:GLU:O	14:BT:5026:PRO:C	2.50	0.49
2:AB:384:ARG:HD3	15:AU:132:LEU:HD13	1.94	0.49
3:BC:5332:GLN:HG3	13:BO:5129:PHE:CE2	2.47	0.49
2:BB:5372:ASP:OD1	2:BB:5374:ASN:N	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:57:SER:HA	4:AD:60:THR:HG22	1.95	0.49
6:AF:41:GLN:HE21	6:AF:41:GLN:N	2.10	0.49
28:AC:519:DGD:O3D	9:AJ:37:GLY:O	2.25	0.49
1:AA:163:ILE:HG12	28:AC:517:DGD:HB31	1.93	0.49
4:AD:279:LEU:HD22	24:AD:401:CLA:HMA2	1.94	0.49
2:BB:5133:LEU:HB3	2:BB:5138:MET:HE1	1.93	0.49
3:BC:5437:PHE:HA	24:BC:5508:CLA:HMC1	1.93	0.49
11:BL:5020:GLY:HA3	12:BM:5022:LEU:CD1	2.43	0.49
13:BO:5178:ARG:HD2	13:BO:5182:PHE:CD1	2.46	0.49
3:BC:5452:ALA:O	3:BC:5454:GLY:N	2.44	0.49
13:AO:147:THR:OG1	13:AO:148:VAL:N	2.46	0.49
1:AA:57:PRO:HD3	1:AA:73:TYR:CE2	2.48	0.49
6:AF:19:ARG:HG3	6:AF:19:ARG:NH1	2.28	0.49
3:BC:5252:ILE:HG22	3:BC:5253:LEU:HD23	1.95	0.49
1:AA:257:ARG:NH1	1:AA:257:ARG:HG3	2.24	0.49
16:BV:5090:PRO:O	16:BV:5092:ARG:HD3	2.13	0.49
13:AO:186:LYS:HE2	13:AO:186:LYS:HA	1.95	0.49
3:AC:276:LEU:HD21	24:AC:508:CLA:HBB1	1.94	0.49
28:AH:101:DGD:O1B	28:AH:101:DGD:HG12	2.12	0.49
2:BB:5252:VAL:HG12	24:BB:5607:CLA:O1A	2.13	0.49
20:AZ:23:VAL:HB	20:AZ:24:PRO:HD3	1.95	0.49
3:AC:155:ASN:CA	3:AC:158:THR:HG22	2.39	0.49
2:AB:44:THR:HB	32:AB:629:LMT:O6'	2.13	0.49
13:AO:178:ARG:HD2	13:AO:182:PHE:CD1	2.48	0.49
1:BA:5077:ILE:HG12	14:BT:5006:TYR:CD1	2.47	0.49
2:BB:5305:ILE:HG22	2:BB:5305:ILE:O	2.11	0.49
4:BD:5161:PRO:HB3	4:BD:5170:ALA:HB2	1.94	0.49
2:AB:41:GLU:HB3	2:AB:60:MET:SD	2.52	0.49
18:AX:24:LEU:O	18:AX:28:VAL:HG23	2.12	0.49
2:AB:251:VAL:O	2:AB:255:THR:HG23	2.12	0.49
24:AB:605:CLA:H141	24:AB:610:CLA:HED2	1.94	0.49
1:BA:5038:ILE:HB	1:BA:5039:PRO:HD3	1.93	0.49
15:BU:5072:TYR:CB	15:BU:5073:PRO:HD3	2.40	0.49
13:AO:126:GLY:O	13:AO:128:ASP:N	2.45	0.49
13:BO:5148:VAL:HA	13:BO:5172:PHE:CD2	2.47	0.49
3:BC:5337:LEU:CD1	13:BO:5131:PRO:HG3	2.41	0.49
29:BA:5413:LHG:HC11	3:BC:5447:ARG:NE	2.27	0.49
9:BJ:5024:ILE:HG23	9:BJ:5025:VAL:N	2.27	0.49
13:AO:59:ASP:C	13:AO:61:SER:H	2.14	0.49
3:AC:346:THR:O	13:AO:40:GLY:HA2	2.13	0.49
1:AA:207:GLY:O	1:AA:210:LEU:HB3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:5308:ASP:C	4:BD:5308:ASP:OD1	2.49	0.49
2:AB:133:LEU:HB3	2:AB:138:MET:HE1	1.94	0.49
2:BB:5008:VAL:HG23	2:BB:5009:HIS:HD2	1.76	0.49
24:BB:5608:CLA:HMC2	24:BB:5615:CLA:H191	1.95	0.49
2:BB:5115:TRP:CZ2	24:BB:5618:CLA:HBA2	2.47	0.49
3:BC:5049:LEU:HD23	3:BC:5149:TYR:OH	2.12	0.49
24:BB:5612:CLA:HMA1	4:BD:5130:PHE:CE1	2.48	0.49
4:BD:5186:GLN:HB2	24:BD:5402:CLA:HBC1	1.95	0.49
13:AO:83:LYS:HE2	2:BB:5338:GLN:HA	1.94	0.49
4:AD:52:THR:HG22	4:AD:67:TYR:CE2	2.48	0.49
3:BC:5089:ILE:N	3:BC:5090:PRO:CD	2.74	0.49
16:BV:5071:ILE:C	16:BV:5071:ILE:HD12	2.33	0.49
3:AC:297:TYR:HA	3:AC:302:TYR:HE2	1.77	0.49
7:AH:44:ILE:HG12	18:AX:19:PHE:CE2	2.48	0.49
10:AK:12:PRO:HB3	20:AZ:62:VAL:HG11	1.93	0.49
9:BJ:5034:ALA:O	9:BJ:5035:GLY:O	2.31	0.49
28:AC:518:DGD:HB22	28:AC:519:DGD:HA21	1.95	0.49
1:AA:22:THR:HG21	8:AI:30:ARG:HE	1.78	0.49
24:AB:608:CLA:HMA1	4:AD:130:PHE:CE1	2.48	0.49
24:AD:404:CLA:C4	18:AX:23:LEU:HA	2.43	0.49
28:BH:5101:DGD:O1B	28:BH:5101:DGD:HG12	2.12	0.49
2:BB:5002:GLY:HA3	11:BL:5009:PRO:HG2	1.94	0.49
3:AC:155:ASN:O	3:AC:158:THR:HG22	2.12	0.49
13:BO:5155:THR:HG23	13:BO:5168:PHE:CE2	2.48	0.49
4:BD:5052:THR:HG22	4:BD:5067:TYR:CE2	2.48	0.49
4:AD:57:SER:CA	4:AD:60:THR:HG22	2.43	0.49
13:AO:66:ILE:HD12	13:AO:121:PHE:CD1	2.48	0.49
13:BO:5240:THR:HA	13:BO:5264:VAL:HA	1.95	0.49
13:AO:71:LEU:HD23	13:AO:265:PHE:HB3	1.94	0.49
2:AB:27:THR:HG23	24:AB:605:CLA:HMC1	1.94	0.49
2:AB:187:PRO:HB3	24:AB:601:CLA:CMB	2.42	0.49
2:AB:8:VAL:HG23	2:AB:9:HIS:HD2	1.77	0.49
3:BC:5271:TYR:CE1	24:BC:5507:CLA:HAC2	2.48	0.49
3:AC:149:TYR:CA	3:AC:156:LYS:HD3	2.42	0.49
15:AU:66:ILE:O	15:AU:66:ILE:CG2	2.61	0.49
1:AA:59:ASP:OD1	1:AA:64:ARG:N	2.46	0.49
3:AC:337:LEU:CD1	13:AO:131:PRO:HG3	2.43	0.49
13:AO:210:ARG:HA	15:AU:39:LEU:CD1	2.43	0.49
3:BC:5346:THR:O	13:BO:5040:GLY:HA2	2.13	0.49
16:AV:45:ILE:HG12	16:AV:46:THR:N	2.27	0.49
18:BX:5043:ILE:HG22	18:BX:5043:ILE:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:139:PHE:CZ	24:AB:609:CLA:HMB3	2.48	0.48
24:AC:505:CLA:HAA1	24:AC:505:CLA:H2	1.95	0.48
2:AB:224:ARG:HG3	7:AH:25:TRP:HA	1.94	0.48
1:BA:5159:LEU:C	1:BA:5162:PRO:HD2	2.34	0.48
24:BA:5408:CLA:HBA2	28:BA:5412:DGD:HB22	1.95	0.48
24:BB:5606:CLA:H191	4:BD:5158:LEU:HB3	1.96	0.48
20:BZ:5023:VAL:HB	20:BZ:5024:PRO:HD3	1.95	0.48
3:BC:5380:ILE:CA	3:BC:5384:ILE:HD11	2.37	0.48
20:BZ:5032:ASP:OD1	20:BZ:5036:SER:HB2	2.13	0.48
1:AA:64:ARG:NH1	1:AA:64:ARG:HG3	2.27	0.48
20:AZ:48:ILE:O	20:AZ:52:LEU:HG	2.13	0.48
20:BZ:5048:ILE:O	20:BZ:5052:LEU:HG	2.13	0.48
5:BE:5026:THR:HB	36:BF:5101:HEM:CAB	2.43	0.48
2:BB:5270:PRO:HG3	2:BB:5312:TYR:CD2	2.48	0.48
2:BB:5384:ARG:HH11	15:BU:5132:LEU:HD13	1.77	0.48
3:BC:5296:VAL:HG23	3:BC:5297:TYR:CD2	2.48	0.48
15:AU:80:VAL:HG22	15:AU:127:ARG:HH21	1.78	0.48
2:BB:5293:ALA:C	2:BB:5295:GLY:H	2.15	0.48
13:BO:5116:ASP:C	13:BO:5116:ASP:OD2	2.50	0.48
24:AB:604:CLA:HMC2	24:AB:611:CLA:H191	1.95	0.48
4:AD:266:TRP:CD1	31:AD:408:LMG:HC1	2.47	0.48
2:BB:5238:LEU:N	24:BB:5616:CLA:HMD3	2.28	0.48
4:BD:5266:TRP:NE1	31:BD:5410:LMG:HC72	2.28	0.48
3:AC:49:LEU:HD23	3:AC:149:TYR:OH	2.13	0.48
1:AA:190:HIS:O	1:AA:298:ASN:HB3	2.13	0.48
2:BB:5324:LEU:CA	4:BD:5293:LEU:HD23	2.38	0.48
3:BC:5249:ILE:O	3:BC:5253:LEU:HG	2.13	0.48
15:BU:5057:LEU:HD11	15:BU:5112:PHE:CB	2.42	0.48
1:BA:5057:PRO:HG3	1:BA:5068:SER:CB	2.43	0.48
2:AB:384:ARG:NH1	15:AU:132:LEU:HD13	2.28	0.48
3:BC:5235:GLY:O	3:BC:5238:ILE:HB	2.13	0.48
13:AO:71:LEU:HD12	13:AO:104:LEU:HD12	1.95	0.48
16:AV:146:LEU:O	16:AV:150:LYS:HG3	2.13	0.48
13:BO:5066:ILE:HD12	13:BO:5121:PHE:CD1	2.48	0.48
1:BA:5092:HIS:CD2	3:BC:5219:GLY:HA3	2.48	0.48
24:BB:5605:CLA:HHC	24:BB:5605:CLA:HBB1	1.94	0.48
4:AD:337:GLU:O	4:AD:338:ASN:C	2.51	0.48
15:AU:73:PRO:HG2	16:AV:107:THR:HB	1.95	0.48
13:BO:5147:THR:OG1	13:BO:5148:VAL:N	2.47	0.48
2:AB:175:THR:O	2:AB:176:GLY:O	2.31	0.48
1:AA:131:TRP:CE3	1:AA:132:GLU:CA	2.97	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BA:5413:LHG:C1	3:BC:5447:ARG:HE	2.26	0.48
29:BA:5413:LHG:HC11	3:BC:5447:ARG:HH21	1.78	0.48
13:AO:159:VAL:HG13	13:AO:159:VAL:O	2.13	0.48
13:BO:5065:ARG:NH1	13:BO:5065:ARG:HB2	2.28	0.48
24:AB:611:CLA:H92	31:AD:407:LMG:H232	1.95	0.48
7:AH:35:MET:SD	27:AX:101:BCR:H322	2.53	0.48
8:BI:5019:PHE:CZ	8:BI:5023:PHE:HE2	2.30	0.48
2:BB:5383:PHE:HE1	13:BO:5194:TYR:CD2	2.30	0.48
2:AB:354:LEU:N	2:AB:354:LEU:HD12	2.28	0.48
20:BZ:5032:ASP:OD1	20:BZ:5033:TRP:N	2.41	0.48
1:AA:254:TYR:CD1	4:AD:132:ILE:HG22	2.48	0.48
1:BA:5330:VAL:CG1	4:BD:5348:ARG:HG2	2.42	0.48
1:AA:318:ALA:HB2	4:AD:75:THR:HG22	1.95	0.48
1:AA:27:ARG:NH1	1:AA:27:ARG:O	2.47	0.48
1:AA:45:THR:CG2	1:AA:46:ILE:N	2.76	0.48
24:AC:506:CLA:HMC2	24:AC:507:CLA:H8	1.95	0.48
2:BB:5004:PRO:CG	2:BB:5007:ARG:HD2	2.35	0.48
4:BD:5087:HIS:HB2	28:BH:5101:DGD:O2D	2.12	0.48
4:BD:5210:LEU:HA	4:BD:5213:ILE:HG22	1.95	0.48
3:AC:155:ASN:HA	3:AC:158:THR:CG2	2.38	0.48
7:BH:5011:LEU:HA	7:BH:5014:LEU:HD12	1.94	0.48
7:AH:11:LEU:C	7:AH:13:PRO:HD2	2.34	0.48
3:AC:337:LEU:HD12	13:AO:131:PRO:CG	2.44	0.48
5:BE:5061:ARG:NH2	16:BV:5153:GLY:HA3	2.28	0.48
13:BO:5135:GLN:HG2	13:BO:5141:ARG:HG3	1.96	0.48
3:AC:94:THR:CG2	3:AC:298:PRO:HD2	2.44	0.48
2:BB:5012:LEU:HD12	2:BB:5019:LEU:HD12	1.96	0.48
1:BA:5220:THR:HG23	4:BD:5141:TYR:CD1	2.49	0.48
24:BC:5511:CLA:H143	20:BZ:5024:PRO:HG2	1.96	0.48
5:BE:5078:THR:O	5:BE:5081:GLU:HB2	2.14	0.48
13:BO:5120:THR:HA	13:BO:5153:ALA:O	2.14	0.48
6:BF:5015:ILE:HG22	6:BF:5016:PHE:CD1	2.47	0.48
1:AA:182:PHE:O	1:AA:186:PHE:HB2	2.14	0.48
9:AJ:34:ALA:O	9:AJ:35:GLY:O	2.31	0.48
2:AB:372:ASP:OD1	2:AB:374:ASN:N	2.46	0.48
3:AC:80:PRO:HB3	3:AC:82:TYR:CE1	2.49	0.48
1:BA:5278:TRP:HA	28:BC:5519:DGD:HAG1	1.96	0.48
1:BA:5022:THR:HG21	8:BI:5030:ARG:HE	1.78	0.48
3:AC:147:PHE:CD2	24:AC:513:CLA:H3A	2.49	0.48
13:AO:155:THR:HG22	13:AO:167:ASP:O	2.14	0.48
3:BC:5418:ASN:HB2	28:BC:5519:DGD:HE2	1.92	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5281:VAL:HG13	28:BC:5519:DGD:HAG3	1.93	0.48
2:AB:245:VAL:HG22	24:AB:612:CLA:H192	1.95	0.48
3:AC:271:TYR:CE1	24:AC:507:CLA:HAC2	2.49	0.48
3:BC:5350:ILE:HG21	3:BC:5359:TRP:HB2	1.96	0.48
24:BC:5501:CLA:CAD	24:BC:5503:CLA:H12	2.44	0.48
10:AK:25:LEU:HB2	10:AK:26:PRO:HD3	1.96	0.48
3:AC:461:ARG:NH2	4:AD:242:GLU:O	2.46	0.48
7:BH:5013:PRO:HG2	7:BH:5014:LEU:H	1.78	0.48
2:AB:172:TYR:O	2:AB:173:GLY:C	2.52	0.48
16:AV:143:GLY:O	16:AV:147:VAL:HG23	2.14	0.48
4:AD:188:PHE:CZ	4:AD:326:ARG:HG2	2.49	0.48
18:AX:22:GLY:HA2	18:AX:25:SER:HG	1.79	0.48
1:AA:248:ILE:CG1	1:AA:248:ILE:O	2.61	0.48
3:AC:214:LEU:HD22	3:AC:214:LEU:N	2.28	0.48
2:BB:5107:LEU:HD21	24:BB:5619:CLA:H42	1.95	0.48
3:BC:5436:PHE:O	24:BC:5508:CLA:HAC1	2.14	0.48
24:BC:5507:CLA:HHC	24:BC:5507:CLA:HBB1	1.96	0.48
5:BE:5069:ARG:HG3	5:BE:5070:PHE:H	1.79	0.48
11:BL:5016:SER:HA	11:BL:5019:LEU:CG	2.44	0.48
15:BU:5066:ILE:O	15:BU:5066:ILE:CG2	2.61	0.48
1:AA:315:ASN:ND2	4:AD:332:GLN:HE22	2.07	0.48
1:BA:5131:TRP:CE3	1:BA:5132:GLU:CA	2.97	0.48
1:BA:5047:CYS:SG	1:BA:5114:LEU:HD22	2.53	0.48
12:AM:1:MET:HG2	12:AM:2:GLU:H	1.79	0.48
16:AV:58:LEU:HD13	16:AV:137:ASP:HB3	1.95	0.48
4:BD:5209:LEU:HD23	4:BD:5209:LEU:C	2.34	0.48
2:AB:222:PRO:HG3	7:AH:27:THR:N	2.25	0.48
2:AB:234:ILE:HD12	2:AB:237:VAL:CG2	2.43	0.48
24:BB:5610:CLA:H52	27:BB:5623:BCR:H321	1.96	0.48
2:BB:5329:PRO:HD2	31:BB:5624:LMG:O4	2.14	0.48
4:BD:5152:VAL:HG11	24:BD:5402:CLA:H11	1.94	0.48
20:AZ:32:ASP:C	20:AZ:34:ASP:H	2.17	0.48
4:AD:218:VAL:HG22	4:AD:244:TYR:CE2	2.49	0.48
18:AX:44:ASP:N	18:AX:44:ASP:OD1	2.46	0.48
2:AB:326:ARG:HD3	2:AB:442:ILE:HG22	1.95	0.48
16:BV:5121:LEU:CD2	16:BV:5138:LEU:HD11	2.44	0.48
3:AC:141:GLU:CD	3:AC:141:GLU:H	2.16	0.48
1:AA:183:MET:HA	24:AA:404:CLA:HMD2	1.96	0.47
1:AA:215:HIS:O	1:AA:216:GLY:C	2.53	0.47
2:AB:15:ASP:N	2:AB:16:PRO:HD3	2.29	0.47
2:AB:12:LEU:HD12	2:AB:19:LEU:HD12	1.94	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:256:PRO:HG2	3:AC:266:TRP:CH2	2.49	0.47
5:AE:69:ARG:HG3	5:AE:70:PHE:H	1.78	0.47
11:AL:20:GLY:HA3	12:AM:22:LEU:CD1	2.44	0.47
24:BA:5406:CLA:HED2	4:BD:5198:MET:SD	2.54	0.47
3:BC:5365:TRP:HA	3:BC:5387:TRP:CH2	2.49	0.47
1:BA:5048:PHE:CA	1:BA:5115:ILE:HD11	2.44	0.47
13:AO:236:GLU:O	13:AO:236:GLU:HG3	2.14	0.47
5:BE:5051:ARG:O	5:BE:5053:ASP:N	2.47	0.47
13:BO:5157:PRO:O	13:BO:5158:ASN:O	2.32	0.47
1:BA:5322:ASN:OD1	3:BC:5412:THR:HA	2.14	0.47
16:AV:81:ARG:NH1	16:AV:81:ARG:HG2	2.29	0.47
15:AU:38:GLU:O	15:AU:39:LEU:O	2.32	0.47
13:BO:5071:LEU:HD12	13:BO:5104:LEU:HD12	1.96	0.47
1:AA:202:VAL:O	1:AA:206:PHE:HB2	2.14	0.47
4:BD:5096:GLU:H	4:BD:5096:GLU:CD	2.17	0.47
1:BA:5281:VAL:HG11	28:BC:5519:DGD:HAV1	1.96	0.47
24:BC:5504:CLA:H192	28:BC:5518:DGD:HBN2	1.96	0.47
1:AA:21:VAL:HG11	1:AA:32:TRP:CE3	2.49	0.47
24:AC:507:CLA:HBB1	24:AC:507:CLA:HHC	1.96	0.47
4:AD:261:PHE:HE1	4:AD:266:TRP:CD1	2.33	0.47
2:BB:5012:LEU:HD22	2:BB:5018:ARG:HB2	1.95	0.47
11:BL:5026:VAL:HG11	31:BL:5101:LMG:H202	1.96	0.47
5:AE:77:GLU:HA	5:AE:80:LEU:HD23	1.96	0.47
20:BZ:5036:SER:HA	20:BZ:5039:LEU:CG	2.40	0.47
4:AD:221:THR:HG23	4:AD:221:THR:O	2.13	0.47
1:AA:10:SER:C	1:AA:12:ASN:H	2.16	0.47
3:BC:5441:HIS:HD2	3:BC:5442:LEU:HD12	1.78	0.47
1:AA:275:LEU:HD13	25:AA:408:MST:C8	2.44	0.47
5:AE:14:ILE:HG22	5:AE:14:ILE:O	2.13	0.47
4:BD:5160:TYR:HB3	4:BD:5161:PRO:CD	2.44	0.47
1:AA:295:PHE:O	3:AC:424:SER:OG	2.32	0.47
20:BZ:5047:TRP:O	20:BZ:5050:LEU:HB2	2.14	0.47
2:AB:24:LEU:HD13	2:AB:111:ALA:N	2.29	0.47
19:AY:11:UNK:C	19:AY:13:UNK:N	2.75	0.47
24:AA:407:CLA:HBA2	28:AA:411:DGD:HB22	1.96	0.47
2:AB:457:VAL:HG12	2:AB:458:PHE:N	2.29	0.47
2:AB:450:TRP:HB3	24:AB:607:CLA:HMB2	1.95	0.47
3:AC:437:PHE:HA	24:AC:508:CLA:HMC1	1.95	0.47
3:AC:330:SER:HB2	13:AO:149:LYS:NZ	2.29	0.47
6:BF:5016:PHE:N	6:BF:5016:PHE:CD1	2.82	0.47
6:BF:5019:ARG:HH11	6:BF:5019:ARG:HG3	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:297:TYR:HD1	3:AC:302:TYR:CE2	2.33	0.47
3:AC:450:ALA:HA	3:AC:455:PHE:CE2	2.49	0.47
4:BD:5084:SER:HB3	5:BE:5068:ASP:HA	1.95	0.47
24:AC:504:CLA:H192	28:AC:518:DGD:HBN2	1.96	0.47
1:AA:153:SER:CB	24:AA:404:CLA:H11	2.45	0.47
24:AB:603:CLA:H2	24:AB:605:CLA:H91	1.96	0.47
24:AB:608:CLA:C1	24:AB:608:CLA:HAA1	2.44	0.47
1:BA:5091:LEU:HD11	1:BA:5163:ILE:HA	1.94	0.47
24:BC:5502:CLA:H122	24:BC:5503:CLA:HMB2	1.96	0.47
3:BC:5147:PHE:CD2	24:BC:5513:CLA:H3A	2.49	0.47
1:BA:5119:PHE:HD1	34:BD:5403:PHO:H92	1.78	0.47
7:BH:5050:ASN:HD22	28:BH:5101:DGD:HA21	1.79	0.47
13:BO:5039:THR:HB	13:BO:5041:LEU:HD22	1.95	0.47
13:AO:155:THR:HG23	13:AO:168:PHE:CD2	2.50	0.47
1:BA:5288:LEU:HD22	3:BC:5432:VAL:HA	1.95	0.47
8:BI:5014:PHE:CE2	8:BI:5018:LEU:HD11	2.49	0.47
2:AB:35:GLY:O	2:AB:38:ALA:HB3	2.14	0.47
28:AC:519:DGD:HE62	9:AJ:40:LEU:CD1	2.45	0.47
29:AA:412:LHG:HC11	3:AC:447:ARG:HH21	1.78	0.47
3:AC:267:SER:O	3:AC:271:TYR:CD2	2.67	0.47
4:AD:274:VAL:HA	35:AD:405:PL9:C25	2.37	0.47
1:BA:5039:PRO:CB	24:BA:5408:CLA:HBB1	2.44	0.47
2:BB:5198:VAL:HG11	24:BB:5607:CLA:HED2	1.97	0.47
24:BC:5506:CLA:HMC2	24:BC:5507:CLA:H8	1.96	0.47
1:BA:5029:TYR:CD2	1:BA:5133:LEU:HD13	2.49	0.47
1:AA:272:HIS:HD2	4:AD:218:VAL:HG21	1.76	0.47
11:BL:5024:ILE:HG21	12:BM:5019:SER:OG	2.14	0.47
12:AM:24:ILE:HD13	31:BM:5102:LMG:H351	1.96	0.47
20:AZ:53:VAL:O	20:AZ:57:LEU:HB2	2.14	0.47
5:BE:5027:ILE:CB	5:BE:5028:PRO:HD3	2.43	0.47
4:AD:253:TRP:HB2	4:AD:260:ALA:HB2	1.96	0.47
1:AA:326:LEU:CD2	3:AC:412:THR:HB	2.44	0.47
4:AD:299:ILE:HG13	11:AL:37:ASN:ND2	2.29	0.47
16:BV:5045:ILE:HG12	16:BV:5046:THR:N	2.29	0.47
19:BY:5011:UNK:C	19:BY:5013:UNK:N	2.76	0.47
3:BC:5327:ASN:HB3	13:BO:5125:ASP:OD1	2.14	0.47
3:BC:5131:TYR:HE1	3:BC:5135:ARG:HD2	1.80	0.47
3:AC:131:TYR:HE1	3:AC:135:ARG:HD2	1.79	0.47
2:AB:54:PRO:HD2	2:AB:57:ARG:HG3	1.95	0.47
4:AD:96:GLU:H	4:AD:96:GLU:CD	2.18	0.47
7:AH:17:GLU:H	7:AH:17:GLU:CD	2.16	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:AB:620:LMG:H202	11:AL:26:VAL:HG11	1.95	0.47
4:BD:5087:HIS:HD2	4:BD:5166:SER:HA	1.72	0.47
7:BH:5025:TRP:O	7:BH:5026:GLY:C	2.53	0.47
1:AA:238:LYS:O	1:AA:241:GLN:HG3	2.14	0.47
13:AO:36:ILE:HG23	13:AO:41:LEU:CB	2.44	0.47
13:AO:39:THR:HB	13:AO:41:LEU:HD22	1.96	0.47
5:AE:9:PRO:O	5:AE:10:PHE:C	2.53	0.47
20:AZ:29:SER:C	20:AZ:31:GLN:H	2.17	0.47
1:AA:13:LEU:N	1:AA:16:ARG:HH11	2.13	0.47
3:BC:5330:SER:HB2	13:BO:5149:LYS:NZ	2.29	0.47
4:BD:5180:ARG:HG3	4:BD:5181:PHE:N	2.29	0.47
5:AE:27:ILE:CB	5:AE:28:PRO:HD3	2.44	0.47
1:AA:43:ALA:HB3	1:AA:118:HIS:HD2	1.80	0.47
15:BU:5099:GLU:HA	15:BU:5102:LYS:HE3	1.97	0.47
1:AA:223:LEU:O	2:AB:482:ILE:HG12	2.13	0.47
2:AB:405:GLU:OE1	2:AB:405:GLU:HA	2.14	0.47
3:AC:416:SER:CA	28:AC:519:DGD:O3E	2.62	0.47
3:AC:437:PHE:HZ	24:AC:510:CLA:HMB3	1.79	0.47
1:AA:119:PHE:HD1	34:AD:402:PHO:H92	1.79	0.47
24:AB:602:CLA:H93	7:AH:46:LEU:HD13	1.96	0.47
1:AA:32:TRP:HB2	8:AI:23:PHE:CZ	2.49	0.47
1:BA:5183:MET:HG3	24:BA:5406:CLA:HBC1	1.96	0.47
24:BC:5510:CLA:H122	24:BC:5510:CLA:H161	1.81	0.47
24:BB:5615:CLA:H92	31:BD:5409:LMG:H232	1.95	0.47
2:BB:5250:PHE:O	28:BH:5101:DGD:HB82	2.15	0.47
2:AB:9:HIS:HB2	24:AB:611:CLA:CBA	2.44	0.47
4:AD:274:VAL:CB	4:AD:275:PRO:HD3	2.44	0.47
24:AD:404:CLA:H42	18:AX:23:LEU:HA	1.96	0.47
1:BA:5153:SER:HB2	24:BA:5405:CLA:H11	1.97	0.47
2:BB:5187:PRO:HG2	2:BB:5188:ASP:H	1.80	0.47
24:BB:5611:CLA:H41	24:BB:5611:CLA:H61	1.74	0.47
3:BC:5271:TYR:HA	3:BC:5274:TYR:CD2	2.49	0.47
4:BD:5263:ASN:O	4:BD:5266:TRP:N	2.47	0.47
5:BE:5015:THR:O	9:BJ:5008:ILE:CD1	2.63	0.47
3:BC:5318:LEU:HD21	3:BC:5380:ILE:HG23	1.97	0.47
1:BA:5059:ASP:OD2	1:BA:5062:GLY:HA2	2.15	0.47
1:AA:64:ARG:NH1	13:AO:98:THR:HG21	2.29	0.47
1:AA:288:LEU:HD22	3:AC:432:VAL:HA	1.96	0.47
1:BA:5015:GLU:O	1:BA:5019:ASN:OD1	2.32	0.47
3:AC:472:LEU:O	3:AC:473:ASP:O	2.32	0.47
2:AB:324:LEU:CA	4:AD:293:LEU:HD23	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:5262:ARG:HH21	32:BC:5522:LMT:C5'	2.26	0.47
13:BO:5236:GLU:HG3	13:BO:5236:GLU:O	2.14	0.47
3:AC:94:THR:HG22	3:AC:298:PRO:HD2	1.95	0.47
3:BC:5075:PHE:CD1	3:BC:5086:LEU:HD21	2.50	0.47
2:AB:325:PHE:CD1	11:AL:34:TYR:HB3	2.49	0.47
2:AB:279:TYR:HE1	7:AH:63:LYS:HE3	1.80	0.47
2:AB:275:TRP:CH2	2:AB:358:ARG:HD3	2.50	0.47
3:BC:5394:GLU:OE2	3:BC:5398:HIS:CD2	2.68	0.47
13:AO:65:ARG:NH1	13:AO:65:ARG:HB2	2.29	0.47
16:AV:148:GLU:OE1	16:AV:148:GLU:HA	2.15	0.47
1:AA:47:CYS:SG	1:AA:114:LEU:HD22	2.54	0.47
1:BA:5248:ILE:O	1:BA:5248:ILE:CG1	2.62	0.47
2:AB:143:LEU:HD12	2:AB:143:LEU:O	2.14	0.47
15:AU:58:ASN:OD1	15:AU:84:PRO:CA	2.61	0.47
1:AA:39:PRO:CB	24:AA:407:CLA:HBB1	2.44	0.47
2:AB:329:PRO:HD2	31:AB:621:LMG:O4	2.15	0.47
1:AA:214:MET:HE1	4:AD:142:ASN:OD1	2.14	0.47
2:AB:250:PHE:O	28:AH:101:DGD:HB82	2.15	0.47
11:AL:17:LEU:HD11	12:AM:23:ILE:HD12	1.97	0.47
1:BA:5135:TYR:HE1	3:BC:5449:ARG:O	1.97	0.47
2:BB:5250:PHE:HD1	28:BH:5101:DGD:HB92	1.80	0.47
4:BD:5086:GLY:O	4:BD:5166:SER:HB2	2.15	0.47
24:BB:5618:CLA:H162	31:BL:5101:LMG:H422	1.96	0.47
3:AC:387:TRP:CE2	3:AC:388:GLN:HG3	2.49	0.47
29:BA:5415:LHG:H102	31:BE:5101:LMG:H142	1.97	0.47
2:AB:384:ARG:HH11	15:AU:132:LEU:HD13	1.79	0.47
16:BV:5143:GLY:O	16:BV:5147:VAL:HG23	2.14	0.47
13:AO:271:PRO:HG2	13:AO:272:ALA:H	1.79	0.47
2:AB:356:VAL:HA	2:AB:370:LEU:CD2	2.45	0.47
4:AD:68:LEU:HD11	5:AE:44:TYR:CE1	2.49	0.47
11:AL:8:GLN:N	11:AL:8:GLN:NE2	2.62	0.47
3:AC:319:ILE:O	3:AC:323:LYS:HG3	2.15	0.47
1:AA:159:LEU:C	1:AA:162:PRO:HD2	2.35	0.47
2:AB:329:PRO:HD3	24:AB:607:CLA:CED	2.44	0.47
3:AC:436:PHE:O	24:AC:508:CLA:HAC1	2.15	0.47
8:AI:11:VAL:CG2	32:AI:102:LMT:H101	2.44	0.47
1:BA:5183:MET:HA	24:BA:5405:CLA:HMD2	1.97	0.47
2:BB:5025:MET:HE2	27:BB:5621:BCR:H393	1.97	0.47
24:BB:5614:CLA:H111	24:BB:5619:CLA:CAA	2.44	0.47
13:BO:5070:CYS:SG	13:BO:5105:ASP:OD1	2.72	0.47
13:BO:5031:LEU:N	13:BO:5031:LEU:CD1	2.72	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BO:5171:GLU:HA	13:BO:5221:GLY:O	2.15	0.47
2:AB:425:ILE:HG22	2:AB:426:PHE:HD2	1.75	0.47
5:BE:5014:ILE:HG22	9:BJ:5013:VAL:HG11	1.96	0.47
2:BB:5369:ILE:C	2:BB:5370:LEU:HD23	2.35	0.47
1:BA:5329:GLU:O	1:BA:5332:HIS:ND1	2.45	0.47
3:AC:193:GLY:O	3:AC:194:GLY:O	2.33	0.47
10:BK:5015:TYR:OH	20:BZ:5058:ASN:ND2	2.48	0.47
2:AB:485:GLU:HG2	2:AB:486:LEU:N	2.29	0.47
3:AC:56:HIS:C	3:AC:58:GLY:N	2.68	0.47
28:BC:5518:DGD:O3D	27:BJ:5101:BCR:H382	2.14	0.47
24:AB:601:CLA:HBC3	7:AH:41:PHE:CE1	2.50	0.47
2:AB:115:TRP:CZ2	24:AB:614:CLA:HBA2	2.50	0.47
2:BB:5183:PRO:HG3	2:BB:5199:VAL:HG12	1.95	0.47
2:BB:5009:HIS:HB2	24:BB:5615:CLA:CBA	2.45	0.47
3:BC:5042:LEU:HD21	24:BC:5511:CLA:H2A	1.97	0.47
3:AC:375:LEU:HB3	3:AC:380:ILE:HD11	1.96	0.47
2:BB:5175:THR:O	2:BB:5176:GLY:O	2.33	0.47
5:BE:5078:THR:HA	5:BE:5081:GLU:CG	2.43	0.47
1:AA:13:LEU:HD12	1:AA:16:ARG:NH1	2.29	0.47
3:BC:5473:ASP:HB2	14:BT:5026:PRO:HB3	1.96	0.47
3:BC:5143:TYR:O	3:BC:5144:SER:CB	2.62	0.47
16:BV:5081:ARG:CZ	16:BV:5157:GLY:HA3	2.45	0.47
3:AC:204:LEU:HD21	3:AC:238:ILE:HG21	1.97	0.47
13:BO:5077:LEU:HB3	13:BO:5091:PHE:HB3	1.97	0.47
15:AU:80:VAL:HG22	15:AU:127:ARG:NH2	2.30	0.47
1:AA:202:VAL:HG11	24:AA:406:CLA:OBD	2.14	0.47
2:AB:24:LEU:HB3	2:AB:111:ALA:HB2	1.97	0.47
3:AC:394:GLU:OE2	3:AC:398:HIS:CD2	2.68	0.47
1:AA:78:ILE:O	1:AA:176:ILE:HB	2.15	0.46
3:AC:264:PHE:CE1	27:AC:516:BCR:H321	2.50	0.46
7:AH:25:TRP:O	7:AH:26:GLY:C	2.53	0.46
2:BB:5112:CYS:HB3	27:BB:5623:BCR:H393	1.96	0.46
24:BC:5510:CLA:HBB1	24:BC:5510:CLA:HHC	1.96	0.46
11:BL:5016:SER:O	11:BL:5019:LEU:HD12	2.14	0.46
24:BD:5405:CLA:C4	18:BX:5023:LEU:HA	2.45	0.46
2:BB:5193:TYR:CD1	2:BB:5260:SER:HA	2.50	0.46
3:BC:5038:GLY:HA3	24:BC:5511:CLA:C2D	2.45	0.46
20:BZ:5023:VAL:HG12	20:BZ:5027:TYR:CE2	2.49	0.46
10:AK:20:PRO:O	10:AK:23:ASP:HB2	2.15	0.46
13:AO:36:ILE:HG23	13:AO:41:LEU:HB2	1.97	0.46
5:BE:5036:LEU:HA	5:BE:5039:SER:OG	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5222:SER:O	1:BA:5246:TYR:HB2	2.14	0.46
15:BU:5072:TYR:O	15:BU:5073:PRO:C	2.51	0.46
3:BC:5432:VAL:HG13	3:BC:5433:LEU:N	2.29	0.46
3:AC:452:ALA:C	3:AC:454:GLY:N	2.68	0.46
3:BC:5420:VAL:HB	3:BC:5425:TRP:HE1	1.80	0.46
24:AB:602:CLA:H191	4:AD:158:LEU:HB3	1.97	0.46
2:BB:5007:ARG:HA	24:BB:5615:CLA:HBA1	1.97	0.46
2:BB:5153:PHE:CZ	2:BB:5158:LEU:HD21	2.50	0.46
18:BX:5012:ILE:CD1	18:BX:5016:LEU:HD12	2.44	0.46
1:AA:240:GLY:HA3	14:AT:29:ILE:HG22	1.98	0.46
10:BK:5043:VAL:HG21	10:BK:5046:ARG:HE	1.80	0.46
15:BU:5073:PRO:HG2	16:BV:5107:THR:HB	1.97	0.46
1:AA:12:ASN:ND2	1:AA:15:GLU:HB2	2.29	0.46
6:AF:24:HIS:HA	6:AF:27:ALA:HB3	1.97	0.46
2:AB:489:GLU:C	2:AB:490:GLN:HG3	2.36	0.46
5:AE:78:THR:O	5:AE:81:GLU:HB2	2.15	0.46
1:BA:5131:TRP:CE3	1:BA:5132:GLU:HA	2.51	0.46
1:BA:5140:ARG:HB2	4:BD:5220:ASN:HA	1.96	0.46
18:BX:5024:LEU:HA	18:BX:5024:LEU:HD12	1.74	0.46
1:AA:210:LEU:HD23	1:AA:210:LEU:C	2.36	0.46
8:AI:33:LYS:O	8:AI:35:LYS:HG2	2.14	0.46
4:BD:5093:TRP:HA	4:BD:5099:GLY:H	1.81	0.46
16:BV:5098:LEU:O	16:BV:5102:MET:HG3	2.14	0.46
1:AA:35:VAL:HA	27:AA:410:BCR:H333	1.95	0.46
24:AB:608:CLA:CAB	4:AD:123:ILE:HG23	2.45	0.46
4:AD:36:LEU:O	4:AD:39:PRO:HD2	2.16	0.46
7:AH:43:LEU:O	7:AH:47:GLU:HG3	2.14	0.46
1:BA:5021:VAL:HG12	1:BA:5022:THR:N	2.30	0.46
2:BB:5243:ALA:HB2	2:BB:5466:HIS:ND1	2.30	0.46
2:BB:5245:VAL:HG22	24:BB:5616:CLA:H192	1.96	0.46
4:BD:5036:LEU:O	4:BD:5039:PRO:HD2	2.15	0.46
2:BB:5005:TRP:CZ2	31:BL:5101:LMG:H291	2.50	0.46
5:BE:5017:VAL:HA	9:BJ:5008:ILE:HD11	1.96	0.46
3:AC:328:VAL:HG23	3:AC:329:GLY:N	2.30	0.46
1:AA:11:ALA:HB1	1:AA:15:GLU:OE1	2.15	0.46
6:AF:15:ILE:HG22	6:AF:16:PHE:N	2.29	0.46
6:BF:5023:VAL:O	6:BF:5027:ALA:CB	2.63	0.46
2:BB:5384:ARG:NH1	15:BU:5132:LEU:HD13	2.30	0.46
4:BD:5299:ILE:HG13	11:BL:5037:ASN:ND2	2.30	0.46
1:BA:5326:LEU:CD2	3:BC:5412:THR:HB	2.46	0.46
13:BO:5086:ARG:O	13:BO:5086:ARG:CG	2.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5138:GLY:HA3	8:BI:5032:PRO:HG2	1.98	0.46
1:AA:214:MET:O	1:AA:215:HIS:C	2.54	0.46
1:AA:21:VAL:HG12	1:AA:22:THR:N	2.29	0.46
31:AA:417:LMG:H301	2:BB:5076:SER:HB3	1.96	0.46
2:AB:112:CYS:HB3	27:AB:619:BCR:H393	1.98	0.46
2:AB:242:ILE:HG22	2:AB:466:HIS:HB2	1.96	0.46
8:AI:30:ARG:O	8:AI:31:ASN:HB3	2.15	0.46
3:BC:5057:ALA:O	3:BC:5061:VAL:HG23	2.15	0.46
24:BC:5511:CLA:H141	20:BZ:5020:VAL:O	2.16	0.46
1:BA:5244:GLU:HG3	1:BA:5246:TYR:H	1.80	0.46
2:AB:298:LEU:HD23	2:AB:402:TYR:CE1	2.51	0.46
20:AZ:36:SER:C	20:AZ:38:GLN:N	2.69	0.46
1:BA:5064:ARG:NH1	13:BO:5098:THR:HG21	2.31	0.46
4:AD:251:ARG:HG2	4:AD:255:GLN:OE1	2.16	0.46
1:AA:275:LEU:HD13	25:AA:408:MST:H83	1.96	0.46
1:AA:48:PHE:CA	1:AA:115:ILE:HD11	2.45	0.46
3:BC:5094:THR:CG2	3:BC:5298:PRO:HD2	2.44	0.46
3:AC:420:VAL:HB	3:AC:425:TRP:HE1	1.79	0.46
16:BV:5148:GLU:OE1	16:BV:5148:GLU:HA	2.15	0.46
4:BD:5136:VAL:O	4:BD:5136:VAL:HG12	2.15	0.46
1:AA:220:THR:CG2	4:AD:141:TYR:HD1	2.29	0.46
2:AB:237:VAL:HB	24:AB:612:CLA:CMD	2.46	0.46
29:AA:412:LHG:HC11	3:AC:447:ARG:NE	2.31	0.46
4:AD:279:LEU:CD2	24:AD:401:CLA:HMA2	2.45	0.46
2:BB:5243:ALA:HB2	2:BB:5466:HIS:CE1	2.50	0.46
4:BD:5250:ASN:ND2	4:BD:5262:SER:HB3	2.28	0.46
20:BZ:5021:ILE:O	20:BZ:5025:VAL:HG22	2.16	0.46
3:BC:5380:ILE:HA	3:BC:5384:ILE:CD1	2.37	0.46
2:AB:179:GLN:HE21	2:AB:179:GLN:CA	2.18	0.46
3:BC:5029:GLU:HA	10:BK:5046:ARG:HH12	1.80	0.46
6:BF:5021:VAL:HG21	30:BF:5102:SQD:H101	1.97	0.46
1:AA:131:TRP:CE3	1:AA:132:GLU:HA	2.50	0.46
13:BO:5072:GLN:O	13:BO:5263:GLY:HA3	2.14	0.46
4:AD:209:LEU:HD23	4:AD:209:LEU:C	2.35	0.46
4:AD:72:ASN:HA	31:AJ:102:LMG:HC72	1.97	0.46
24:AA:407:CLA:HMA2	28:AA:411:DGD:HB42	1.98	0.46
24:AB:610:CLA:H111	24:AB:615:CLA:CAA	2.43	0.46
3:AC:239:TRP:CE3	3:AC:243:ILE:HD11	2.28	0.46
3:AC:288:CYS:HB3	28:AC:517:DGD:HG2	1.98	0.46
4:AD:210:LEU:HA	4:AD:213:ILE:HG22	1.97	0.46
1:AA:214:MET:HE1	34:AD:403:PHO:OBD	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:88:SER:HA	7:AH:50:ASN:OD1	2.15	0.46
30:BB:5601:SQD:H141	24:BB:5618:CLA:H143	1.97	0.46
3:BC:5266:TRP:HZ3	24:BC:5507:CLA:HBC2	1.80	0.46
1:AA:84:PRO:HA	1:AA:112:TYR:CG	2.50	0.46
20:BZ:5032:ASP:C	20:BZ:5034:ASP:H	2.17	0.46
1:BA:5010:SER:C	1:BA:5012:ASN:H	2.19	0.46
2:BB:5124:ARG:HD3	2:BB:5131:PRO:N	2.30	0.46
4:AD:67:TYR:CE1	4:AD:76:VAL:HG11	2.51	0.46
4:BD:5253:TRP:HA	4:BD:5256:ILE:CG2	2.45	0.46
1:BA:5140:ARG:HD3	4:BD:5219:GLU:O	2.15	0.46
13:BO:5071:LEU:HD23	13:BO:5265:PHE:CB	2.45	0.46
2:AB:334:ASP:HB3	13:AO:202:GLN:HG3	1.98	0.46
4:AD:155:SER:HA	4:AD:159:ILE:HG13	1.98	0.46
3:AC:418:ASN:HB2	28:AC:519:DGD:HE2	1.98	0.46
1:AA:153:SER:HB2	24:AA:404:CLA:H11	1.98	0.46
24:AA:405:CLA:H72	31:AB:620:LMG:C25	2.46	0.46
2:AB:135:LEU:HD21	2:AB:234:ILE:HD13	1.98	0.46
2:AB:229:LEU:O	2:AB:230:ARG:C	2.54	0.46
4:AD:119:ALA:O	4:AD:123:ILE:HG13	2.16	0.46
1:AA:32:TRP:CB	8:AI:23:PHE:CZ	2.98	0.46
1:BA:5149:ALA:HB1	1:BA:5283:VAL:CG1	2.45	0.46
2:BB:5012:LEU:HB2	24:BB:5616:CLA:HMC2	1.98	0.46
3:BC:5213:LEU:HD21	27:BC:5516:BCR:C19	2.46	0.46
3:BC:5267:SER:O	3:BC:5271:TYR:CD2	2.69	0.46
4:BD:5210:LEU:HD13	4:BD:5271:MET:HG2	1.98	0.46
16:BV:5059:PHE:HA	16:BV:5063:CYS:SG	2.56	0.46
3:AC:57:ALA:O	3:AC:61:VAL:HG23	2.16	0.46
2:BB:5371:THR:HG22	2:BB:5377:VAL:CA	2.42	0.46
5:AE:26:THR:HB	36:AF:101:HEM:C3B	2.51	0.46
6:BF:5031:ILE:HG12	36:BF:5101:HEM:HMC2	1.97	0.46
4:BD:5057:SER:HA	4:BD:5060:THR:HG22	1.97	0.46
1:AA:210:LEU:C	1:AA:210:LEU:CD2	2.84	0.46
2:BB:5490:GLN:OE1	2:BB:5490:GLN:O	2.33	0.46
3:BC:5319:ILE:O	3:BC:5323:LYS:HG3	2.15	0.46
2:AB:12:LEU:HD22	2:AB:18:ARG:HB2	1.96	0.46
2:AB:107:LEU:HD21	24:AB:615:CLA:H42	1.97	0.46
1:AA:135:TYR:HE1	3:AC:449:ARG:O	1.99	0.46
4:AD:162:LEU:HD21	4:AD:167:TRP:CH2	2.50	0.46
1:BA:5179:THR:HG22	1:BA:5183:MET:CE	2.46	0.46
3:BC:5272:LEU:HA	24:BC:5509:CLA:HMD3	1.97	0.46
24:BB:5612:CLA:CAB	4:BD:5123:ILE:HG23	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BA:5406:CLA:H61	34:BD:5403:PHO:HMB3	1.97	0.46
3:AC:62:PHE:HZ	10:AK:28:ILE:CD1	2.29	0.46
2:BB:5179:GLN:CA	2:BB:5179:GLN:HE21	2.17	0.46
3:AC:164:HIS:HA	3:AC:167:VAL:HG23	1.97	0.46
4:BD:5217:THR:O	4:BD:5221:THR:HB	2.15	0.46
4:AD:180:ARG:HG3	4:AD:181:PHE:N	2.31	0.46
2:BB:5384:ARG:HD3	15:BU:5132:LEU:HD13	1.98	0.46
2:BB:5356:VAL:HG22	2:BB:5370:LEU:HD21	1.97	0.46
2:AB:363:PHE:HD1	4:AD:326:ARG:HD2	1.80	0.46
4:AD:30:VAL:HG12	4:AD:31:GLY:N	2.30	0.46
8:AI:24:LEU:O	8:AI:26:GLY:N	2.41	0.46
2:AB:152:GLY:C	24:AB:606:CLA:HMC3	2.36	0.46
2:AB:187:PRO:HG2	2:AB:188:ASP:H	1.80	0.46
3:AC:215:LYS:HZ3	3:AC:226:SER:CB	2.28	0.46
3:AC:271:TYR:HA	3:AC:274:TYR:CD2	2.50	0.46
11:AL:22:LEU:HD13	14:AT:16:LEU:HD23	1.98	0.46
1:BA:5151:LEU:HD21	1:BA:5155:PHE:HE2	1.81	0.46
2:BB:5012:LEU:O	2:BB:5014:ASN:N	2.49	0.46
30:BB:5601:SQD:H92	24:BB:5618:CLA:H42	1.98	0.46
9:AJ:11:TRP:CE3	10:AK:42:ALA:HB2	2.51	0.46
9:BJ:5003:SER:CA	9:BJ:5007:ARG:HH22	2.29	0.46
4:BD:5323:GLU:HG2	13:BO:5194:TYR:OH	2.16	0.46
2:AB:121:GLU:HG2	7:AH:4:ARG:CD	2.43	0.46
20:AZ:33:TRP:O	20:AZ:33:TRP:CD1	2.67	0.46
2:BB:5121:GLU:HG2	7:BH:5004:ARG:CD	2.42	0.46
3:BC:5335:THR:HA	13:BO:5178:ARG:CD	2.46	0.46
2:BB:5425:ILE:HG22	2:BB:5426:PHE:HD2	1.78	0.46
3:BC:5465:PRO:O	3:BC:5469:MET:HE3	2.16	0.46
13:BO:5086:ARG:O	13:BO:5086:ARG:CD	2.64	0.46
13:BO:5159:VAL:O	13:BO:5159:VAL:HG13	2.16	0.46
1:BA:5114:LEU:HD23	1:BA:5114:LEU:C	2.37	0.46
1:AA:107:TYR:CD1	13:AO:141:ARG:NH1	2.84	0.46
4:BD:5193:LEU:O	4:BD:5193:LEU:HG	2.16	0.46
2:AB:226:TYR:HA	2:AB:231:MET:HE2	1.97	0.46
2:AB:9:HIS:HB2	24:AB:611:CLA:CGA	2.46	0.46
3:AC:272:LEU:HA	24:AC:509:CLA:HMD3	1.97	0.46
1:AA:159:LEU:HD11	28:AC:517:DGD:HB51	1.97	0.46
1:BA:5021:VAL:HG11	1:BA:5032:TRP:CE3	2.51	0.46
35:BD:5406:PL9:H303	35:BD:5406:PL9:H262	1.97	0.46
3:BC:5460:ASP:O	3:BC:5461:ARG:C	2.54	0.46
3:AC:107:ASP:OD2	3:AC:110:PRO:HD3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BO:5036:ILE:HG23	13:BO:5041:LEU:CB	2.46	0.46
2:BB:5354:LEU:HD21	2:BB:5378:LYS:CB	2.46	0.46
12:BM:5019:SER:O	12:BM:5023:ILE:HD13	2.16	0.46
7:BH:5006:TRP:O	7:BH:5010:ILE:HG13	2.16	0.46
13:BO:5271:PRO:HG2	13:BO:5272:ALA:H	1.81	0.46
4:BD:5084:SER:HB3	5:BE:5068:ASP:CA	2.46	0.46
2:AB:485:GLU:CG	2:AB:486:LEU:N	2.78	0.46
4:AD:93:TRP:HA	4:AD:99:GLY:H	1.81	0.46
2:BB:5485:GLU:CG	2:BB:5486:LEU:N	2.79	0.46
1:BA:5318:ALA:HB2	4:BD:5075:THR:HG22	1.97	0.46
2:BB:5285:ASN:HD22	2:BB:5285:ASN:N	2.14	0.46
3:BC:5185:LEU:HD12	3:BC:5230:LEU:HD12	1.97	0.46
31:AC:520:LMG:H202	9:AJ:22:ILE:HG21	1.97	0.45
2:AB:16:PRO:HB3	2:AB:133:LEU:HD21	1.99	0.45
24:AB:604:CLA:H111	24:AB:615:CLA:H2	1.97	0.45
3:BC:5229:ASN:ND2	3:BC:5231:GLU:HB2	2.31	0.45
14:BT:5014:ILE:HD13	14:BT:5017:PHE:CD2	2.52	0.45
1:BA:5084:PRO:HA	1:BA:5112:TYR:CG	2.49	0.45
1:AA:244:GLU:HG3	1:AA:246:TYR:H	1.80	0.45
1:AA:10:SER:C	1:AA:12:ASN:N	2.69	0.45
13:BO:5215:ARG:HD2	15:BU:5039:LEU:HD22	1.98	0.45
2:BB:5356:VAL:HA	2:BB:5370:LEU:CD2	2.45	0.45
2:AB:398:THR:HG22	2:AB:412:THR:HG22	1.96	0.45
4:AD:136:VAL:HG12	4:AD:136:VAL:O	2.16	0.45
11:AL:7:ARG:HD2	11:AL:7:ARG:O	2.16	0.45
3:BC:5414:ILE:HG22	3:BC:5415:ASN:N	2.32	0.45
1:BA:5214:MET:HE1	34:BD:5404:PHO:OBD	2.16	0.45
1:BA:5042:LEU:HD21	30:BA:5401:SQD:H152	1.97	0.45
2:BB:5016:PRO:HB3	2:BB:5133:LEU:HD21	1.97	0.45
2:BB:5329:PRO:HD3	24:BB:5611:CLA:CED	2.46	0.45
3:BC:5435:PHE:O	3:BC:5438:LEU:N	2.47	0.45
4:BD:5119:ALA:O	4:BD:5123:ILE:HG13	2.16	0.45
3:AC:55:ALA:HB1	27:AC:514:BCR:C37	2.43	0.45
1:AA:29:TYR:HD2	1:AA:133:LEU:HB2	1.80	0.45
6:BF:5016:PHE:N	6:BF:5016:PHE:HD1	2.14	0.45
2:AB:144:PHE:CE1	2:AB:210:ILE:CG2	2.99	0.45
3:AC:75:PHE:CD1	3:AC:86:LEU:HD21	2.51	0.45
16:BV:5141:ILE:O	16:BV:5145:ILE:HG13	2.16	0.45
4:AD:126:MET:HE1	4:AD:147:SER:HA	1.99	0.45
2:AB:366:PHE:CD1	2:AB:367:PRO:HD2	2.52	0.45
3:BC:5450:ALA:HA	3:BC:5455:PHE:CE2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AT:18:PHE:CB	27:AT:101:BCR:HC8	2.47	0.45
2:BB:5102:VAL:HB	24:BB:5610:CLA:H91	1.98	0.45
3:BC:5438:LEU:HD23	28:BC:5517:DGD:HAW2	1.97	0.45
11:BL:5022:LEU:HG	31:BL:5101:LMG:C19	2.46	0.45
2:AB:179:GLN:HA	2:AB:179:GLN:NE2	2.22	0.45
3:AC:318:LEU:HD21	3:AC:380:ILE:HG23	1.97	0.45
20:BZ:5036:SER:C	20:BZ:5038:GLN:N	2.70	0.45
3:BC:5055:ALA:HB1	27:BC:5514:BCR:C37	2.41	0.45
13:BO:5114:ASN:HD21	13:BO:5120:THR:CG2	2.29	0.45
16:BV:5130:MET:SD	16:BV:5133:LEU:HD22	2.56	0.45
4:BD:5079:SER:HA	4:BD:5172:SER:HB3	1.97	0.45
3:BC:5202:PRO:HB2	3:BC:5235:GLY:HA2	1.98	0.45
7:BH:5044:ILE:HG12	18:BX:5019:PHE:CE2	2.51	0.45
1:BA:5292:THR:HB	28:BC:5518:DGD:HAH2	1.99	0.45
2:AB:112:CYS:O	2:AB:116:VAL:HG23	2.16	0.45
24:AC:510:CLA:HHC	24:AC:510:CLA:HBB1	1.98	0.45
35:AD:405:PL9:H262	35:AD:405:PL9:H303	1.98	0.45
24:BA:5408:CLA:HMA2	28:BA:5412:DGD:HB42	1.98	0.45
24:BB:5612:CLA:HAA1	24:BB:5612:CLA:C1	2.45	0.45
4:BD:5088:SER:HA	7:BH:5050:ASN:OD1	2.16	0.45
6:AF:24:HIS:NE2	36:AF:101:HEM:NB	2.65	0.45
4:AD:291:LEU:O	4:AD:292:ASN:HB2	2.16	0.45
4:BD:5057:SER:CA	4:BD:5060:THR:HG22	2.46	0.45
16:AV:118:HIS:ND1	16:AV:119:PRO:HD2	2.31	0.45
1:AA:342:ASP:HB2	4:AD:352:LEU:HD21	1.98	0.45
13:AO:135:GLN:HB3	13:AO:135:GLN:HE21	1.48	0.45
8:BI:5024:LEU:O	8:BI:5026:GLY:N	2.41	0.45
1:BA:5041:LEU:HD21	1:BA:5122:GLY:HA3	1.99	0.45
2:BB:5041:GLU:HB3	2:BB:5060:MET:SD	2.55	0.45
1:AA:234:ASN:HD21	4:AD:266:TRP:CA	2.30	0.45
2:AB:153:PHE:O	2:AB:157:HIS:HB3	2.17	0.45
24:AB:612:CLA:H13	24:AB:613:CLA:CBB	2.47	0.45
24:AC:507:CLA:O1D	24:AC:509:CLA:H101	2.17	0.45
3:AC:213:LEU:HD21	27:AC:516:BCR:C19	2.47	0.45
1:BA:5045:THR:CG2	1:BA:5046:ILE:N	2.79	0.45
1:BA:5096:ILE:HD12	24:BA:5408:CLA:HMD1	1.98	0.45
1:BA:5216:GLY:O	1:BA:5220:THR:HG22	2.17	0.45
2:BB:5007:ARG:HG2	24:BB:5615:CLA:HED1	1.97	0.45
24:BB:5608:CLA:H111	24:BB:5619:CLA:H2	1.99	0.45
5:AE:17:VAL:HG22	9:AJ:8:ILE:CD1	2.47	0.45
18:AX:43:ILE:O	18:AX:43:ILE:CG2	2.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:36:LEU:HA	5:AE:39:SER:OG	2.16	0.45
2:BB:5172:TYR:O	2:BB:5173:GLY:C	2.52	0.45
10:BK:5021:LEU:HD11	27:BK:5102:BCR:HC42	1.99	0.45
13:AO:215:ARG:HD2	15:AU:39:LEU:HD22	1.97	0.45
4:AD:19:ASP:O	4:AD:20:ASP:C	2.55	0.45
1:AA:65:GLU:N	1:AA:66:PRO:HD3	2.32	0.45
2:AB:226:TYR:HA	2:AB:231:MET:CE	2.47	0.45
2:BB:5153:PHE:O	2:BB:5157:HIS:HB3	2.17	0.45
2:BB:5234:ILE:HD12	2:BB:5237:VAL:CG2	2.45	0.45
32:BB:5627:LMT:H92	7:BH:5035:MET:HE2	1.98	0.45
24:BA:5408:CLA:HBC1	31:BI:5101:LMG:H361	1.98	0.45
9:BJ:5003:SER:CB	9:BJ:5007:ARG:HH22	2.30	0.45
3:AC:365:TRP:HA	3:AC:387:TRP:CH2	2.51	0.45
2:BB:5279:TYR:HE1	7:BH:5063:LYS:HE3	1.80	0.45
4:BD:5038:PHE:CE2	4:BD:5128:ARG:NH2	2.85	0.45
20:AZ:30:PRO:HA	20:AZ:33:TRP:CE3	2.51	0.45
1:AA:29:TYR:CD2	1:AA:133:LEU:HB2	2.51	0.45
4:BD:5251:ARG:HG2	4:BD:5255:GLN:OE1	2.17	0.45
2:BB:5390:TYR:HD2	4:BD:5344:GLU:OE1	2.00	0.45
5:AE:51:ARG:O	5:AE:53:ASP:N	2.49	0.45
16:AV:103:LYS:O	16:AV:122:ARG:HG2	2.17	0.45
4:BD:5176:ALA:HA	4:BD:5179:PHE:CD2	2.52	0.45
2:BB:5278:SER:HB3	2:BB:5281:GLN:NE2	2.31	0.45
13:BO:5210:ARG:HA	15:BU:5039:LEU:HD13	1.97	0.45
16:BV:5081:ARG:HG2	16:BV:5081:ARG:NH1	2.31	0.45
5:AE:14:ILE:HG22	9:AJ:13:VAL:HG11	1.99	0.45
3:BC:5193:GLY:O	3:BC:5194:GLY:O	2.34	0.45
15:BU:5056:ASP:OD2	15:BU:5115:THR:OG1	2.34	0.45
32:BD:5411:LMT:O2'	18:BX:5021:ILE:HG21	2.15	0.45
6:BF:5030:THR:HG22	6:BF:5034:LEU:CD1	2.47	0.45
12:BM:5003:VAL:HG11	14:BT:5002:GLU:HG2	1.99	0.45
13:BO:5184:ASP:HB2	13:BO:5185:PRO:HD2	1.99	0.45
28:AC:518:DGD:O3D	27:AJ:101:BCR:H382	2.16	0.45
1:AA:157:VAL:HG11	24:AA:405:CLA:HMC3	1.99	0.45
1:AA:205:VAL:HG21	24:AA:404:CLA:HMA2	1.99	0.45
8:AI:10:ILE:HG21	32:AI:102:LMT:H82	1.98	0.45
27:AB:617:BCR:HC41	12:AM:9:ILE:HG23	1.98	0.45
1:BA:5180:PHE:O	1:BA:5184:ILE:HG13	2.17	0.45
2:BB:5010:THR:C	2:BB:5012:LEU:N	2.70	0.45
2:BB:5112:CYS:O	2:BB:5116:VAL:HG23	2.16	0.45
3:BC:5276:LEU:HD23	3:BC:5276:LEU:HA	1.75	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:5035:ILE:O	24:BD:5405:CLA:HBB2	2.16	0.45
12:BM:5033:GLN:HG2	12:BM:5034:LYS:N	2.32	0.45
10:BK:5011:LEU:HD12	10:BK:5019:ASP:HA	1.98	0.45
20:BZ:5009:LEU:HD13	20:BZ:5054:VAL:HG11	1.98	0.45
3:AC:38:GLY:HA3	24:AC:511:CLA:C2D	2.46	0.45
20:AZ:9:LEU:HD13	20:AZ:54:VAL:HG11	1.97	0.45
4:BD:5337:GLU:O	4:BD:5338:ASN:C	2.55	0.45
15:BU:5066:ILE:CG1	15:BU:5072:TYR:CD1	3.00	0.45
13:AO:171:GLU:HA	13:AO:221:GLY:O	2.17	0.45
1:BA:5013:LEU:CA	1:BA:5016:ARG:HH11	2.30	0.45
13:BO:5126:GLY:O	13:BO:5128:ASP:N	2.50	0.45
8:AI:14:PHE:CE2	8:AI:18:LEU:HD11	2.52	0.45
16:BV:5124:ALA:HB1	16:BV:5131:ARG:CG	2.47	0.45
1:BA:5295:PHE:O	3:BC:5424:SER:OG	2.31	0.45
1:AA:103:ASP:OD1	31:AA:417:LMG:H342	2.16	0.45
3:AC:435:PHE:O	3:AC:438:LEU:N	2.49	0.45
4:AD:277:THR:HG22	35:AD:405:PL9:H272	1.98	0.45
2:BB:5229:LEU:O	2:BB:5231:MET:N	2.50	0.45
24:BB:5612:CLA:HBA1	30:BB:5625:SQD:H102	1.98	0.45
3:BC:5095:LEU:HD21	24:BC:5501:CLA:OBD	2.16	0.45
3:BC:5239:TRP:CE3	3:BC:5243:ILE:HD11	2.27	0.45
7:BH:5055:LEU:HB2	7:BH:5058:VAL:CG1	2.46	0.45
2:BB:5357:ARG:NH2	4:BD:5337:GLU:OE1	2.50	0.45
13:AO:147:THR:O	13:AO:172:PHE:CE2	2.70	0.45
3:AC:249:ILE:O	3:AC:253:LEU:HG	2.17	0.45
4:BD:5067:TYR:CE1	4:BD:5076:VAL:HG11	2.51	0.45
13:AO:83:LYS:HG2	13:AO:84:ASN:N	2.28	0.45
3:AC:472:LEU:HG	4:AD:251:ARG:HH12	1.80	0.45
6:AF:37:ILE:HG22	9:AJ:28:PHE:CE1	2.52	0.45
2:BB:5088:PRO:HD2	28:BB:5602:DGD:O4D	2.17	0.45
13:AO:91:PHE:CD1	13:AO:260:LYS:HB2	2.51	0.45
13:AO:71:LEU:HD23	13:AO:265:PHE:CB	2.47	0.45
13:AO:56:TYR:O	13:AO:161:SER:HA	2.17	0.45
13:BO:5056:TYR:O	13:BO:5161:SER:HA	2.17	0.45
1:BA:5235:TYR:C	1:BA:5237:TYR:H	2.20	0.45
1:AA:176:ILE:HD12	24:AA:405:CLA:HED3	1.98	0.45
1:AA:179:THR:HG22	1:AA:183:MET:CE	2.47	0.45
2:AB:112:CYS:HA	27:AB:617:BCR:H282	1.98	0.45
2:AB:69:LEU:HD21	24:AB:603:CLA:OBD	2.17	0.45
8:AI:19:PHE:CE1	8:AI:23:PHE:CE2	3.00	0.45
2:BB:5008:VAL:HG22	24:BB:5615:CLA:O1A	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BB:5620:CLA:HHC	24:BB:5620:CLA:HBB1	1.99	0.45
3:BC:5256:PRO:HG2	3:BC:5266:TRP:CH2	2.51	0.45
24:AC:511:CLA:H2	24:AC:511:CLA:H61	1.86	0.45
3:BC:5328:VAL:HG23	3:BC:5329:GLY:N	2.31	0.45
2:AB:345:VAL:HG21	2:AB:402:TYR:HE2	1.82	0.45
13:AO:168:PHE:O	13:AO:224:SER:HA	2.17	0.45
3:AC:347:GLY:CA	13:AO:43:ASN:HB2	2.45	0.45
18:AX:24:LEU:HA	18:AX:24:LEU:HD12	1.69	0.45
18:BX:5043:ILE:O	18:BX:5043:ILE:CG2	2.64	0.45
12:AM:5:GLN:HE22	32:AM:102:LMT:H3'	1.82	0.45
7:AH:18:TYR:CD1	7:AH:18:TYR:C	2.89	0.45
3:AC:414:ILE:HG22	3:AC:415:ASN:N	2.31	0.45
24:AB:611:CLA:H52	24:AB:614:CLA:HBC2	1.99	0.45
2:BB:5009:HIS:HB2	24:BB:5615:CLA:CGA	2.47	0.45
3:BC:5164:HIS:HA	3:BC:5167:VAL:HG23	1.98	0.45
24:BD:5405:CLA:H41	18:BX:5023:LEU:CD1	2.42	0.45
16:AV:63:CYS:O	16:AV:64:ALA:C	2.55	0.45
24:BC:5511:CLA:H151	20:BZ:5024:PRO:CG	2.45	0.45
2:AB:476:ARG:CZ	2:AB:476:ARG:HB3	2.46	0.45
20:BZ:5030:PRO:HB3	20:BZ:5033:TRP:CZ3	2.51	0.45
31:BM:5102:LMG:O9	31:BM:5102:LMG:O8	2.35	0.45
3:BC:5472:LEU:O	3:BC:5473:ASP:O	2.35	0.45
2:AB:124:ARG:HD3	2:AB:131:PRO:N	2.32	0.45
2:AB:172:TYR:O	2:AB:174:LEU:HG	2.17	0.45
3:AC:453:ALA:C	8:AI:34:ARG:HB2	2.38	0.45
2:BB:5073:GLY:O	2:BB:5093:PHE:CD1	2.70	0.45
1:AA:224:ILE:H	1:AA:224:ILE:HG13	1.55	0.45
4:AD:70:GLY:O	9:AJ:37:GLY:CA	2.64	0.44
1:AA:93:PHE:CE2	24:AA:407:CLA:HBA1	2.52	0.44
2:AB:223:GLN:HG3	2:AB:227:LYS:CE	2.41	0.44
31:AB:620:LMG:C19	11:AL:22:LEU:HG	2.46	0.44
18:AX:12:ILE:CD1	18:AX:16:LEU:HD12	2.47	0.44
30:BB:5625:SQD:H281	32:BB:5627:LMT:H82	1.98	0.44
3:BC:5437:PHE:HZ	24:BC:5510:CLA:HMB3	1.82	0.44
2:AB:193:TYR:CD1	2:AB:260:SER:HA	2.52	0.44
13:BO:5155:THR:HG23	13:BO:5168:PHE:CD2	2.52	0.44
4:BD:5052:THR:HG22	4:BD:5067:TYR:CZ	2.53	0.44
4:BD:5053:THR:CB	4:BD:5067:TYR:HD2	2.30	0.44
6:AF:31:ILE:HG12	36:AF:101:HEM:HMC2	1.99	0.44
1:BA:5271:LEU:CD1	25:BA:5409:MST:H162	2.45	0.44
16:BV:5092:ARG:HG3	16:BV:5092:ARG:NH1	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BE:5051:ARG:O	5:BE:5054:SER:N	2.50	0.44
3:AC:452:ALA:O	3:AC:453:ALA:C	2.56	0.44
2:BB:5435:GLU:O	2:BB:5436:THR:C	2.56	0.44
1:AA:187:GLN:HG2	4:AD:183:LEU:HD21	2.00	0.44
2:BB:5035:GLY:O	2:BB:5038:ALA:HB3	2.16	0.44
2:AB:15:ASP:O	2:AB:17:GLY:N	2.50	0.44
4:AD:87:HIS:HD2	4:AD:166:SER:HA	1.74	0.44
1:BA:5032:TRP:CZ2	8:BI:5022:GLY:HA2	2.52	0.44
4:BD:5261:PHE:CG	4:BD:5267:LEU:HD12	2.53	0.44
24:BC:5511:CLA:C14	20:BZ:5024:PRO:HG2	2.47	0.44
4:BD:5218:VAL:HG22	4:BD:5244:TYR:CD2	2.53	0.44
2:BB:5173:GLY:N	2:BB:5265:ILE:HD11	2.33	0.44
1:BA:5011:ALA:O	1:BA:5012:ASN:HB3	2.17	0.44
6:AF:15:ILE:HG23	36:AF:101:HEM:HAA1	1.98	0.44
1:BA:5343:LEU:O	1:BA:5344:ALA:CB	2.64	0.44
13:BO:5184:ASP:OD2	13:BO:5188:ARG:HB2	2.17	0.44
16:AV:121:LEU:CD2	16:AV:138:LEU:HD11	2.47	0.44
2:BB:5399:VAL:HG12	2:BB:5417:VAL:HG22	1.99	0.44
13:AO:72:GLN:O	13:AO:263:GLY:HA3	2.17	0.44
15:AU:89:GLU:H	15:AU:89:GLU:CD	2.21	0.44
2:AB:248:ALA:CA	24:AB:603:CLA:H42	2.32	0.44
3:AC:437:PHE:CD2	24:AC:508:CLA:HMC2	2.52	0.44
31:AD:408:LMG:HC71	11:AL:15:THR:HG23	1.98	0.44
14:AT:22:PHE:C	14:AT:23:PHE:CD2	2.91	0.44
18:AX:12:ILE:H	27:AX:101:BCR:C29	2.30	0.44
1:BA:5042:LEU:HD23	1:BA:5042:LEU:HA	1.76	0.44
24:BC:5507:CLA:O1D	24:BC:5509:CLA:H101	2.17	0.44
8:BI:5030:ARG:O	8:BI:5031:ASN:HB3	2.17	0.44
31:BI:5101:LMG:H132	32:BI:5102:LMT:H42	1.98	0.44
13:BO:5055:ALA:HA	13:BO:5230:VAL:HG11	1.99	0.44
31:AA:414:LMG:H142	29:AA:415:LHG:H102	1.99	0.44
5:BE:5009:PRO:O	5:BE:5010:PHE:C	2.55	0.44
5:BE:5078:THR:O	5:BE:5082:GLN:OE1	2.36	0.44
12:BM:5001:MET:CG	12:BM:5002:GLU:N	2.81	0.44
12:AM:28:GLN:HB3	12:BM:5027:VAL:HG12	1.99	0.44
9:AJ:24:ILE:HG23	9:AJ:25:VAL:N	2.32	0.44
1:BA:5051:ALA:HA	27:BA:5411:BCR:H381	1.99	0.44
2:BB:5485:GLU:HG2	2:BB:5486:LEU:N	2.31	0.44
3:BC:5056:HIS:C	3:BC:5058:GLY:N	2.70	0.44
2:BB:5045:PHE:HE2	2:BB:5047:PRO:HB3	1.83	0.44
4:AD:78:VAL:HG11	4:AD:114:ILE:HD12	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:BX:5030:LEU:HD23	18:BX:5030:LEU:HA	1.87	0.44
4:AD:127:LEU:HD23	4:AD:127:LEU:HA	1.80	0.44
11:AL:24:ILE:HG21	12:AM:19:SER:OG	2.17	0.44
1:BA:5153:SER:CB	24:BA:5405:CLA:H11	2.47	0.44
13:BO:5080:GLU:O	13:BO:5089:ALA:CB	2.65	0.44
5:BE:5015:THR:CG2	9:BJ:5006:GLY:HA2	2.47	0.44
1:BA:5261:GLN:CD	2:BB:5489:GLU:HG3	2.36	0.44
7:BH:5019:GLY:O	7:BH:5021:VAL:CG1	2.66	0.44
5:BE:5026:THR:HB	36:BF:5101:HEM:C3B	2.53	0.44
3:BC:5166:ILE:HG13	3:BC:5248:GLY:HA3	1.99	0.44
4:BD:5291:LEU:O	4:BD:5292:ASN:HB2	2.17	0.44
6:BF:5030:THR:HG22	6:BF:5034:LEU:HD12	1.99	0.44
4:BD:5126:MET:HE1	4:BD:5147:SER:HA	2.00	0.44
3:BC:5205:ASP:OD1	3:BC:5207:ARG:HB3	2.17	0.44
13:BO:5109:GLY:HA3	13:BO:5122:VAL:O	2.16	0.44
2:BB:5334:ASP:HB3	13:BO:5202:GLN:HG3	2.00	0.44
3:AC:414:ILE:HD11	16:AV:163:TYR:CG	2.53	0.44
1:AA:91:LEU:HD11	1:AA:163:ILE:HA	1.99	0.44
2:AB:139:PHE:HZ	24:AB:609:CLA:HMB3	1.83	0.44
2:AB:252:VAL:HG12	24:AB:603:CLA:O1A	2.17	0.44
3:AC:165:LEU:HD11	24:AC:506:CLA:CHC	2.47	0.44
3:AC:438:LEU:HD23	28:AC:517:DGD:HAW2	1.99	0.44
11:AL:17:LEU:HD12	12:AM:22:LEU:HB3	2.00	0.44
1:BA:5215:HIS:O	1:BA:5216:GLY:C	2.56	0.44
2:BB:5222:PRO:HG3	7:BH:5027:THR:N	2.30	0.44
24:BD:5402:CLA:H2	34:BD:5404:PHO:HBB1	2.00	0.44
11:BL:5016:SER:HA	11:BL:5019:LEU:CD1	2.48	0.44
18:BX:5012:ILE:HD13	18:BX:5016:LEU:HD12	1.98	0.44
15:BU:5058:ASN:OD1	15:BU:5084:PRO:CA	2.65	0.44
3:AC:42:LEU:HD21	24:AC:511:CLA:H2A	1.98	0.44
2:BB:5413:ASP:O	2:BB:5414:PRO:C	2.55	0.44
1:AA:11:ALA:O	1:AA:12:ASN:HB3	2.18	0.44
1:AA:59:ASP:OD2	1:AA:62:GLY:HA2	2.17	0.44
3:BC:5452:ALA:C	3:BC:5454:GLY:N	2.68	0.44
5:AE:49:THR:HA	5:AE:50:PRO:HD3	1.86	0.44
3:BC:5081:MET:HE2	3:BC:5090:PRO:HD3	2.00	0.44
13:AO:210:ARG:HA	15:AU:39:LEU:HD13	1.99	0.44
4:AD:195:PRO:HD3	11:AL:34:TYR:CE1	2.52	0.44
2:AB:11:VAL:HG23	11:AL:6:ASN:O	2.18	0.44
1:AA:113:GLN:HB3	1:AA:117:PHE:CE2	2.52	0.44
15:AU:56:ASP:OD2	15:AU:115:THR:OG1	2.36	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AB:606:CLA:H52	27:AB:619:BCR:H321	2.00	0.44
4:AD:122:LEU:HB3	4:AD:150:ILE:HD11	1.99	0.44
1:AA:214:MET:CE	4:AD:142:ASN:OD1	2.65	0.44
4:AD:186:GLN:HB2	24:AD:401:CLA:HBC1	2.00	0.44
2:BB:5466:HIS:HE1	24:BB:5612:CLA:C4D	2.30	0.44
24:BB:5607:CLA:H2	24:BB:5609:CLA:H91	2.00	0.44
3:BC:5057:ALA:CB	24:BC:5512:CLA:HED2	2.48	0.44
4:BD:5221:THR:O	4:BD:5221:THR:HG23	2.16	0.44
4:AD:323:GLU:HG2	13:AO:194:TYR:OH	2.18	0.44
4:AD:346:LEU:O	4:AD:348:ARG:HG3	2.18	0.44
1:AA:12:ASN:O	1:AA:15:GLU:HB3	2.17	0.44
3:AC:344:SER:HB2	3:AC:345:PRO:CD	2.48	0.44
12:AM:20:VAL:HG11	12:BM:5020:VAL:HG22	2.00	0.44
6:AF:17:THR:O	6:AF:21:VAL:HG23	2.18	0.44
28:BB:5602:DGD:C6E	32:BB:5626:LMT:H2'	2.47	0.44
18:AX:22:GLY:HA2	18:AX:25:SER:OG	2.18	0.44
2:BB:5054:PRO:HD2	2:BB:5057:ARG:HG3	2.00	0.44
3:BC:5176:VAL:O	3:BC:5180:MET:HG3	2.17	0.44
3:AC:363:GLY:O	3:AC:364:PRO:C	2.56	0.44
1:AA:41:LEU:HD21	1:AA:122:GLY:HA3	2.00	0.44
3:AC:205:ASP:OD1	3:AC:207:ARG:HB3	2.18	0.44
13:AO:184:ASP:HB2	13:AO:185:PRO:HD2	1.99	0.44
1:BA:5210:LEU:C	1:BA:5210:LEU:HD23	2.38	0.44
3:AC:217:PRO:O	28:AC:517:DGD:HB21	2.17	0.44
1:BA:5135:TYR:HD2	1:BA:5136:ARG:HH11	1.64	0.44
3:BC:5053:HIS:HB3	24:BC:5512:CLA:OBD	2.17	0.44
3:BC:5053:HIS:ND1	24:BC:5509:CLA:H141	2.33	0.44
3:BC:5116:VAL:CG2	3:BC:5117:VAL:N	2.81	0.44
8:BI:5028:PRO:O	8:BI:5031:ASN:ND2	2.51	0.44
8:BI:5011:VAL:CG2	32:BI:5102:LMT:H101	2.46	0.44
31:BD:5410:LMG:HC71	11:BL:5015:THR:HG23	1.99	0.44
10:BK:5025:LEU:HB2	10:BK:5026:PRO:HD3	2.00	0.44
4:BD:5145:ALA:HB2	4:BD:5272:LEU:CD2	2.47	0.44
13:BO:5036:ILE:HG23	13:BO:5041:LEU:HB2	2.00	0.44
2:AB:483:ASP:OD2	2:AB:484:PRO:HD2	2.18	0.44
20:BZ:5002:THR:O	20:BZ:5005:PHE:HB3	2.18	0.44
3:AC:296:VAL:HG23	3:AC:297:TYR:CD2	2.53	0.44
10:AK:12:PRO:CB	20:AZ:62:VAL:HG11	2.48	0.44
13:AO:94:THR:HB	13:AO:135:GLN:O	2.18	0.44
2:AB:435:GLU:O	2:AB:436:THR:C	2.56	0.44
2:AB:63:LEU:N	2:AB:64:PRO:HD2	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:292:THR:HB	28:AC:518:DGD:HAH2	1.99	0.44
1:BA:5210:LEU:C	1:BA:5210:LEU:CD2	2.86	0.44
1:BA:5304:HIS:CD2	1:BA:5313:VAL:HG11	2.52	0.44
24:AB:614:CLA:H162	31:AB:620:LMG:H422	1.98	0.44
3:AC:208:VAL:O	3:AC:209:ILE:C	2.56	0.44
4:AD:14:TRP:CG	4:AD:15:PHE:N	2.85	0.44
11:AL:16:SER:O	11:AL:19:LEU:HD12	2.17	0.44
12:AM:18:PRO:O	12:AM:21:PHE:HB3	2.18	0.44
3:BC:5264:PHE:CE1	27:BC:5516:BCR:H321	2.49	0.44
35:BD:5406:PL9:H103	35:BD:5406:PL9:HC72	1.77	0.44
1:BA:5272:HIS:CD2	4:BD:5218:VAL:HG11	2.53	0.44
10:BK:5044:GLY:O	10:BK:5045:PHE:C	2.56	0.44
1:BA:5059:ASP:OD1	1:BA:5064:ARG:N	2.50	0.44
2:BB:5144:PHE:CE1	2:BB:5210:ILE:CG2	3.01	0.44
2:BB:5363:PHE:CD1	4:BD:5326:ARG:HD2	2.52	0.44
4:AD:161:PRO:CB	4:AD:170:ALA:HB2	2.47	0.44
13:AO:141:ARG:HH11	13:AO:141:ARG:HG2	1.83	0.44
4:BD:5126:MET:HE2	4:BD:5146:PHE:HB3	2.00	0.44
2:BB:5326:ARG:HD3	2:BB:5442:ILE:HG22	1.98	0.44
3:BC:5416:SER:CA	28:BC:5519:DGD:O3E	2.66	0.44
2:AB:10:THR:C	2:AB:12:LEU:N	2.71	0.44
2:AB:153:PHE:CZ	2:AB:158:LEU:HD21	2.53	0.44
2:AB:12:LEU:HB2	24:AB:612:CLA:HMC2	1.98	0.44
2:AB:7:ARG:HG2	24:AB:611:CLA:HED1	1.99	0.44
28:AA:411:DGD:HA82	3:AC:223:TRP:CH2	2.53	0.44
24:BA:5406:CLA:H72	31:BL:5101:LMG:C25	2.47	0.44
4:BD:5279:LEU:CD2	24:BD:5402:CLA:HMA2	2.48	0.44
3:BC:5028:GLN:HB2	24:BC:5511:CLA:HED1	1.99	0.44
3:BC:5029:GLU:CB	10:BK:5046:ARG:NH1	2.79	0.44
7:AH:19:GLY:O	7:AH:21:VAL:CG1	2.66	0.44
1:BA:5131:TRP:HZ3	1:BA:5132:GLU:HG3	1.83	0.44
4:AD:253:TRP:HA	4:AD:256:ILE:CG2	2.48	0.44
1:BA:5107:TYR:CD1	13:BO:5141:ARG:NH1	2.86	0.44
2:BB:5049:ASP:HA	2:BB:5050:PRO:HD2	1.81	0.44
3:BC:5080:PRO:HB3	3:BC:5082:TYR:CE1	2.53	0.44
1:BA:5276:ALA:HB2	4:BD:5215:GLY:HA3	2.00	0.44
1:AA:205:VAL:HG21	24:AA:404:CLA:HMA1	2.00	0.43
1:BA:5214:MET:O	1:BA:5215:HIS:C	2.54	0.43
2:BB:5226:TYR:HA	2:BB:5231:MET:CE	2.48	0.43
24:BB:5607:CLA:CGA	24:BB:5607:CLA:H3A	2.48	0.43
2:BB:5091:TRP:CE3	24:BB:5610:CLA:O1A	2.71	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:5039:PRO:HB3	24:BD:5405:CLA:HMC3	2.00	0.43
24:AB:607:CLA:HMD3	27:BT:5101:BCR:H271	2.00	0.43
3:AC:311:GLN:OE1	3:AC:355:THR:CG2	2.66	0.43
4:AD:128:ARG:CG	4:AD:129:GLN:N	2.81	0.43
2:BB:5137:LYS:HG3	2:BB:5220:ARG:NH2	2.32	0.43
3:BC:5347:GLY:CA	13:BO:5043:ASN:HB2	2.47	0.43
30:AB:627:SQD:H45	14:BT:5023:PHE:CD1	2.52	0.43
5:BE:5008:ARG:HB2	6:BF:5013:TYR:CB	2.47	0.43
2:AB:246:PHE:CD2	2:AB:463:PHE:HA	2.53	0.43
4:BD:5253:TRP:HB2	4:BD:5260:ALA:CB	2.48	0.43
2:AB:169:SER:O	7:AH:65:LEU:HG	2.18	0.43
13:AO:51:THR:OG1	13:AO:52:ALA:N	2.50	0.43
13:BO:5190:LEU:HB2	13:BO:5214:LYS:HB2	2.00	0.43
2:AB:433:ASP:OD1	2:AB:433:ASP:C	2.55	0.43
4:BD:5183:LEU:HD23	4:BD:5183:LEU:HA	1.87	0.43
1:AA:157:VAL:HG21	24:AA:405:CLA:HMC1	2.00	0.43
24:AB:608:CLA:HBA1	30:AB:622:SQD:H102	2.00	0.43
4:AD:266:TRP:HE1	31:AD:408:LMG:HC72	1.82	0.43
2:AB:250:PHE:HB3	28:AH:101:DGD:HB82	2.00	0.43
14:AT:23:PHE:CD1	30:BB:5601:SQD:H45	2.53	0.43
1:BA:5093:PHE:CE2	24:BA:5408:CLA:HBA1	2.52	0.43
24:BB:5614:CLA:H2	24:BB:5614:CLA:H61	1.88	0.43
24:BB:5616:CLA:H13	24:BB:5617:CLA:CBB	2.47	0.43
9:AJ:3:SER:CA	9:AJ:7:ARG:HH22	2.32	0.43
3:AC:116:VAL:CG2	3:AC:117:VAL:N	2.81	0.43
1:AA:309:ALA:HB3	16:AV:27:ALA:O	2.17	0.43
15:AU:72:TYR:CB	15:AU:73:PRO:HD3	2.40	0.43
2:AB:137:LYS:HG3	2:AB:220:ARG:NH2	2.33	0.43
11:AL:9:PRO:HB3	31:BM:5102:LMG:O2	2.18	0.43
4:BD:5081:PRO:HB2	4:BD:5085:MET:HG3	1.99	0.43
5:BE:5008:ARG:NH2	9:BJ:5004:GLU:HB2	2.34	0.43
3:AC:143:TYR:O	3:AC:144:SER:CB	2.65	0.43
4:BD:5190:ASN:HB2	4:BD:5296:TYR:CE1	2.53	0.43
2:AB:247:PHE:O	2:AB:251:VAL:HG23	2.19	0.43
24:AA:405:CLA:H61	34:AD:402:PHO:HMB3	2.00	0.43
18:AX:20:PHE:HZ	27:AX:101:BCR:H371	1.84	0.43
1:BA:5234:ASN:HD21	4:BD:5266:TRP:CA	2.30	0.43
2:BB:5222:PRO:O	2:BB:5223:GLN:C	2.56	0.43
31:AM:101:LMG:H132	24:BB:5618:CLA:H12	2.00	0.43
3:BC:5224:ILE:HG22	3:BC:5289:PHE:CZ	2.53	0.43
2:BB:5222:PRO:CG	7:BH:5027:THR:H	2.26	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BM:5021:PHE:CD2	12:BM:5022:LEU:HD23	2.53	0.43
16:AV:64:ALA:O	16:AV:65:SER:C	2.56	0.43
3:BC:5161:LEU:HD23	3:BC:5251:HIS:HD2	1.84	0.43
13:AO:230:VAL:CG1	13:AO:231:ASP:N	2.73	0.43
3:AC:166:ILE:HG13	3:AC:248:GLY:HA3	2.01	0.43
1:BA:5010:SER:C	1:BA:5012:ASN:N	2.71	0.43
13:BO:5155:THR:HG22	13:BO:5167:ASP:O	2.18	0.43
1:BA:5193:LEU:CD1	4:BD:5179:PHE:HB3	2.47	0.43
16:AV:54:GLU:O	16:AV:58:LEU:HG	2.18	0.43
3:AC:185:LEU:HD12	3:AC:230:LEU:HD12	2.00	0.43
2:BB:5024:LEU:HD13	2:BB:5111:ALA:N	2.34	0.43
3:BC:5407:VAL:HA	28:BC:5519:DGD:O2E	2.18	0.43
3:AC:438:LEU:HD12	3:AC:438:LEU:O	2.18	0.43
31:AI:101:LMG:H132	32:AI:102:LMT:H42	2.00	0.43
27:AT:101:BCR:H271	24:BB:5611:CLA:HMD3	2.01	0.43
2:BB:5260:SER:HG	2:BB:5262:THR:HG22	1.77	0.43
2:BB:5476:ARG:CZ	2:BB:5476:ARG:HB3	2.44	0.43
2:BB:5179:GLN:NE2	2:BB:5179:GLN:HA	2.22	0.43
5:BE:5007:GLU:O	5:BE:5009:PRO:HD3	2.17	0.43
13:BO:5168:PHE:O	13:BO:5224:SER:HA	2.18	0.43
14:AT:25:GLU:O	14:AT:26:PRO:C	2.54	0.43
1:BA:5309:ALA:HB3	5:BE:5053:ASP:HA	2.01	0.43
2:BB:5356:VAL:HG22	2:BB:5370:LEU:CD2	2.48	0.43
2:BB:5075:TRP:CZ3	28:BB:5602:DGD:HB32	2.54	0.43
13:BO:5135:GLN:HE21	13:BO:5135:GLN:HB3	1.53	0.43
13:AO:184:ASP:OD2	13:AO:188:ARG:HB2	2.17	0.43
2:BB:5343:HIS:O	2:BB:5401:PHE:HA	2.18	0.43
28:BC:5519:DGD:HE62	9:BJ:5040:LEU:CD1	2.48	0.43
14:AT:18:PHE:CD1	27:AT:101:BCR:HC8	2.54	0.43
24:BB:5607:CLA:HMB1	24:BB:5607:CLA:HAB	1.81	0.43
3:BC:5266:TRP:HB3	3:BC:5271:TYR:OH	2.17	0.43
3:AC:29:GLU:CD	3:AC:29:GLU:N	2.72	0.43
4:AD:17:ILE:CG2	18:AX:42:GLN:HG2	2.42	0.43
27:AC:514:BCR:H11C	27:AK:102:BCR:H322	2.00	0.43
1:AA:271:LEU:HD21	25:AA:408:MST:H83	2.00	0.43
2:BB:5348:ASN:O	2:BB:5349:LYS:C	2.56	0.43
2:AB:37:MET:O	2:AB:41:GLU:HG3	2.18	0.43
16:AV:148:GLU:N	16:AV:149:PRO:HD2	2.34	0.43
4:BD:5078:VAL:HG11	4:BD:5114:ILE:HD12	2.01	0.43
1:AA:281:VAL:HG13	1:AA:282:GLY:N	2.33	0.43
2:AB:230:ARG:HD2	2:AB:230:ARG:H	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:5:TRP:CZ2	31:AB:620:LMG:H291	2.53	0.43
2:AB:68:ARG:NH1	24:AB:604:CLA:HED1	2.30	0.43
2:AB:90:PHE:HE2	2:AB:91:TRP:CZ3	2.35	0.43
24:AC:510:CLA:H122	24:AC:510:CLA:H161	1.85	0.43
1:BA:5078:ILE:O	1:BA:5176:ILE:HB	2.18	0.43
1:BA:5149:ALA:HB1	1:BA:5283:VAL:HG12	2.00	0.43
24:BC:5502:CLA:HBB1	24:BC:5502:CLA:HHC	2.01	0.43
24:BC:5505:CLA:HAA2	24:BC:5505:CLA:HBD	2.00	0.43
24:BC:5507:CLA:O1A	24:BC:5509:CLA:H2	2.19	0.43
7:BH:5043:LEU:O	7:BH:5047:GLU:HG3	2.17	0.43
19:BY:5023:UNK:O	19:BY:5024:UNK:C	2.67	0.43
14:AT:31:LYS:O	14:AT:32:LYS:HB2	2.18	0.43
3:AC:380:ILE:CA	3:AC:384:ILE:HD11	2.40	0.43
2:BB:5159:THR:OG1	2:BB:5161:LEU:HD13	2.19	0.43
1:AA:222:SER:O	1:AA:246:TYR:HB2	2.19	0.43
5:BE:5082:GLN:O	5:BE:5083:LEU:C	2.56	0.43
3:AC:377:LEU:CD2	13:AO:126:GLY:HA2	2.48	0.43
1:BA:5013:LEU:HA	1:BA:5016:ARG:NH1	2.33	0.43
6:AF:15:ILE:HG22	6:AF:16:PHE:CD1	2.50	0.43
3:BC:5466:VAL:HA	3:BC:5469:MET:CE	2.48	0.43
13:AO:180:ALA:HB2	15:AU:120:ALA:O	2.18	0.43
3:BC:5203:THR:O	3:BC:5235:GLY:HA3	2.19	0.43
24:AA:405:CLA:HED2	4:AD:198:MET:SD	2.58	0.43
27:AA:410:BCR:H312	8:AI:15:PHE:CE1	2.54	0.43
2:AB:12:LEU:CD1	2:AB:19:LEU:HA	2.36	0.43
30:AB:622:SQD:H281	32:AB:624:LMT:H82	2.00	0.43
3:AC:95:LEU:HD21	24:AC:501:CLA:OBD	2.18	0.43
24:AC:505:CLA:HMD2	27:AC:516:BCR:H343	2.01	0.43
2:BB:5098:LEU:O	2:BB:5102:VAL:HG23	2.18	0.43
2:BB:5457:VAL:HG12	2:BB:5458:PHE:N	2.33	0.43
1:BA:5214:MET:CE	4:BD:5142:ASN:OD1	2.66	0.43
4:BD:5261:PHE:HE1	4:BD:5266:TRP:CD1	2.37	0.43
8:BI:5027:ASP:N	8:BI:5028:PRO:HD3	2.33	0.43
24:AC:511:CLA:H141	20:AZ:20:VAL:O	2.18	0.43
3:AC:315:MET:HE2	3:AC:365:TRP:HZ3	1.83	0.43
15:AU:66:ILE:HG12	15:AU:72:TYR:CD1	2.54	0.43
3:BC:5452:ALA:O	3:BC:5453:ALA:C	2.57	0.43
11:BL:5024:ILE:HG22	11:BL:5025:LEU:N	2.33	0.43
4:AD:52:THR:HG22	4:AD:67:TYR:CZ	2.53	0.43
14:BT:5029:ILE:O	14:BT:5031:LYS:N	2.52	0.43
3:BC:5404:LEU:HD12	3:BC:5404:LEU:HA	1.73	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:228:THR:CG2	1:AA:229:GLU:N	2.81	0.43
3:BC:5324:LEU:HB3	15:BU:5062:ILE:HD13	2.01	0.43
4:AD:253:TRP:HB2	4:AD:260:ALA:CB	2.49	0.43
1:BA:5342:ASP:HB2	4:BD:5352:LEU:HD21	1.99	0.43
2:AB:358:ARG:O	2:AB:360:PRO:HD3	2.18	0.43
3:BC:5071:GLU:OE2	3:BC:5088:LEU:HG	2.19	0.43
13:AO:127:ILE:H	13:AO:127:ILE:HG12	1.64	0.43
1:AA:281:VAL:HG11	28:AC:519:DGD:CIA	2.49	0.43
2:AB:249:ALA:O	2:AB:252:VAL:HG22	2.19	0.43
4:AD:203:GLY:O	4:AD:207:GLY:N	2.52	0.43
4:AD:263:ASN:O	4:AD:265:ARG:N	2.52	0.43
2:BB:5229:LEU:O	2:BB:5230:ARG:C	2.56	0.43
24:BB:5616:CLA:H12	24:BB:5619:CLA:HAA2	2.01	0.43
1:AA:325:ASN:HA	1:AA:328:MET:CE	2.31	0.43
16:BV:5063:CYS:O	16:BV:5064:ALA:C	2.56	0.43
3:AC:460:ASP:O	3:AC:461:ARG:C	2.55	0.43
5:AE:15:THR:CG2	9:AJ:6:GLY:HA2	2.49	0.43
1:BA:5013:LEU:HD12	1:BA:5016:ARG:NH1	2.33	0.43
4:BD:5171:PRO:HG3	4:BD:5181:PHE:CE1	2.53	0.43
2:BB:5011:VAL:CG2	11:BL:5007:ARG:HA	2.49	0.43
2:AB:271:THR:N	2:AB:274:GLN:OE1	2.47	0.43
1:AA:248:ILE:HG12	1:AA:248:ILE:O	2.18	0.43
2:BB:5024:LEU:HB3	2:BB:5111:ALA:HB2	2.00	0.43
1:BA:5299:GLY:O	3:BC:5403:SER:HB2	2.18	0.43
5:BE:5057:ALA:H	5:BE:5060:GLN:NE2	2.17	0.43
6:AF:30:THR:HG22	6:AF:34:LEU:CD1	2.48	0.43
4:AD:43:LEU:HD23	4:AD:117:HIS:CE1	2.53	0.43
1:BA:5065:GLU:N	1:BA:5066:PRO:HD3	2.34	0.43
24:AC:504:CLA:H141	28:AC:518:DGD:HBT1	2.01	0.43
3:BC:5415:ASN:O	3:BC:5416:SER:CB	2.63	0.43
1:AA:51:ALA:HA	27:AA:410:BCR:H381	2.01	0.43
1:AA:42:LEU:HA	1:AA:45:THR:HG22	2.00	0.43
2:AB:68:ARG:NH2	24:AB:604:CLA:HED1	2.29	0.43
2:AB:102:VAL:HG13	27:AB:618:BCR:H401	2.00	0.43
1:BA:5176:ILE:HD12	24:BA:5406:CLA:HED3	2.01	0.43
3:BC:5438:LEU:HD12	3:BC:5438:LEU:O	2.19	0.43
3:BC:5062:PHE:HZ	10:BK:5028:ILE:CD1	2.29	0.43
3:BC:5313:GLN:HB2	3:BC:5313:GLN:HE21	1.54	0.43
5:AE:16:SER:HB2	9:AJ:3:SER:O	2.18	0.43
24:AC:512:CLA:H122	24:AC:512:CLA:H162	1.87	0.43
2:AB:354:LEU:HD21	2:AB:378:LYS:CB	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AZ:30:PRO:C	20:AZ:32:ASP:N	2.73	0.43
4:AD:217:THR:O	4:AD:221:THR:HB	2.18	0.43
27:BC:5514:BCR:H11C	27:BK:5102:BCR:H322	2.00	0.43
13:BO:5147:THR:O	13:BO:5172:PHE:CE2	2.71	0.43
13:AO:120:THR:HA	13:AO:153:ALA:O	2.19	0.43
3:AC:466:VAL:HA	3:AC:469:MET:CE	2.48	0.43
16:AV:130:MET:SD	16:AV:133:LEU:HD22	2.58	0.43
16:BV:5071:ILE:CD1	16:BV:5072:THR:N	2.81	0.43
2:BB:5011:VAL:HG23	11:BL:5007:ARG:HA	2.01	0.43
15:BU:5130:ASN:O	15:BU:5132:LEU:HD23	2.18	0.43
1:AA:77:ILE:HG12	14:AT:6:TYR:CD1	2.54	0.43
10:AK:44:GLY:O	10:AK:45:PHE:C	2.57	0.43
1:BA:5113:GLN:HB3	1:BA:5117:PHE:CE2	2.54	0.43
1:BA:5207:GLY:HA3	1:BA:5278:TRP:HE1	1.84	0.43
1:AA:18:CYS:O	1:AA:22:THR:CG2	2.65	0.43
1:AA:286:THR:HG23	24:AA:404:CLA:HED3	2.01	0.43
2:AB:222:PRO:HB3	7:AH:26:GLY:N	2.34	0.43
24:AB:603:CLA:H3A	24:AB:603:CLA:CGA	2.49	0.43
4:AD:39:PRO:HB3	24:AD:404:CLA:HMC3	2.00	0.43
11:AL:16:SER:HA	11:AL:19:LEU:CG	2.45	0.43
1:BA:5157:VAL:HG21	24:BA:5406:CLA:HMC1	2.00	0.43
24:BB:5609:CLA:H143	24:BB:5614:CLA:HBA1	2.01	0.43
1:BA:5032:TRP:HB2	8:BI:5023:PHE:CZ	2.54	0.43
19:BY:5023:UNK:O	19:BY:5025:UNK:N	2.52	0.43
4:BD:5272:LEU:O	4:BD:5276:VAL:HG23	2.19	0.43
13:AO:32:THR:OG1	13:AO:33:TYR:N	2.52	0.43
2:AB:345:VAL:HG21	2:AB:402:TYR:CE2	2.53	0.43
20:AZ:32:ASP:CG	20:AZ:33:TRP:N	2.68	0.43
20:AZ:31:GLN:HG3	20:AZ:32:ASP:OD2	2.19	0.43
2:AB:315:ILE:HG22	2:AB:426:PHE:HB3	2.00	0.43
13:AO:92:VAL:HG12	13:AO:93:PRO:CD	2.49	0.43
1:BA:5239:PHE:HB3	14:BT:5028:ARG:O	2.18	0.43
4:AD:171:PRO:HG3	4:AD:181:PHE:CE2	2.54	0.43
5:BE:5008:ARG:HB2	6:BF:5013:TYR:HB3	2.00	0.43
3:BC:5366:LEU:HD21	3:BC:5370:ARG:NH2	2.34	0.43
18:AX:44:ASP:O	18:AX:45:LYS:HB3	2.18	0.43
1:AA:295:PHE:HD2	3:AC:291:TRP:CD2	2.37	0.43
2:BB:5037:MET:O	2:BB:5041:GLU:HG3	2.19	0.43
10:BK:5014:ALA:HB2	20:BZ:5061:VAL:HG12	2.00	0.43
3:AC:417:VAL:O	3:AC:417:VAL:HG13	2.19	0.43
3:AC:232:ASP:OD2	3:AC:232:ASP:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BE:5035:TRP:C	5:BE:5035:TRP:CD1	2.92	0.43
13:AO:109:GLY:HA3	13:AO:122:VAL:O	2.18	0.43
1:BA:5281:VAL:HG11	28:BC:5519:DGD:CHA	2.48	0.42
2:AB:250:PHE:HD1	28:AH:101:DGD:HB92	1.83	0.42
2:AB:102:VAL:HB	24:AB:606:CLA:H91	2.00	0.42
24:AD:404:CLA:H41	18:AX:23:LEU:CD1	2.43	0.42
2:BB:5135:LEU:HD21	2:BB:5234:ILE:HD13	2.01	0.42
24:BB:5609:CLA:H41	24:BB:5609:CLA:H61	1.83	0.42
3:BC:5239:TRP:O	3:BC:5243:ILE:HD12	2.19	0.42
3:BC:5437:PHE:CD2	24:BC:5508:CLA:HMC2	2.54	0.42
19:BY:5021:UNK:O	19:BY:5022:UNK:C	2.66	0.42
3:BC:5042:LEU:CD1	24:BC:5511:CLA:HMA3	2.50	0.42
13:BO:5069:LEU:HD12	13:BO:5070:CYS:N	2.33	0.42
6:BF:5025:THR:O	6:BF:5029:PRO:HG2	2.18	0.42
3:BC:5466:VAL:HA	3:BC:5469:MET:HE1	2.01	0.42
2:AB:490:GLN:O	2:AB:491:VAL:O	2.37	0.42
2:AB:144:PHE:HE1	2:AB:210:ILE:CG2	2.31	0.42
16:AV:92:ARG:HG3	16:AV:92:ARG:NH1	2.33	0.42
3:AC:404:LEU:HA	3:AC:404:LEU:HD12	1.69	0.42
2:BB:5437:LEU:N	2:BB:5437:LEU:HD12	2.34	0.42
16:BV:5121:LEU:HD21	16:BV:5138:LEU:HD11	2.01	0.42
7:BH:5040:VAL:O	7:BH:5044:ILE:HG13	2.19	0.42
2:BB:5169:SER:O	7:BH:5065:LEU:HG	2.19	0.42
23:AA:403[A]:CL:CL	4:AD:317:LYS:HD3	2.56	0.42
13:BO:5127:ILE:H	13:BO:5127:ILE:HG12	1.65	0.42
1:AA:303:ASN:O	1:AA:304:HIS:HB2	2.20	0.42
28:BC:5518:DGD:HBT2	27:BJ:5101:BCR:H342	2.01	0.42
1:AA:96:ILE:HD12	24:AA:407:CLA:HMD1	2.00	0.42
4:AD:266:TRP:NE1	31:AD:408:LMG:HC72	2.34	0.42
2:BB:5015:ASP:N	2:BB:5016:PRO:CD	2.81	0.42
3:BC:5165:LEU:HD11	24:BC:5506:CLA:CHC	2.48	0.42
3:BC:5243:ILE:O	24:BC:5506:CLA:HMC1	2.19	0.42
4:BD:5210:LEU:HD21	35:BD:5406:PL9:H13	2.00	0.42
1:BA:5259:ILE:N	1:BA:5259:ILE:CD1	2.69	0.42
15:BU:5072:TYR:CG	15:BU:5073:PRO:N	2.84	0.42
2:BB:5137:LYS:HE2	7:BH:5017:GLU:CG	2.49	0.42
10:AK:14:ALA:HB2	20:AZ:61:VAL:HG12	2.01	0.42
16:AV:90:PRO:O	16:AV:92:ARG:CD	2.67	0.42
29:BA:5413:LHG:HC62	3:BC:5443:TRP:HH2	1.85	0.42
2:BB:5358:ARG:O	2:BB:5360:PRO:HD3	2.19	0.42
13:BO:5075:THR:HG21	13:BO:5077:LEU:HD21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BO:5051:THR:OG1	13:BO:5052:ALA:N	2.52	0.42
3:BC:5426:LEU:HA	3:BC:5426:LEU:HD23	1.86	0.42
3:AC:415:ASN:CB	9:AJ:39:SER:OG	2.67	0.42
1:AA:20:TRP:O	1:AA:23:SER:HB3	2.18	0.42
24:AB:614:CLA:HMB1	24:AB:614:CLA:HAB	1.89	0.42
31:AM:101:LMG:O8	31:AM:101:LMG:O9	2.37	0.42
2:BB:5234:ILE:C	2:BB:5236:THR:H	2.23	0.42
24:BB:5607:CLA:H203	24:BB:5613:CLA:H92	2.00	0.42
4:BD:5122:LEU:HD21	24:BD:5402:CLA:C9	2.41	0.42
3:AC:369:LEU:HD21	3:AC:384:ILE:HD13	2.01	0.42
3:AC:385:GLN:O	3:AC:388:GLN:HB2	2.19	0.42
2:AB:297:THR:OG1	2:AB:298:LEU:N	2.52	0.42
2:BB:5345:VAL:HG21	2:BB:5402:TYR:CE2	2.54	0.42
1:AA:288:LEU:CD1	3:AC:432:VAL:HG23	2.44	0.42
2:BB:5141:ILE:O	2:BB:5144:PHE:HB3	2.20	0.42
30:AB:627:SQD:H45	14:BT:5023:PHE:HD1	1.85	0.42
3:AC:304:PRO:HB3	3:AC:395:TYR:CG	2.54	0.42
4:AD:181:PHE:CZ	4:AD:185:PHE:CE1	3.07	0.42
3:BC:5321:ASP:OD2	15:BU:5129:ASN:HB2	2.19	0.42
13:AO:135:GLN:HG2	13:AO:141:ARG:HG3	2.00	0.42
4:BD:5155:SER:HA	4:BD:5159:ILE:HG13	2.01	0.42
4:BD:5164:GLN:NE2	4:BD:5290:ALA:O	2.53	0.42
2:BB:5477:ASP:OD2	2:BB:5478:VAL:HG13	2.19	0.42
28:AC:518:DGD:HBT2	27:AJ:101:BCR:H342	2.02	0.42
2:AB:162:PHE:O	24:AB:606:CLA:HMD3	2.19	0.42
2:AB:466:HIS:CE1	24:AB:608:CLA:ND	2.87	0.42
24:AB:613:CLA:H41	24:AB:613:CLA:H61	1.63	0.42
27:AC:516:BCR:HC41	8:AI:20:VAL:CG1	2.48	0.42
1:BA:5042:LEU:HA	1:BA:5045:THR:HG22	2.01	0.42
2:BB:5230:ARG:HD2	2:BB:5230:ARG:H	1.84	0.42
24:BB:5618:CLA:HAA2	24:BB:5618:CLA:HBD	2.01	0.42
10:BK:5018:PHE:O	10:BK:5019:ASP:C	2.57	0.42
9:AJ:3:SER:CB	9:AJ:7:ARG:HH22	2.32	0.42
2:BB:5298:LEU:HD23	2:BB:5402:TYR:CE1	2.54	0.42
13:BO:5178:ARG:HG3	13:BO:5178:ARG:NH1	2.28	0.42
2:BB:5144:PHE:HE1	2:BB:5210:ILE:CG2	2.33	0.42
32:BC:5522:LMT:H41	8:BI:5021:PHE:HE1	1.84	0.42
1:BA:5131:TRP:CZ3	1:BA:5132:GLU:HG3	2.53	0.42
1:AA:322:ASN:OD1	3:AC:412:THR:HA	2.19	0.42
13:BO:5141:ARG:HH11	13:BO:5141:ARG:HG2	1.83	0.42
15:BU:5056:ASP:HB3	15:BU:5060:THR:H	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AO:57:PRO:HA	13:AO:161:SER:OG	2.19	0.42
2:AB:12:LEU:HD13	2:AB:19:LEU:CA	2.38	0.42
3:AC:229:ASN:O	3:AC:233:VAL:HG23	2.18	0.42
1:BA:5217:SER:HB2	4:BD:5141:TYR:O	2.19	0.42
3:BC:5217:PRO:O	28:BC:5517:DGD:HB21	2.20	0.42
5:BE:5069:ARG:CG	5:BE:5070:PHE:N	2.82	0.42
19:BY:5018:UNK:O	19:BY:5022:UNK:N	2.52	0.42
13:BO:5081:GLU:HA	13:BO:5082:PRO:HD3	1.88	0.42
10:AK:16:ALA:O	10:AK:19:ASP:HB2	2.19	0.42
16:BV:5062:ALA:O	36:BV:5201:HEM:HAB	2.20	0.42
13:AO:70:CYS:SG	13:AO:105:ASP:OD1	2.77	0.42
2:AB:357:ARG:NH2	4:AD:337:GLU:OE1	2.53	0.42
2:BB:5274:GLN:HG2	2:BB:5279:TYR:CD2	2.54	0.42
20:BZ:5030:PRO:C	20:BZ:5032:ASP:N	2.72	0.42
2:AB:124:ARG:NH1	2:AB:124:ARG:HG3	2.33	0.42
1:AA:257:ARG:NH1	2:AB:489:GLU:OE2	2.52	0.42
13:BO:5091:PHE:CD1	13:BO:5260:LYS:HB2	2.55	0.42
15:AU:56:ASP:HB3	15:AU:60:THR:H	1.85	0.42
13:AO:73:PRO:HG3	13:AO:146:PHE:CE2	2.54	0.42
3:AC:390:ARG:CZ	16:AV:126:ILE:HG21	2.50	0.42
2:AB:466:HIS:HE1	24:AB:608:CLA:C4D	2.31	0.42
2:AB:450:TRP:NE1	24:AB:607:CLA:HBA2	2.34	0.42
2:AB:224:ARG:CZ	32:AB:624:LMT:H2'	2.50	0.42
3:AC:266:TRP:HB3	3:AC:271:TYR:OH	2.20	0.42
4:AD:263:ASN:O	4:AD:266:TRP:N	2.50	0.42
14:AT:14:ILE:HD13	14:AT:17:PHE:CD2	2.55	0.42
2:BB:5112:CYS:HA	27:BB:5621:BCR:H282	2.01	0.42
2:BB:5238:LEU:CD2	2:BB:5469:HIS:CD2	3.03	0.42
3:BC:5272:LEU:CA	24:BC:5509:CLA:HMD3	2.50	0.42
8:BI:5019:PHE:CE1	8:BI:5023:PHE:CE2	3.02	0.42
10:AK:43:VAL:O	10:AK:46:ARG:HG3	2.20	0.42
6:AF:27:ALA:CB	36:AF:101:HEM:HBC2	2.46	0.42
8:AI:21:PHE:HA	8:AI:21:PHE:HD1	1.76	0.42
3:AC:337:LEU:HA	13:AO:131:PRO:HG3	2.01	0.42
2:BB:5246:PHE:CD2	2:BB:5463:PHE:HA	2.54	0.42
1:BA:5069:GLY:HA2	1:BA:5075:ASN:HD21	1.83	0.42
13:BO:5094:THR:HB	13:BO:5135:GLN:O	2.20	0.42
4:AD:164:GLN:NE2	4:AD:290:ALA:O	2.53	0.42
1:BA:5207:GLY:O	1:BA:5210:LEU:HB3	2.19	0.42
2:AB:234:ILE:C	2:AB:236:THR:H	2.23	0.42
2:AB:91:TRP:CE3	24:AB:606:CLA:O1A	2.73	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AB:607:CLA:HAB	24:AB:607:CLA:HMB1	1.88	0.42
3:AC:269:GLU:O	3:AC:272:LEU:HB3	2.19	0.42
24:AA:405:CLA:H62	34:AD:402:PHO:HMA1	2.01	0.42
1:BA:5118:HIS:HE1	24:BA:5408:CLA:C1A	2.32	0.42
1:BA:5157:VAL:HG13	1:BA:5172:MET:HB2	2.00	0.42
2:BB:5188:ASP:HA	7:BH:5058:VAL:HG23	2.02	0.42
3:BC:5223:TRP:CH2	3:BC:5224:ILE:HD11	2.54	0.42
10:AK:34:ALA:O	10:AK:37:PHE:HB2	2.19	0.42
1:AA:259:ILE:N	1:AA:259:ILE:CD1	2.71	0.42
3:AC:324:LEU:HB3	15:AU:62:ILE:HD13	2.01	0.42
4:AD:79:SER:HA	4:AD:172:SER:HB3	2.02	0.42
3:BC:5142:GLU:C	3:BC:5144:SER:H	2.22	0.42
13:BO:5059:ASP:O	13:BO:5061:SER:N	2.53	0.42
13:AO:56:TYR:CD1	13:AO:235:GLY:HA2	2.55	0.42
13:AO:190:LEU:HB2	13:AO:214:LYS:HB2	2.02	0.42
28:AC:518:DGD:O1B	28:AC:518:DGD:C1G	2.68	0.42
3:BC:5418:ASN:HB2	28:BC:5519:DGD:O4E	2.20	0.42
1:AA:149:ALA:HB1	1:AA:283:VAL:CG1	2.49	0.42
3:AC:276:LEU:HA	3:AC:276:LEU:HD23	1.76	0.42
2:BB:5238:LEU:CA	24:BB:5616:CLA:HMD3	2.50	0.42
4:BD:5014:TRP:CG	4:BD:5015:PHE:N	2.88	0.42
2:AB:413:ASP:O	2:AB:414:PRO:C	2.57	0.42
3:BC:5318:LEU:C	3:BC:5318:LEU:HD23	2.40	0.42
1:AA:262:TYR:HE1	31:AA:414:LMG:HO5	1.66	0.42
1:AA:288:LEU:CD2	3:AC:432:VAL:HG23	2.49	0.42
7:BH:5019:GLY:O	7:BH:5021:VAL:HG13	2.20	0.42
6:AF:20:TRP:NE1	6:AF:24:HIS:CE1	2.88	0.42
6:BF:5023:VAL:O	6:BF:5027:ALA:HB2	2.20	0.42
1:BA:5240:GLY:HA3	14:BT:5029:ILE:CG2	2.48	0.42
2:AB:270:PRO:HG3	2:AB:312:TYR:CD2	2.51	0.42
9:BJ:5021:VAL:HA	9:BJ:5024:ILE:HG22	2.02	0.42
4:AD:68:LEU:HB2	6:AF:40:MET:HE1	2.02	0.42
3:AC:366:LEU:HD23	3:AC:366:LEU:O	2.20	0.42
13:AO:141:ARG:NH1	13:AO:141:ARG:HG2	2.35	0.42
2:BB:5475:PHE:HB3	2:BB:5478:VAL:HG22	2.02	0.42
1:BA:5225:ARG:CA	2:BB:5481:GLY:HA3	2.50	0.42
1:AA:292:THR:HB	28:AC:518:DGD:CDA	2.49	0.42
1:BA:5200:LEU:HD12	1:BA:5285:PHE:CG	2.54	0.42
1:AA:96:ILE:C	1:AA:98:GLU:H	2.23	0.42
2:AB:19:LEU:HA	2:AB:19:LEU:HD12	1.80	0.42
18:AX:16:LEU:HD13	18:AX:16:LEU:C	2.39	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:5286:THR:HG23	24:BA:5405:CLA:HED3	2.02	0.42
2:BB:5162:PHE:O	24:BB:5610:CLA:HMD3	2.20	0.42
4:BD:5203:GLY:O	4:BD:5207:GLY:N	2.51	0.42
4:BD:5274:VAL:CB	4:BD:5275:PRO:HD3	2.47	0.42
24:BA:5405:CLA:H111	34:BD:5403:PHO:H3A	2.00	0.42
8:BI:5027:ASP:O	8:BI:5028:PRO:C	2.56	0.42
32:BB:5603:LMT:H5'	32:BB:5603:LMT:H1B	1.79	0.42
20:BZ:5031:GLN:HG3	20:BZ:5032:ASP:OD2	2.18	0.42
20:AZ:30:PRO:HB3	20:AZ:33:TRP:CZ3	2.54	0.42
4:AD:128:ARG:HE	4:AD:128:ARG:HB2	1.66	0.42
1:AA:254:TYR:OH	4:AD:129:GLN:HB3	2.20	0.42
2:AB:356:VAL:HG21	2:AB:424:ALA:CB	2.50	0.42
4:BD:5161:PRO:HG3	4:BD:5170:ALA:HB2	2.02	0.42
4:AD:303:ILE:HG21	12:AM:2:GLU:HG2	2.02	0.42
6:AF:30:THR:HG22	6:AF:34:LEU:HD12	2.01	0.42
2:AB:264:PRO:HG2	2:AB:267:LEU:HB2	2.02	0.42
1:AA:281:VAL:HG11	28:AC:519:DGD:HAG3	2.01	0.42
2:AB:450:TRP:CZ3	24:AB:607:CLA:H2	2.55	0.42
3:AC:243:ILE:O	24:AC:506:CLA:HAC1	2.20	0.42
14:AT:14:ILE:HD13	14:AT:14:ILE:HA	1.88	0.42
1:BA:5183:MET:HG3	24:BA:5406:CLA:CBC	2.50	0.42
2:BB:5135:LEU:HB2	2:BB:5136:PRO:CD	2.41	0.42
2:BB:5237:VAL:HB	24:BB:5616:CLA:CMD	2.50	0.42
2:BB:5450:TRP:NE1	24:BB:5611:CLA:HBA2	2.35	0.42
2:BB:5224:ARG:NH1	32:BB:5627:LMT:H2'	2.35	0.42
3:BC:5128:GLY:HA3	24:BC:5513:CLA:C3C	2.50	0.42
3:BC:5160:ILE:HA	3:BC:5163:PHE:CD2	2.54	0.42
24:BC:5509:CLA:HHC	24:BC:5509:CLA:HBB1	2.02	0.42
5:BE:5015:THR:O	9:BJ:5008:ILE:HD13	2.19	0.42
5:AE:72:ALA:O	5:AE:76:VAL:HG23	2.20	0.42
1:BA:5133:LEU:HD23	4:BD:5252:PHE:HD1	1.81	0.42
20:AZ:38:GLN:O	20:AZ:42:LEU:HG	2.19	0.42
1:AA:13:LEU:CA	1:AA:16:ARG:HH11	2.33	0.42
3:AC:335:THR:HA	13:AO:178:ARG:HD3	2.02	0.42
3:AC:45:LEU:O	3:AC:46:SER:C	2.58	0.42
5:AE:78:THR:HA	5:AE:81:GLU:CG	2.49	0.42
3:BC:5269:GLU:OE1	3:BC:5447:ARG:HD3	2.20	0.42
3:BC:5141:GLU:HA	3:BC:5148:GLY:HA3	2.02	0.42
13:AO:59:ASP:O	13:AO:61:SER:N	2.53	0.42
1:BA:5147:TYR:CG	1:BA:5147:TYR:O	2.73	0.42
1:AA:220:THR:HG23	4:AD:141:TYR:CD1	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:187:PRO:HG2	2:AB:188:ASP:N	2.35	0.41
24:AB:616:CLA:HHC	24:AB:616:CLA:HBB1	2.01	0.41
1:BA:5032:TRP:CB	8:BI:5023:PHE:CZ	3.03	0.41
2:BB:5152:GLY:C	24:BB:5610:CLA:HMC3	2.40	0.41
24:BB:5606:CLA:H93	7:BH:5046:LEU:HD13	2.02	0.41
2:BB:5466:HIS:CE1	24:BB:5612:CLA:ND	2.87	0.41
24:BB:5615:CLA:H52	24:BB:5618:CLA:HBC2	2.01	0.41
3:BC:5229:ASN:O	3:BC:5233:VAL:HG23	2.19	0.41
3:BC:5307:PRO:O	3:BC:5311:GLN:HG2	2.20	0.41
3:AC:160:ILE:HA	3:AC:163:PHE:CD2	2.55	0.41
32:AB:629:LMT:H51	14:BT:5004:ILE:CG1	2.42	0.41
2:BB:5324:LEU:HD13	4:BD:5293:LEU:CD2	2.50	0.41
20:BZ:5005:PHE:HA	20:BZ:5057:LEU:CD2	2.50	0.41
2:AB:390:TYR:HD2	4:AD:344:GLU:OE1	2.02	0.41
1:AA:317:TRP:HZ3	4:AD:180:ARG:HD3	1.85	0.41
16:BV:5090:PRO:O	16:BV:5092:ARG:CD	2.67	0.41
1:AA:343:LEU:O	1:AA:344:ALA:CB	2.66	0.41
1:BA:5191:ASN:ND2	1:BA:5194:MET:HB2	2.35	0.41
4:BD:5318:ASN:O	4:BD:5321:LEU:HB2	2.20	0.41
27:BA:5411:BCR:H312	8:BI:5015:PHE:CE1	2.54	0.41
1:AA:232:SER:HB3	1:AA:235:TYR:CD2	2.55	0.41
13:BO:5065:ARG:CB	13:BO:5065:ARG:HH11	2.33	0.41
13:BO:5141:ARG:HG2	13:BO:5141:ARG:NH1	2.35	0.41
2:AB:363:PHE:CD1	4:AD:326:ARG:HD2	2.55	0.41
15:AU:89:GLU:N	15:AU:89:GLU:CD	2.74	0.41
1:AA:278:TRP:HB3	1:AA:279:PRO:CD	2.46	0.41
9:AJ:32:ALA:HA	31:AJ:102:LMG:O3	2.20	0.41
2:AB:12:LEU:O	2:AB:14:ASN:N	2.53	0.41
2:AB:198:VAL:HG11	24:AB:603:CLA:HED2	2.02	0.41
24:AB:603:CLA:H203	24:AB:609:CLA:H92	2.02	0.41
3:AC:225:VAL:O	3:AC:225:VAL:HG12	2.20	0.41
24:AC:502:CLA:HAA2	24:AC:502:CLA:HBD	2.01	0.41
31:AM:101:LMG:H132	24:BB:5618:CLA:C1	2.51	0.41
12:AM:17:VAL:HG12	12:AM:18:PRO:N	2.34	0.41
2:BB:5225:LEU:O	2:BB:5226:TYR:C	2.59	0.41
2:BB:5185:TRP:HD1	24:BB:5606:CLA:HBB2	1.85	0.41
24:BB:5618:CLA:H162	31:BL:5101:LMG:C42	2.50	0.41
3:BC:5215:LYS:HZ3	3:BC:5226:SER:CB	2.32	0.41
12:BM:5018:PRO:O	12:BM:5021:PHE:HB3	2.20	0.41
3:BC:5062:PHE:CD2	10:BK:5029:PRO:HG3	2.50	0.41
2:AB:338:GLN:HB2	2:AB:431:GLU:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AC:511:CLA:H143	20:AZ:24:PRO:HG2	2.02	0.41
16:BV:5062:ALA:O	36:BV:5201:HEM:CAB	2.68	0.41
18:AX:42:GLN:O	18:AX:43:ILE:HG13	2.20	0.41
3:AC:441:HIS:HD2	3:AC:442:LEU:HD12	1.85	0.41
7:BH:5018:TYR:CD1	7:BH:5018:TYR:C	2.94	0.41
13:AO:114:ASN:HD21	13:AO:120:THR:CG2	2.29	0.41
3:BC:5337:LEU:HD23	3:BC:5342:MET:HE1	2.01	0.41
3:BC:5337:LEU:HA	13:BO:5131:PRO:HG3	2.02	0.41
7:BH:5017:GLU:CD	7:BH:5017:GLU:N	2.72	0.41
4:AD:53:THR:HA	4:AD:67:TYR:CD2	2.56	0.41
1:BA:5239:PHE:O	14:BT:5030:THR:N	2.53	0.41
1:BA:5243:GLU:HA	4:BD:5240:ALA:O	2.20	0.41
1:AA:306:VAL:HG22	1:AA:314:ILE:HB	2.03	0.41
2:AB:348:ASN:O	2:AB:349:LYS:C	2.58	0.41
1:AA:140:ARG:HB2	4:AD:220:ASN:HA	2.01	0.41
13:AO:46:PRO:HB2	13:AO:266:TYR:CD2	2.55	0.41
4:BD:5161:PRO:CB	4:BD:5170:ALA:HB2	2.50	0.41
13:BO:5106:GLN:HE21	13:BO:5106:GLN:HB3	1.68	0.41
28:BC:5519:DGD:HD3	9:BJ:5032:ALA:O	2.20	0.41
2:AB:238:LEU:CA	24:AB:612:CLA:HMD3	2.50	0.41
24:AB:614:CLA:HAA2	24:AB:614:CLA:HBD	2.01	0.41
24:AB:615:CLA:HHC	24:AB:615:CLA:HBB1	2.02	0.41
4:AD:199:MET:HG2	35:AD:405:PL9:H312	2.03	0.41
1:BA:5096:ILE:C	1:BA:5098:GLU:H	2.24	0.41
24:BA:5406:CLA:H72	31:BL:5101:LMG:H241	2.02	0.41
14:AT:23:PHE:HD1	30:BB:5601:SQD:H45	1.85	0.41
2:BB:5224:ARG:CZ	32:BB:5627:LMT:H2'	2.50	0.41
1:BA:5135:TYR:CE1	3:BC:5449:ARG:HB3	2.55	0.41
7:BH:5035:MET:SD	27:BX:5101:BCR:H322	2.61	0.41
1:BA:5321:ILE:HG22	1:BA:5325:ASN:ND2	2.35	0.41
20:BZ:5022:GLY:O	20:BZ:5023:VAL:C	2.58	0.41
5:AE:8:ARG:NH2	9:AJ:4:GLU:HB2	2.35	0.41
9:BJ:5003:SER:CB	9:BJ:5007:ARG:NH2	2.83	0.41
3:BC:5466:VAL:HG21	4:BD:5248:THR:OG1	2.20	0.41
1:BA:5048:PHE:HA	1:BA:5115:ILE:CD1	2.48	0.41
3:AC:142:GLU:C	3:AC:144:SER:H	2.24	0.41
13:AO:157:PRO:O	13:AO:158:ASN:O	2.38	0.41
13:AO:77:LEU:HB3	13:AO:91:PHE:HB3	2.02	0.41
3:AC:204:LEU:HA	3:AC:204:LEU:HD23	1.79	0.41
2:AB:373:LYS:HG3	2:AB:374:ASN:N	2.35	0.41
16:BV:5069:GLY:O	16:BV:5156:TRP:O	2.38	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:5019:ASP:O	4:BD:5020:ASP:C	2.57	0.41
3:BC:5417:VAL:HG13	3:BC:5417:VAL:O	2.19	0.41
13:AO:156:GLN:OE1	13:AO:156:GLN:HA	2.20	0.41
28:AC:519:DGD:HD3	9:AJ:32:ALA:O	2.20	0.41
1:BA:5278:TRP:HB3	1:BA:5279:PRO:CD	2.42	0.41
12:AM:21:PHE:CD2	12:AM:22:LEU:HD23	2.55	0.41
1:BA:5119:PHE:CZ	24:BA:5405:CLA:H101	2.52	0.41
2:BB:5034:ALA:HB2	24:BB:5609:CLA:C2D	2.51	0.41
5:BE:5069:ARG:HG3	5:BE:5070:PHE:CD1	2.55	0.41
7:BH:5063:LYS:O	7:BH:5064:ALA:HB3	2.20	0.41
13:BO:5120:THR:HG22	13:BO:5154:SER:CB	2.50	0.41
1:AA:57:PRO:HA	1:AA:68:SER:HA	2.03	0.41
6:BF:5024:HIS:NE2	36:BF:5101:HEM:NB	2.67	0.41
4:AD:53:THR:CB	4:AD:67:TYR:HD2	2.34	0.41
1:BA:5306:VAL:HG22	1:BA:5314:ILE:HB	2.02	0.41
1:AA:296:ASN:HB3	3:AC:401:LEU:HD13	2.02	0.41
3:AC:367:GLU:OE1	3:AC:367:GLU:HA	2.18	0.41
1:BA:5138:GLY:CA	8:BI:5032:PRO:HG2	2.51	0.41
15:BU:5077:LYS:O	15:BU:5081:LYS:HB2	2.21	0.41
1:AA:36:ILE:HD13	1:AA:36:ILE:HA	1.89	0.41
1:AA:200:LEU:HD21	28:AC:519:DGD:CCA	2.50	0.41
1:BA:5292:THR:HB	28:BC:5518:DGD:CDA	2.50	0.41
9:BJ:5038:SER:OG	9:BJ:5039:SER:N	2.53	0.41
2:AB:252:VAL:HG23	2:AB:253:ALA:N	2.35	0.41
3:AC:244:CYS:HA	24:AC:506:CLA:CMC	2.51	0.41
3:AC:449:ARG:HE	24:AC:505:CLA:HED1	1.86	0.41
4:AD:259:ILE:HD13	14:AT:21:ILE:HG12	2.02	0.41
7:AH:42:LEU:HA	7:AH:42:LEU:HD12	1.83	0.41
18:AX:12:ILE:CA	27:AX:101:BCR:H401	2.48	0.41
1:BA:5172:MET:HA	1:BA:5173:PRO:HD3	1.97	0.41
2:BB:5026:HIS:HB2	24:BB:5616:CLA:HMB2	2.01	0.41
1:BA:5092:HIS:HE1	3:BC:5359:TRP:CZ2	2.38	0.41
3:BC:5244:CYS:HA	24:BC:5506:CLA:CMC	2.51	0.41
3:AC:62:PHE:CD2	10:AK:29:PRO:HG3	2.50	0.41
19:BY:5025:UNK:C	19:BY:5027:UNK:N	2.82	0.41
3:AC:42:LEU:CD1	24:AC:511:CLA:HMA3	2.50	0.41
4:BD:5272:LEU:HD22	4:BD:5276:VAL:HG21	2.03	0.41
2:BB:5271:THR:N	2:BB:5274:GLN:OE1	2.45	0.41
2:AB:483:ASP:CB	2:AB:484:PRO:CD	2.94	0.41
2:BB:5298:LEU:HD12	2:BB:5298:LEU:HA	1.89	0.41
4:AD:218:VAL:HG22	4:AD:244:TYR:CD2	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AK:21:LEU:HD11	27:AK:102:BCR:HC42	2.03	0.41
7:BH:5016:SER:C	7:BH:5018:TYR:H	2.23	0.41
1:BA:5340:PRO:HG3	15:BU:5133:TYR:CD1	2.55	0.41
10:AK:11:LEU:O	10:AK:12:PRO:C	2.59	0.41
9:AJ:36:LEU:C	9:AJ:38:SER:H	2.24	0.41
1:AA:184:ILE:CD1	4:AD:186:GLN:HG2	2.51	0.41
24:AA:405:CLA:H72	31:AB:620:LMG:H241	2.01	0.41
24:AB:605:CLA:H143	24:AB:610:CLA:HBA1	2.02	0.41
2:AB:4:PRO:CG	2:AB:7:ARG:HD2	2.42	0.41
24:AC:505:CLA:HAA2	24:AC:505:CLA:HBD	2.02	0.41
3:AC:437:PHE:CD2	24:AC:508:CLA:CMC	3.04	0.41
4:AD:202:ALA:HB3	35:AD:405:PL9:C30	2.49	0.41
1:BA:5020:TRP:O	1:BA:5023:SER:HB3	2.19	0.41
1:BA:5044:ALA:HB1	34:BD:5403:PHO:H91	2.02	0.41
2:BB:5112:CYS:CB	27:BB:5623:BCR:H393	2.51	0.41
2:BB:5135:LEU:HD23	2:BB:5138:MET:CE	2.50	0.41
24:BB:5615:CLA:HBB1	24:BB:5615:CLA:HHC	2.03	0.41
2:BB:5193:TYR:CE1	2:BB:5260:SER:HA	2.55	0.41
3:AC:149:TYR:HB3	3:AC:156:LYS:HD3	2.02	0.41
20:BZ:5032:ASP:HA	20:BZ:5034:ASP:OD2	2.21	0.41
15:BU:5072:TYR:CB	15:BU:5073:PRO:CD	2.98	0.41
2:BB:5489:GLU:CB	5:BE:5003:GLY:N	2.76	0.41
3:AC:459:ILE:HG21	3:AC:464:GLU:HG3	2.02	0.41
13:AO:168:PHE:HB2	13:AO:225:LEU:HB2	2.03	0.41
3:AC:466:VAL:HG13	4:AD:251:ARG:CD	2.50	0.41
2:AB:278:SER:HB3	2:AB:281:GLN:NE2	2.32	0.41
3:AC:71:GLU:OE2	3:AC:88:LEU:HG	2.21	0.41
4:AD:84:SER:HB3	5:AE:68:ASP:HA	2.03	0.41
2:AB:105:GLY:O	2:AB:108:PHE:HB3	2.20	0.41
1:AA:278:TRP:CD2	28:AC:519:DGD:CIA	2.96	0.41
27:AJ:101:BCR:H20C	27:AJ:101:BCR:H361	1.91	0.41
1:AA:119:PHE:CZ	24:AA:404:CLA:H101	2.53	0.41
2:AB:12:LEU:HD13	2:AB:19:LEU:HD12	2.03	0.41
24:AB:612:CLA:H12	24:AB:615:CLA:HAA2	2.03	0.41
3:AC:229:ASN:ND2	3:AC:231:GLU:HB2	2.36	0.41
3:AC:243:ILE:O	24:AC:506:CLA:HMC1	2.20	0.41
29:AA:412:LHG:C1	3:AC:447:ARG:HE	2.34	0.41
4:AD:261:PHE:CG	4:AD:267:LEU:HD12	2.56	0.41
10:BK:5019:ASP:N	10:BK:5020:PRO:CD	2.81	0.41
16:AV:59:PHE:HA	16:AV:63:CYS:SG	2.60	0.41
3:BC:5038:GLY:HA3	24:BC:5511:CLA:CMD	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:5311:GLN:OE1	3:BC:5355:THR:CG2	2.68	0.41
3:BC:5384:ILE:H	3:BC:5384:ILE:HG12	1.75	0.41
3:AC:48:LYS:HE2	3:AC:138:GLU:OE2	2.20	0.41
4:AD:128:ARG:O	4:AD:129:GLN:C	2.59	0.41
6:BF:5015:ILE:HG23	36:BF:5101:HEM:HAA1	2.03	0.41
1:BA:5129:ARG:NH2	4:BD:5256:ILE:O	2.54	0.41
2:AB:369:ILE:HD13	4:AD:340:VAL:O	2.21	0.41
18:BX:5044:ASP:C	18:BX:5045:LYS:HD3	2.41	0.41
7:AH:40:VAL:O	7:AH:44:ILE:HG13	2.21	0.41
4:BD:5030:VAL:HG12	4:BD:5031:GLY:N	2.35	0.41
1:BA:5224:ILE:H	1:BA:5224:ILE:HG13	1.57	0.41
24:AA:404:CLA:H111	34:AD:402:PHO:H3A	2.02	0.41
28:BA:5412:DGD:HA82	3:BC:5223:TRP:CH2	2.56	0.41
2:BB:5103:LEU:O	2:BB:5107:LEU:HG	2.20	0.41
24:BC:5513:CLA:NB	27:BC:5515:BCR:H383	2.36	0.41
24:BC:5505:CLA:HMD2	27:BC:5516:BCR:H343	2.01	0.41
4:BD:5162:LEU:HD21	4:BD:5167:TRP:CH2	2.56	0.41
19:AY:23:UNK:O	19:AY:24:UNK:C	2.68	0.41
10:BK:5030:VAL:CG1	10:BK:5031:LEU:N	2.84	0.41
4:AD:272:LEU:O	4:AD:276:VAL:HG23	2.21	0.41
27:AC:515:BCR:H331	27:AC:515:BCR:H342	2.02	0.41
5:AE:10:PHE:N	5:AE:10:PHE:CD2	2.89	0.41
4:BD:5128:ARG:O	4:BD:5129:GLN:C	2.59	0.41
20:AZ:36:SER:C	20:AZ:38:GLN:H	2.24	0.41
7:BH:5018:TYR:CG	7:BH:5019:GLY:N	2.89	0.41
3:BC:5466:VAL:HG13	4:BD:5251:ARG:CD	2.51	0.41
2:AB:324:LEU:HA	4:AD:293:LEU:HD21	1.99	0.41
2:AB:113:TRP:NE1	2:AB:117:TYR:CD1	2.89	0.41
4:BD:5056:THR:OG1	4:BD:5057:SER:N	2.53	0.41
13:AO:86:ARG:O	13:AO:86:ARG:CG	2.69	0.41
3:AC:332:GLN:HG3	13:AO:129:PHE:CE2	2.56	0.41
3:AC:189:TRP:O	3:AC:190:ALA:C	2.59	0.41
2:AB:73:GLY:O	2:AB:93:PHE:CD1	2.74	0.41
4:AD:168:PHE:CD2	4:AD:168:PHE:O	2.74	0.41
1:BA:5289:GLY:HA2	1:BA:5292:THR:CG2	2.51	0.41
1:BA:5278:TRP:HA	28:BC:5519:DGD:CIA	2.51	0.41
9:BJ:5036:LEU:C	9:BJ:5038:SER:H	2.22	0.41
1:AA:38:ILE:O	1:AA:42:LEU:HG	2.20	0.41
3:AC:272:LEU:CA	24:AC:509:CLA:HMD3	2.51	0.41
4:AD:162:LEU:HD22	28:AH:101:DGD:O1A	2.21	0.41
14:BT:5018:PHE:CD1	27:BT:5101:BCR:HC8	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:151:LEU:HD21	1:AA:155:PHE:HE2	1.85	0.41
2:AB:329:PRO:CD	24:AB:607:CLA:HED1	2.49	0.41
2:AB:26:HIS:HB2	24:AB:612:CLA:HMB2	2.03	0.41
2:AB:224:ARG:NH1	32:AB:624:LMT:H2'	2.35	0.41
24:AB:611:CLA:HMD1	31:AD:407:LMG:HC92	2.02	0.41
24:AB:602:CLA:C9	7:AH:46:LEU:HD22	2.51	0.41
11:AL:24:ILE:HG22	11:AL:25:LEU:N	2.35	0.41
1:BA:5092:HIS:HE1	3:BC:5359:TRP:HZ2	1.68	0.41
1:BA:5205:VAL:HG21	24:BA:5405:CLA:HMA2	2.03	0.41
2:BB:5150:CYS:HB2	24:BB:5607:CLA:CMC	2.47	0.41
27:AT:101:BCR:H372	27:BB:5621:BCR:H353	2.03	0.41
4:BD:5214:HIS:HA	35:BD:5406:PL9:O2	2.21	0.41
24:AB:607:CLA:HAC2	27:BT:5101:BCR:H393	2.02	0.41
19:BY:5021:UNK:HA	19:BY:5024:UNK:CB	2.51	0.41
13:BO:5162:ILE:O	13:BO:5230:VAL:HG11	2.20	0.41
3:AC:114:VAL:CG2	31:AC:521:LMG:H141	2.50	0.41
4:BD:5145:ALA:CB	4:BD:5272:LEU:HD21	2.51	0.41
10:BK:5043:VAL:CG2	10:BK:5046:ARG:HE	2.34	0.41
2:BB:5137:LYS:HE3	7:BH:5014:LEU:O	2.21	0.41
2:AB:168:VAL:O	2:AB:176:GLY:HA2	2.20	0.41
2:AB:173:GLY:N	2:AB:265:ILE:HD11	2.36	0.41
13:BO:5078:VAL:HG22	13:BO:5259:VAL:HG22	2.03	0.41
4:BD:5179:PHE:HA	4:BD:5182:LEU:HD12	2.03	0.41
27:BD:5407:BCR:H392	9:BJ:5025:VAL:HG21	2.03	0.41
6:AF:40:MET:O	6:AF:43:ILE:HG13	2.21	0.41
16:BV:5148:GLU:N	16:BV:5149:PRO:HD2	2.36	0.41
3:BC:5455:PHE:C	3:BC:5457:LYS:H	2.24	0.41
10:BK:5014:ALA:HB2	20:BZ:5061:VAL:CG1	2.51	0.41
16:BV:5039:ASN:HD21	16:BV:5043:LYS:HB3	1.86	0.41
16:AV:98:LEU:O	16:AV:102:MET:HG3	2.20	0.41
24:AC:504:CLA:H2	28:AC:518:DGD:C2A	2.51	0.41
28:BC:5518:DGD:C1G	28:BC:5518:DGD:O1B	2.69	0.41
4:BD:5070:GLY:O	9:BJ:5037:GLY:CA	2.69	0.41
2:AB:222:PRO:O	2:AB:223:GLN:C	2.58	0.41
3:AC:266:TRP:HZ3	24:AC:507:CLA:HBC2	1.86	0.41
4:AD:250:ASN:ND2	4:AD:262:SER:HB3	2.33	0.41
2:BB:5005:TRP:CE3	24:BB:5615:CLA:H42	2.56	0.41
2:BB:5187:PRO:C	2:BB:5189:GLY:H	2.24	0.41
2:BB:5328:GLY:O	24:BB:5611:CLA:HBA1	2.21	0.41
24:BB:5606:CLA:H161	28:BH:5101:DGD:HAW1	2.02	0.41
32:BB:5627:LMT:H92	7:BH:5035:MET:HE1	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:5202:ALA:HB3	35:BD:5406:PL9:C30	2.51	0.41
10:AK:30:VAL:CG1	10:AK:31:LEU:N	2.84	0.41
19:AY:23:UNK:O	19:AY:25:UNK:N	2.54	0.41
13:AO:55:ALA:HA	13:AO:230:VAL:HG11	2.03	0.41
3:BC:5305:THR:HG23	3:BC:5307:PRO:HG2	2.03	0.41
29:BA:5415:LHG:H272	10:BK:5045:PHE:CE2	2.56	0.41
1:BA:5258:LEU:HD12	4:BD:5128:ARG:CG	2.51	0.41
2:BB:5297:THR:OG1	2:BB:5298:LEU:N	2.54	0.41
2:BB:5377:VAL:HG11	4:BD:5342:PRO:CG	2.51	0.41
1:AA:29:TYR:CG	1:AA:133:LEU:HD13	2.56	0.41
6:BF:5024:HIS:HA	6:BF:5027:ALA:HB3	2.03	0.41
3:BC:5472:LEU:HD11	4:BD:5255:GLN:CD	2.40	0.41
8:AI:25:SER:HA	32:AI:103:LMT:H6D	2.02	0.41
2:BB:5348:ASN:O	2:BB:5350:GLU:N	2.54	0.41
32:BM:5101:LMT:H5'	32:BM:5101:LMT:H1B	1.97	0.41
3:AC:203:THR:O	3:AC:235:GLY:HA3	2.20	0.41
4:AD:126:MET:HE2	4:AD:146:PHE:HB3	2.02	0.41
13:BO:5056:TYR:CD1	13:BO:5235:GLY:HA2	2.55	0.41
3:BC:5172:ALA:O	3:BC:5176:VAL:HG23	2.21	0.41
3:AC:390:ARG:NE	16:AV:126:ILE:CG2	2.84	0.41
2:AB:447:PRO:O	2:AB:448:ARG:C	2.60	0.41
2:AB:45:PHE:HE2	2:AB:47:PRO:HB3	1.86	0.41
3:AC:282:MET:SD	24:AC:503:CLA:H142	2.61	0.40
3:AC:269:GLU:OE1	3:AC:447:ARG:HD3	2.21	0.40
24:AC:509:CLA:HBB1	24:AC:509:CLA:HHC	2.03	0.40
24:AB:602:CLA:H93	7:AH:46:LEU:HD22	2.02	0.40
8:AI:11:VAL:O	8:AI:15:PHE:HD2	2.04	0.40
1:BA:5184:ILE:CD1	4:BD:5186:GLN:HG2	2.51	0.40
2:BB:5004:PRO:HB2	2:BB:5006:TYR:CE1	2.56	0.40
2:BB:5238:LEU:CD2	2:BB:5469:HIS:HD2	2.34	0.40
2:BB:5328:GLY:N	24:BB:5611:CLA:O1A	2.49	0.40
4:BD:5263:ASN:O	4:BD:5265:ARG:N	2.54	0.40
2:AB:431:GLU:OE2	13:BO:5084:ASN:ND2	2.54	0.40
2:BB:5172:TYR:O	2:BB:5174:LEU:HG	2.21	0.40
6:AF:29:PRO:O	6:AF:32:PHE:HB3	2.21	0.40
1:BA:5012:ASN:O	1:BA:5015:GLU:HB3	2.22	0.40
16:AV:71:ILE:CD1	16:AV:72:THR:N	2.82	0.40
1:AA:333:GLU:HB2	1:AA:337:HIS:CE1	2.53	0.40
1:AA:340:PRO:HG3	15:AU:133:TYR:CD1	2.56	0.40
7:AH:63:LYS:C	7:AH:65:LEU:N	2.73	0.40
1:BA:5295:PHE:HD2	3:BC:5291:TRP:CD2	2.39	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:76:ASN:ND2	11:AL:33:SER:HB3	2.37	0.40
9:AJ:10:LEU:HD12	9:AJ:10:LEU:HA	1.86	0.40
1:BA:5206:PHE:HD2	1:BA:5206:PHE:HA	1.77	0.40
1:AA:278:TRP:HA	28:AC:519:DGD:HAG1	2.02	0.40
4:BD:5277:THR:HG22	35:BD:5406:PL9:H272	2.02	0.40
11:BL:5008:GLN:H	11:BL:5008:GLN:HE21	1.68	0.40
14:AT:29:ILE:HG22	14:AT:30:THR:H	1.86	0.40
9:BJ:5008:ILE:HD12	9:BJ:5008:ILE:H	1.85	0.40
3:AC:113:VAL:CG1	31:AC:521:LMG:H132	2.49	0.40
13:BO:5032:THR:OG1	13:BO:5033:TYR:N	2.54	0.40
2:AB:121:GLU:CG	7:AH:4:ARG:CA	2.94	0.40
2:BB:5161:LEU:N	2:BB:5161:LEU:CD1	2.84	0.40
1:BA:5029:TYR:HD2	1:BA:5133:LEU:HB2	1.87	0.40
15:AU:72:TYR:CG	15:AU:73:PRO:N	2.89	0.40
13:AO:83:LYS:CG	13:AO:84:ASN:H	2.29	0.40
6:AF:15:ILE:CG2	6:AF:16:PHE:HD1	2.33	0.40
1:AA:129:ARG:C	1:AA:131:TRP:H	2.23	0.40
28:BB:5602:DGD:HE61	32:BB:5626:LMT:H2'	2.02	0.40
27:AD:406:BCR:H392	9:AJ:25:VAL:HG21	2.03	0.40
16:AV:121:LEU:HD21	16:AV:138:LEU:HD11	2.02	0.40
10:AK:15:TYR:OH	20:AZ:58:ASN:ND2	2.52	0.40
3:AC:34:ALA:HB2	4:AD:230:SER:CB	2.51	0.40
15:AU:75:LEU:HA	15:AU:75:LEU:HD23	1.85	0.40
1:BA:5200:LEU:HD11	28:BC:5519:DGD:CCA	2.27	0.40
1:AA:217:SER:O	1:AA:220:THR:HG22	2.22	0.40
2:AB:238:LEU:CD2	2:AB:469:HIS:CD2	3.05	0.40
24:AB:603:CLA:HMB1	24:AB:603:CLA:HAB	1.80	0.40
35:AD:405:PL9:H103	35:AD:405:PL9:HC72	1.74	0.40
5:AE:69:ARG:CG	5:AE:70:PHE:N	2.83	0.40
24:BC:5502:CLA:HAA2	24:BC:5502:CLA:HBD	2.03	0.40
24:BC:5505:CLA:C2	24:BC:5505:CLA:HAA1	2.51	0.40
24:BC:5507:CLA:H122	27:BC:5516:BCR:H362	2.03	0.40
3:AC:161:LEU:HD23	3:AC:251:HIS:HD2	1.85	0.40
10:AK:46:ARG:HB2	10:AK:46:ARG:NH1	2.36	0.40
4:BD:5148:ALA:HB3	4:BD:5149:PRO:CD	2.41	0.40
32:AB:629:LMT:H5'	32:AB:629:LMT:H1B	1.80	0.40
15:BU:5072:TYR:CD2	15:BU:5073:PRO:N	2.90	0.40
4:AD:180:ARG:NH1	4:AD:333:ASP:OD1	2.54	0.40
1:BA:5069:GLY:CA	1:BA:5075:ASN:ND2	2.84	0.40
2:BB:5385:ARG:O	2:BB:5386:ALA:C	2.60	0.40
2:BB:5151:PHE:CE1	2:BB:5203:ILE:HG23	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:200:LEU:CD2	28:AC:519:DGD:CCA	2.99	0.40
1:AA:278:TRP:HE3	28:AC:519:DGD:HAG1	1.83	0.40
15:AU:83:ALA:CB	15:AU:84:PRO:HD2	2.17	0.40
1:AA:39:PRO:HG3	27:AA:410:BCR:HC8	2.04	0.40
24:AC:502:CLA:HBB1	24:AC:502:CLA:HHC	2.03	0.40
4:AD:210:LEU:HD21	35:AD:405:PL9:H13	2.03	0.40
4:AD:262:SER:N	31:AD:408:LMG:O3	2.55	0.40
27:AT:101:BCR:H393	24:BB:5611:CLA:HAC2	2.03	0.40
24:BB:5615:CLA:HMD1	31:BD:5409:LMG:HC92	2.03	0.40
3:BC:5278:ALA:HB1	24:BC:5501:CLA:H142	2.03	0.40
13:BO:5081:GLU:C	13:BO:5083:LYS:H	2.25	0.40
14:AT:30:THR:HB	14:AT:31:LYS:NZ	2.35	0.40
3:AC:134:ILE:HD11	24:AC:511:CLA:C9	2.49	0.40
3:AC:38:GLY:HA3	24:AC:511:CLA:CMD	2.50	0.40
27:BK:5102:BCR:H332	20:BZ:5017:PHE:CD1	2.56	0.40
8:BI:5007:THR:O	8:BI:5008:VAL:C	2.59	0.40
3:BC:5447:ARG:HG2	3:BC:5447:ARG:HH11	1.86	0.40
4:AD:313:THR:H	4:AD:316:THR:HG23	1.86	0.40
15:AU:51:TYR:HE1	15:AU:60:THR:HG1	1.66	0.40
1:BA:5238:LYS:O	1:BA:5241:GLN:HG3	2.21	0.40
2:AB:285:ASN:N	2:AB:285:ASN:HD22	2.18	0.40
18:AX:30:LEU:HD23	18:AX:30:LEU:HA	1.88	0.40
2:AB:243:ALA:O	24:AB:608:CLA:HBC3	2.22	0.40
7:AH:41:PHE:O	7:AH:45:ILE:HG12	2.21	0.40
24:BA:5406:CLA:H62	34:BD:5403:PHO:HMA1	2.02	0.40
24:BB:5607:CLA:HMB2	24:BB:5607:CLA:H52	2.02	0.40
24:BB:5619:CLA:HBB1	24:BB:5619:CLA:HHC	2.03	0.40
4:BD:5261:PHE:HB2	35:BD:5406:PL9:H522	2.03	0.40
4:BD:5262:SER:N	31:BD:5410:LMG:O3	2.54	0.40
24:AC:511:CLA:H151	20:AZ:24:PRO:CG	2.50	0.40
3:AC:307:PRO:O	3:AC:311:GLN:HG2	2.21	0.40
13:BO:5132:VAL:HG12	13:BO:5133:THR:N	2.37	0.40
1:BA:5011:ALA:HB1	1:BA:5015:GLU:OE1	2.21	0.40
6:BF:5029:PRO:O	6:BF:5032:PHE:HB3	2.22	0.40
6:AF:21:VAL:HG21	30:AF:102:SQD:H101	2.02	0.40
6:BF:5020:TRP:NE1	6:BF:5024:HIS:CE1	2.89	0.40
1:AA:271:LEU:CD1	25:AA:408:MST:H162	2.48	0.40
1:BA:5296:ASN:HB3	3:BC:5401:LEU:HD13	2.04	0.40
2:BB:5170:ASP:CB	2:BB:5171:PRO:CD	2.97	0.40
3:AC:202:PRO:HB2	3:AC:235:GLY:HA2	2.02	0.40
13:BO:5065:ARG:CB	13:BO:5065:ARG:NH1	2.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:24:ARG:NH2	18:AX:44:ASP:O	2.55	0.40
2:AB:283:GLU:O	2:AB:287:ARG:HG3	2.21	0.40
4:BD:5095:PRO:HG3	18:BX:5015:SER:HB3	2.03	0.40
5:AE:38:VAL:HG21	6:AF:36:ALA:O	2.21	0.40
12:BM:5016:LEU:HA	12:BM:5016:LEU:HD23	1.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	333/344 (97%)	284 (85%)	42 (13%)	7 (2%)	9	46
1	BA	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	9	46
2	AB	488/510 (96%)	418 (86%)	54 (11%)	16 (3%)	5	32
2	BB	488/510 (96%)	422 (86%)	51 (10%)	15 (3%)	5	34
3	AC	445/461 (96%)	371 (83%)	58 (13%)	16 (4%)	4	30
3	BC	445/461 (96%)	372 (84%)	56 (13%)	17 (4%)	4	28
4	AD	339/352 (96%)	286 (84%)	44 (13%)	9 (3%)	6	39
4	BD	339/352 (96%)	288 (85%)	43 (13%)	8 (2%)	7	43
5	AE	80/84 (95%)	71 (89%)	6 (8%)	3 (4%)	4	28
5	BE	80/84 (95%)	70 (88%)	7 (9%)	3 (4%)	4	28
6	AF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	5	35
6	BF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	5	35
7	AH	63/66 (96%)	47 (75%)	11 (18%)	5 (8%)	1	8
7	BH	63/66 (96%)	48 (76%)	11 (18%)	4 (6%)	2	13
8	AI	33/38 (87%)	20 (61%)	11 (33%)	2 (6%)	2	15
8	BI	33/38 (87%)	21 (64%)	10 (30%)	2 (6%)	2	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AJ	36/40 (90%)	27 (75%)	6 (17%)	3 (8%)	1	7
9	BJ	36/40 (90%)	25 (69%)	8 (22%)	3 (8%)	1	7
10	AK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	2	17
10	BK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	2	17
11	AL	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	BL	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	AM	32/36 (89%)	24 (75%)	8 (25%)	0	100	100
12	BM	32/36 (89%)	24 (75%)	8 (25%)	0	100	100
13	AO	241/247 (98%)	198 (82%)	31 (13%)	12 (5%)	3	21
13	BO	241/247 (98%)	199 (83%)	31 (13%)	11 (5%)	3	23
14	AT	30/32 (94%)	26 (87%)	3 (10%)	1 (3%)	5	32
14	BT	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	5	32
15	AU	95/104 (91%)	78 (82%)	12 (13%)	5 (5%)	2	19
15	BU	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	3	26
16	AV	135/137 (98%)	111 (82%)	23 (17%)	1 (1%)	26	72
16	BV	135/137 (98%)	112 (83%)	22 (16%)	1 (1%)	26	72
17	Ay	26/46 (56%)	15 (58%)	7 (27%)	4 (15%)	0	1
17	By	26/46 (56%)	14 (54%)	9 (35%)	3 (12%)	0	3
18	AX	35/41 (85%)	26 (74%)	5 (14%)	4 (11%)	0	3
18	BX	35/41 (85%)	27 (77%)	4 (11%)	4 (11%)	0	3
20	AZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	3	21
20	BZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	3	21
All	All	5148/5438 (95%)	4279 (83%)	686 (13%)	183 (4%)	4	30

All (183) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	12	ASN
1	AA	141	PRO
1	AA	142	TRP
2	AB	176	GLY
2	AB	230	ARG
2	AB	484	PRO
2	AB	488	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	AB	490	GLN
3	AC	144	SER
3	AC	257	PHE
3	AC	416	SER
3	AC	452	ALA
4	AD	239	GLN
4	AD	240	ALA
4	AD	262	SER
7	AH	18	TYR
8	AI	25	SER
9	AJ	35	GLY
13	AO	52	ALA
14	AT	30	THR
15	AU	72	TYR
15	AU	83	ALA
16	AV	75	ASN
17	Ay	43	ARG
18	AX	45	LYS
20	AZ	32	ASP
1	BA	5012	ASN
1	BA	5141	PRO
1	BA	5142	TRP
2	BB	5176	GLY
2	BB	5230	ARG
2	BB	5484	PRO
2	BB	5488	PRO
3	BC	5144	SER
3	BC	5257	PHE
3	BC	5416	SER
3	BC	5452	ALA
4	BD	5239	GLN
4	BD	5240	ALA
4	BD	5262	SER
7	BH	5018	TYR
8	BI	5025	SER
9	BJ	5035	GLY
13	BO	5052	ALA
14	BT	5030	THR
15	BU	5072	TYR
15	BU	5083	ALA
17	By	5043	ARG
18	BX	5045	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	BZ	5032	ASP
2	AB	349	LYS
3	AC	46	SER
3	AC	136	GLY
3	AC	194	GLY
3	AC	209	ILE
3	AC	456	GLU
4	AD	234	ALA
4	AD	264	LYS
7	AH	26	GLY
9	AJ	38	SER
13	AO	231	ASP
15	AU	39	LEU
15	AU	73	PRO
17	Ay	25	ILE
18	AX	43	ILE
2	BB	5349	LYS
2	BB	5436	THR
3	BC	5136	GLY
3	BC	5141	GLU
3	BC	5194	GLY
4	BD	5234	ALA
7	BH	5026	GLY
9	BJ	5038	SER
13	BO	5158	ASN
13	BO	5231	ASP
15	BU	5073	PRO
16	BV	5075	ASN
18	BX	5043	ILE
2	AB	13	ILE
2	AB	127	ARG
2	AB	183	PRO
2	AB	414	PRO
2	AB	436	THR
3	AC	32	GLY
3	AC	141	GLU
3	AC	375	LEU
3	AC	453	ALA
4	AD	263	ASN
5	AE	9	PRO
7	AH	16	SER
10	AK	13	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	AK	45	PHE
13	AO	60	SER
13	AO	158	ASN
13	AO	165	SER
20	AZ	24	PRO
20	AZ	28	ALA
2	BB	5013	ILE
2	BB	5127	ARG
2	BB	5183	PRO
2	BB	5414	PRO
3	BC	5032	GLY
3	BC	5046	SER
3	BC	5209	ILE
3	BC	5375	LEU
3	BC	5411	ALA
3	BC	5456	GLU
4	BD	5263	ASN
4	BD	5264	LYS
5	BE	5009	PRO
7	BH	5016	SER
10	BK	5013	GLU
10	BK	5045	PHE
13	BO	5165	SER
17	By	5025	ILE
20	BZ	5024	PRO
20	BZ	5028	ALA
2	AB	173	GLY
2	AB	231	MET
3	AC	154	LYS
4	AD	73	PHE
5	AE	10	PHE
13	AO	51	THR
13	AO	82	PRO
17	Ay	24	MET
18	AX	44	ASP
2	BB	5235	GLU
5	BE	5010	PHE
13	BO	5060	SER
13	BO	5082	PRO
1	AA	97	TRP
2	AB	235	GLU
3	AC	462	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	AF	41	GLN
7	AH	6	TRP
15	AU	42	VAL
2	BB	5435	GLU
2	BB	5490	GLN
3	BC	5453	ALA
3	BC	5462	GLU
4	BD	5252	PHE
6	BF	5041	GLN
7	BH	5006	TRP
13	BO	5085	LYS
13	BO	5088	GLU
15	BU	5042	VAL
17	By	5024	MET
18	BX	5044	ASP
1	AA	334	ARG
2	AB	435	GLU
4	AD	351	ALA
13	AO	88	GLU
18	AX	12	ILE
1	BA	5097	TRP
1	BA	5334	ARG
2	BB	5173	GLY
3	BC	5382	ASN
4	BD	5351	ALA
5	BE	5052	PRO
13	BO	5051	THR
13	BO	5159	VAL
18	BX	5012	ILE
1	AA	21	VAL
2	AB	16	PRO
9	AJ	5	GLY
13	AO	159	VAL
1	BA	5021	VAL
3	AC	201	ASN
17	Ay	35	ILE
3	BC	5201	ASN
5	AE	52	PRO
7	AH	60	VAL
8	AI	32	PRO
13	AO	232	GLY
2	BB	5016	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	BI	5032	PRO
1	AA	176	ILE
4	AD	160	TYR
13	AO	127	ILE
1	BA	5039	PRO
13	AO	152	VAL
9	BJ	5005	GLY
13	BO	5152	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	271/280 (97%)	250 (92%)	21 (8%)	16	54
1	BA	271/280 (97%)	253 (93%)	18 (7%)	21	61
2	AB	390/407 (96%)	372 (95%)	18 (5%)	33	74
2	BB	390/407 (96%)	374 (96%)	16 (4%)	37	76
3	AC	347/362 (96%)	326 (94%)	21 (6%)	23	64
3	BC	347/362 (96%)	325 (94%)	22 (6%)	22	63
4	AD	275/283 (97%)	249 (90%)	26 (10%)	11	40
4	BD	275/283 (97%)	249 (90%)	26 (10%)	11	40
5	AE	72/73 (99%)	66 (92%)	6 (8%)	14	49
5	BE	72/73 (99%)	66 (92%)	6 (8%)	14	49
6	AF	29/39 (74%)	27 (93%)	2 (7%)	19	59
6	BF	29/39 (74%)	28 (97%)	1 (3%)	44	80
7	AH	53/55 (96%)	42 (79%)	11 (21%)	1	7
7	BH	53/55 (96%)	43 (81%)	10 (19%)	2	10
8	AI	32/35 (91%)	32 (100%)	0	100	100
8	BI	32/35 (91%)	31 (97%)	1 (3%)	47	82
9	AJ	25/28 (89%)	24 (96%)	1 (4%)	38	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	BJ	25/28 (89%)	24 (96%)	1 (4%)	38	77
10	AK	30/30 (100%)	29 (97%)	1 (3%)	45	81
10	BK	30/30 (100%)	29 (97%)	1 (3%)	45	81
11	AL	35/35 (100%)	33 (94%)	2 (6%)	25	67
11	BL	35/35 (100%)	32 (91%)	3 (9%)	13	46
12	AM	31/33 (94%)	30 (97%)	1 (3%)	46	81
12	BM	31/33 (94%)	29 (94%)	2 (6%)	21	61
13	AO	202/208 (97%)	187 (93%)	15 (7%)	17	56
13	BO	202/208 (97%)	187 (93%)	15 (7%)	17	56
14	AT	29/29 (100%)	28 (97%)	1 (3%)	44	80
14	BT	29/29 (100%)	27 (93%)	2 (7%)	19	59
15	AU	84/89 (94%)	76 (90%)	8 (10%)	11	40
15	BU	84/89 (94%)	76 (90%)	8 (10%)	11	40
16	AV	116/117 (99%)	111 (96%)	5 (4%)	35	75
16	BV	116/117 (99%)	110 (95%)	6 (5%)	29	69
17	Ay	20/37 (54%)	15 (75%)	5 (25%)	1	2
17	By	20/37 (54%)	15 (75%)	5 (25%)	1	2
18	AX	30/34 (88%)	29 (97%)	1 (3%)	45	81
18	BX	30/34 (88%)	29 (97%)	1 (3%)	45	81
20	AZ	52/52 (100%)	49 (94%)	3 (6%)	25	66
20	BZ	52/52 (100%)	48 (92%)	4 (8%)	16	54
All	All	4246/4452 (95%)	3950 (93%)	296 (7%)	19	58

All (296) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	13	LEU
1	AA	30	VAL
1	AA	32	TRP
1	AA	56	PRO
1	AA	121	LEU
1	AA	129	ARG
1	AA	145	VAL
1	AA	170	ASP
1	AA	202	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	206	PHE
1	AA	210	LEU
1	AA	218	LEU
1	AA	226	GLU
1	AA	243	GLU
1	AA	245	THR
1	AA	247	ASN
1	AA	259	ILE
1	AA	266	ASN
1	AA	286	THR
1	AA	298	ASN
1	AA	335	ASN
2	AB	16	PRO
2	AB	18	ARG
2	AB	62	VAL
2	AB	79	SER
2	AB	121	GLU
2	AB	161	LEU
2	AB	179	GLN
2	AB	245	VAL
2	AB	246	PHE
2	AB	297	THR
2	AB	311	PHE
2	AB	433	ASP
2	AB	439	SER
2	AB	467	ILE
2	AB	484	PRO
2	AB	485	GLU
2	AB	488	PRO
2	AB	490	GLN
3	AC	27	ASP
3	AC	29	GLU
3	AC	78	GLU
3	AC	97	TRP
3	AC	121	SER
3	AC	165	LEU
3	AC	188	THR
3	AC	228	ASN
3	AC	244	CYS
3	AC	259	TRP
3	AC	289	PHE
3	AC	295	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	AC	318	LEU
3	AC	321	ASP
3	AC	324	LEU
3	AC	355	THR
3	AC	424	SER
3	AC	430	HIS
3	AC	456	GLU
3	AC	461	ARG
3	AC	473	ASP
4	AD	14	TRP
4	AD	43	LEU
4	AD	84	SER
4	AD	91	LEU
4	AD	110	LEU
4	AD	112	THR
4	AD	130	PHE
4	AD	166	SER
4	AD	180	ARG
4	AD	201	VAL
4	AD	205	LEU
4	AD	242	GLU
4	AD	256	ILE
4	AD	259	ILE
4	AD	262	SER
4	AD	264	LYS
4	AD	272	LEU
4	AD	279	LEU
4	AD	282	SER
4	AD	291	LEU
4	AD	293	LEU
4	AD	316	THR
4	AD	323	GLU
4	AD	331	PRO
4	AD	345	VAL
4	AD	346	LEU
5	AE	9	PRO
5	AE	10	PHE
5	AE	52	PRO
5	AE	60	GLN
5	AE	68	ASP
5	AE	84	LYS
6	AF	18	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	AF	19	ARG
7	AH	12	ARG
7	AH	14	LEU
7	AH	21	VAL
7	AH	25	TRP
7	AH	27	THR
7	AH	42	LEU
7	AH	43	LEU
7	AH	45	ILE
7	AH	49	TYR
7	AH	56	ASP
7	AH	60	VAL
9	AJ	7	ARG
10	AK	19	ASP
11	AL	8	GLN
11	AL	15	THR
12	AM	25	LEU
13	AO	31	LEU
13	AO	41	LEU
13	AO	60	SER
13	AO	65	ARG
13	AO	84	ASN
13	AO	86	ARG
13	AO	97	VAL
13	AO	106	GLN
13	AO	141	ARG
13	AO	152	VAL
13	AO	158	ASN
13	AO	165	SER
13	AO	171	GLU
13	AO	207	GLU
13	AO	224	SER
14	AT	29	ILE
15	AU	44	ASP
15	AU	53	GLU
15	AU	61	ASN
15	AU	98	THR
15	AU	103	GLN
15	AU	114	VAL
15	AU	119	THR
15	AU	132	LEU
16	AV	32	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	AV	40	SER
16	AV	68	VAL
16	AV	89	THR
16	AV	92	ARG
17	Ay	21	GLN
17	Ay	28	ILE
17	Ay	34	MET
17	Ay	35	ILE
17	Ay	36	ILE
18	AX	45	LYS
20	AZ	33	TRP
20	AZ	58	ASN
20	AZ	62	VAL
1	BA	5013	LEU
1	BA	5030	VAL
1	BA	5032	TRP
1	BA	5121	LEU
1	BA	5129	ARG
1	BA	5145	VAL
1	BA	5202	VAL
1	BA	5206	PHE
1	BA	5210	LEU
1	BA	5218	LEU
1	BA	5226	GLU
1	BA	5243	GLU
1	BA	5245	THR
1	BA	5247	ASN
1	BA	5259	ILE
1	BA	5286	THR
1	BA	5298	ASN
1	BA	5335	ASN
2	BB	5016	PRO
2	BB	5018	ARG
2	BB	5062	VAL
2	BB	5121	GLU
2	BB	5161	LEU
2	BB	5179	GLN
2	BB	5246	PHE
2	BB	5297	THR
2	BB	5311	PHE
2	BB	5433	ASP
2	BB	5439	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	BB	5467	ILE
2	BB	5484	PRO
2	BB	5485	GLU
2	BB	5488	PRO
2	BB	5490	GLN
3	BC	5027	ASP
3	BC	5029	GLU
3	BC	5078	GLU
3	BC	5097	TRP
3	BC	5121	SER
3	BC	5165	LEU
3	BC	5188	THR
3	BC	5228	ASN
3	BC	5244	CYS
3	BC	5259	TRP
3	BC	5289	PHE
3	BC	5295	THR
3	BC	5318	LEU
3	BC	5321	ASP
3	BC	5324	LEU
3	BC	5355	THR
3	BC	5424	SER
3	BC	5430	HIS
3	BC	5432	VAL
3	BC	5456	GLU
3	BC	5461	ARG
3	BC	5473	ASP
4	BD	5014	TRP
4	BD	5043	LEU
4	BD	5084	SER
4	BD	5091	LEU
4	BD	5110	LEU
4	BD	5112	THR
4	BD	5128	ARG
4	BD	5130	PHE
4	BD	5166	SER
4	BD	5180	ARG
4	BD	5201	VAL
4	BD	5205	LEU
4	BD	5242	GLU
4	BD	5259	ILE
4	BD	5262	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	BD	5264	LYS
4	BD	5272	LEU
4	BD	5279	LEU
4	BD	5282	SER
4	BD	5291	LEU
4	BD	5293	LEU
4	BD	5316	THR
4	BD	5323	GLU
4	BD	5331	PRO
4	BD	5345	VAL
4	BD	5346	LEU
5	BE	5009	PRO
5	BE	5010	PHE
5	BE	5052	PRO
5	BE	5060	GLN
5	BE	5068	ASP
5	BE	5084	LYS
6	BF	5018	VAL
7	BH	5012	ARG
7	BH	5021	VAL
7	BH	5025	TRP
7	BH	5027	THR
7	BH	5042	LEU
7	BH	5043	LEU
7	BH	5045	ILE
7	BH	5049	TYR
7	BH	5056	ASP
7	BH	5060	VAL
8	BI	5032	PRO
9	BJ	5007	ARG
10	BK	5023	ASP
11	BL	5008	GLN
11	BL	5009	PRO
11	BL	5015	THR
12	BM	5025	LEU
12	BM	5034	LYS
13	BO	5031	LEU
13	BO	5041	LEU
13	BO	5060	SER
13	BO	5065	ARG
13	BO	5084	ASN
13	BO	5086	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	BO	5097	VAL
13	BO	5106	GLN
13	BO	5141	ARG
13	BO	5152	VAL
13	BO	5158	ASN
13	BO	5165	SER
13	BO	5171	GLU
13	BO	5207	GLU
13	BO	5224	SER
14	BT	5029	ILE
14	BT	5032	LYS
15	BU	5044	ASP
15	BU	5053	GLU
15	BU	5061	ASN
15	BU	5098	THR
15	BU	5103	GLN
15	BU	5114	VAL
15	BU	5119	THR
15	BU	5132	LEU
16	BV	5032	GLU
16	BV	5040	SER
16	BV	5068	VAL
16	BV	5089	THR
16	BV	5092	ARG
16	BV	5125	ASP
17	By	5021	GLN
17	By	5028	ILE
17	By	5034	MET
17	By	5035	ILE
17	By	5036	ILE
18	BX	5045	LYS
20	BZ	5025	VAL
20	BZ	5033	TRP
20	BZ	5058	ASN
20	BZ	5062	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	12	ASN
1	AA	19	ASN
1	AA	75	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	92	HIS
1	AA	118	HIS
1	AA	199	GLN
1	AA	234	ASN
1	AA	241	GLN
1	AA	247	ASN
1	AA	272	HIS
1	AA	315	ASN
1	AA	337	HIS
1	AA	338	ASN
2	AB	53	ASN
2	AB	157	HIS
2	AB	179	GLN
2	AB	201	HIS
2	AB	216	HIS
2	AB	281	GLN
2	AB	282	GLN
2	AB	285	ASN
2	AB	331	ASN
2	AB	490	GLN
3	AC	155	ASN
3	AC	201	ASN
3	AC	228	ASN
3	AC	322	GLN
3	AC	388	GLN
3	AC	398	HIS
4	AD	83	ASN
4	AD	129	GLN
4	AD	332	GLN
5	AE	60	GLN
5	AE	75	GLN
6	AF	41	GLN
11	AL	8	GLN
11	AL	37	ASN
12	AM	5	GLN
12	AM	32	GLN
13	AO	62	GLN
13	AO	84	ASN
13	AO	87	GLN
13	AO	106	GLN
13	AO	114	ASN
13	AO	135	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	AO	150	ASN
13	AO	173	ASN
13	AO	181	ASN
13	AO	202	GLN
13	AO	222	GLN
18	AX	47	GLN
20	AZ	58	ASN
1	BA	5012	ASN
1	BA	5019	ASN
1	BA	5075	ASN
1	BA	5092	HIS
1	BA	5118	HIS
1	BA	5199	GLN
1	BA	5234	ASN
1	BA	5241	GLN
1	BA	5247	ASN
1	BA	5272	HIS
1	BA	5312	ASN
1	BA	5315	ASN
1	BA	5337	HIS
1	BA	5338	ASN
2	BB	5053	ASN
2	BB	5157	HIS
2	BB	5179	GLN
2	BB	5201	HIS
2	BB	5216	HIS
2	BB	5281	GLN
2	BB	5282	GLN
2	BB	5285	ASN
2	BB	5331	ASN
2	BB	5338	GLN
2	BB	5469	HIS
2	BB	5490	GLN
3	BC	5155	ASN
3	BC	5201	ASN
3	BC	5228	ASN
3	BC	5322	GLN
3	BC	5388	GLN
3	BC	5398	HIS
3	BC	5418	ASN
4	BD	5083	ASN
4	BD	5129	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	BD	5250	ASN
4	BD	5332	GLN
5	BE	5060	GLN
5	BE	5075	GLN
6	BF	5041	GLN
11	BL	5008	GLN
11	BL	5037	ASN
12	BM	5005	GLN
12	BM	5028	GLN
12	BM	5032	GLN
13	BO	5062	GLN
13	BO	5084	ASN
13	BO	5087	GLN
13	BO	5106	GLN
13	BO	5114	ASN
13	BO	5135	GLN
13	BO	5150	ASN
13	BO	5173	ASN
13	BO	5181	ASN
13	BO	5202	GLN
13	BO	5222	GLN
16	BV	5060	GLN
18	BX	5042	GLN
18	BX	5047	GLN
20	BZ	5058	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 196 ligands modelled in this entry, 12 are monoatomic - leaving 184 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
22	BCT	AA	402	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	AA	404	-	55,73,73	2.48	12 (21%)	61,113,113	1.58	15 (24%)
24	CLA	AA	405	-	55,73,73	2.54	16 (29%)	61,113,113	2.12	18 (29%)
24	CLA	AA	406	-	55,73,73	2.50	14 (25%)	61,113,113	1.98	16 (26%)
24	CLA	AA	407	-	55,73,73	2.49	13 (23%)	61,113,113	1.78	17 (27%)
25	MST	AA	408	-	16,16,16	0.52	0	21,22,22	4.03	8 (38%)
26	OEC	AA	409	1,3	0,0,13	0.00	-	0,0,27	0.00	-
27	BCR	AA	410	-	41,41,41	1.62	7 (17%)	56,56,56	2.11	22 (39%)
28	DGD	AA	411	-	57,57,67	1.76	14 (24%)	71,71,81	3.75	25 (35%)
29	LHG	AA	412	-	38,38,48	1.91	5 (13%)	39,44,54	1.40	4 (10%)
30	SQD	AA	413	-	50,51,54	2.41	25 (50%)	58,62,65	3.03	20 (34%)
31	LMG	AA	414	-	44,44,55	1.08	3 (6%)	52,52,63	1.51	6 (11%)
29	LHG	AA	415	-	36,36,48	1.04	2 (5%)	37,42,54	1.15	3 (8%)
30	SQD	AA	416	-	53,54,54	2.40	29 (54%)	61,65,65	2.99	19 (31%)
31	LMG	AA	417	-	42,42,55	1.06	5 (11%)	50,50,63	2.37	12 (24%)
24	CLA	AB	601	-	55,73,73	2.85	15 (27%)	61,113,113	1.56	9 (14%)
24	CLA	AB	602	-	55,73,73	2.48	13 (23%)	61,113,113	1.60	12 (19%)
24	CLA	AB	603	-	55,73,73	2.61	13 (23%)	61,113,113	1.96	18 (29%)
24	CLA	AB	604	-	55,73,73	2.55	14 (25%)	61,113,113	1.58	15 (24%)
24	CLA	AB	605	-	55,73,73	2.67	13 (23%)	61,113,113	1.78	14 (22%)
24	CLA	AB	606	-	55,73,73	2.68	14 (25%)	61,113,113	1.72	16 (26%)
24	CLA	AB	607	-	55,73,73	2.59	16 (29%)	61,113,113	2.01	18 (29%)
24	CLA	AB	608	-	55,73,73	2.77	16 (29%)	61,113,113	2.04	17 (27%)
24	CLA	AB	609	-	55,73,73	2.64	12 (21%)	61,113,113	1.66	14 (22%)
24	CLA	AB	610	-	55,73,73	2.49	11 (20%)	61,113,113	1.62	11 (18%)
24	CLA	AB	611	-	55,73,73	2.52	13 (23%)	61,113,113	1.85	20 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	AB	612	-	55,73,73	2.54	12 (21%)	61,113,113	1.76	12 (19%)
24	CLA	AB	613	-	55,73,73	2.31	11 (20%)	61,113,113	1.49	12 (19%)
24	CLA	AB	614	-	55,73,73	2.71	13 (23%)	61,113,113	1.90	15 (24%)
24	CLA	AB	615	-	55,73,73	2.51	12 (21%)	61,113,113	1.61	11 (18%)
24	CLA	AB	616	-	55,73,73	2.62	11 (20%)	61,113,113	1.54	9 (14%)
27	BCR	AB	617	-	41,41,41	1.58	6 (14%)	56,56,56	2.16	19 (33%)
27	BCR	AB	618	-	41,41,41	1.93	7 (17%)	56,56,56	2.13	16 (28%)
27	BCR	AB	619	-	41,41,41	1.84	8 (19%)	56,56,56	2.01	19 (33%)
31	LMG	AB	620	-	51,51,55	1.30	3 (5%)	59,59,63	2.01	13 (22%)
31	LMG	AB	621	-	49,49,55	0.77	1 (2%)	57,57,63	1.90	15 (26%)
30	SQD	AB	622	-	42,43,54	2.62	20 (47%)	50,54,65	3.13	14 (28%)
32	LMT	AB	623	-	36,36,36	1.73	8 (22%)	47,47,47	0.98	2 (4%)
32	LMT	AB	624	-	36,36,36	1.62	7 (19%)	47,47,47	0.93	2 (4%)
33	DMS	AB	625	-	3,3,3	0.71	0	3,3,3	1.36	0
33	DMS	AB	626	-	3,3,3	0.66	0	3,3,3	0.99	0
30	SQD	AB	627	-	46,47,54	2.50	23 (50%)	54,58,65	2.97	14 (25%)
28	DGD	AB	628	-	53,53,67	1.42	7 (13%)	67,67,81	2.12	13 (19%)
32	LMT	AB	629	-	36,36,36	1.56	7 (19%)	47,47,47	1.38	5 (10%)
32	LMT	AB	630	-	36,36,36	1.70	9 (25%)	47,47,47	1.00	1 (2%)
24	CLA	AC	501	-	55,73,73	2.58	15 (27%)	61,113,113	1.75	13 (21%)
24	CLA	AC	502	-	55,73,73	2.52	12 (21%)	61,113,113	1.67	13 (21%)
24	CLA	AC	503	-	55,73,73	2.55	13 (23%)	61,113,113	1.80	16 (26%)
24	CLA	AC	504	-	55,73,73	2.47	15 (27%)	61,113,113	1.85	14 (22%)
24	CLA	AC	505	-	55,73,73	2.83	16 (29%)	61,113,113	1.85	13 (21%)
24	CLA	AC	506	-	55,73,73	2.71	14 (25%)	61,113,113	1.68	14 (22%)
24	CLA	AC	507	-	55,73,73	2.42	13 (23%)	61,113,113	1.62	12 (19%)
24	CLA	AC	508	-	55,73,73	2.49	12 (21%)	61,113,113	1.80	15 (24%)
24	CLA	AC	509	-	55,73,73	2.46	11 (20%)	61,113,113	1.69	12 (19%)
24	CLA	AC	510	-	55,73,73	2.48	11 (20%)	61,113,113	1.59	11 (18%)
24	CLA	AC	511	3	55,73,73	2.65	12 (21%)	61,113,113	1.92	15 (24%)
24	CLA	AC	512	-	55,73,73	2.58	12 (21%)	61,113,113	1.55	10 (16%)
24	CLA	AC	513	-	55,73,73	2.70	11 (20%)	61,113,113	1.69	14 (22%)
27	BCR	AC	514	-	41,41,41	1.62	7 (17%)	56,56,56	2.19	25 (44%)
27	BCR	AC	515	-	41,41,41	1.75	7 (17%)	56,56,56	2.29	22 (39%)
27	BCR	AC	516	-	41,41,41	1.64	8 (19%)	56,56,56	2.31	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	DGD	AC	517	-	54,54,67	1.32	7 (12%)	68,68,81	2.84	22 (32%)
28	DGD	AC	518	-	63,63,67	1.20	6 (9%)	77,77,81	2.94	25 (32%)
28	DGD	AC	519	-	67,67,67	1.47	11 (16%)	81,81,81	3.41	31 (38%)
31	LMG	AC	520	-	48,48,55	1.04	5 (10%)	56,56,63	1.93	18 (32%)
31	LMG	AC	521	-	45,45,55	1.07	2 (4%)	53,53,63	1.98	14 (26%)
24	CLA	AD	401	-	55,73,73	2.47	13 (23%)	61,113,113	1.67	14 (22%)
34	PHO	AD	402	-	67,69,69	2.30	13 (19%)	84,99,99	1.39	14 (16%)
34	PHO	AD	403	-	67,69,69	2.40	15 (22%)	84,99,99	1.52	15 (17%)
24	CLA	AD	404	-	55,73,73	2.60	15 (27%)	61,113,113	1.74	12 (19%)
35	PL9	AD	405	-	55,55,55	4.40	18 (32%)	68,69,69	2.90	24 (35%)
27	BCR	AD	406	-	41,41,41	1.65	7 (17%)	56,56,56	2.40	24 (42%)
31	LMG	AD	407	-	49,49,55	0.73	1 (2%)	57,57,63	2.72	20 (35%)
31	LMG	AD	408	-	48,48,55	0.94	4 (8%)	56,56,63	2.10	12 (21%)
32	LMT	AD	409	-	32,32,36	1.71	7 (21%)	43,43,47	1.23	2 (4%)
28	DGD	AE	101	-	64,64,67	1.52	13 (20%)	78,78,81	1.49	10 (12%)
36	HEM	AF	101	5,6	30,50,50	2.83	13 (43%)	24,82,82	3.89	13 (54%)
30	SQD	AF	102	-	44,45,54	2.53	21 (47%)	52,56,65	3.25	16 (30%)
28	DGD	AH	101	-	59,59,67	1.31	10 (16%)	73,73,81	2.10	19 (26%)
31	LMG	AI	101	-	43,43,55	1.01	2 (4%)	51,51,63	1.74	7 (13%)
32	LMT	AI	102	-	36,36,36	1.58	7 (19%)	47,47,47	1.00	2 (4%)
32	LMT	AI	103	-	36,36,36	1.42	6 (16%)	47,47,47	1.75	9 (19%)
27	BCR	AJ	101	-	41,41,41	2.47	13 (31%)	56,56,56	3.30	26 (46%)
31	LMG	AJ	102	-	46,46,55	0.95	3 (6%)	54,54,63	2.62	16 (29%)
27	BCR	AK	102	-	41,41,41	1.78	6 (14%)	56,56,56	2.52	25 (44%)
31	LMG	AM	101	-	42,42,55	0.94	2 (4%)	50,50,63	1.70	7 (14%)
32	LMT	AM	102	-	36,36,36	1.71	10 (27%)	47,47,47	0.90	1 (2%)
27	BCR	AT	101	-	41,41,41	1.63	6 (14%)	56,56,56	2.29	24 (42%)
33	DMS	AU	201	-	3,3,3	0.90	0	3,3,3	1.08	0
36	HEM	AV	201	16	30,50,50	2.80	14 (46%)	24,82,82	3.88	13 (54%)
33	DMS	AV	202	-	3,3,3	0.74	0	3,3,3	1.00	0
27	BCR	AX	101	-	41,41,41	1.86	8 (19%)	56,56,56	2.26	22 (39%)
30	SQD	BA	5401	-	53,54,54	2.43	28 (52%)	61,65,65	2.98	19 (31%)
31	LMG	BA	5402	-	42,42,55	1.06	3 (7%)	50,50,63	2.38	12 (24%)
22	BCT	BA	5403	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	BA	5405	-	55,73,73	2.47	13 (23%)	61,113,113	1.54	14 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	BA	5406	-	55,73,73	2.64	15 (27%)	61,113,113	2.13	16 (26%)
24	CLA	BA	5407	-	55,73,73	2.61	15 (27%)	61,113,113	1.96	15 (24%)
24	CLA	BA	5408	-	55,73,73	2.59	13 (23%)	61,113,113	1.77	14 (22%)
25	MST	BA	5409	-	16,16,16	0.49	0	21,22,22	3.94	8 (38%)
26	OEC	BA	5410	1,3	0,0,13	0.00	-	0,0,27	0.00	-
27	BCR	BA	5411	-	41,41,41	1.68	7 (17%)	56,56,56	2.13	21 (37%)
28	DGD	BA	5412	-	57,57,67	1.79	12 (21%)	71,71,81	3.76	24 (33%)
29	LHG	BA	5413	-	38,38,48	1.90	5 (13%)	39,44,54	1.37	4 (10%)
30	SQD	BA	5414	-	50,51,54	2.50	26 (52%)	58,62,65	3.02	19 (32%)
29	LHG	BA	5415	-	36,36,48	1.04	2 (5%)	37,42,54	1.15	3 (8%)
30	SQD	BB	5601	-	46,47,54	2.50	23 (50%)	54,58,65	2.97	15 (27%)
28	DGD	BB	5602	-	53,53,67	1.46	7 (13%)	67,67,81	2.14	13 (19%)
32	LMT	BB	5603	-	36,36,36	1.56	7 (19%)	47,47,47	1.38	5 (10%)
32	LMT	BB	5604	-	36,36,36	1.68	9 (25%)	47,47,47	1.00	1 (2%)
24	CLA	BB	5605	-	55,73,73	2.86	14 (25%)	61,113,113	1.54	9 (14%)
24	CLA	BB	5606	-	55,73,73	2.51	12 (21%)	61,113,113	1.62	10 (16%)
24	CLA	BB	5607	-	55,73,73	2.57	12 (21%)	61,113,113	1.98	17 (27%)
24	CLA	BB	5608	-	55,73,73	2.49	13 (23%)	61,113,113	1.60	14 (22%)
24	CLA	BB	5609	-	55,73,73	2.60	14 (25%)	61,113,113	1.75	14 (22%)
24	CLA	BB	5610	-	55,73,73	2.71	15 (27%)	61,113,113	1.75	16 (26%)
24	CLA	BB	5611	-	55,73,73	2.51	14 (25%)	61,113,113	2.02	19 (31%)
24	CLA	BB	5612	-	55,73,73	2.74	16 (29%)	61,113,113	2.03	17 (27%)
24	CLA	BB	5613	-	55,73,73	2.64	13 (23%)	61,113,113	1.69	16 (26%)
24	CLA	BB	5614	-	55,73,73	2.47	11 (20%)	61,113,113	1.59	12 (19%)
24	CLA	BB	5615	-	55,73,73	2.58	13 (23%)	61,113,113	1.86	20 (32%)
24	CLA	BB	5616	-	55,73,73	2.60	12 (21%)	61,113,113	1.78	12 (19%)
24	CLA	BB	5617	-	55,73,73	2.34	13 (23%)	61,113,113	1.50	12 (19%)
24	CLA	BB	5618	-	55,73,73	2.70	12 (21%)	61,113,113	1.90	13 (21%)
24	CLA	BB	5619	-	55,73,73	2.46	12 (21%)	61,113,113	1.61	11 (18%)
24	CLA	BB	5620	-	55,73,73	2.63	12 (21%)	61,113,113	1.57	9 (14%)
27	BCR	BB	5621	-	41,41,41	1.51	7 (17%)	56,56,56	2.15	19 (33%)
27	BCR	BB	5622	-	41,41,41	1.88	7 (17%)	56,56,56	2.11	16 (28%)
27	BCR	BB	5623	-	41,41,41	1.71	8 (19%)	56,56,56	1.98	17 (30%)
31	LMG	BB	5624	-	49,49,55	0.79	1 (2%)	57,57,63	1.90	15 (26%)
30	SQD	BB	5625	-	42,43,54	2.63	20 (47%)	50,54,65	3.19	14 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMT	BB	5626	-	36,36,36	1.73	9 (25%)	47,47,47	0.99	2 (4%)
32	LMT	BB	5627	-	36,36,36	1.58	8 (22%)	47,47,47	0.92	2 (4%)
33	DMS	BB	5628	-	3,3,3	0.69	0	3,3,3	1.08	0
33	DMS	BB	5629	-	3,3,3	0.67	0	3,3,3	1.14	0
24	CLA	BC	5501	-	55,73,73	2.68	13 (23%)	61,113,113	1.75	13 (21%)
24	CLA	BC	5502	-	55,73,73	2.60	13 (23%)	61,113,113	1.69	13 (21%)
24	CLA	BC	5503	-	55,73,73	2.62	13 (23%)	61,113,113	1.76	16 (26%)
24	CLA	BC	5504	-	55,73,73	2.60	14 (25%)	61,113,113	1.86	14 (22%)
24	CLA	BC	5505	-	55,73,73	2.87	15 (27%)	61,113,113	1.81	13 (21%)
24	CLA	BC	5506	-	55,73,73	2.73	14 (25%)	61,113,113	1.68	15 (24%)
24	CLA	BC	5507	-	55,73,73	2.50	12 (21%)	61,113,113	1.64	11 (18%)
24	CLA	BC	5508	-	55,73,73	2.57	13 (23%)	61,113,113	1.84	14 (22%)
24	CLA	BC	5509	-	55,73,73	2.65	14 (25%)	61,113,113	1.67	13 (21%)
24	CLA	BC	5510	-	55,73,73	2.53	11 (20%)	61,113,113	1.60	11 (18%)
24	CLA	BC	5511	3	55,73,73	2.76	15 (27%)	61,113,113	1.90	14 (22%)
24	CLA	BC	5512	-	55,73,73	2.66	12 (21%)	61,113,113	1.52	10 (16%)
24	CLA	BC	5513	-	55,73,73	2.77	14 (25%)	61,113,113	1.68	11 (18%)
27	BCR	BC	5514	-	41,41,41	1.80	6 (14%)	56,56,56	2.14	24 (42%)
27	BCR	BC	5515	-	41,41,41	1.89	8 (19%)	56,56,56	2.29	23 (41%)
27	BCR	BC	5516	-	41,41,41	1.78	7 (17%)	56,56,56	2.27	20 (35%)
28	DGD	BC	5517	-	54,54,67	1.41	8 (14%)	68,68,81	2.84	21 (30%)
28	DGD	BC	5518	-	63,63,67	1.23	6 (9%)	77,77,81	2.91	24 (31%)
28	DGD	BC	5519	-	67,67,67	1.50	12 (17%)	81,81,81	3.41	30 (37%)
31	LMG	BC	5520	-	48,48,55	1.08	3 (6%)	56,56,63	1.90	17 (30%)
31	LMG	BC	5521	-	45,45,55	1.01	2 (4%)	53,53,63	1.98	13 (24%)
32	LMT	BC	5522	-	36,36,36	1.48	7 (19%)	47,47,47	1.74	8 (17%)
24	CLA	BD	5402	-	55,73,73	2.55	13 (23%)	61,113,113	1.69	14 (22%)
34	PHO	BD	5403	-	67,69,69	2.40	14 (20%)	84,99,99	1.41	16 (19%)
34	PHO	BD	5404	-	67,69,69	2.44	14 (20%)	84,99,99	1.57	17 (20%)
24	CLA	BD	5405	-	55,73,73	2.63	13 (23%)	61,113,113	1.72	11 (18%)
35	PL9	BD	5406	-	55,55,55	4.52	20 (36%)	68,69,69	2.92	24 (35%)
27	BCR	BD	5407	-	41,41,41	1.82	9 (21%)	56,56,56	2.38	24 (42%)
31	LMG	BD	5408	-	46,46,55	0.95	3 (6%)	54,54,63	2.61	16 (29%)
31	LMG	BD	5409	-	49,49,55	0.70	0	57,57,63	2.73	21 (36%)
31	LMG	BD	5410	-	48,48,55	0.93	2 (4%)	56,56,63	2.11	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMT	BD	5411	-	32,32,36	1.69	7 (21%)	43,43,47	1.24	2 (4%)
31	LMG	BE	5101	-	44,44,55	1.07	2 (4%)	52,52,63	1.52	6 (11%)
28	DGD	BE	5102	-	64,64,67	1.49	13 (20%)	78,78,81	1.48	10 (12%)
36	HEM	BF	5101	5,6	30,50,50	2.91	14 (46%)	24,82,82	3.93	13 (54%)
30	SQD	BF	5102	-	44,45,54	2.54	21 (47%)	52,56,65	3.27	17 (32%)
28	DGD	BH	5101	-	59,59,67	1.29	8 (13%)	73,73,81	2.11	19 (26%)
31	LMG	BI	5101	-	43,43,55	1.00	3 (6%)	51,51,63	1.72	7 (13%)
32	LMT	BI	5102	-	36,36,36	1.62	8 (22%)	47,47,47	1.00	2 (4%)
27	BCR	BJ	5101	-	41,41,41	2.41	14 (34%)	56,56,56	3.28	25 (44%)
27	BCR	BK	5102	-	41,41,41	1.91	8 (19%)	56,56,56	2.48	24 (42%)
31	LMG	BL	5101	-	51,51,55	1.34	3 (5%)	59,59,63	2.00	13 (22%)
32	LMT	BM	5101	-	36,36,36	1.72	9 (25%)	47,47,47	0.90	2 (4%)
31	LMG	BM	5102	-	42,42,55	0.99	3 (7%)	50,50,63	1.70	8 (16%)
27	BCR	BT	5101	-	41,41,41	1.77	6 (14%)	56,56,56	2.29	24 (42%)
36	HEM	BV	5201	16	30,50,50	2.96	14 (46%)	24,82,82	3.84	13 (54%)
33	DMS	BV	5202	-	3,3,3	0.84	0	3,3,3	0.93	0
33	DMS	BV	5203	-	3,3,3	0.82	0	3,3,3	1.12	0
27	BCR	BX	5101	-	41,41,41	1.89	9 (21%)	56,56,56	2.29	22 (39%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCT	AA	402	21	-	0/0/0/0	0/0/0/0
24	CLA	AA	404	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AA	405	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AA	406	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AA	407	-	4/4/20/25	0/37/135/135	0/0/9/9
25	MST	AA	408	-	-	0/10/10/10	0/1/1/1
26	OEC	AA	409	1,3	-	0/0/0/54	0/0/0/5
27	BCR	AA	410	-	-	0/29/63/63	0/2/2/2
28	DGD	AA	411	-	-	0/45/85/95	0/2/2/2
29	LHG	AA	412	-	-	0/43/43/53	0/0/0/0
30	SQD	AA	413	-	-	0/46/66/69	0/1/1/1
31	LMG	AA	414	-	-	0/39/59/70	0/1/1/1
29	LHG	AA	415	-	-	0/41/41/53	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SQD	AA	416	-	-	0/49/69/69	0/1/1/1
31	LMG	AA	417	-	-	0/37/57/70	0/1/1/1
24	CLA	AB	601	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	602	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	603	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	604	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	605	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	606	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	607	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	608	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	609	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	610	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	611	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	612	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	613	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	614	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	615	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	616	-	4/4/20/25	0/37/135/135	0/0/9/9
27	BCR	AB	617	-	-	0/29/63/63	0/2/2/2
27	BCR	AB	618	-	-	0/29/63/63	0/2/2/2
27	BCR	AB	619	-	-	0/29/63/63	0/2/2/2
31	LMG	AB	620	-	-	0/46/66/70	0/1/1/1
31	LMG	AB	621	-	-	0/44/64/70	0/1/1/1
30	SQD	AB	622	-	-	0/38/58/69	0/1/1/1
32	LMT	AB	623	-	-	0/21/61/61	0/2/2/2
32	LMT	AB	624	-	-	0/21/61/61	0/2/2/2
33	DMS	AB	625	-	-	0/0/0/0	0/0/0/0
33	DMS	AB	626	-	-	0/0/0/0	0/0/0/0
30	SQD	AB	627	-	-	0/42/62/69	0/1/1/1
28	DGD	AB	628	-	-	0/41/81/95	0/2/2/2
32	LMT	AB	629	-	-	0/21/61/61	0/2/2/2
32	LMT	AB	630	-	-	0/21/61/61	0/2/2/2
24	CLA	AC	501	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	502	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	503	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	504	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	505	-	4/4/20/25	0/37/135/135	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	AC	506	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	507	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	508	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	509	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	510	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	511	3	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	512	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	513	-	4/4/20/25	0/37/135/135	0/0/9/9
27	BCR	AC	514	-	-	0/29/63/63	0/2/2/2
27	BCR	AC	515	-	-	0/29/63/63	0/2/2/2
27	BCR	AC	516	-	-	0/29/63/63	0/2/2/2
28	DGD	AC	517	-	-	0/42/82/95	0/2/2/2
28	DGD	AC	518	-	1/1/13/13	0/51/91/95	0/2/2/2
28	DGD	AC	519	-	1/1/13/13	0/55/95/95	0/2/2/2
31	LMG	AC	520	-	-	0/43/63/70	0/1/1/1
31	LMG	AC	521	-	-	0/40/60/70	0/1/1/1
24	CLA	AD	401	-	4/4/20/25	0/37/135/135	0/0/9/9
34	PHO	AD	402	-	1/1/17/22	0/53/103/103	0/1/6/6
34	PHO	AD	403	-	1/1/17/22	0/53/103/103	0/1/6/6
24	CLA	AD	404	-	4/4/20/25	0/37/135/135	0/0/9/9
35	PL9	AD	405	-	-	2/53/73/73	0/1/1/1
27	BCR	AD	406	-	-	0/29/63/63	0/2/2/2
31	LMG	AD	407	-	-	0/44/64/70	0/1/1/1
31	LMG	AD	408	-	-	0/43/63/70	0/1/1/1
32	LMT	AD	409	-	-	0/17/57/61	0/2/2/2
28	DGD	AE	101	-	-	0/52/92/95	0/2/2/2
36	HEM	AF	101	5,6	-	0/10/54/54	0/0/8/8
30	SQD	AF	102	-	-	0/40/60/69	0/1/1/1
28	DGD	AH	101	-	-	0/47/87/95	0/2/2/2
31	LMG	AI	101	-	-	0/38/58/70	0/1/1/1
32	LMT	AI	102	-	-	0/21/61/61	0/2/2/2
32	LMT	AI	103	-	-	0/21/61/61	0/2/2/2
27	BCR	AJ	101	-	-	0/29/63/63	0/2/2/2
31	LMG	AJ	102	-	-	0/41/61/70	0/1/1/1
27	BCR	AK	102	-	-	0/29/63/63	0/2/2/2
31	LMG	AM	101	-	-	0/37/57/70	0/1/1/1
32	LMT	AM	102	-	-	0/21/61/61	0/2/2/2
27	BCR	AT	101	-	-	0/29/63/63	0/2/2/2
33	DMS	AU	201	-	-	0/0/0/0	0/0/0/0
36	HEM	AV	201	16	-	0/10/54/54	0/0/8/8

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	DMS	AV	202	-	-	0/0/0/0	0/0/0/0
27	BCR	AX	101	-	-	0/29/63/63	0/2/2/2
30	SQD	BA	5401	-	-	0/49/69/69	0/1/1/1
31	LMG	BA	5402	-	-	0/37/57/70	0/1/1/1
22	BCT	BA	5403	21	-	0/0/0/0	0/0/0/0
24	CLA	BA	5405	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BA	5406	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BA	5407	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BA	5408	-	4/4/20/25	0/37/135/135	0/0/9/9
25	MST	BA	5409	-	-	0/10/10/10	0/1/1/1
26	OEC	BA	5410	1,3	-	0/0/0/54	0/0/0/5
27	BCR	BA	5411	-	-	0/29/63/63	0/2/2/2
28	DGD	BA	5412	-	-	0/45/85/95	0/2/2/2
29	LHG	BA	5413	-	-	0/43/43/53	0/0/0/0
30	SQD	BA	5414	-	-	0/46/66/69	0/1/1/1
29	LHG	BA	5415	-	-	0/41/41/53	0/0/0/0
30	SQD	BB	5601	-	-	0/42/62/69	0/1/1/1
28	DGD	BB	5602	-	-	0/41/81/95	0/2/2/2
32	LMT	BB	5603	-	-	0/21/61/61	0/2/2/2
32	LMT	BB	5604	-	-	0/21/61/61	0/2/2/2
24	CLA	BB	5605	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5606	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5607	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5608	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5609	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5610	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5611	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5612	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5613	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5614	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5615	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5616	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5617	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5618	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5619	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5620	-	4/4/20/25	0/37/135/135	0/0/9/9
27	BCR	BB	5621	-	-	0/29/63/63	0/2/2/2
27	BCR	BB	5622	-	-	0/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	BB	5623	-	-	0/29/63/63	0/2/2/2
31	LMG	BB	5624	-	-	0/44/64/70	0/1/1/1
30	SQD	BB	5625	-	-	0/38/58/69	0/1/1/1
32	LMT	BB	5626	-	-	0/21/61/61	0/2/2/2
32	LMT	BB	5627	-	-	0/21/61/61	0/2/2/2
33	DMS	BB	5628	-	-	0/0/0/0	0/0/0/0
33	DMS	BB	5629	-	-	0/0/0/0	0/0/0/0
24	CLA	BC	5501	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5502	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5503	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5504	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5505	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5506	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5507	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5508	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5509	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5510	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5511	3	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5512	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5513	-	4/4/20/25	0/37/135/135	0/0/9/9
27	BCR	BC	5514	-	-	0/29/63/63	0/2/2/2
27	BCR	BC	5515	-	-	0/29/63/63	0/2/2/2
27	BCR	BC	5516	-	-	0/29/63/63	0/2/2/2
28	DGD	BC	5517	-	-	0/42/82/95	0/2/2/2
28	DGD	BC	5518	-	1/1/13/13	0/51/91/95	0/2/2/2
28	DGD	BC	5519	-	1/1/13/13	0/55/95/95	0/2/2/2
31	LMG	BC	5520	-	-	0/43/63/70	0/1/1/1
31	LMG	BC	5521	-	-	0/40/60/70	0/1/1/1
32	LMT	BC	5522	-	-	0/21/61/61	0/2/2/2
24	CLA	BD	5402	-	4/4/20/25	0/37/135/135	0/0/9/9
34	PHO	BD	5403	-	1/1/17/22	0/53/103/103	0/1/6/6
34	PHO	BD	5404	-	1/1/17/22	0/53/103/103	0/1/6/6
24	CLA	BD	5405	-	4/4/20/25	0/37/135/135	0/0/9/9
35	PL9	BD	5406	-	-	1/53/73/73	0/1/1/1
27	BCR	BD	5407	-	-	0/29/63/63	0/2/2/2
31	LMG	BD	5408	-	-	0/41/61/70	0/1/1/1
31	LMG	BD	5409	-	-	0/44/64/70	0/1/1/1
31	LMG	BD	5410	-	-	0/43/63/70	0/1/1/1
32	LMT	BD	5411	-	-	0/17/57/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	BE	5101	-	-	0/39/59/70	0/1/1/1
28	DGD	BE	5102	-	-	0/52/92/95	0/2/2/2
36	HEM	BF	5101	5,6	-	0/10/54/54	0/0/8/8
30	SQD	BF	5102	-	-	0/40/60/69	0/1/1/1
28	DGD	BH	5101	-	-	0/47/87/95	0/2/2/2
31	LMG	BI	5101	-	-	0/38/58/70	0/1/1/1
32	LMT	BI	5102	-	-	0/21/61/61	0/2/2/2
27	BCR	BJ	5101	-	-	0/29/63/63	0/2/2/2
27	BCR	BK	5102	-	-	0/29/63/63	0/2/2/2
31	LMG	BL	5101	-	-	0/46/66/70	0/1/1/1
32	LMT	BM	5101	-	-	0/21/61/61	0/2/2/2
31	LMG	BM	5102	-	-	0/37/57/70	0/1/1/1
27	BCR	BT	5101	-	-	0/29/63/63	0/2/2/2
36	HEM	BV	5201	16	-	0/10/54/54	0/0/8/8
33	DMS	BV	5202	-	-	0/0/0/0	0/0/0/0
33	DMS	BV	5203	-	-	0/0/0/0	0/0/0/0
27	BCR	BX	5101	-	-	0/29/63/63	0/2/2/2

All (1822) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BV	5201	HEM	C3B-C4B	-7.11	1.45	1.51
36	BF	5101	HEM	C3B-C4B	-6.40	1.46	1.51
36	AF	101	HEM	C3B-C4B	-6.34	1.46	1.51
36	BF	5101	HEM	C2D-C3D	-6.13	1.36	1.54
36	BV	5201	HEM	C2D-C3D	-5.81	1.37	1.54
36	AV	201	HEM	C2D-C3D	-5.77	1.37	1.54
24	AC	505	CLA	CAA-C2A	-5.68	1.42	1.54
36	AF	101	HEM	C2D-C3D	-5.61	1.37	1.54
31	BL	5101	LMG	O7-C8	-5.57	1.32	1.46
36	AV	201	HEM	C3B-C4B	-5.46	1.47	1.51
31	AB	620	LMG	O7-C8	-5.20	1.33	1.46
36	BV	5201	HEM	C3B-CAB	-4.97	1.42	1.51
24	BC	5505	CLA	CAA-C2A	-4.76	1.44	1.54
36	AV	201	HEM	C3B-CAB	-4.68	1.42	1.51
35	BD	5406	PL9	C6-C1	-4.59	1.39	1.48
35	AD	405	PL9	C6-C1	-4.52	1.39	1.48
32	BB	5603	LMT	C1B-C2B	-4.30	1.39	1.52
32	BD	5411	LMT	C1B-C2B	-4.30	1.39	1.52
32	AB	624	LMT	C1B-C2B	-4.30	1.39	1.52
32	AB	629	LMT	C1B-C2B	-4.30	1.39	1.52
32	AD	409	LMT	C1B-C2B	-4.29	1.39	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	AI	103	LMT	C1B-C2B	-4.28	1.39	1.52
32	BB	5627	LMT	C1B-C2B	-4.28	1.39	1.52
32	BB	5604	LMT	C1B-C2B	-4.28	1.39	1.52
32	BM	5101	LMT	C1B-C2B	-4.27	1.39	1.52
32	AI	102	LMT	C1B-C2B	-4.27	1.39	1.52
32	AB	630	LMT	C1B-C2B	-4.27	1.39	1.52
32	BI	5102	LMT	C1B-C2B	-4.26	1.39	1.52
32	AM	102	LMT	C1B-C2B	-4.26	1.39	1.52
32	BB	5626	LMT	C1B-C2B	-4.25	1.39	1.52
32	BC	5522	LMT	C1B-C2B	-4.24	1.39	1.52
32	AB	623	LMT	C1B-C2B	-4.23	1.39	1.52
28	AC	519	DGD	O5D-C6D	-4.16	1.36	1.43
36	BF	5101	HEM	CAD-C3D	-4.15	1.45	1.54
35	BD	5406	PL9	C37-C38	-3.93	1.39	1.50
35	BD	5406	PL9	C32-C33	-3.88	1.39	1.50
35	AD	405	PL9	C32-C33	-3.87	1.39	1.50
28	AC	518	DGD	C2A-C1A	-3.82	1.39	1.50
36	AF	101	HEM	CAD-C3D	-3.82	1.46	1.54
28	BC	5518	DGD	C2A-C1A	-3.81	1.39	1.50
36	AV	201	HEM	C2B-C1B	-3.81	1.39	1.51
36	BV	5201	HEM	CAD-C3D	-3.80	1.46	1.54
36	AF	101	HEM	C2B-C1B	-3.77	1.39	1.51
28	BC	5517	DGD	C2A-C1A	-3.77	1.39	1.50
28	AC	519	DGD	C2A-C1A	-3.76	1.39	1.50
36	BF	5101	HEM	C2B-C1B	-3.76	1.39	1.51
36	BV	5201	HEM	C2B-C1B	-3.75	1.39	1.51
28	BH	5101	DGD	C2A-C1A	-3.75	1.39	1.50
35	AD	405	PL9	C37-C38	-3.74	1.40	1.50
28	AC	517	DGD	C2A-C1A	-3.73	1.39	1.50
28	BC	5519	DGD	C2A-C1A	-3.73	1.39	1.50
28	AB	628	DGD	C2A-C1A	-3.71	1.39	1.50
28	AH	101	DGD	C2A-C1A	-3.71	1.39	1.50
28	AE	101	DGD	C2A-C1A	-3.69	1.39	1.50
28	BB	5602	DGD	C2A-C1A	-3.67	1.39	1.50
36	AV	201	HEM	CAD-C3D	-3.67	1.46	1.54
28	BE	5102	DGD	C2A-C1A	-3.67	1.39	1.50
28	AA	411	DGD	C2A-C1A	-3.66	1.39	1.50
28	BA	5412	DGD	C2A-C1A	-3.64	1.39	1.50
32	AM	102	LMT	C6B-C5B	-3.51	1.39	1.51
32	AD	409	LMT	C6B-C5B	-3.51	1.39	1.51
32	BD	5411	LMT	C6B-C5B	-3.50	1.39	1.51
32	AB	623	LMT	C6B-C5B	-3.50	1.39	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	BB	5604	LMT	C6B-C5B	-3.49	1.39	1.51
32	AI	103	LMT	C6B-C5B	-3.49	1.39	1.51
32	AB	624	LMT	C6B-C5B	-3.48	1.39	1.51
32	BC	5522	LMT	C6B-C5B	-3.48	1.39	1.51
32	AI	102	LMT	C6B-C5B	-3.48	1.39	1.51
32	BB	5603	LMT	C6B-C5B	-3.48	1.39	1.51
32	AB	630	LMT	C6B-C5B	-3.48	1.39	1.51
32	BM	5101	LMT	C6B-C5B	-3.48	1.39	1.51
32	BB	5627	LMT	C6B-C5B	-3.48	1.39	1.51
32	BI	5102	LMT	C6B-C5B	-3.47	1.39	1.51
32	BB	5626	LMT	C6B-C5B	-3.47	1.39	1.51
32	AB	629	LMT	C6B-C5B	-3.45	1.39	1.51
36	AF	101	HEM	C3B-CAB	-3.32	1.45	1.51
36	BF	5101	HEM	C3B-CAB	-3.27	1.45	1.51
30	AA	413	SQD	O6-C44	-3.15	1.37	1.43
24	AB	612	CLA	C2A-C1A	-3.02	1.46	1.52
24	BB	5616	CLA	C2A-C1A	-3.02	1.46	1.52
28	BC	5519	DGD	O5D-C6D	-3.00	1.38	1.43
24	AC	505	CLA	CAA-CBA	-2.98	1.42	1.52
28	BA	5412	DGD	O5D-C6D	-2.96	1.38	1.43
34	AD	402	PHO	C1B-C2B	-2.89	1.39	1.45
24	BB	5615	CLA	C2A-C1A	-2.86	1.46	1.52
28	AA	411	DGD	O5D-C6D	-2.86	1.38	1.43
34	AD	403	PHO	C1B-C2B	-2.86	1.39	1.45
31	AJ	102	LMG	O7-C8	-2.85	1.39	1.46
24	AA	405	CLA	C3D-C2D	-2.85	1.33	1.40
31	BD	5408	LMG	O7-C8	-2.84	1.39	1.46
30	BB	5625	SQD	C12-C11	-2.82	1.35	1.51
34	BD	5403	PHO	C1B-C2B	-2.81	1.39	1.45
30	BA	5414	SQD	O6-C44	-2.81	1.38	1.43
34	BD	5404	PHO	C1B-C2B	-2.80	1.39	1.45
30	AB	622	SQD	C12-C11	-2.78	1.35	1.51
24	BA	5406	CLA	C3D-C2D	-2.76	1.33	1.40
30	AA	413	SQD	C17-C16	-2.76	1.35	1.51
30	BB	5625	SQD	C11-C10	-2.75	1.35	1.51
30	BB	5601	SQD	C12-C11	-2.75	1.35	1.51
24	BC	5505	CLA	CAA-CBA	-2.75	1.43	1.52
34	BD	5403	PHO	C4D-CHA	-2.75	1.37	1.44
30	AB	627	SQD	C15-C14	-2.73	1.35	1.51
30	BB	5601	SQD	C15-C14	-2.72	1.35	1.51
28	AC	517	DGD	O3G-C3G	-2.72	1.38	1.43
30	BB	5601	SQD	C16-C15	-2.71	1.35	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	AB	627	SQD	C20-C19	-2.71	1.35	1.51
30	BA	5414	SQD	C17-C16	-2.70	1.35	1.51
30	AA	413	SQD	C15-C14	-2.70	1.35	1.51
30	AB	622	SQD	C11-C10	-2.70	1.35	1.51
30	AB	627	SQD	C16-C15	-2.69	1.36	1.51
30	AB	627	SQD	C12-C11	-2.69	1.36	1.51
30	BF	5102	SQD	C17-C16	-2.68	1.36	1.51
30	BA	5414	SQD	C33-C32	-2.68	1.36	1.51
30	BA	5414	SQD	C15-C14	-2.68	1.36	1.51
30	BB	5601	SQD	C20-C19	-2.67	1.36	1.51
24	AB	611	CLA	C2A-C1A	-2.66	1.46	1.52
30	AB	627	SQD	C19-C18	-2.66	1.36	1.51
30	BB	5601	SQD	C11-C10	-2.66	1.36	1.51
30	AB	627	SQD	C14-C13	-2.66	1.36	1.51
30	AA	413	SQD	C16-C15	-2.65	1.36	1.51
30	BB	5601	SQD	C14-C13	-2.64	1.36	1.51
30	BA	5414	SQD	C16-C15	-2.63	1.36	1.51
30	AA	413	SQD	C33-C32	-2.63	1.36	1.51
30	BF	5102	SQD	C11-C10	-2.62	1.36	1.51
30	AB	627	SQD	C11-C10	-2.61	1.36	1.51
30	BB	5601	SQD	C17-C16	-2.61	1.36	1.51
30	BF	5102	SQD	C16-C15	-2.61	1.36	1.51
27	BB	5621	BCR	C23-C22	-2.60	1.40	1.45
24	AB	608	CLA	C2A-C1A	-2.60	1.47	1.52
30	AB	627	SQD	C13-C12	-2.59	1.36	1.51
30	AF	102	SQD	C17-C16	-2.59	1.36	1.51
27	BC	5516	BCR	C19-C18	-2.59	1.40	1.45
30	BB	5601	SQD	C19-C18	-2.59	1.36	1.51
30	AF	102	SQD	C11-C10	-2.59	1.36	1.51
30	BA	5414	SQD	C11-C10	-2.59	1.36	1.51
30	AA	416	SQD	C17-C16	-2.59	1.36	1.51
30	BB	5601	SQD	C13-C12	-2.58	1.36	1.51
30	BA	5414	SQD	C12-C11	-2.57	1.36	1.51
30	BA	5414	SQD	C19-C18	-2.56	1.36	1.51
30	BF	5102	SQD	C15-C14	-2.55	1.36	1.51
30	AB	627	SQD	C17-C16	-2.55	1.36	1.51
30	AA	413	SQD	C19-C18	-2.54	1.36	1.51
30	BB	5625	SQD	C16-C15	-2.54	1.36	1.51
34	AD	402	PHO	C4D-CHA	-2.54	1.37	1.44
30	AF	102	SQD	C12-C11	-2.54	1.36	1.51
30	AA	416	SQD	C16-C15	-2.54	1.36	1.51
30	BF	5102	SQD	C12-C11	-2.54	1.36	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BA	5401	SQD	C36-C35	-2.53	1.36	1.51
30	AA	413	SQD	C12-C11	-2.53	1.36	1.51
30	AB	622	SQD	C16-C15	-2.51	1.37	1.51
30	AA	416	SQD	C19-C18	-2.51	1.37	1.51
30	AA	416	SQD	C12-C11	-2.50	1.37	1.51
24	AB	608	CLA	CAA-C2A	-2.50	1.49	1.54
30	AF	102	SQD	C15-C14	-2.49	1.37	1.51
30	BA	5401	SQD	C12-C11	-2.49	1.37	1.51
30	AA	413	SQD	C32-C31	-2.49	1.37	1.51
30	AB	622	SQD	C13-C12	-2.48	1.37	1.51
30	AF	102	SQD	C16-C15	-2.48	1.37	1.51
30	BA	5401	SQD	C33-C32	-2.48	1.37	1.51
30	BB	5625	SQD	C13-C12	-2.48	1.37	1.51
30	AA	416	SQD	C36-C35	-2.48	1.37	1.51
30	BA	5414	SQD	C14-C13	-2.47	1.37	1.51
27	AC	516	BCR	C19-C18	-2.46	1.40	1.45
30	BA	5401	SQD	C17-C16	-2.46	1.37	1.51
30	BA	5401	SQD	C15-C14	-2.46	1.37	1.51
24	BB	5608	CLA	C2A-C1A	-2.46	1.47	1.52
30	AA	413	SQD	C14-C13	-2.46	1.37	1.51
30	AA	413	SQD	C11-C10	-2.46	1.37	1.51
30	BA	5401	SQD	C16-C15	-2.45	1.37	1.51
30	AA	413	SQD	C18-C17	-2.44	1.37	1.51
30	AA	413	SQD	C20-C19	-2.44	1.37	1.51
27	AB	619	BCR	C23-C22	-2.44	1.40	1.45
30	BB	5601	SQD	C18-C17	-2.44	1.37	1.51
30	BA	5414	SQD	C20-C19	-2.43	1.37	1.51
30	AA	416	SQD	C15-C14	-2.42	1.37	1.51
30	AA	416	SQD	C33-C32	-2.42	1.37	1.51
27	BC	5515	BCR	C19-C18	-2.42	1.40	1.45
30	BA	5414	SQD	C32-C31	-2.42	1.37	1.51
30	BB	5625	SQD	C15-C14	-2.41	1.37	1.51
30	AB	622	SQD	C15-C14	-2.40	1.37	1.51
30	BA	5401	SQD	C13-C12	-2.40	1.37	1.51
30	BA	5401	SQD	C32-C31	-2.39	1.37	1.51
30	BB	5625	SQD	C14-C13	-2.38	1.37	1.51
30	BA	5414	SQD	C13-C12	-2.38	1.37	1.51
30	BA	5414	SQD	C18-C17	-2.38	1.37	1.51
24	BB	5612	CLA	CAA-C2A	-2.38	1.49	1.54
24	AB	607	CLA	C3B-CAB	-2.38	1.42	1.47
30	AB	627	SQD	C18-C17	-2.37	1.37	1.51
30	AA	416	SQD	C11-C10	-2.37	1.37	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	5612	CLA	C2A-C1A	-2.37	1.47	1.52
28	BC	5519	DGD	O3E-C3E	-2.37	1.37	1.43
30	AF	102	SQD	C14-C13	-2.36	1.37	1.51
30	BA	5401	SQD	C34-C33	-2.36	1.37	1.51
30	AB	622	SQD	C14-C13	-2.35	1.37	1.51
30	AA	416	SQD	C20-C19	-2.35	1.37	1.51
30	BA	5401	SQD	C14-C13	-2.35	1.37	1.51
30	AA	413	SQD	C13-C12	-2.35	1.38	1.51
30	AA	416	SQD	C32-C31	-2.35	1.38	1.51
30	AF	102	SQD	C13-C12	-2.34	1.38	1.51
30	BA	5401	SQD	C35-C34	-2.34	1.38	1.51
24	BA	5407	CLA	C3D-C2D	-2.34	1.34	1.40
30	AA	416	SQD	C13-C12	-2.32	1.38	1.51
30	BF	5102	SQD	C14-C13	-2.31	1.38	1.51
30	BA	5401	SQD	C19-C18	-2.31	1.38	1.51
30	BA	5401	SQD	C20-C19	-2.31	1.38	1.51
30	AA	416	SQD	C35-C34	-2.31	1.38	1.51
27	BB	5623	BCR	C23-C22	-2.29	1.40	1.45
30	BF	5102	SQD	C13-C12	-2.29	1.38	1.51
30	BA	5401	SQD	C11-C10	-2.28	1.38	1.51
30	AA	416	SQD	C34-C33	-2.27	1.38	1.51
30	AA	416	SQD	C18-C17	-2.27	1.38	1.51
30	AA	416	SQD	C14-C13	-2.27	1.38	1.51
31	AA	417	LMG	O7-C8	-2.27	1.40	1.46
24	AC	505	CLA	C2A-C1A	-2.26	1.47	1.52
28	AC	519	DGD	C1E-C2E	-2.25	1.45	1.52
24	AD	404	CLA	C2A-C1A	-2.22	1.47	1.52
24	BC	5502	CLA	C2A-C1A	-2.22	1.47	1.52
36	AV	201	HEM	C2D-C1D	-2.21	1.44	1.51
31	AD	407	LMG	O7-C8	-2.19	1.41	1.46
24	BC	5505	CLA	C2A-C1A	-2.18	1.47	1.52
30	BB	5625	SQD	C17-C16	-2.16	1.35	1.51
30	AA	416	SQD	O6-C44	-2.16	1.39	1.43
31	AD	408	LMG	O3-C3	-2.16	1.37	1.43
24	BA	5405	CLA	C2A-C1A	-2.16	1.47	1.52
31	BA	5402	LMG	O7-C8	-2.15	1.41	1.46
30	AB	622	SQD	C17-C16	-2.15	1.35	1.51
27	AC	514	BCR	C23-C22	-2.14	1.41	1.45
31	AD	408	LMG	O7-C8	-2.14	1.41	1.46
30	AB	627	SQD	C21-C20	-2.12	1.35	1.51
27	AC	515	BCR	C19-C18	-2.12	1.41	1.45
28	BC	5519	DGD	C6A-C5A	-2.11	1.39	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	AC	519	DGD	C6A-C5A	-2.11	1.39	1.51
30	BA	5401	SQD	C18-C17	-2.11	1.39	1.51
32	BB	5603	LMT	C10-C9	-2.10	1.39	1.51
30	BB	5601	SQD	C21-C20	-2.10	1.36	1.51
28	AC	518	DGD	C6A-C5A	-2.10	1.39	1.51
28	BC	5518	DGD	C6A-C5A	-2.10	1.39	1.51
32	BB	5604	LMT	C10-C9	-2.10	1.39	1.51
32	AI	102	LMT	C10-C9	-2.10	1.39	1.51
32	AB	629	LMT	C10-C9	-2.10	1.39	1.51
28	BC	5518	DGD	CEB-CDB	-2.10	1.39	1.51
24	AC	501	CLA	C3D-CAD	-2.10	1.39	1.45
28	AA	411	DGD	C6A-C5A	-2.09	1.39	1.51
28	AH	101	DGD	C6A-C5A	-2.09	1.39	1.51
28	AC	518	DGD	CEB-CDB	-2.09	1.39	1.51
28	BA	5412	DGD	C6A-C5A	-2.09	1.39	1.51
28	BC	5517	DGD	C6A-C5A	-2.09	1.39	1.51
24	AC	507	CLA	C3B-CAB	-2.09	1.43	1.47
32	AI	103	LMT	C10-C9	-2.09	1.39	1.51
32	BC	5522	LMT	C10-C9	-2.09	1.39	1.51
28	AC	517	DGD	C6A-C5A	-2.09	1.39	1.51
28	AE	101	DGD	CEB-CDB	-2.09	1.39	1.51
28	BH	5101	DGD	C6A-C5A	-2.09	1.39	1.51
24	BC	5508	CLA	C2A-C1A	-2.09	1.48	1.52
28	AB	628	DGD	C6A-C5A	-2.08	1.39	1.51
28	BE	5102	DGD	CEB-CDB	-2.08	1.39	1.51
32	AB	630	LMT	C10-C9	-2.08	1.39	1.51
32	AB	623	LMT	C10-C9	-2.08	1.39	1.51
32	BI	5102	LMT	C10-C9	-2.08	1.39	1.51
28	BB	5602	DGD	C6A-C5A	-2.08	1.39	1.51
32	AB	624	LMT	C10-C9	-2.08	1.39	1.51
24	AB	606	CLA	C2A-C1A	-2.08	1.48	1.52
32	BB	5626	LMT	C10-C9	-2.08	1.39	1.51
27	AA	410	BCR	C19-C18	-2.08	1.41	1.45
32	BM	5101	LMT	C10-C9	-2.08	1.39	1.51
34	AD	403	PHO	C4D-CHA	-2.08	1.38	1.44
32	AM	102	LMT	C10-C9	-2.08	1.39	1.51
28	AE	101	DGD	C6A-C5A	-2.07	1.39	1.51
28	BC	5519	DGD	CEB-CDB	-2.07	1.39	1.51
28	AC	519	DGD	CEB-CDB	-2.07	1.39	1.51
30	BA	5401	SQD	O6-C44	-2.07	1.39	1.43
28	BE	5102	DGD	C6A-C5A	-2.07	1.39	1.51
32	BB	5627	LMT	C10-C9	-2.06	1.39	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	504	CLA	C2A-C1A	-2.05	1.48	1.52
24	AB	614	CLA	C2A-C1A	-2.05	1.48	1.52
24	AB	604	CLA	C2A-C1A	-2.05	1.48	1.52
30	AA	416	SQD	C37-C36	-2.03	1.36	1.51
31	BD	5410	LMG	O7-C8	-2.03	1.41	1.46
28	AA	411	DGD	C4D-C3D	-2.02	1.47	1.52
24	BB	5619	CLA	C3D-CAD	-2.02	1.40	1.45
27	BD	5407	BCR	C23-C22	-2.01	1.41	1.45
27	BA	5411	BCR	C19-C18	-2.01	1.41	1.45
30	BA	5414	SQD	C34-C33	-2.01	1.36	1.51
24	BB	5609	CLA	C2A-C1A	-2.01	1.48	1.52
24	AC	503	CLA	C2A-C1A	-2.01	1.48	1.52
28	AA	411	DGD	O2D-C2D	-2.00	1.38	1.43
24	AA	407	CLA	CHC-C1C	2.00	1.41	1.35
28	AB	628	DGD	O6D-C5D	2.00	1.49	1.44
27	AJ	101	BCR	C4-C5	2.00	1.55	1.51
27	BX	5101	BCR	C24-C23	2.01	1.38	1.33
32	BB	5626	LMT	O5B-C5B	2.01	1.49	1.44
24	BC	5513	CLA	CAC-C3C	2.01	1.56	1.51
24	BC	5513	CLA	C4-C3	2.01	1.55	1.50
24	AB	610	CLA	O2A-CGA	2.02	1.39	1.33
24	BC	5511	CLA	C4B-CHC	2.02	1.45	1.39
32	AM	102	LMT	O5'-C5'	2.02	1.49	1.44
30	AB	622	SQD	C24-C23	2.02	1.56	1.50
31	AC	520	LMG	O7-C10	2.02	1.40	1.34
27	BC	5515	BCR	C38-C26	2.02	1.54	1.51
30	BB	5625	SQD	C24-C23	2.02	1.56	1.50
31	AA	414	LMG	O8-C9	2.02	1.49	1.45
31	BI	5101	LMG	C4-C5	2.02	1.57	1.53
24	AB	609	CLA	CBA-CGA	2.03	1.56	1.50
24	AD	404	CLA	CBA-CGA	2.03	1.56	1.50
24	AC	508	CLA	C1C-NC	2.03	1.41	1.37
28	BC	5519	DGD	O4D-C4D	2.03	1.47	1.43
24	AA	404	CLA	C1C-NC	2.03	1.41	1.37
24	AC	502	CLA	CMC-C2C	2.03	1.55	1.50
24	BC	5511	CLA	CBA-CGA	2.03	1.56	1.50
24	AC	505	CLA	C1C-NC	2.03	1.41	1.37
32	AD	409	LMT	O5'-C1'	2.04	1.47	1.41
28	AH	101	DGD	C3G-C2G	2.04	1.56	1.50
36	BF	5101	HEM	FE-NB	2.04	2.08	1.97
24	AB	613	CLA	C4C-NC	2.04	1.41	1.37
24	BB	5612	CLA	CHC-C1C	2.04	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BJ	5101	BCR	C4-C5	2.04	1.55	1.51
30	BF	5102	SQD	C44-C45	2.04	1.56	1.50
24	AB	616	CLA	C5-C3	2.04	1.55	1.51
24	BB	5605	CLA	CBD-CHA	2.05	1.63	1.52
27	BJ	5101	BCR	C11-C12	2.05	1.39	1.34
24	BC	5509	CLA	OBD-CAD	2.05	1.25	1.22
28	BE	5102	DGD	C4D-C5D	2.05	1.57	1.53
31	AC	520	LMG	C4-C5	2.05	1.57	1.53
24	BB	5610	CLA	CHC-C1C	2.05	1.41	1.35
24	BD	5405	CLA	CHC-C1C	2.05	1.41	1.35
24	AC	511	CLA	C4C-NC	2.06	1.41	1.37
24	BB	5613	CLA	C1C-NC	2.06	1.41	1.37
34	BD	5403	PHO	CMD-C2D	2.06	1.55	1.50
24	AC	501	CLA	C4C-NC	2.06	1.41	1.37
24	BB	5610	CLA	CBA-CGA	2.07	1.56	1.50
24	AB	601	CLA	CBA-CGA	2.07	1.56	1.50
24	AC	501	CLA	C1C-NC	2.07	1.41	1.37
28	AH	101	DGD	O6D-C5D	2.07	1.49	1.44
24	BC	5509	CLA	C4C-NC	2.07	1.41	1.37
24	AB	601	CLA	CAC-C3C	2.07	1.56	1.51
28	BB	5602	DGD	C3E-C2E	2.07	1.57	1.52
32	BM	5101	LMT	O5'-C1'	2.07	1.47	1.41
24	BB	5615	CLA	C1C-NC	2.07	1.41	1.37
32	BB	5627	LMT	O1B-C4'	2.08	1.49	1.43
35	BD	5406	PL9	C10-C9	2.08	1.55	1.50
30	BA	5414	SQD	O6-C1	2.08	1.43	1.40
27	AC	516	BCR	C33-C5	2.08	1.54	1.51
31	AC	520	LMG	O7-C8	2.08	1.51	1.46
24	AB	601	CLA	CBD-CGD	2.08	1.59	1.52
24	BB	5605	CLA	CAC-C3C	2.09	1.56	1.51
24	AC	506	CLA	CHC-C1C	2.09	1.41	1.35
28	BC	5517	DGD	O6E-C1E	2.09	1.47	1.41
24	BB	5620	CLA	C5-C3	2.09	1.56	1.51
24	AD	401	CLA	O2A-CGA	2.09	1.39	1.33
24	BC	5511	CLA	C5-C3	2.09	1.56	1.51
28	AE	101	DGD	C4E-C5E	2.09	1.57	1.53
31	AM	101	LMG	O7-C10	2.10	1.40	1.34
27	AB	619	BCR	C33-C5	2.10	1.54	1.51
30	AB	627	SQD	C24-C23	2.10	1.56	1.50
27	BD	5407	BCR	C14-C13	2.11	1.38	1.35
24	AC	502	CLA	CHC-C1C	2.11	1.41	1.35
31	BC	5520	LMG	O7-C8	2.11	1.51	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BC	5509	CLA	C1C-NC	2.11	1.41	1.37
27	AB	618	BCR	C33-C5	2.11	1.54	1.51
34	AD	403	PHO	C4A-NA	2.11	1.40	1.34
24	AB	602	CLA	CHC-C1C	2.11	1.41	1.35
28	AC	517	DGD	C3G-C2G	2.12	1.56	1.50
27	BJ	5101	BCR	C7-C6	2.12	1.53	1.45
24	AD	404	CLA	CAC-C3C	2.12	1.57	1.51
32	AI	103	LMT	C4'-C5'	2.12	1.58	1.52
27	AJ	101	BCR	C7-C6	2.12	1.53	1.45
36	AV	201	HEM	CHC-C1C	2.12	1.41	1.36
24	BB	5609	CLA	CHC-C1C	2.12	1.41	1.35
24	BB	5618	CLA	C1C-NC	2.12	1.41	1.37
28	BE	5102	DGD	O6D-C5D	2.12	1.49	1.44
24	AB	611	CLA	C1C-NC	2.13	1.41	1.37
30	AF	102	SQD	C8-C7	2.13	1.57	1.50
35	AD	405	PL9	C47-C48	2.14	1.56	1.50
24	AA	406	CLA	C4C-NC	2.14	1.41	1.37
28	AC	518	DGD	O2G-C1B	2.14	1.40	1.34
24	AA	406	CLA	O2A-CGA	2.14	1.39	1.33
24	AC	504	CLA	C5-C3	2.14	1.56	1.51
34	BD	5404	PHO	C4A-NA	2.15	1.40	1.34
24	BB	5614	CLA	C1C-NC	2.15	1.41	1.37
24	BC	5504	CLA	C5-C3	2.16	1.56	1.51
31	AI	101	LMG	O1-C1	2.16	1.44	1.40
28	AA	411	DGD	C1G-C2G	2.16	1.56	1.50
32	BI	5102	LMT	O1B-C4'	2.16	1.49	1.43
28	BC	5519	DGD	C6E-C5E	2.16	1.59	1.51
24	AC	504	CLA	C1C-NC	2.16	1.41	1.37
24	BB	5620	CLA	C1C-NC	2.16	1.41	1.37
24	BC	5505	CLA	CHC-C1C	2.17	1.42	1.35
35	BD	5406	PL9	C11-C9	2.17	1.56	1.51
36	AV	201	HEM	CAA-C2A	2.17	1.55	1.52
24	AA	404	CLA	C4C-NC	2.17	1.41	1.37
24	BB	5611	CLA	C1C-NC	2.17	1.41	1.37
24	AC	507	CLA	C1C-NC	2.18	1.41	1.37
36	BV	5201	HEM	C2A-C3A	2.18	1.44	1.37
24	BC	5502	CLA	CHC-C1C	2.18	1.42	1.35
24	AB	613	CLA	CMC-C2C	2.19	1.55	1.50
24	BB	5615	CLA	CHC-C1C	2.19	1.42	1.35
34	BD	5404	PHO	C4C-NC	2.19	1.42	1.37
24	BB	5613	CLA	CBA-CGA	2.19	1.57	1.50
31	AA	417	LMG	C4-C5	2.19	1.57	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	BC	5522	LMT	O1'-C1'	2.19	1.44	1.40
32	AB	623	LMT	C4'-C5'	2.19	1.59	1.52
28	AC	519	DGD	O4D-C4D	2.20	1.48	1.43
27	AD	406	BCR	C38-C26	2.20	1.54	1.51
27	BX	5101	BCR	C38-C26	2.20	1.54	1.51
31	AJ	102	LMG	O6-C1	2.20	1.47	1.41
24	AC	505	CLA	CHC-C1C	2.20	1.42	1.35
35	BD	5406	PL9	C47-C48	2.20	1.56	1.50
24	BB	5609	CLA	C1C-NC	2.20	1.41	1.37
32	AM	102	LMT	O5'-C1'	2.20	1.47	1.41
24	AA	406	CLA	O1D-CGD	2.21	1.26	1.21
30	AA	413	SQD	O6-C1	2.21	1.44	1.40
27	AX	101	BCR	C14-C13	2.21	1.38	1.35
28	AC	519	DGD	O5D-C1E	2.21	1.44	1.40
28	AC	519	DGD	C6E-C5E	2.21	1.59	1.51
24	BB	5611	CLA	CHC-C1C	2.21	1.42	1.35
24	AC	509	CLA	CHC-C1C	2.22	1.42	1.35
24	BB	5611	CLA	O1D-CGD	2.22	1.26	1.21
27	BD	5407	BCR	C38-C26	2.23	1.54	1.51
24	BC	5503	CLA	OBD-CAD	2.23	1.25	1.22
27	AJ	101	BCR	C17-C18	2.23	1.38	1.35
30	AF	102	SQD	C44-C45	2.23	1.57	1.50
24	BB	5617	CLA	CHC-C1C	2.23	1.42	1.35
24	AA	406	CLA	C1C-NC	2.23	1.41	1.37
32	BD	5411	LMT	O5'-C1'	2.24	1.47	1.41
31	AA	417	LMG	O8-C9	2.24	1.50	1.45
36	BV	5201	HEM	CAA-C2A	2.24	1.55	1.52
28	BC	5517	DGD	C3G-C2G	2.24	1.57	1.50
32	BC	5522	LMT	O1B-C1B	2.24	1.47	1.41
28	AH	101	DGD	O3G-C1D	2.24	1.44	1.40
27	BK	5102	BCR	C38-C26	2.24	1.54	1.51
24	BC	5506	CLA	CHC-C1C	2.24	1.42	1.35
24	BC	5513	CLA	C4C-NC	2.24	1.41	1.37
24	BB	5614	CLA	O1D-CGD	2.24	1.26	1.21
24	AB	608	CLA	CHC-C1C	2.24	1.42	1.35
31	BI	5101	LMG	O1-C1	2.24	1.44	1.40
24	BC	5508	CLA	C1C-NC	2.24	1.41	1.37
24	BB	5605	CLA	C1C-NC	2.24	1.41	1.37
24	BB	5608	CLA	CHC-C1C	2.25	1.42	1.35
30	BB	5601	SQD	C24-C23	2.25	1.57	1.50
32	AI	102	LMT	O1B-C1B	2.25	1.47	1.41
30	BF	5102	SQD	C8-C7	2.25	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	606	CLA	CMC-C2C	2.25	1.55	1.50
32	AI	102	LMT	O5'-C1'	2.26	1.47	1.41
28	BC	5517	DGD	O6D-C5D	2.26	1.50	1.44
28	BH	5101	DGD	O3G-C1D	2.26	1.44	1.40
32	AB	629	LMT	O1B-C4'	2.26	1.49	1.43
24	BC	5511	CLA	C4C-NC	2.27	1.41	1.37
34	AD	403	PHO	O2A-CGA	2.27	1.40	1.33
24	AC	511	CLA	CMC-C2C	2.28	1.55	1.50
31	BM	5102	LMG	O6-C1	2.28	1.47	1.41
24	AB	611	CLA	CHC-C1C	2.28	1.42	1.35
24	BB	5610	CLA	OBD-CAD	2.29	1.25	1.22
28	BA	5412	DGD	O3G-C1D	2.29	1.44	1.40
24	BC	5501	CLA	C1C-NC	2.29	1.41	1.37
32	AM	102	LMT	O1B-C1B	2.29	1.47	1.41
24	AC	512	CLA	O2A-CGA	2.29	1.40	1.33
24	BA	5408	CLA	O2A-CGA	2.29	1.40	1.33
31	AC	520	LMG	O1-C1	2.29	1.44	1.40
30	AA	416	SQD	C6-S	2.29	1.81	1.77
27	BB	5623	BCR	C33-C5	2.30	1.54	1.51
24	BC	5507	CLA	C1C-NC	2.30	1.41	1.37
31	AA	417	LMG	O1-C1	2.30	1.44	1.40
24	BD	5405	CLA	C1C-NC	2.31	1.41	1.37
32	BB	5626	LMT	O1B-C1B	2.31	1.48	1.41
32	AD	409	LMT	C4'-C5'	2.31	1.59	1.52
24	BB	5609	CLA	C4C-NC	2.31	1.41	1.37
32	BB	5627	LMT	O5'-C1'	2.31	1.47	1.41
24	AA	405	CLA	CHC-C1C	2.32	1.42	1.35
36	AF	101	HEM	CHC-C1C	2.32	1.41	1.36
28	BA	5412	DGD	C1G-C2G	2.32	1.57	1.50
34	BD	5404	PHO	O1D-CGD	2.32	1.27	1.21
32	BB	5604	LMT	C4'-C5'	2.33	1.59	1.52
24	AA	404	CLA	CHC-C1C	2.33	1.42	1.35
24	BC	5508	CLA	O2A-CGA	2.33	1.40	1.33
24	AA	407	CLA	O2A-CGA	2.33	1.40	1.33
24	AC	503	CLA	C1C-NC	2.34	1.41	1.37
31	BM	5102	LMG	O7-C10	2.34	1.41	1.34
32	AI	103	LMT	O1B-C1B	2.34	1.48	1.41
32	BB	5604	LMT	O5'-C1'	2.34	1.47	1.41
24	AC	501	CLA	CBA-CGA	2.34	1.57	1.50
24	AB	614	CLA	C1C-NC	2.35	1.41	1.37
24	BB	5610	CLA	C1C-NC	2.35	1.41	1.37
32	AB	624	LMT	C4'-C5'	2.35	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	BC	5517	DGD	O3G-C1D	2.35	1.44	1.40
28	BC	5518	DGD	O2G-C1B	2.35	1.41	1.34
24	BC	5510	CLA	C1C-NC	2.35	1.41	1.37
24	BB	5617	CLA	C4C-NC	2.35	1.41	1.37
24	AA	405	CLA	OBD-CAD	2.36	1.26	1.22
24	AC	508	CLA	O1D-CGD	2.36	1.27	1.21
32	AB	630	LMT	C4'-C5'	2.36	1.59	1.52
24	AC	506	CLA	CBA-CGA	2.36	1.57	1.50
24	BC	5506	CLA	CBA-CGA	2.36	1.57	1.50
28	AC	519	DGD	C4E-C3E	2.36	1.58	1.52
24	AC	505	CLA	O1D-CGD	2.37	1.27	1.21
24	AC	504	CLA	O1D-CGD	2.37	1.27	1.21
24	BA	5405	CLA	CHC-C1C	2.37	1.42	1.35
24	AC	509	CLA	O2A-CGA	2.38	1.40	1.33
24	AB	604	CLA	CHC-C1C	2.38	1.42	1.35
28	BE	5102	DGD	O6E-C5E	2.39	1.50	1.44
30	AA	416	SQD	C8-C7	2.39	1.57	1.50
27	BK	5102	BCR	C14-C13	2.39	1.38	1.35
34	AD	403	PHO	O1D-CGD	2.39	1.27	1.21
30	BB	5625	SQD	C44-C45	2.40	1.57	1.50
34	BD	5403	PHO	O2A-CGA	2.40	1.40	1.33
24	AC	506	CLA	C1C-NC	2.40	1.41	1.37
30	BA	5401	SQD	C6-S	2.40	1.81	1.77
24	AC	507	CLA	CMC-C2C	2.40	1.55	1.50
27	AX	101	BCR	C38-C26	2.40	1.55	1.51
30	AF	102	SQD	C24-C23	2.40	1.57	1.50
24	AB	613	CLA	C1C-NC	2.40	1.41	1.37
28	AA	411	DGD	C4E-C3E	2.41	1.58	1.52
32	BI	5102	LMT	O5'-C1'	2.41	1.48	1.41
24	BB	5612	CLA	C1C-NC	2.41	1.41	1.37
24	BC	5511	CLA	CMC-C2C	2.41	1.55	1.50
24	BC	5513	CLA	CMC-C2C	2.41	1.55	1.50
30	BF	5102	SQD	C24-C23	2.41	1.57	1.50
28	BE	5102	DGD	O2G-C2G	2.41	1.52	1.46
24	BB	5606	CLA	O1D-CGD	2.42	1.27	1.21
32	BB	5627	LMT	C4'-C5'	2.42	1.59	1.52
24	BA	5407	CLA	C1C-NC	2.42	1.41	1.37
24	AB	603	CLA	C4C-NC	2.42	1.41	1.37
32	BC	5522	LMT	C4'-C5'	2.42	1.59	1.52
24	BB	5619	CLA	C4C-NC	2.43	1.41	1.37
24	AC	501	CLA	C5-C3	2.43	1.56	1.51
24	AA	406	CLA	CMC-C2C	2.43	1.56	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BX	5101	BCR	C14-C13	2.43	1.39	1.35
24	AB	609	CLA	CMC-C2C	2.43	1.56	1.50
24	AC	507	CLA	O1D-CGD	2.43	1.27	1.21
24	AB	604	CLA	O1D-CGD	2.43	1.27	1.21
34	AD	403	PHO	CHC-C1C	2.44	1.43	1.38
32	BB	5626	LMT	C4'-C5'	2.44	1.59	1.52
27	BJ	5101	BCR	C17-C18	2.44	1.39	1.35
24	BA	5407	CLA	CHC-C1C	2.44	1.42	1.35
24	AC	510	CLA	CMC-C2C	2.44	1.56	1.50
24	AB	602	CLA	O2A-CGA	2.45	1.40	1.33
24	AB	610	CLA	O1D-CGD	2.45	1.27	1.21
31	AM	101	LMG	O1-C1	2.46	1.44	1.40
24	AB	606	CLA	C1C-NC	2.46	1.42	1.37
28	AE	101	DGD	O2G-C2G	2.46	1.52	1.46
24	AB	606	CLA	OBD-CAD	2.46	1.26	1.22
24	AB	614	CLA	O1D-CGD	2.47	1.27	1.21
30	AB	627	SQD	O6-C1	2.47	1.44	1.40
24	BB	5617	CLA	O2A-CGA	2.47	1.40	1.33
32	AI	102	LMT	O1'-C1'	2.47	1.44	1.40
24	BB	5611	CLA	CMC-C2C	2.47	1.56	1.50
31	BD	5408	LMG	O6-C1	2.47	1.48	1.41
31	BM	5102	LMG	O1-C1	2.48	1.44	1.40
24	AB	607	CLA	CHC-C1C	2.48	1.43	1.35
24	AC	508	CLA	O2A-CGA	2.48	1.40	1.33
32	BD	5411	LMT	C4'-C5'	2.48	1.59	1.52
30	BA	5414	SQD	C8-C7	2.48	1.58	1.50
24	AB	605	CLA	C4C-NC	2.48	1.41	1.37
36	BF	5101	HEM	CHC-C1C	2.48	1.42	1.36
24	AB	605	CLA	CHC-C1C	2.48	1.43	1.35
24	AB	614	CLA	CMC-C2C	2.49	1.56	1.50
24	BB	5616	CLA	CHC-C1C	2.49	1.43	1.35
31	AC	520	LMG	O6-C1	2.49	1.48	1.41
24	BB	5616	CLA	CMC-C2C	2.50	1.56	1.50
24	BA	5407	CLA	O2A-CGA	2.50	1.40	1.33
24	BC	5509	CLA	CHC-C1C	2.50	1.43	1.35
24	BC	5503	CLA	C1C-NC	2.50	1.42	1.37
24	AD	404	CLA	O2A-CGA	2.50	1.40	1.33
24	AC	513	CLA	CMC-C2C	2.50	1.56	1.50
24	BD	5402	CLA	O1D-CGD	2.50	1.27	1.21
24	BC	5504	CLA	O1D-CGD	2.50	1.27	1.21
24	AC	504	CLA	CHC-C1C	2.50	1.43	1.35
24	AC	505	CLA	C4C-NC	2.50	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BC	5507	CLA	CMC-C2C	2.50	1.56	1.50
32	AB	623	LMT	O1B-C1B	2.50	1.48	1.41
24	BA	5408	CLA	CHC-C1C	2.51	1.43	1.35
24	BA	5406	CLA	O2A-CGA	2.51	1.40	1.33
30	BA	5401	SQD	C8-C7	2.51	1.58	1.50
24	AC	501	CLA	O1D-CGD	2.51	1.27	1.21
24	BC	5512	CLA	O2A-CGA	2.52	1.40	1.33
24	BC	5507	CLA	C4C-NC	2.52	1.42	1.37
35	AD	405	PL9	C3-C4	2.52	1.53	1.49
24	AD	404	CLA	C1C-NC	2.52	1.42	1.37
27	AA	410	BCR	C5-C6	2.52	1.38	1.34
24	AC	506	CLA	CMC-C2C	2.52	1.56	1.50
24	AC	504	CLA	O2A-CGA	2.52	1.40	1.33
28	BH	5101	DGD	O6E-C1E	2.53	1.48	1.41
27	BJ	5101	BCR	C24-C23	2.53	1.40	1.33
34	BD	5404	PHO	CHC-C1C	2.53	1.43	1.38
24	AB	607	CLA	C4C-NC	2.53	1.42	1.37
24	AC	508	CLA	CHC-C1C	2.54	1.43	1.35
24	AB	602	CLA	O1D-CGD	2.54	1.27	1.21
24	BB	5617	CLA	CMC-C2C	2.54	1.56	1.50
24	AB	607	CLA	CMC-C2C	2.54	1.56	1.50
24	AC	504	CLA	CMC-C2C	2.54	1.56	1.50
24	BD	5402	CLA	CHC-C1C	2.54	1.43	1.35
35	AD	405	PL9	C7-C3	2.54	1.53	1.51
28	AE	101	DGD	C1G-C2G	2.54	1.57	1.50
27	AJ	101	BCR	C24-C23	2.54	1.40	1.33
32	BB	5626	LMT	O5'-C1'	2.54	1.48	1.41
24	BA	5407	CLA	C4C-NC	2.54	1.42	1.37
36	BV	5201	HEM	CHC-C1C	2.55	1.42	1.36
34	AD	403	PHO	CMC-C2C	2.55	1.56	1.50
24	AB	603	CLA	CMC-C2C	2.55	1.56	1.50
24	BB	5608	CLA	CMC-C2C	2.55	1.56	1.50
28	AE	101	DGD	O6D-C5D	2.55	1.50	1.44
24	BB	5613	CLA	C4C-NC	2.55	1.42	1.37
32	BB	5603	LMT	O1B-C4'	2.56	1.50	1.43
27	AT	101	BCR	C26-C25	2.56	1.38	1.34
24	AC	512	CLA	C1C-NC	2.56	1.42	1.37
24	BC	5507	CLA	O1D-CGD	2.56	1.27	1.21
24	BB	5607	CLA	CMC-C2C	2.56	1.56	1.50
31	AD	408	LMG	O6-C1	2.56	1.48	1.41
36	BF	5101	HEM	CAA-C2A	2.56	1.56	1.52
24	BB	5606	CLA	O2A-CGA	2.56	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	AB	630	LMT	O5'-C1'	2.56	1.48	1.41
24	BB	5610	CLA	O2A-CGA	2.56	1.41	1.33
24	AB	607	CLA	O1D-CGD	2.57	1.27	1.21
30	BB	5601	SQD	O5-C1	2.57	1.48	1.41
31	BC	5520	LMG	O1-C1	2.57	1.44	1.40
27	AC	516	BCR	C29-C30	2.57	1.60	1.54
24	AD	401	CLA	O1D-CGD	2.57	1.27	1.21
24	AA	405	CLA	C4C-NC	2.58	1.42	1.37
24	AB	608	CLA	O1D-CGD	2.58	1.27	1.21
28	BA	5412	DGD	O6D-C5D	2.58	1.50	1.44
24	BC	5502	CLA	CMC-C2C	2.58	1.56	1.50
35	BD	5406	PL9	C7-C3	2.58	1.53	1.51
28	AH	101	DGD	O6E-C1E	2.58	1.48	1.41
24	AD	401	CLA	CHC-C1C	2.58	1.43	1.35
31	AB	621	LMG	O6-C1	2.58	1.48	1.41
30	AB	627	SQD	O5-C1	2.59	1.48	1.41
24	BB	5610	CLA	CMC-C2C	2.59	1.56	1.50
24	AB	605	CLA	C1C-NC	2.59	1.42	1.37
24	BC	5505	CLA	C4C-NC	2.59	1.42	1.37
24	BD	5402	CLA	O2A-CGA	2.59	1.41	1.33
28	BE	5102	DGD	C1G-C2G	2.59	1.58	1.50
32	BB	5604	LMT	O1'-C1'	2.60	1.44	1.40
24	BB	5608	CLA	O2A-CGA	2.60	1.41	1.33
24	AB	612	CLA	O1D-CGD	2.60	1.27	1.21
24	AC	503	CLA	O1D-CGD	2.60	1.27	1.21
24	AB	615	CLA	O1D-CGD	2.60	1.27	1.21
24	BB	5610	CLA	C4C-NC	2.60	1.42	1.37
24	BC	5508	CLA	O1D-CGD	2.60	1.27	1.21
24	BB	5611	CLA	CBA-CGA	2.60	1.58	1.50
31	AD	408	LMG	O1-C1	2.61	1.44	1.40
24	AA	407	CLA	C4C-NC	2.61	1.42	1.37
32	BD	5411	LMT	O1B-C1B	2.61	1.48	1.41
24	BB	5613	CLA	CMC-C2C	2.61	1.56	1.50
32	AB	630	LMT	O1'-C1'	2.62	1.44	1.40
24	BA	5406	CLA	C1C-NC	2.62	1.42	1.37
27	BC	5514	BCR	C5-C6	2.62	1.38	1.34
28	AC	517	DGD	O6D-C5D	2.62	1.50	1.44
30	AB	622	SQD	O5-C1	2.63	1.48	1.41
28	AC	519	DGD	O3G-C3G	2.63	1.48	1.43
32	AB	624	LMT	O5'-C1'	2.63	1.48	1.41
24	BC	5504	CLA	CHC-C1C	2.64	1.43	1.35
30	BB	5625	SQD	O5-C1	2.64	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	604	CLA	C1C-NC	2.64	1.42	1.37
24	BA	5406	CLA	O1D-CGD	2.64	1.27	1.21
24	AB	611	CLA	O1D-CGD	2.64	1.27	1.21
24	AB	608	CLA	C1C-NC	2.64	1.42	1.37
24	BB	5618	CLA	O1D-CGD	2.64	1.27	1.21
24	BB	5606	CLA	C1C-NC	2.65	1.42	1.37
31	AI	101	LMG	O6-C1	2.65	1.48	1.41
31	BD	5410	LMG	O6-C1	2.65	1.48	1.41
24	BB	5612	CLA	O1D-CGD	2.65	1.27	1.21
24	BC	5506	CLA	C1C-NC	2.65	1.42	1.37
32	BM	5101	LMT	O1B-C1B	2.65	1.48	1.41
31	BE	5101	LMG	O1-C1	2.65	1.44	1.40
24	AB	607	CLA	CBA-CGA	2.65	1.58	1.50
24	AB	612	CLA	O2A-CGA	2.66	1.41	1.33
24	BC	5501	CLA	CBA-CGA	2.66	1.58	1.50
24	BA	5406	CLA	C4C-C3C	2.66	1.49	1.45
28	AE	101	DGD	O6E-C5E	2.66	1.51	1.44
24	AA	405	CLA	C1C-NC	2.66	1.42	1.37
32	AB	623	LMT	O5'-C1'	2.67	1.48	1.41
28	AE	101	DGD	O6D-C1D	2.67	1.48	1.41
27	AB	617	BCR	C1-C6	2.67	1.57	1.53
27	AC	514	BCR	C5-C6	2.68	1.38	1.34
34	BD	5404	PHO	CMC-C2C	2.68	1.56	1.50
24	AB	615	CLA	C4C-NC	2.68	1.42	1.37
32	BI	5102	LMT	O1B-C1B	2.68	1.49	1.41
24	BB	5609	CLA	CMC-C2C	2.68	1.56	1.50
27	BB	5621	BCR	C30-C25	2.68	1.57	1.53
24	AA	406	CLA	CHC-C1C	2.68	1.43	1.35
24	BC	5501	CLA	C4C-NC	2.68	1.42	1.37
28	BA	5412	DGD	C3G-C2G	2.68	1.58	1.50
31	BB	5624	LMG	O6-C1	2.68	1.48	1.41
24	BB	5619	CLA	CMC-C2C	2.68	1.56	1.50
24	AB	604	CLA	O2A-CGA	2.68	1.41	1.33
24	AC	510	CLA	C1C-NC	2.69	1.42	1.37
24	BC	5510	CLA	CMC-C2C	2.69	1.56	1.50
24	AA	407	CLA	CMC-C2C	2.69	1.56	1.50
28	BE	5102	DGD	O6D-C1D	2.69	1.48	1.41
27	AD	406	BCR	C5-C6	2.69	1.38	1.34
30	AB	622	SQD	C44-C45	2.69	1.58	1.50
32	BI	5102	LMT	O1'-C1'	2.70	1.45	1.40
24	BB	5612	CLA	CBA-CGA	2.70	1.58	1.50
32	AB	630	LMT	O1B-C1B	2.70	1.49	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	BA	5402	LMG	O1-C1	2.70	1.45	1.40
27	BB	5621	BCR	C1-C6	2.70	1.57	1.53
28	AH	101	DGD	C1G-C2G	2.71	1.58	1.50
24	BD	5405	CLA	O2A-CGA	2.71	1.41	1.33
24	BB	5612	CLA	C4C-NC	2.71	1.42	1.37
24	BB	5615	CLA	O2A-CGA	2.71	1.41	1.33
24	AB	607	CLA	C1C-NC	2.71	1.42	1.37
24	AB	613	CLA	O1D-CGD	2.71	1.28	1.21
24	AC	507	CLA	C4C-NC	2.71	1.42	1.37
24	BC	5513	CLA	CHC-C1C	2.72	1.43	1.35
28	BC	5519	DGD	O5D-C1E	2.72	1.45	1.40
24	BC	5508	CLA	CHC-C1C	2.72	1.43	1.35
24	AB	608	CLA	CBA-CGA	2.72	1.58	1.50
24	BB	5620	CLA	O2A-CGA	2.72	1.41	1.33
35	BD	5406	PL9	C3-C4	2.72	1.54	1.49
31	BI	5101	LMG	O6-C1	2.72	1.48	1.41
24	AA	407	CLA	O1D-CGD	2.73	1.28	1.21
32	BM	5101	LMT	C4'-C5'	2.73	1.60	1.52
30	AA	413	SQD	C8-C7	2.73	1.58	1.50
24	AB	612	CLA	CMC-C2C	2.73	1.56	1.50
24	AB	615	CLA	O2A-CGA	2.74	1.41	1.33
28	AA	411	DGD	O6D-C5D	2.74	1.51	1.44
31	AA	417	LMG	O6-C1	2.74	1.48	1.41
24	AB	603	CLA	CHC-C1C	2.74	1.43	1.35
24	AB	606	CLA	C4C-NC	2.74	1.42	1.37
30	BB	5601	SQD	O3-C3	2.74	1.49	1.43
24	AB	601	CLA	C1C-NC	2.74	1.42	1.37
28	AE	101	DGD	C3G-C2G	2.75	1.58	1.50
24	AC	512	CLA	O1D-CGD	2.75	1.28	1.21
35	AD	405	PL9	C27-C28	2.75	1.58	1.50
24	AB	601	CLA	CMC-C2C	2.75	1.56	1.50
24	BC	5509	CLA	O2A-CGA	2.75	1.41	1.33
28	BC	5519	DGD	O6E-C1E	2.75	1.48	1.41
34	BD	5403	PHO	CMC-C2C	2.75	1.56	1.50
24	BA	5408	CLA	O1D-CGD	2.75	1.28	1.21
32	AB	629	LMT	O5'-C1'	2.76	1.48	1.41
32	AD	409	LMT	O1B-C1B	2.76	1.49	1.41
27	AK	102	BCR	C2-C1	2.76	1.60	1.54
30	BB	5601	SQD	O6-C1	2.76	1.45	1.40
24	BC	5504	CLA	C1C-NC	2.76	1.42	1.37
24	BC	5503	CLA	O1D-CGD	2.77	1.28	1.21
24	AB	602	CLA	C1C-NC	2.77	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	603	CLA	CBA-CGA	2.77	1.58	1.50
24	BB	5605	CLA	CMC-C2C	2.77	1.56	1.50
36	AV	201	HEM	C3C-CAC	2.77	1.56	1.51
24	BB	5619	CLA	O1D-CGD	2.77	1.28	1.21
24	BB	5608	CLA	O1D-CGD	2.77	1.28	1.21
24	AB	612	CLA	CHC-C1C	2.77	1.44	1.35
32	BD	5411	LMT	O1'-C1'	2.77	1.45	1.40
27	BB	5622	BCR	C14-C13	2.78	1.39	1.35
24	BB	5607	CLA	O1D-CGD	2.78	1.28	1.21
28	BH	5101	DGD	C1G-C2G	2.78	1.58	1.50
32	BB	5604	LMT	O1B-C1B	2.78	1.49	1.41
24	AB	615	CLA	C1C-NC	2.78	1.42	1.37
36	AF	101	HEM	CAA-C2A	2.78	1.56	1.52
24	BB	5614	CLA	C4C-NC	2.78	1.42	1.37
24	BB	5618	CLA	CMC-C2C	2.78	1.56	1.50
24	AB	602	CLA	CMC-C2C	2.78	1.56	1.50
24	BB	5607	CLA	CBA-CGA	2.79	1.59	1.50
28	BE	5102	DGD	O6E-C1E	2.79	1.49	1.41
24	AB	607	CLA	CBB-CAB	2.79	1.49	1.28
24	AB	610	CLA	C4C-NC	2.79	1.42	1.37
24	AB	603	CLA	O1D-CGD	2.79	1.28	1.21
31	BC	5520	LMG	O6-C1	2.80	1.49	1.41
30	BF	5102	SQD	O3-C3	2.80	1.49	1.43
28	AA	411	DGD	C3G-C2G	2.80	1.58	1.50
31	BA	5402	LMG	O6-C1	2.80	1.49	1.41
24	BC	5503	CLA	CMC-C2C	2.80	1.56	1.50
27	AC	514	BCR	C2-C1	2.81	1.60	1.54
24	BB	5619	CLA	O2A-CGA	2.81	1.41	1.33
27	AX	101	BCR	C2-C1	2.82	1.60	1.54
24	AB	615	CLA	CMC-C2C	2.82	1.56	1.50
34	AD	402	PHO	O2A-CGA	2.82	1.41	1.33
24	BB	5610	CLA	O1D-CGD	2.82	1.28	1.21
24	AC	512	CLA	CMC-C2C	2.82	1.56	1.50
24	BB	5611	CLA	CBB-CAB	2.83	1.49	1.28
24	BC	5504	CLA	CMC-C2C	2.83	1.56	1.50
24	AB	608	CLA	CMC-C2C	2.83	1.56	1.50
24	AC	513	CLA	CHC-C1C	2.83	1.44	1.35
35	BD	5406	PL9	C27-C28	2.83	1.58	1.50
24	BB	5609	CLA	O1D-CGD	2.84	1.28	1.21
27	BC	5516	BCR	C29-C30	2.84	1.60	1.54
24	AA	405	CLA	O2A-CGA	2.84	1.41	1.33
24	AC	511	CLA	O1D-CGD	2.84	1.28	1.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	5411	BCR	C2-C1	2.84	1.60	1.54
31	BC	5521	LMG	O6-C1	2.84	1.49	1.41
24	BD	5402	CLA	C4C-NC	2.84	1.42	1.37
27	BC	5515	BCR	C2-C1	2.85	1.61	1.54
24	BA	5406	CLA	C4C-NC	2.85	1.42	1.37
24	AC	510	CLA	O1D-CGD	2.86	1.28	1.21
24	AC	506	CLA	O1D-CGD	2.86	1.28	1.21
31	AB	620	LMG	O6-C1	2.86	1.49	1.41
24	AA	407	CLA	C1C-NC	2.86	1.42	1.37
24	AC	510	CLA	C4C-NC	2.86	1.42	1.37
28	BE	5102	DGD	C3G-C2G	2.86	1.58	1.50
24	BC	5506	CLA	O1D-CGD	2.86	1.28	1.21
24	BB	5617	CLA	CBB-CAB	2.87	1.49	1.28
24	AA	405	CLA	O1D-CGD	2.87	1.28	1.21
27	AD	406	BCR	C1-C6	2.87	1.57	1.53
24	BB	5615	CLA	C4C-C3C	2.87	1.50	1.45
36	BV	5201	HEM	C4C-NC	2.88	1.39	1.36
32	AM	102	LMT	C4'-C5'	2.88	1.60	1.52
36	AV	201	HEM	FE-NC	2.88	2.07	1.95
27	AX	101	BCR	C5-C6	2.88	1.38	1.34
24	AC	504	CLA	C4C-NC	2.89	1.42	1.37
24	BB	5607	CLA	CHC-C1C	2.89	1.44	1.35
24	AB	605	CLA	CMC-C2C	2.89	1.56	1.50
30	AF	102	SQD	O3-C3	2.89	1.49	1.43
28	BH	5101	DGD	O6D-C1D	2.89	1.49	1.41
24	AD	404	CLA	O1D-CGD	2.90	1.28	1.21
24	AB	613	CLA	CBB-CAB	2.90	1.49	1.28
30	AA	413	SQD	O5-C1	2.90	1.49	1.41
24	AC	507	CLA	O2A-CGA	2.90	1.42	1.33
24	BC	5506	CLA	CMC-C2C	2.90	1.57	1.50
28	AE	101	DGD	O6E-C1E	2.90	1.49	1.41
24	AB	611	CLA	O2A-CGA	2.90	1.42	1.33
24	AA	405	CLA	C4C-C3C	2.90	1.50	1.45
31	BC	5521	LMG	O1-C1	2.91	1.45	1.40
24	AC	502	CLA	O1D-CGD	2.91	1.28	1.21
32	BB	5603	LMT	O5'-C1'	2.91	1.49	1.41
24	BB	5608	CLA	C4C-NC	2.91	1.42	1.37
24	AB	616	CLA	C4C-NC	2.92	1.42	1.37
24	BA	5405	CLA	O1D-CGD	2.92	1.28	1.21
24	BB	5606	CLA	CMC-C2C	2.93	1.57	1.50
32	AB	630	LMT	O1B-C4'	2.94	1.51	1.43
27	AA	410	BCR	C2-C1	2.94	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BC	5504	CLA	O2A-CGA	2.94	1.42	1.33
24	AC	508	CLA	C4C-C3C	2.94	1.50	1.45
32	AB	624	LMT	O5B-C1B	2.94	1.49	1.41
24	AB	616	CLA	O2A-CGA	2.94	1.42	1.33
24	AC	503	CLA	CMC-C2C	2.94	1.57	1.50
24	BA	5405	CLA	CMC-C2C	2.94	1.57	1.50
24	BC	5509	CLA	CMC-C2C	2.94	1.57	1.50
24	BC	5507	CLA	O2A-CGA	2.95	1.42	1.33
24	BC	5502	CLA	O1D-CGD	2.95	1.28	1.21
32	AM	102	LMT	O1'-C1'	2.95	1.45	1.40
27	BB	5621	BCR	C29-C30	2.95	1.61	1.54
24	AC	509	CLA	CMC-C2C	2.95	1.57	1.50
24	AC	511	CLA	CBB-CAB	2.95	1.50	1.28
30	AB	627	SQD	O3-C3	2.95	1.50	1.43
27	BB	5623	BCR	C26-C25	2.95	1.39	1.34
30	BA	5414	SQD	O3-C3	2.95	1.50	1.43
36	BF	5101	HEM	C3C-CAC	2.95	1.56	1.51
28	BC	5519	DGD	C4E-C3E	2.95	1.60	1.52
24	AB	606	CLA	O2A-CGA	2.96	1.42	1.33
31	BE	5101	LMG	O6-C1	2.96	1.49	1.41
32	BM	5101	LMT	O1'-C1'	2.96	1.45	1.40
24	BC	5508	CLA	C4C-C3C	2.96	1.50	1.45
24	BA	5407	CLA	CMC-C2C	2.96	1.57	1.50
24	AB	614	CLA	CBB-CAB	2.96	1.50	1.28
24	AD	401	CLA	C4C-NC	2.96	1.42	1.37
24	AB	609	CLA	C4C-NC	2.97	1.42	1.37
24	AA	407	CLA	CBB-CAB	2.97	1.50	1.28
31	AA	414	LMG	O6-C1	2.97	1.49	1.41
24	BC	5501	CLA	CMC-C2C	2.97	1.57	1.50
24	BB	5613	CLA	O1D-CGD	2.98	1.28	1.21
24	BC	5510	CLA	O1D-CGD	2.98	1.28	1.21
24	BA	5405	CLA	C1C-NC	2.98	1.42	1.37
28	AH	101	DGD	O6D-C1D	2.98	1.49	1.41
24	BD	5402	CLA	CMC-C2C	2.98	1.57	1.50
32	BB	5627	LMT	O1'-C1'	2.98	1.45	1.40
24	AC	513	CLA	O2A-CGA	2.98	1.42	1.33
24	AC	513	CLA	O1D-CGD	2.99	1.28	1.21
24	BB	5607	CLA	CBB-CAB	2.99	1.50	1.28
24	BC	5511	CLA	CBB-CAB	2.99	1.50	1.28
24	AC	511	CLA	O2A-CGA	2.99	1.42	1.33
27	AA	410	BCR	C29-C30	2.99	1.61	1.54
24	BB	5618	CLA	CBB-CAB	2.99	1.50	1.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	BA	5412	DGD	O1G-C1A	2.99	1.42	1.33
27	BT	5101	BCR	C26-C25	2.99	1.39	1.34
24	BB	5615	CLA	O1D-CGD	2.99	1.28	1.21
34	AD	402	PHO	O1D-CGD	3.00	1.28	1.21
27	BA	5411	BCR	C29-C30	3.00	1.61	1.54
27	AD	406	BCR	C2-C1	3.00	1.61	1.54
24	BB	5611	CLA	C5-C3	3.00	1.58	1.51
24	AC	502	CLA	C4C-C3C	3.00	1.50	1.45
32	AD	409	LMT	O1'-C1'	3.00	1.45	1.40
24	BB	5612	CLA	CMC-C2C	3.00	1.57	1.50
24	BB	5617	CLA	O1D-CGD	3.01	1.28	1.21
24	BC	5511	CLA	O2A-CGA	3.01	1.42	1.33
30	BA	5401	SQD	O3-C3	3.01	1.50	1.43
24	BC	5512	CLA	CMC-C2C	3.01	1.57	1.50
24	BA	5408	CLA	CBB-CAB	3.01	1.50	1.28
24	AD	401	CLA	C1C-NC	3.01	1.42	1.37
24	AA	404	CLA	O1D-CGD	3.02	1.28	1.21
30	AA	413	SQD	O3-C3	3.02	1.50	1.43
32	BB	5627	LMT	O5B-C1B	3.02	1.49	1.41
24	AC	504	CLA	CBB-CAB	3.02	1.50	1.28
24	BA	5408	CLA	C4C-NC	3.03	1.42	1.37
24	AB	609	CLA	O1D-CGD	3.04	1.28	1.21
24	BC	5504	CLA	CBB-CAB	3.04	1.50	1.28
34	AD	402	PHO	CMC-C2C	3.04	1.57	1.50
24	BC	5501	CLA	O1D-CGD	3.04	1.28	1.21
27	BD	5407	BCR	C1-C6	3.04	1.58	1.53
24	BA	5406	CLA	OBD-CAD	3.04	1.27	1.22
24	AB	606	CLA	O1D-CGD	3.05	1.28	1.21
31	BD	5408	LMG	O1-C1	3.05	1.45	1.40
27	AB	617	BCR	C29-C30	3.05	1.61	1.54
29	AA	412	LHG	O7-C7	3.05	1.43	1.34
36	BV	5201	HEM	FE-NC	3.05	2.07	1.95
24	BB	5613	CLA	O2A-CGA	3.05	1.42	1.33
28	AB	628	DGD	O6E-C1E	3.06	1.49	1.41
30	AA	416	SQD	O5-C1	3.06	1.49	1.41
30	BA	5414	SQD	O5-C1	3.06	1.49	1.41
24	AB	605	CLA	O1D-CGD	3.06	1.28	1.21
24	AB	610	CLA	CMC-C2C	3.07	1.57	1.50
27	BK	5102	BCR	C2-C1	3.07	1.61	1.54
27	BB	5622	BCR	C5-C6	3.07	1.39	1.34
24	BB	5611	CLA	O2A-CGA	3.07	1.42	1.33
24	BB	5617	CLA	C1C-NC	3.07	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	612	CLA	CBB-CAB	3.07	1.51	1.28
30	AA	413	SQD	O7-S	3.07	1.54	1.45
24	AB	608	CLA	C4C-C3C	3.07	1.50	1.45
24	AB	611	CLA	CBB-CAB	3.08	1.51	1.28
24	BB	5616	CLA	O2A-CGA	3.08	1.42	1.33
28	BB	5602	DGD	O6E-C1E	3.08	1.49	1.41
36	BF	5101	HEM	FE-NC	3.08	2.08	1.95
24	AC	501	CLA	CMC-C2C	3.08	1.57	1.50
27	AB	617	BCR	C30-C25	3.08	1.58	1.53
28	AA	411	DGD	O1G-C1A	3.09	1.42	1.33
24	AC	501	CLA	O2A-CGA	3.09	1.42	1.33
31	AA	414	LMG	O1-C1	3.09	1.45	1.40
24	BC	5513	CLA	O2A-CGA	3.09	1.42	1.33
31	BL	5101	LMG	O6-C1	3.09	1.49	1.41
27	AC	515	BCR	C2-C1	3.09	1.61	1.54
24	BC	5512	CLA	C1C-NC	3.09	1.43	1.37
30	BB	5625	SQD	O6-C1	3.10	1.45	1.40
36	AF	101	HEM	C3C-CAC	3.10	1.57	1.51
24	AC	511	CLA	CHC-C1C	3.10	1.45	1.35
24	AB	603	CLA	CBB-CAB	3.10	1.51	1.28
24	BC	5509	CLA	O1D-CGD	3.10	1.29	1.21
27	AT	101	BCR	C2-C1	3.10	1.61	1.54
24	AB	608	CLA	C4C-NC	3.10	1.42	1.37
27	BD	5407	BCR	C2-C1	3.11	1.61	1.54
27	AC	514	BCR	C29-C30	3.11	1.61	1.54
24	BD	5405	CLA	C4C-NC	3.11	1.42	1.37
24	BC	5512	CLA	O1D-CGD	3.11	1.29	1.21
24	AA	407	CLA	C4C-C3C	3.11	1.50	1.45
24	AC	503	CLA	O2A-CGA	3.12	1.42	1.33
24	BB	5614	CLA	CMC-C2C	3.12	1.57	1.50
27	BC	5514	BCR	C2-C1	3.12	1.61	1.54
24	BB	5612	CLA	C4C-C3C	3.12	1.50	1.45
24	BA	5408	CLA	CMC-C2C	3.13	1.57	1.50
24	BC	5509	CLA	CBB-CAB	3.13	1.51	1.28
27	BT	5101	BCR	C29-C30	3.13	1.61	1.54
24	BB	5616	CLA	CBB-CAB	3.13	1.51	1.28
24	AB	604	CLA	C4C-NC	3.13	1.43	1.37
24	AB	607	CLA	C5-C3	3.14	1.58	1.51
24	AB	604	CLA	CMC-C2C	3.14	1.57	1.50
24	AC	512	CLA	C4C-NC	3.14	1.43	1.37
29	BA	5413	LHG	O8-C23	3.14	1.42	1.33
30	AA	416	SQD	O3-C3	3.14	1.50	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AD	404	CLA	CBB-CAB	3.14	1.51	1.28
24	BC	5511	CLA	CHC-C1C	3.14	1.45	1.35
24	AA	406	CLA	CBA-CGA	3.15	1.60	1.50
24	BD	5405	CLA	CBB-CAB	3.15	1.51	1.28
24	BB	5615	CLA	CBB-CAB	3.15	1.51	1.28
27	AC	516	BCR	C2-C1	3.16	1.61	1.54
27	BJ	5101	BCR	C21-C22	3.16	1.39	1.35
24	BD	5405	CLA	O1D-CGD	3.16	1.29	1.21
31	AC	521	LMG	O1-C1	3.16	1.45	1.40
24	BC	5503	CLA	O2A-CGA	3.17	1.42	1.33
24	BC	5508	CLA	CBB-CAB	3.17	1.51	1.28
24	AA	404	CLA	CMC-C2C	3.17	1.57	1.50
24	AC	503	CLA	C4C-NC	3.17	1.43	1.37
27	AC	516	BCR	C26-C25	3.18	1.39	1.34
30	BA	5401	SQD	O5-C1	3.18	1.50	1.41
24	BB	5616	CLA	O1D-CGD	3.19	1.29	1.21
24	AA	404	CLA	CBB-CAB	3.19	1.51	1.28
30	AA	413	SQD	O48-C23	3.19	1.42	1.33
24	BC	5505	CLA	O1D-CGD	3.19	1.29	1.21
32	AB	624	LMT	O1'-C1'	3.19	1.45	1.40
24	BD	5402	CLA	CBB-CAB	3.19	1.51	1.28
24	AB	602	CLA	C4C-NC	3.19	1.43	1.37
24	AB	607	CLA	O2A-CGA	3.20	1.42	1.33
32	AM	102	LMT	O1B-C4'	3.20	1.51	1.43
24	BB	5610	CLA	CBB-CAB	3.20	1.52	1.28
27	BA	5411	BCR	C5-C6	3.20	1.39	1.34
27	AC	515	BCR	C29-C30	3.20	1.61	1.54
24	BB	5609	CLA	C4C-C3C	3.20	1.50	1.45
24	AC	502	CLA	CBB-CAB	3.20	1.52	1.28
27	BJ	5101	BCR	C2-C1	3.21	1.61	1.54
27	BK	5102	BCR	C29-C30	3.21	1.61	1.54
24	BA	5406	CLA	CMC-C2C	3.21	1.57	1.50
24	AC	509	CLA	CBB-CAB	3.21	1.52	1.28
24	AC	508	CLA	CBB-CAB	3.22	1.52	1.28
24	BC	5502	CLA	O2A-CGA	3.22	1.43	1.33
24	AA	405	CLA	CMC-C2C	3.22	1.57	1.50
34	BD	5403	PHO	O1D-CGD	3.22	1.29	1.21
27	BD	5407	BCR	C5-C6	3.22	1.39	1.34
24	AC	503	CLA	CBB-CAB	3.23	1.52	1.28
27	BX	5101	BCR	C2-C1	3.23	1.61	1.54
32	AB	629	LMT	O1B-C1B	3.23	1.50	1.41
27	AB	617	BCR	C2-C1	3.23	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	AD	402	PHO	C4C-C3C	3.23	1.51	1.45
30	AA	416	SQD	O7-S	3.23	1.55	1.45
27	AJ	101	BCR	C21-C22	3.24	1.40	1.35
30	BF	5102	SQD	O5-C1	3.24	1.50	1.41
24	AC	506	CLA	O2A-CGA	3.24	1.43	1.33
27	BC	5514	BCR	C26-C25	3.24	1.39	1.34
31	AC	521	LMG	O6-C1	3.24	1.50	1.41
24	AC	508	CLA	C4C-NC	3.24	1.43	1.37
24	BD	5405	CLA	CMC-C2C	3.24	1.57	1.50
24	AB	606	CLA	CBB-CAB	3.24	1.52	1.28
27	AT	101	BCR	C29-C30	3.25	1.61	1.54
27	BB	5622	BCR	C29-C30	3.25	1.61	1.54
27	BC	5514	BCR	C29-C30	3.25	1.61	1.54
32	AI	103	LMT	O5B-C1B	3.25	1.50	1.41
24	AB	610	CLA	CBB-CAB	3.25	1.52	1.28
24	AB	605	CLA	C4C-C3C	3.25	1.50	1.45
24	BA	5407	CLA	CBA-CGA	3.25	1.60	1.50
24	BC	5507	CLA	CBB-CAB	3.26	1.52	1.28
27	BC	5516	BCR	C26-C25	3.26	1.39	1.34
24	AC	507	CLA	CBB-CAB	3.26	1.52	1.28
24	AD	401	CLA	CBB-CAB	3.26	1.52	1.28
24	BB	5609	CLA	O2A-CGA	3.26	1.43	1.33
34	AD	402	PHO	C3D-C4D	3.26	1.52	1.43
27	AJ	101	BCR	C2-C1	3.26	1.62	1.54
27	AC	516	BCR	C30-C25	3.27	1.58	1.53
24	BB	5614	CLA	CBB-CAB	3.27	1.52	1.28
32	BB	5604	LMT	O1B-C4'	3.27	1.52	1.43
32	BB	5603	LMT	O1B-C1B	3.27	1.50	1.41
24	BB	5620	CLA	CBB-CAB	3.28	1.52	1.28
32	BM	5101	LMT	O1B-C4'	3.28	1.52	1.43
30	AB	622	SQD	O3-C3	3.28	1.50	1.43
24	BC	5510	CLA	C4C-NC	3.28	1.43	1.37
24	BC	5513	CLA	O1D-CGD	3.28	1.29	1.21
24	BA	5405	CLA	CBB-CAB	3.28	1.52	1.28
30	AA	416	SQD	O6-C1	3.28	1.46	1.40
35	AD	405	PL9	C38-C39	3.28	1.39	1.33
34	AD	403	PHO	C3D-C4D	3.29	1.52	1.43
27	BB	5621	BCR	C2-C1	3.29	1.62	1.54
24	AC	502	CLA	C4C-NC	3.29	1.43	1.37
24	AB	616	CLA	O1D-CGD	3.30	1.29	1.21
24	BC	5501	CLA	O2A-CGA	3.30	1.43	1.33
24	AC	512	CLA	CBB-CAB	3.30	1.52	1.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BC	5512	CLA	CBB-CAB	3.30	1.52	1.28
24	AD	404	CLA	C4C-NC	3.30	1.43	1.37
24	BB	5606	CLA	CBB-CAB	3.30	1.52	1.28
24	BB	5619	CLA	C4C-C3C	3.30	1.51	1.45
24	AB	605	CLA	O2A-CGA	3.30	1.43	1.33
24	BC	5510	CLA	CBB-CAB	3.30	1.52	1.28
24	AC	510	CLA	CBB-CAB	3.30	1.52	1.28
24	AA	406	CLA	O2D-CGD	3.30	1.41	1.33
24	BB	5608	CLA	CBB-CAB	3.30	1.52	1.28
27	AB	619	BCR	C2-C1	3.30	1.62	1.54
24	BC	5506	CLA	CBB-CAB	3.31	1.52	1.28
27	BB	5623	BCR	C29-C30	3.31	1.62	1.54
28	BB	5602	DGD	O3G-C1D	3.31	1.46	1.40
24	BC	5502	CLA	CBB-CAB	3.31	1.52	1.28
24	AC	506	CLA	CBB-CAB	3.31	1.52	1.28
34	BD	5403	PHO	C3D-C4D	3.32	1.53	1.43
24	AD	401	CLA	CMC-C2C	3.32	1.57	1.50
27	BT	5101	BCR	C2-C1	3.32	1.62	1.54
24	AB	609	CLA	CBB-CAB	3.32	1.52	1.28
27	AB	619	BCR	C26-C25	3.32	1.39	1.34
36	AF	101	HEM	FE-NC	3.32	2.08	1.95
27	AD	406	BCR	C29-C30	3.32	1.62	1.54
24	AB	609	CLA	O2A-CGA	3.32	1.43	1.33
24	AA	405	CLA	CBA-CGA	3.33	1.60	1.50
24	AB	608	CLA	CBB-CAB	3.33	1.52	1.28
28	BH	5101	DGD	O2G-C2G	3.33	1.55	1.46
34	BD	5404	PHO	C3D-C4D	3.33	1.53	1.43
30	BA	5401	SQD	O6-C1	3.33	1.46	1.40
24	BB	5620	CLA	C4C-NC	3.33	1.43	1.37
35	AD	405	PL9	C18-C19	3.33	1.39	1.33
24	BB	5620	CLA	O1D-CGD	3.33	1.29	1.21
24	AC	513	CLA	CBB-CAB	3.33	1.53	1.28
24	BC	5503	CLA	CBB-CAB	3.33	1.53	1.28
30	BB	5601	SQD	O48-C23	3.33	1.43	1.33
30	AA	413	SQD	C6-S	3.34	1.82	1.77
30	BA	5414	SQD	O48-C23	3.34	1.43	1.33
35	BD	5406	PL9	C18-C19	3.34	1.39	1.33
24	AB	602	CLA	CBB-CAB	3.34	1.53	1.28
27	AB	618	BCR	C29-C30	3.35	1.62	1.54
24	BC	5505	CLA	C4C-C3C	3.35	1.51	1.45
32	AM	102	LMT	O5B-C1B	3.35	1.50	1.41
30	BF	5102	SQD	O7-S	3.36	1.55	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BC	5511	CLA	O1D-CGD	3.36	1.29	1.21
24	BB	5605	CLA	C4C-NC	3.36	1.43	1.37
24	BB	5612	CLA	CBB-CAB	3.36	1.53	1.28
28	AH	101	DGD	O2G-C2G	3.36	1.55	1.46
24	AB	616	CLA	CBB-CAB	3.37	1.53	1.28
24	AA	406	CLA	CBB-CAB	3.37	1.53	1.28
24	BB	5606	CLA	C4C-NC	3.37	1.43	1.37
27	BB	5623	BCR	C5-C6	3.37	1.39	1.34
27	AK	102	BCR	C1-C6	3.37	1.58	1.53
27	BX	5101	BCR	C5-C6	3.37	1.39	1.34
27	AB	619	BCR	C29-C30	3.37	1.62	1.54
30	BB	5625	SQD	O3-C3	3.37	1.51	1.43
24	AB	601	CLA	O2A-CGA	3.38	1.43	1.33
24	BC	5513	CLA	CBB-CAB	3.39	1.53	1.28
24	BA	5406	CLA	CBB-CAB	3.39	1.53	1.28
27	BB	5623	BCR	C2-C1	3.39	1.62	1.54
24	AB	615	CLA	CBB-CAB	3.39	1.53	1.28
24	BC	5504	CLA	C4C-NC	3.39	1.43	1.37
32	BD	5411	LMT	O5B-C1B	3.39	1.50	1.41
24	AC	504	CLA	C4C-C3C	3.40	1.51	1.45
24	BB	5619	CLA	CBB-CAB	3.40	1.53	1.28
24	AC	505	CLA	CMC-C2C	3.40	1.58	1.50
32	BB	5603	LMT	O5B-C1B	3.40	1.50	1.41
27	BC	5515	BCR	C29-C30	3.40	1.62	1.54
30	AA	416	SQD	O48-C23	3.41	1.43	1.33
24	BC	5512	CLA	C4C-NC	3.41	1.43	1.37
35	BD	5406	PL9	C38-C39	3.41	1.39	1.33
28	BA	5412	DGD	O2G-C1B	3.41	1.44	1.34
24	BA	5406	CLA	CBA-CGA	3.41	1.60	1.50
30	AB	622	SQD	O6-C1	3.41	1.46	1.40
24	AC	501	CLA	CBB-CAB	3.41	1.53	1.28
24	AC	509	CLA	O1D-CGD	3.42	1.29	1.21
30	AF	102	SQD	O5-C1	3.42	1.50	1.41
24	BA	5407	CLA	CBB-CAB	3.43	1.53	1.28
32	BB	5626	LMT	O1'-C1'	3.43	1.46	1.40
28	AA	411	DGD	O2G-C1B	3.43	1.44	1.34
24	BC	5506	CLA	O2A-CGA	3.43	1.43	1.33
24	AB	604	CLA	CBB-CAB	3.43	1.53	1.28
24	BC	5502	CLA	C4C-C3C	3.44	1.51	1.45
24	BB	5613	CLA	CBB-CAB	3.44	1.53	1.28
32	BC	5522	LMT	O5B-C1B	3.44	1.50	1.41
24	BB	5609	CLA	CBB-CAB	3.44	1.53	1.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BC	5502	CLA	C4C-NC	3.44	1.43	1.37
24	BA	5406	CLA	O2D-CGD	3.45	1.42	1.33
30	BA	5401	SQD	O7-S	3.46	1.56	1.45
24	BB	5605	CLA	CBB-CAB	3.46	1.53	1.28
24	AB	605	CLA	CBB-CAB	3.47	1.54	1.28
30	BB	5625	SQD	O7-S	3.47	1.56	1.45
30	AF	102	SQD	O7-S	3.47	1.56	1.45
24	BB	5618	CLA	CHC-C1C	3.47	1.46	1.35
34	AD	402	PHO	C1C-C2C	3.47	1.53	1.45
24	BC	5501	CLA	CBB-CAB	3.47	1.54	1.28
32	AB	629	LMT	O5B-C1B	3.48	1.50	1.41
24	BA	5405	CLA	C4C-NC	3.48	1.43	1.37
30	BB	5601	SQD	O47-C7	3.48	1.44	1.34
31	AJ	102	LMG	O1-C1	3.48	1.46	1.40
30	AF	102	SQD	O8-S	3.48	1.55	1.46
24	AB	611	CLA	C4C-C3C	3.48	1.51	1.45
24	AA	405	CLA	CBB-CAB	3.49	1.54	1.28
27	AB	618	BCR	C2-C1	3.49	1.62	1.54
27	BJ	5101	BCR	C10-C9	3.49	1.40	1.35
24	BB	5605	CLA	O2A-CGA	3.49	1.43	1.33
24	BA	5407	CLA	O2D-CGD	3.49	1.42	1.33
24	BB	5605	CLA	O1D-CGD	3.49	1.30	1.21
30	AB	627	SQD	O47-C7	3.49	1.44	1.34
24	AB	614	CLA	CHC-C1C	3.50	1.46	1.35
28	BC	5518	DGD	O5D-C1E	3.50	1.46	1.40
28	AC	518	DGD	O5D-C1E	3.51	1.46	1.40
27	AK	102	BCR	C29-C30	3.51	1.62	1.54
30	AA	413	SQD	O5-C5	3.51	1.53	1.44
24	BA	5407	CLA	O1D-CGD	3.51	1.30	1.21
30	AA	413	SQD	C1-C2	3.52	1.63	1.52
29	BA	5413	LHG	P-O6	3.52	1.75	1.59
27	AC	514	BCR	C26-C25	3.52	1.39	1.34
27	BB	5621	BCR	C5-C6	3.52	1.39	1.34
24	AD	404	CLA	CMC-C2C	3.52	1.58	1.50
24	BC	5503	CLA	C4C-NC	3.53	1.43	1.37
34	BD	5403	PHO	C1C-C2C	3.53	1.53	1.45
34	BD	5404	PHO	C1C-C2C	3.53	1.53	1.45
24	AB	601	CLA	CBB-CAB	3.53	1.54	1.28
36	BV	5201	HEM	C3C-CAC	3.54	1.58	1.51
24	AC	505	CLA	CBB-CAB	3.54	1.54	1.28
24	BC	5505	CLA	CMC-C2C	3.54	1.58	1.50
32	BI	5102	LMT	O5B-C1B	3.54	1.50	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	5617	CLA	C4C-C3C	3.54	1.51	1.45
24	BC	5505	CLA	CBB-CAB	3.54	1.54	1.28
28	BB	5602	DGD	O6D-C1D	3.55	1.50	1.41
27	AB	619	BCR	C5-C6	3.55	1.40	1.34
32	BM	5101	LMT	O5B-C1B	3.55	1.50	1.41
24	AB	601	CLA	C4C-NC	3.56	1.43	1.37
24	BA	5408	CLA	C4C-C3C	3.57	1.51	1.45
34	AD	403	PHO	C1C-C2C	3.57	1.53	1.45
27	BC	5516	BCR	C2-C1	3.57	1.62	1.54
28	AB	628	DGD	O6D-C1D	3.57	1.51	1.41
24	BB	5618	CLA	O2A-CGA	3.58	1.44	1.33
24	BB	5611	CLA	O2D-CGD	3.58	1.42	1.33
24	BA	5408	CLA	C1C-NC	3.58	1.43	1.37
27	BA	5411	BCR	C26-C25	3.58	1.40	1.34
29	BA	5413	LHG	O7-C7	3.58	1.45	1.34
32	BB	5604	LMT	O5B-C1B	3.59	1.51	1.41
24	AC	505	CLA	C4C-C3C	3.60	1.51	1.45
27	AB	618	BCR	C5-C6	3.60	1.40	1.34
24	AC	502	CLA	O2A-CGA	3.61	1.44	1.33
30	BA	5401	SQD	O48-C23	3.61	1.44	1.33
24	AB	607	CLA	C4C-C3C	3.61	1.51	1.45
24	BC	5506	CLA	C4C-NC	3.61	1.43	1.37
32	AD	409	LMT	O5B-C1B	3.62	1.51	1.41
27	BB	5622	BCR	C2-C1	3.63	1.62	1.54
28	BE	5102	DGD	O5D-C1E	3.63	1.46	1.40
24	AC	511	CLA	C4C-C3C	3.63	1.51	1.45
30	BA	5414	SQD	C1-C2	3.64	1.63	1.52
24	BA	5407	CLA	C4C-C3C	3.64	1.51	1.45
24	BC	5508	CLA	C4C-NC	3.65	1.43	1.37
24	AB	611	CLA	C4C-NC	3.65	1.43	1.37
30	AB	627	SQD	O48-C23	3.65	1.44	1.33
32	AI	102	LMT	O5B-C1B	3.66	1.51	1.41
30	BA	5401	SQD	C1-C2	3.66	1.63	1.52
28	BC	5519	DGD	C3E-C2E	3.66	1.62	1.52
24	BB	5607	CLA	C4C-C3C	3.67	1.51	1.45
24	AB	614	CLA	O2A-CGA	3.67	1.44	1.33
24	AC	506	CLA	C4C-NC	3.68	1.43	1.37
32	AB	623	LMT	O1'-C1'	3.68	1.46	1.40
27	AC	516	BCR	C1-C6	3.69	1.59	1.53
24	AC	501	CLA	C4C-C3C	3.69	1.51	1.45
24	AB	601	CLA	O1D-CGD	3.69	1.30	1.21
24	AB	604	CLA	O2D-CGD	3.69	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	AC	515	BCR	C5-C6	3.69	1.40	1.34
24	BB	5608	CLA	C4C-C3C	3.70	1.51	1.45
24	BB	5612	CLA	O2D-CGD	3.70	1.42	1.33
29	AA	412	LHG	O8-C23	3.70	1.44	1.33
24	AB	613	CLA	O2D-CGD	3.71	1.42	1.33
30	AA	416	SQD	C1-C2	3.71	1.63	1.52
28	AC	517	DGD	O5D-C1E	3.72	1.46	1.40
24	BD	5402	CLA	C1C-NC	3.72	1.44	1.37
30	BA	5414	SQD	C6-S	3.72	1.83	1.77
30	AB	627	SQD	O7-S	3.73	1.56	1.45
27	BD	5407	BCR	C29-C30	3.74	1.63	1.54
30	BF	5102	SQD	O6-C1	3.75	1.46	1.40
27	BX	5101	BCR	C29-C30	3.75	1.63	1.54
24	AC	509	CLA	C4C-C3C	3.75	1.51	1.45
24	AA	406	CLA	C4C-C3C	3.76	1.51	1.45
30	BA	5401	SQD	O8-S	3.77	1.56	1.46
30	BB	5625	SQD	O48-C23	3.78	1.44	1.33
32	BB	5626	LMT	O5B-C1B	3.78	1.51	1.41
24	AB	607	CLA	O2D-CGD	3.78	1.42	1.33
24	AB	612	CLA	C4C-C3C	3.79	1.51	1.45
28	AB	628	DGD	O3G-C1D	3.79	1.47	1.40
24	BC	5511	CLA	C4C-C3C	3.79	1.51	1.45
30	AB	622	SQD	O7-S	3.80	1.57	1.45
27	AJ	101	BCR	C10-C9	3.80	1.40	1.35
24	AB	603	CLA	C4C-C3C	3.81	1.51	1.45
24	AB	609	CLA	C4C-C3C	3.82	1.51	1.45
28	BA	5412	DGD	O6E-C1E	3.82	1.51	1.41
36	AF	101	HEM	C1C-NC	3.83	1.40	1.36
30	BA	5414	SQD	O7-S	3.83	1.57	1.45
24	AB	612	CLA	O2D-CGD	3.83	1.43	1.33
24	AB	608	CLA	O2D-CGD	3.83	1.43	1.33
30	BB	5601	SQD	O7-S	3.83	1.57	1.45
28	AB	628	DGD	O5D-C1E	3.84	1.47	1.40
29	AA	415	LHG	O7-C7	3.84	1.45	1.34
30	AF	102	SQD	O6-C1	3.84	1.47	1.40
27	BJ	5101	BCR	C29-C30	3.84	1.63	1.54
28	AE	101	DGD	O5D-C1E	3.85	1.47	1.40
27	AB	617	BCR	C5-C6	3.85	1.40	1.34
30	BA	5414	SQD	O5-C5	3.85	1.54	1.44
30	BF	5102	SQD	O48-C23	3.86	1.44	1.33
27	AA	410	BCR	C26-C25	3.86	1.40	1.34
27	BC	5516	BCR	C30-C25	3.86	1.59	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	5614	CLA	O2D-CGD	3.87	1.43	1.33
28	AH	101	DGD	O5D-C1E	3.87	1.47	1.40
24	BB	5611	CLA	C4C-C3C	3.87	1.52	1.45
24	AA	405	CLA	O2D-CGD	3.87	1.43	1.33
24	BC	5510	CLA	C4C-C3C	3.88	1.52	1.45
30	BF	5102	SQD	C6-S	3.88	1.83	1.77
30	BB	5625	SQD	C6-S	3.88	1.83	1.77
29	BA	5415	LHG	O7-C7	3.89	1.45	1.34
24	BD	5405	CLA	C4C-C3C	3.89	1.52	1.45
24	AC	505	CLA	O2D-CGD	3.89	1.43	1.33
24	BB	5615	CLA	C4C-NC	3.90	1.44	1.37
27	BK	5102	BCR	C1-C6	3.90	1.59	1.53
30	AB	622	SQD	C6-S	3.90	1.83	1.77
30	AB	627	SQD	C6-S	3.90	1.83	1.77
24	BC	5506	CLA	C4C-C3C	3.90	1.52	1.45
27	AX	101	BCR	C29-C30	3.90	1.63	1.54
24	AC	503	CLA	C4C-C3C	3.91	1.52	1.45
30	AB	627	SQD	C1-C2	3.92	1.64	1.52
27	AC	515	BCR	C1-C6	3.92	1.59	1.53
24	AB	615	CLA	C4C-C3C	3.92	1.52	1.45
36	AV	201	HEM	CBB-CAB	3.92	1.51	1.29
24	BC	5505	CLA	O2A-CGA	3.92	1.45	1.33
24	BB	5613	CLA	C4C-C3C	3.93	1.52	1.45
32	AB	630	LMT	O5B-C1B	3.93	1.51	1.41
24	AB	604	CLA	C4C-C3C	3.93	1.52	1.45
24	BC	5504	CLA	C4C-C3C	3.93	1.52	1.45
24	AB	616	CLA	C4C-C3C	3.93	1.52	1.45
24	AD	401	CLA	O2D-CGD	3.93	1.43	1.33
30	AF	102	SQD	C6-S	3.94	1.83	1.77
30	AA	416	SQD	O8-S	3.95	1.56	1.46
34	BD	5404	PHO	C4C-C3C	3.95	1.52	1.45
30	AB	622	SQD	C1-C2	3.96	1.64	1.52
24	BB	5617	CLA	O2D-CGD	3.96	1.43	1.33
30	AB	627	SQD	O5-C5	3.96	1.54	1.44
28	AE	101	DGD	O3G-C1D	3.96	1.47	1.40
24	AD	404	CLA	O2D-CGD	3.96	1.43	1.33
24	AC	504	CLA	O2D-CGD	3.96	1.43	1.33
27	AT	101	BCR	C30-C25	3.97	1.59	1.53
30	BB	5601	SQD	C1-C2	3.97	1.64	1.52
27	AJ	101	BCR	C29-C30	3.97	1.63	1.54
24	BC	5509	CLA	C4C-C3C	3.98	1.52	1.45
30	BF	5102	SQD	C1-C2	3.99	1.64	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	AA	412	LHG	P-O6	3.99	1.77	1.59
24	AC	503	CLA	O2D-CGD	4.00	1.43	1.33
30	AB	622	SQD	O48-C23	4.00	1.45	1.33
32	AB	623	LMT	O5B-C1B	4.00	1.52	1.41
28	BH	5101	DGD	O5D-C1E	4.00	1.47	1.40
30	AF	102	SQD	O47-C7	4.00	1.46	1.34
36	AV	201	HEM	C1C-NC	4.01	1.41	1.36
24	BC	5503	CLA	C4C-C3C	4.01	1.52	1.45
30	AA	416	SQD	O47-C7	4.01	1.46	1.34
24	AD	401	CLA	C4C-C3C	4.01	1.52	1.45
27	BB	5621	BCR	C26-C25	4.02	1.40	1.34
28	AA	411	DGD	O6E-C1E	4.02	1.52	1.41
27	AC	516	BCR	C5-C6	4.05	1.40	1.34
24	BB	5605	CLA	C4C-C3C	4.05	1.52	1.45
24	BC	5501	CLA	C4C-C3C	4.05	1.52	1.45
24	AD	404	CLA	C4C-C3C	4.05	1.52	1.45
30	AF	102	SQD	O48-C23	4.06	1.45	1.33
24	AC	505	CLA	O2A-CGA	4.06	1.45	1.33
30	BB	5601	SQD	C6-S	4.06	1.84	1.77
30	BB	5625	SQD	C1-C2	4.06	1.64	1.52
30	AB	622	SQD	O47-C7	4.06	1.46	1.34
36	AF	101	HEM	CBC-CAC	4.09	1.52	1.29
24	BB	5620	CLA	C4C-C3C	4.09	1.52	1.45
34	AD	402	PHO	O2D-CGD	4.09	1.43	1.33
30	BF	5102	SQD	O8-S	4.09	1.57	1.46
24	AC	513	CLA	C4C-C3C	4.10	1.52	1.45
27	AK	102	BCR	C26-C25	4.11	1.40	1.34
24	AB	615	CLA	O2D-CGD	4.12	1.43	1.33
24	AA	404	CLA	C4C-C3C	4.12	1.52	1.45
30	BB	5601	SQD	O5-C5	4.12	1.54	1.44
24	AC	501	CLA	O2D-CGD	4.13	1.43	1.33
34	BD	5403	PHO	C4C-C3C	4.14	1.52	1.45
30	AA	416	SQD	O5-C5	4.14	1.54	1.44
27	AA	410	BCR	C30-C25	4.14	1.59	1.53
24	AC	506	CLA	C4C-C3C	4.15	1.52	1.45
24	BA	5408	CLA	O2D-CGD	4.15	1.43	1.33
29	BA	5415	LHG	O8-C23	4.15	1.45	1.33
24	BB	5607	CLA	O2A-CGA	4.15	1.45	1.33
24	BB	5616	CLA	O2D-CGD	4.15	1.43	1.33
27	AB	617	BCR	C26-C25	4.16	1.41	1.34
24	BB	5606	CLA	C4C-C3C	4.16	1.52	1.45
27	BK	5102	BCR	C26-C25	4.16	1.41	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AA	407	CLA	O2D-CGD	4.16	1.43	1.33
30	AB	622	SQD	O5-C5	4.17	1.54	1.44
24	AB	614	CLA	C4C-C3C	4.17	1.52	1.45
24	BB	5619	CLA	O2D-CGD	4.17	1.43	1.33
30	BB	5625	SQD	O5-C5	4.17	1.54	1.44
24	AB	613	CLA	C4C-C3C	4.18	1.52	1.45
29	AA	415	LHG	O8-C23	4.18	1.45	1.33
24	AB	603	CLA	O2D-CGD	4.19	1.43	1.33
30	AA	413	SQD	O47-C7	4.19	1.46	1.34
36	BV	5201	HEM	CBB-CAB	4.19	1.53	1.29
30	AB	627	SQD	O8-S	4.20	1.57	1.46
30	BA	5414	SQD	O8-S	4.20	1.57	1.46
36	AF	101	HEM	CBB-CAB	4.20	1.53	1.29
24	AC	511	CLA	O2D-CGD	4.20	1.43	1.33
30	AA	413	SQD	O8-S	4.20	1.57	1.46
36	BF	5101	HEM	C4C-NC	4.21	1.41	1.36
24	BB	5608	CLA	O2D-CGD	4.21	1.43	1.33
36	BV	5201	HEM	C1C-NC	4.23	1.41	1.36
27	AD	406	BCR	C30-C25	4.23	1.59	1.53
24	AC	512	CLA	O2D-CGD	4.23	1.44	1.33
27	BX	5101	BCR	C1-C6	4.24	1.59	1.53
27	BT	5101	BCR	C30-C25	4.24	1.59	1.53
36	BF	5101	HEM	CBC-CAC	4.24	1.53	1.29
30	BA	5401	SQD	O47-C7	4.24	1.47	1.34
24	BC	5513	CLA	C4C-C3C	4.26	1.52	1.45
27	AT	101	BCR	C5-C6	4.26	1.41	1.34
24	AB	611	CLA	O2D-CGD	4.26	1.44	1.33
24	AC	510	CLA	C4C-C3C	4.26	1.52	1.45
24	BB	5618	CLA	C4C-C3C	4.27	1.52	1.45
30	AF	102	SQD	C1-C2	4.27	1.65	1.52
36	BF	5101	HEM	CBB-CAB	4.27	1.53	1.29
24	BC	5503	CLA	O2D-CGD	4.27	1.44	1.33
24	AB	606	CLA	C4C-C3C	4.28	1.52	1.45
24	AB	602	CLA	O2D-CGD	4.28	1.44	1.33
24	AC	512	CLA	C4C-C3C	4.28	1.52	1.45
24	BB	5620	CLA	C1C-C2C	4.29	1.53	1.44
27	BB	5622	BCR	C26-C25	4.29	1.41	1.34
24	AC	510	CLA	O2D-CGD	4.29	1.44	1.33
24	AC	507	CLA	O2D-CGD	4.29	1.44	1.33
24	BC	5512	CLA	O2D-CGD	4.29	1.44	1.33
27	AC	514	BCR	C1-C6	4.29	1.59	1.53
24	BC	5507	CLA	C4C-C3C	4.29	1.52	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	502	CLA	C1C-C2C	4.29	1.53	1.44
27	BJ	5101	BCR	C14-C13	4.29	1.41	1.35
24	BC	5505	CLA	O2D-CGD	4.30	1.44	1.33
28	AC	517	DGD	O6D-C1D	4.30	1.52	1.41
24	BB	5610	CLA	C4C-C3C	4.30	1.52	1.45
24	AB	601	CLA	C4C-C3C	4.30	1.52	1.45
34	AD	403	PHO	C4C-C3C	4.31	1.53	1.45
24	BB	5610	CLA	C1C-C2C	4.31	1.53	1.44
24	BB	5615	CLA	C1C-C2C	4.31	1.53	1.44
24	AB	606	CLA	C1C-C2C	4.32	1.53	1.44
30	BA	5414	SQD	O47-C7	4.32	1.47	1.34
30	BB	5601	SQD	O8-S	4.33	1.57	1.46
24	BD	5402	CLA	O2D-CGD	4.33	1.44	1.33
24	BB	5605	CLA	C1C-C2C	4.33	1.53	1.44
29	AA	412	LHG	P-O3	4.33	1.78	1.59
30	BF	5102	SQD	O47-C7	4.33	1.47	1.34
27	BC	5515	BCR	C5-C6	4.33	1.41	1.34
24	AC	504	CLA	C1C-C2C	4.33	1.53	1.44
24	BC	5501	CLA	C1C-C2C	4.33	1.53	1.44
24	BD	5405	CLA	C1C-C2C	4.34	1.53	1.44
36	BV	5201	HEM	CBC-CAC	4.34	1.54	1.29
24	BB	5619	CLA	C1C-C2C	4.34	1.53	1.44
24	BB	5606	CLA	O2D-CGD	4.34	1.44	1.33
28	AA	411	DGD	O6D-C1D	4.34	1.53	1.41
36	AV	201	HEM	CBC-CAC	4.34	1.54	1.29
24	BB	5609	CLA	C1C-C2C	4.35	1.53	1.44
24	BB	5614	CLA	C1C-C2C	4.35	1.53	1.44
24	AC	501	CLA	C1C-C2C	4.35	1.53	1.44
24	AC	512	CLA	C1C-C2C	4.35	1.53	1.44
24	BB	5606	CLA	C1C-C2C	4.35	1.53	1.44
24	BB	5608	CLA	C1C-C2C	4.35	1.53	1.44
27	AK	102	BCR	C5-C6	4.35	1.41	1.34
24	BA	5407	CLA	C1C-C2C	4.35	1.53	1.44
24	AB	603	CLA	O2A-CGA	4.35	1.46	1.33
24	BC	5504	CLA	O2D-CGD	4.36	1.44	1.33
24	AB	615	CLA	C1C-C2C	4.36	1.53	1.44
24	BB	5617	CLA	C1C-C2C	4.36	1.53	1.44
24	BC	5512	CLA	C1C-C2C	4.36	1.53	1.44
24	AB	616	CLA	C1C-C2C	4.36	1.53	1.44
24	AB	610	CLA	C1C-C2C	4.36	1.53	1.44
24	AB	601	CLA	C1C-C2C	4.37	1.53	1.44
24	BC	5503	CLA	C1C-C2C	4.37	1.53	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	507	CLA	C1C-C2C	4.37	1.53	1.44
24	AB	612	CLA	C1C-C2C	4.37	1.53	1.44
24	BC	5509	CLA	C1C-C2C	4.37	1.53	1.44
27	AC	515	BCR	C26-C25	4.37	1.41	1.34
24	AC	510	CLA	C1C-C2C	4.37	1.53	1.44
24	BC	5507	CLA	C1C-C2C	4.37	1.53	1.44
24	BB	5607	CLA	C1C-C2C	4.37	1.53	1.44
24	AB	609	CLA	C1C-C2C	4.38	1.53	1.44
24	AC	508	CLA	C1C-C2C	4.38	1.53	1.44
24	BB	5612	CLA	C1C-C2C	4.38	1.53	1.44
24	AB	611	CLA	C1C-C2C	4.38	1.53	1.44
27	BA	5411	BCR	C30-C25	4.38	1.60	1.53
24	AB	602	CLA	C1C-C2C	4.38	1.53	1.44
24	BC	5502	CLA	C1C-C2C	4.38	1.53	1.44
24	BB	5616	CLA	C1C-C2C	4.38	1.53	1.44
24	AB	603	CLA	C1C-C2C	4.38	1.53	1.44
24	AA	406	CLA	C1C-C2C	4.38	1.53	1.44
24	AB	613	CLA	C1C-C2C	4.38	1.53	1.44
24	BB	5613	CLA	C1C-C2C	4.38	1.53	1.44
24	BB	5616	CLA	C4C-C3C	4.38	1.52	1.45
24	AC	503	CLA	C1C-C2C	4.39	1.53	1.44
24	AD	404	CLA	C1C-C2C	4.39	1.53	1.44
34	BD	5404	PHO	O2D-CGD	4.39	1.44	1.33
30	AF	102	SQD	O5-C5	4.39	1.55	1.44
24	BC	5508	CLA	C1C-C2C	4.39	1.53	1.44
24	AB	605	CLA	C1C-C2C	4.39	1.53	1.44
27	BB	5623	BCR	C30-C25	4.39	1.60	1.53
36	AF	101	HEM	C4C-NC	4.39	1.41	1.36
24	AC	511	CLA	C1C-C2C	4.39	1.53	1.44
30	BA	5401	SQD	O5-C5	4.40	1.55	1.44
24	AA	404	CLA	C1C-C2C	4.40	1.53	1.44
24	AA	407	CLA	C1C-C2C	4.40	1.53	1.44
24	BD	5402	CLA	C4C-C3C	4.40	1.53	1.45
24	BC	5504	CLA	C1C-C2C	4.40	1.53	1.44
24	AB	602	CLA	C4C-C3C	4.40	1.53	1.45
24	AB	607	CLA	C1C-C2C	4.40	1.53	1.44
24	AB	608	CLA	C1C-C2C	4.41	1.53	1.44
24	AC	509	CLA	C1C-C2C	4.41	1.53	1.44
24	BB	5611	CLA	C1C-C2C	4.41	1.53	1.44
24	AC	502	CLA	O2D-CGD	4.41	1.44	1.33
27	BC	5515	BCR	C26-C25	4.41	1.41	1.34
36	AV	201	HEM	C4C-NC	4.42	1.41	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	513	CLA	C1C-C2C	4.42	1.53	1.44
24	BA	5405	CLA	C4C-C3C	4.42	1.53	1.45
24	BC	5511	CLA	C1C-C2C	4.42	1.53	1.44
24	AB	610	CLA	C4C-C3C	4.42	1.53	1.45
24	AB	604	CLA	C1C-C2C	4.42	1.53	1.44
30	BF	5102	SQD	O5-C5	4.42	1.55	1.44
24	BC	5510	CLA	C1C-C2C	4.43	1.53	1.44
24	BC	5505	CLA	C1C-C2C	4.43	1.53	1.44
24	AA	405	CLA	C1C-C2C	4.43	1.53	1.44
24	AC	506	CLA	C1C-C2C	4.44	1.53	1.44
24	BC	5506	CLA	C1C-C2C	4.44	1.53	1.44
29	BA	5413	LHG	P-O3	4.45	1.79	1.59
24	BA	5408	CLA	C1C-C2C	4.45	1.53	1.44
28	BE	5102	DGD	O3G-C1D	4.45	1.48	1.40
24	AB	614	CLA	C1C-C2C	4.45	1.53	1.44
24	BC	5513	CLA	C1C-C2C	4.45	1.53	1.44
28	AC	518	DGD	O6D-C1D	4.46	1.53	1.41
24	BA	5406	CLA	C1C-C2C	4.46	1.53	1.44
30	BB	5625	SQD	O47-C7	4.46	1.47	1.34
24	BB	5618	CLA	C1C-C2C	4.47	1.53	1.44
24	BA	5405	CLA	C1C-C2C	4.47	1.53	1.44
24	AC	505	CLA	C1C-C2C	4.48	1.53	1.44
30	BB	5625	SQD	O8-S	4.49	1.58	1.46
27	BJ	5101	BCR	C26-C25	4.49	1.41	1.34
24	BC	5512	CLA	C4C-C3C	4.49	1.53	1.45
24	AC	508	CLA	O2D-CGD	4.49	1.44	1.33
24	BA	5405	CLA	O2D-CGD	4.49	1.44	1.33
24	AD	401	CLA	C1C-C2C	4.50	1.53	1.44
27	AJ	101	BCR	C26-C25	4.50	1.41	1.34
34	AD	403	PHO	O2D-CGD	4.51	1.44	1.33
34	AD	403	PHO	CBB-CAB	4.53	1.52	1.30
24	BD	5402	CLA	C1C-C2C	4.53	1.53	1.44
24	BD	5405	CLA	O2D-CGD	4.54	1.44	1.33
34	AD	402	PHO	CBB-CAB	4.55	1.52	1.30
34	BD	5403	PHO	CBB-CAB	4.55	1.52	1.30
24	BC	5511	CLA	O2D-CGD	4.57	1.44	1.33
27	AX	101	BCR	C1-C6	4.57	1.60	1.53
24	BC	5509	CLA	O2D-CGD	4.58	1.44	1.33
24	BC	5510	CLA	O2D-CGD	4.59	1.44	1.33
24	BB	5610	CLA	O2D-CGD	4.59	1.44	1.33
24	BB	5614	CLA	C4C-C3C	4.59	1.53	1.45
24	BC	5502	CLA	O2D-CGD	4.62	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	BC	5517	DGD	O6D-C1D	4.62	1.53	1.41
30	AB	622	SQD	O8-S	4.63	1.58	1.46
24	AB	614	CLA	O2D-CGD	4.64	1.45	1.33
24	BB	5615	CLA	O2D-CGD	4.65	1.45	1.33
34	BD	5404	PHO	CBB-CAB	4.65	1.53	1.30
27	AA	410	BCR	C1-C6	4.66	1.60	1.53
24	AB	603	CLA	C3B-C2B	4.67	1.46	1.40
28	BC	5518	DGD	O6D-C1D	4.67	1.53	1.41
36	BF	5101	HEM	C1C-NC	4.67	1.41	1.36
24	AB	608	CLA	O2A-CGA	4.70	1.47	1.33
24	BB	5613	CLA	O2D-CGD	4.71	1.45	1.33
24	BB	5607	CLA	O2D-CGD	4.71	1.45	1.33
24	BC	5501	CLA	O2D-CGD	4.72	1.45	1.33
24	BB	5612	CLA	O2A-CGA	4.73	1.47	1.33
27	AT	101	BCR	C1-C6	4.73	1.60	1.53
24	AB	616	CLA	O2D-CGD	4.73	1.45	1.33
24	AC	507	CLA	C4C-C3C	4.74	1.53	1.45
28	BC	5517	DGD	O5D-C1E	4.75	1.48	1.40
24	AB	609	CLA	O2D-CGD	4.77	1.45	1.33
27	BC	5516	BCR	C5-C6	4.78	1.42	1.34
24	AB	610	CLA	O2D-CGD	4.78	1.45	1.33
27	AJ	101	BCR	C14-C13	4.78	1.42	1.35
28	BB	5602	DGD	O5D-C1E	4.78	1.48	1.40
34	BD	5403	PHO	O2D-CGD	4.79	1.45	1.33
28	BC	5519	DGD	O6D-C1D	4.79	1.54	1.41
27	AD	406	BCR	C26-C25	4.80	1.42	1.34
27	BC	5516	BCR	C1-C6	4.80	1.60	1.53
24	BB	5611	CLA	C3C-C2C	4.81	1.47	1.36
24	AA	404	CLA	O2D-CGD	4.82	1.45	1.33
27	AX	101	BCR	C30-C25	4.83	1.60	1.53
24	AB	606	CLA	O2D-CGD	4.84	1.45	1.33
27	BJ	5101	BCR	C1-C6	4.84	1.60	1.53
24	BC	5507	CLA	O2D-CGD	4.85	1.45	1.33
24	BB	5620	CLA	O2D-CGD	4.87	1.45	1.33
24	BB	5609	CLA	O2D-CGD	4.88	1.45	1.33
28	AC	519	DGD	O6D-C1D	4.88	1.54	1.41
27	BB	5623	BCR	C1-C6	4.89	1.60	1.53
27	BT	5101	BCR	C5-C6	4.89	1.42	1.34
27	BB	5622	BCR	C30-C25	4.90	1.60	1.53
24	BB	5618	CLA	O2D-CGD	4.91	1.45	1.33
24	BB	5607	CLA	C3B-C2B	4.91	1.46	1.40
27	AB	618	BCR	C30-C25	4.91	1.60	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	AB	618	BCR	C26-C25	4.94	1.42	1.34
28	BA	5412	DGD	O6D-C1D	4.97	1.54	1.41
27	AC	514	BCR	C30-C25	4.98	1.60	1.53
24	AC	513	CLA	O2D-CGD	5.03	1.46	1.33
27	BK	5102	BCR	C5-C6	5.03	1.42	1.34
24	AC	509	CLA	O2D-CGD	5.04	1.46	1.33
24	AC	506	CLA	O2D-CGD	5.04	1.46	1.33
27	BD	5407	BCR	C26-C25	5.05	1.42	1.34
27	BX	5101	BCR	C30-C25	5.07	1.61	1.53
27	BC	5515	BCR	C1-C6	5.09	1.61	1.53
24	BC	5506	CLA	O2D-CGD	5.10	1.46	1.33
27	AJ	101	BCR	C1-C6	5.13	1.61	1.53
27	BA	5411	BCR	C1-C6	5.14	1.61	1.53
24	AA	405	CLA	C3C-C2C	5.17	1.47	1.36
24	AB	607	CLA	C3B-C2B	5.19	1.47	1.40
24	BB	5617	CLA	C3B-C2B	5.21	1.47	1.40
24	AB	616	CLA	C3C-C2C	5.21	1.48	1.36
31	AB	620	LMG	O1-C1	5.23	1.49	1.40
24	BB	5609	CLA	C3C-C2C	5.24	1.48	1.36
27	AC	515	BCR	C30-C25	5.24	1.61	1.53
24	BC	5513	CLA	O2D-CGD	5.25	1.46	1.33
24	AB	605	CLA	O2D-CGD	5.26	1.46	1.33
24	BC	5507	CLA	C3C-C2C	5.26	1.48	1.36
27	AB	619	BCR	C1-C6	5.28	1.61	1.53
27	BD	5407	BCR	C30-C25	5.29	1.61	1.53
27	AK	102	BCR	C30-C25	5.32	1.61	1.53
24	AC	507	CLA	C3C-C2C	5.32	1.48	1.36
27	BC	5515	BCR	C30-C25	5.33	1.61	1.53
27	AX	101	BCR	C26-C25	5.35	1.42	1.34
24	AB	611	CLA	C3C-C2C	5.36	1.48	1.36
27	BT	5101	BCR	C1-C6	5.37	1.61	1.53
27	AB	618	BCR	C1-C6	5.41	1.61	1.53
31	BL	5101	LMG	O1-C1	5.41	1.49	1.40
27	BC	5514	BCR	C30-C25	5.41	1.61	1.53
27	BX	5101	BCR	C26-C25	5.42	1.43	1.34
24	AC	502	CLA	C3C-C2C	5.44	1.48	1.36
24	BB	5605	CLA	O2D-CGD	5.46	1.47	1.33
24	AB	605	CLA	C3C-C2C	5.47	1.48	1.36
24	BB	5613	CLA	C3C-C2C	5.48	1.48	1.36
24	BB	5620	CLA	C3C-C2C	5.49	1.48	1.36
24	BC	5508	CLA	O2D-CGD	5.49	1.47	1.33
24	AA	406	CLA	C3C-C2C	5.50	1.48	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	613	CLA	C3C-C2C	5.54	1.48	1.36
24	BB	5617	CLA	C3C-C2C	5.56	1.48	1.36
27	BK	5102	BCR	C30-C25	5.56	1.61	1.53
27	BB	5622	BCR	C1-C6	5.56	1.61	1.53
24	AC	510	CLA	C3C-C2C	5.57	1.48	1.36
27	AB	619	BCR	C30-C25	5.62	1.61	1.53
24	BB	5615	CLA	C3C-C2C	5.67	1.49	1.36
27	AJ	101	BCR	C5-C6	5.68	1.43	1.34
24	BB	5619	CLA	C3C-C2C	5.68	1.49	1.36
24	AB	601	CLA	O2D-CGD	5.68	1.47	1.33
28	AA	411	DGD	O5D-C1E	5.71	1.50	1.40
24	AB	609	CLA	C3C-C2C	5.72	1.49	1.36
27	BC	5514	BCR	C1-C6	5.72	1.61	1.53
24	AB	607	CLA	C3C-C2C	5.74	1.49	1.36
34	BD	5403	PHO	C3C-C2C	5.74	1.49	1.36
24	BC	5508	CLA	C3C-C2C	5.75	1.49	1.36
24	AB	613	CLA	C3B-C2B	5.77	1.47	1.40
24	BB	5608	CLA	C3C-C2C	5.80	1.49	1.36
27	BJ	5101	BCR	C5-C6	5.80	1.43	1.34
24	BA	5406	CLA	C3C-C2C	5.82	1.49	1.36
24	AC	501	CLA	C3C-C2C	5.83	1.49	1.36
24	AB	614	CLA	C3C-C2C	5.85	1.49	1.36
24	AC	508	CLA	C3C-C2C	5.85	1.49	1.36
28	BA	5412	DGD	O5D-C1E	5.89	1.50	1.40
24	AC	503	CLA	C3C-C2C	5.90	1.49	1.36
24	AB	606	CLA	C3C-C2C	5.91	1.49	1.36
24	AC	506	CLA	C3C-C2C	5.93	1.49	1.36
24	AC	509	CLA	C3C-C2C	5.93	1.49	1.36
24	BC	5503	CLA	C3C-C2C	5.94	1.49	1.36
24	AB	602	CLA	C3C-C2C	5.95	1.49	1.36
24	BC	5510	CLA	C3C-C2C	5.95	1.49	1.36
34	AD	402	PHO	C3C-C2C	5.96	1.49	1.36
24	AC	512	CLA	C3C-C2C	6.04	1.49	1.36
24	AD	401	CLA	C3C-C2C	6.05	1.49	1.36
24	BB	5606	CLA	C3C-C2C	6.06	1.49	1.36
24	AB	610	CLA	C3C-C2C	6.12	1.50	1.36
24	BC	5501	CLA	C3C-C2C	6.12	1.50	1.36
24	BB	5610	CLA	C3C-C2C	6.12	1.50	1.36
24	BB	5614	CLA	C3C-C2C	6.13	1.50	1.36
24	BA	5407	CLA	C3C-C2C	6.13	1.50	1.36
34	AD	403	PHO	C3C-C2C	6.14	1.50	1.36
24	AA	407	CLA	C3C-C2C	6.14	1.50	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BD	5402	CLA	C3C-C2C	6.15	1.50	1.36
24	AB	612	CLA	C3C-C2C	6.16	1.50	1.36
24	AB	608	CLA	C3C-C2C	6.17	1.50	1.36
24	AC	504	CLA	C3C-C2C	6.19	1.50	1.36
24	BC	5506	CLA	C3C-C2C	6.19	1.50	1.36
24	BB	5618	CLA	C3C-C2C	6.19	1.50	1.36
24	AB	615	CLA	C3C-C2C	6.21	1.50	1.36
24	BB	5607	CLA	C3C-C2C	6.24	1.50	1.36
24	AC	505	CLA	C3C-C2C	6.31	1.50	1.36
24	BC	5505	CLA	C3C-C2C	6.34	1.50	1.36
34	AD	402	PHO	C3B-C2B	6.34	1.50	1.36
24	BB	5616	CLA	C3C-C2C	6.36	1.50	1.36
24	BC	5502	CLA	C3C-C2C	6.37	1.50	1.36
24	BB	5612	CLA	C3C-C2C	6.37	1.50	1.36
24	AA	404	CLA	C3C-C2C	6.38	1.50	1.36
24	BA	5408	CLA	C3C-C2C	6.39	1.50	1.36
24	BC	5512	CLA	C3C-C2C	6.40	1.50	1.36
24	BA	5405	CLA	C3C-C2C	6.41	1.50	1.36
24	AC	511	CLA	C3C-C2C	6.48	1.50	1.36
24	BC	5509	CLA	C3C-C2C	6.48	1.50	1.36
24	BB	5611	CLA	C3B-C2B	6.49	1.48	1.40
24	AB	604	CLA	C3C-C2C	6.51	1.50	1.36
27	BJ	5101	BCR	C30-C25	6.53	1.63	1.53
24	AB	606	CLA	C3B-C2B	6.53	1.48	1.40
24	BD	5405	CLA	C3C-C2C	6.57	1.50	1.36
24	AC	513	CLA	C3C-C2C	6.59	1.51	1.36
34	BD	5404	PHO	C3C-C2C	6.61	1.51	1.36
24	BC	5511	CLA	C3C-C2C	6.67	1.51	1.36
34	AD	403	PHO	C3B-C2B	6.68	1.50	1.36
24	AB	603	CLA	C3C-C2C	6.69	1.51	1.36
24	BC	5513	CLA	C3C-C2C	6.71	1.51	1.36
24	AA	405	CLA	C3B-C2B	6.72	1.49	1.40
24	AC	507	CLA	C3B-C2B	6.78	1.49	1.40
24	BC	5504	CLA	C3C-C2C	6.80	1.51	1.36
24	AD	404	CLA	C3C-C2C	6.81	1.51	1.36
35	AD	405	PL9	O2-C1	6.83	1.43	1.24
35	BD	5406	PL9	O2-C1	6.86	1.43	1.24
24	BB	5612	CLA	C3B-C2B	6.88	1.49	1.40
27	AJ	101	BCR	C30-C25	6.89	1.63	1.53
24	AC	508	CLA	C3B-C2B	6.91	1.49	1.40
24	BB	5605	CLA	C3C-C2C	6.94	1.51	1.36
30	AA	413	SQD	C4-C3	6.97	1.70	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	BD	5403	PHO	C3B-C2B	6.98	1.51	1.36
24	AB	601	CLA	C3C-C2C	7.01	1.51	1.36
24	AB	602	CLA	C3B-C2B	7.01	1.49	1.40
24	AD	401	CLA	C3B-C2B	7.10	1.49	1.40
24	BC	5504	CLA	C3B-C2B	7.13	1.49	1.40
24	AA	404	CLA	C3B-C2B	7.17	1.49	1.40
24	AC	504	CLA	C3B-C2B	7.18	1.49	1.40
30	AF	102	SQD	C4-C3	7.19	1.71	1.52
24	AA	407	CLA	C3B-C2B	7.25	1.49	1.40
24	AC	502	CLA	C3B-C2B	7.25	1.49	1.40
24	BC	5508	CLA	C3B-C2B	7.27	1.49	1.40
24	BB	5610	CLA	C3B-C2B	7.32	1.50	1.40
24	BB	5606	CLA	C3B-C2B	7.33	1.50	1.40
30	BF	5102	SQD	C4-C3	7.33	1.71	1.52
24	AC	509	CLA	C3B-C2B	7.35	1.50	1.40
34	BD	5404	PHO	C3B-C2B	7.36	1.52	1.36
24	BA	5408	CLA	C3B-C2B	7.37	1.50	1.40
24	BB	5616	CLA	C3B-C2B	7.39	1.50	1.40
35	AD	405	PL9	C48-C49	7.40	1.55	1.32
24	BD	5402	CLA	C3B-C2B	7.44	1.50	1.40
24	AB	611	CLA	C3B-C2B	7.46	1.50	1.40
24	AB	608	CLA	C3B-C2B	7.46	1.50	1.40
30	AA	416	SQD	C4-C3	7.47	1.72	1.52
24	AB	612	CLA	C3B-C2B	7.49	1.50	1.40
30	BB	5601	SQD	C4-C3	7.51	1.72	1.52
24	BB	5620	CLA	C3B-C2B	7.51	1.50	1.40
24	BA	5405	CLA	C3B-C2B	7.52	1.50	1.40
24	AC	501	CLA	C3B-C2B	7.57	1.50	1.40
30	BA	5414	SQD	C4-C3	7.57	1.72	1.52
35	BD	5406	PL9	C48-C49	7.59	1.55	1.32
24	BD	5405	CLA	C3B-C2B	7.61	1.50	1.40
24	BB	5608	CLA	C3B-C2B	7.64	1.50	1.40
29	BA	5413	LHG	P-O5	7.66	1.79	1.51
24	AD	404	CLA	C3B-C2B	7.66	1.50	1.40
30	BA	5401	SQD	C4-C3	7.66	1.72	1.52
24	AB	610	CLA	C3B-C2B	7.68	1.50	1.40
24	BC	5507	CLA	C3B-C2B	7.69	1.50	1.40
24	BB	5615	CLA	C3B-C2B	7.69	1.50	1.40
24	BB	5618	CLA	C3B-C2B	7.70	1.50	1.40
24	AB	604	CLA	C3B-C2B	7.70	1.50	1.40
30	AB	627	SQD	C4-C3	7.72	1.72	1.52
24	AB	614	CLA	C3B-C2B	7.72	1.50	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	AA	412	LHG	P-O5	7.72	1.79	1.51
24	AC	510	CLA	C3B-C2B	7.78	1.50	1.40
24	AA	406	CLA	C3B-C2B	7.82	1.50	1.40
24	AC	511	CLA	C3B-C2B	7.84	1.50	1.40
24	BC	5502	CLA	C3B-C2B	7.91	1.50	1.40
24	AC	503	CLA	C3B-C2B	7.94	1.50	1.40
24	AB	615	CLA	C3B-C2B	7.98	1.50	1.40
24	BB	5614	CLA	C3B-C2B	8.03	1.50	1.40
30	AB	622	SQD	C4-C3	8.08	1.73	1.52
24	AB	616	CLA	C3B-C2B	8.11	1.51	1.40
24	BC	5510	CLA	C3B-C2B	8.12	1.51	1.40
24	AB	609	CLA	C3B-C2B	8.21	1.51	1.40
24	BC	5506	CLA	C3B-C2B	8.21	1.51	1.40
24	BA	5407	CLA	C3B-C2B	8.21	1.51	1.40
24	AC	513	CLA	C3B-C2B	8.23	1.51	1.40
24	BB	5613	CLA	C3B-C2B	8.25	1.51	1.40
24	BC	5511	CLA	C3B-C2B	8.25	1.51	1.40
30	BB	5625	SQD	C4-C3	8.28	1.74	1.52
24	BB	5619	CLA	C3B-C2B	8.29	1.51	1.40
24	BB	5609	CLA	C3B-C2B	8.31	1.51	1.40
24	AC	506	CLA	C3B-C2B	8.34	1.51	1.40
24	BC	5501	CLA	C3B-C2B	8.42	1.51	1.40
24	BC	5503	CLA	C3B-C2B	8.44	1.51	1.40
24	AB	605	CLA	C3B-C2B	8.50	1.51	1.40
35	AD	405	PL9	C2-C3	8.54	1.57	1.34
24	AC	512	CLA	C3B-C2B	8.55	1.51	1.40
35	BD	5406	PL9	C2-C3	8.65	1.57	1.34
24	BC	5509	CLA	C3B-C2B	8.67	1.51	1.40
24	BC	5513	CLA	C3B-C2B	8.73	1.51	1.40
24	BC	5512	CLA	C3B-C2B	8.76	1.51	1.40
24	BA	5406	CLA	C3B-C2B	8.83	1.51	1.40
24	AC	505	CLA	C3B-C2B	9.16	1.52	1.40
24	AB	601	CLA	C3B-C2B	9.25	1.52	1.40
24	BC	5505	CLA	C3B-C2B	9.47	1.52	1.40
24	BA	5405	CLA	C2-C3	9.54	1.51	1.33
24	BB	5605	CLA	C3B-C2B	9.75	1.53	1.40
35	AD	405	PL9	C23-C24	10.47	1.53	1.33
24	BB	5619	CLA	C2-C3	10.48	1.53	1.33
24	BB	5614	CLA	C2-C3	10.54	1.53	1.33
24	AB	615	CLA	C2-C3	10.55	1.53	1.33
24	AC	507	CLA	C2-C3	10.60	1.53	1.33
24	AC	509	CLA	C2-C3	10.69	1.54	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	610	CLA	C2-C3	10.70	1.54	1.33
24	AA	404	CLA	C2-C3	10.72	1.54	1.33
24	AB	613	CLA	C2-C3	10.78	1.54	1.33
24	AC	504	CLA	C2-C3	10.78	1.54	1.33
24	BB	5608	CLA	C2-C3	10.82	1.54	1.33
24	AD	401	CLA	C2-C3	10.83	1.54	1.33
24	BB	5617	CLA	C2-C3	10.83	1.54	1.33
24	BC	5510	CLA	C2-C3	10.88	1.54	1.33
35	AD	405	PL9	C43-C44	10.92	1.54	1.33
24	AC	512	CLA	C2-C3	10.92	1.54	1.33
24	AB	604	CLA	C2-C3	10.93	1.54	1.33
24	AB	602	CLA	C2-C3	10.94	1.54	1.33
35	AD	405	PL9	C8-C9	10.95	1.54	1.33
24	AC	510	CLA	C2-C3	10.98	1.54	1.33
24	BA	5407	CLA	C2-C3	10.98	1.54	1.33
24	BC	5512	CLA	C2-C3	11.00	1.54	1.33
24	AD	404	CLA	C2-C3	11.01	1.54	1.33
24	BC	5507	CLA	C2-C3	11.02	1.54	1.33
24	BD	5402	CLA	C2-C3	11.03	1.54	1.33
24	AC	503	CLA	C2-C3	11.03	1.54	1.33
24	BB	5616	CLA	C2-C3	11.07	1.54	1.33
35	BD	5406	PL9	C8-C9	11.07	1.54	1.33
24	BC	5503	CLA	C2-C3	11.07	1.54	1.33
24	AA	407	CLA	C2-C3	11.08	1.54	1.33
24	BB	5606	CLA	C2-C3	11.11	1.54	1.33
24	BC	5504	CLA	C2-C3	11.13	1.54	1.33
24	AB	612	CLA	C2-C3	11.20	1.55	1.33
24	BC	5502	CLA	C2-C3	11.21	1.55	1.33
24	AA	406	CLA	C2-C3	11.22	1.55	1.33
35	AD	405	PL9	C33-C34	11.22	1.55	1.33
24	AC	508	CLA	C2-C3	11.23	1.55	1.33
35	BD	5406	PL9	C43-C44	11.29	1.55	1.33
34	AD	402	PHO	C2-C3	11.33	1.55	1.33
24	AB	611	CLA	C2-C3	11.34	1.55	1.33
24	BA	5406	CLA	C2-C3	11.34	1.55	1.33
24	AA	405	CLA	C2-C3	11.38	1.55	1.33
24	BC	5508	CLA	C2-C3	11.39	1.55	1.33
24	BC	5509	CLA	C2-C3	11.41	1.55	1.33
24	BA	5408	CLA	C2-C3	11.43	1.55	1.33
24	BC	5501	CLA	C2-C3	11.49	1.55	1.33
24	AB	601	CLA	C2-C3	11.51	1.55	1.33
24	BB	5609	CLA	C2-C3	11.53	1.55	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AC	502	CLA	C2-C3	11.54	1.55	1.33
24	BD	5405	CLA	C2-C3	11.56	1.55	1.33
35	BD	5406	PL9	C33-C34	11.57	1.55	1.33
24	AC	501	CLA	C2-C3	11.59	1.55	1.33
24	BC	5513	CLA	C2-C3	11.60	1.55	1.33
24	AC	513	CLA	C2-C3	11.63	1.55	1.33
24	AB	605	CLA	C2-C3	11.63	1.55	1.33
34	BD	5403	PHO	C2-C3	11.67	1.55	1.33
24	AC	505	CLA	C2-C3	11.68	1.55	1.33
34	BD	5404	PHO	C2-C3	11.68	1.55	1.33
35	AD	405	PL9	C13-C14	11.70	1.55	1.33
35	BD	5406	PL9	C23-C24	11.72	1.56	1.33
24	BB	5618	CLA	C2-C3	11.74	1.56	1.33
35	BD	5406	PL9	C28-C29	11.74	1.56	1.33
24	BB	5605	CLA	C2-C3	11.75	1.56	1.33
24	BB	5611	CLA	C2-C3	11.75	1.56	1.33
24	BB	5615	CLA	C2-C3	11.76	1.56	1.33
24	AC	506	CLA	C2-C3	11.76	1.56	1.33
34	AD	403	PHO	C2-C3	11.80	1.56	1.33
35	BD	5406	PL9	C13-C14	11.84	1.56	1.33
24	BB	5607	CLA	C2-C3	11.87	1.56	1.33
24	BC	5506	CLA	C2-C3	11.88	1.56	1.33
24	AB	609	CLA	C2-C3	11.91	1.56	1.33
35	AD	405	PL9	C28-C29	11.92	1.56	1.33
24	BC	5505	CLA	C2-C3	11.96	1.56	1.33
24	AB	603	CLA	C2-C3	12.09	1.56	1.33
24	AC	511	CLA	C2-C3	12.16	1.56	1.33
24	AB	616	CLA	C2-C3	12.16	1.56	1.33
24	BB	5613	CLA	C2-C3	12.17	1.56	1.33
24	AB	614	CLA	C2-C3	12.17	1.56	1.33
24	BC	5511	CLA	C2-C3	12.41	1.57	1.33
24	BB	5620	CLA	C2-C3	12.43	1.57	1.33
24	AB	607	CLA	C2-C3	12.43	1.57	1.33
24	BB	5610	CLA	C2-C3	12.79	1.58	1.33
24	AB	606	CLA	C2-C3	12.81	1.58	1.33
24	BB	5612	CLA	C2-C3	12.81	1.58	1.33
24	AB	608	CLA	C2-C3	12.82	1.58	1.33

All (2457) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BJ	5101	BCR	C32-C1-C6	-10.33	94.11	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AJ	101	BCR	C32-C1-C6	-10.27	94.20	110.30
28	BA	5412	DGD	O3G-C1D-C2D	-9.80	95.67	108.04
28	AC	519	DGD	C3G-O3G-C1D	-9.79	93.25	113.82
28	AA	411	DGD	O3G-C1D-C2D	-9.69	95.80	108.04
28	BC	5519	DGD	C3G-O3G-C1D	-9.62	93.61	113.82
36	AV	201	HEM	C3C-CAC-CBC	-9.07	110.55	124.46
27	BJ	5101	BCR	C32-C1-C31	-8.97	79.64	108.37
27	AJ	101	BCR	C32-C1-C31	-8.92	79.78	108.37
36	BV	5201	HEM	C3C-CAC-CBC	-8.84	110.90	124.46
28	AA	411	DGD	O3G-C3G-C2G	-8.56	90.62	110.99
36	BF	5101	HEM	CMA-C3A-C2A	-8.56	107.34	125.24
28	BA	5412	DGD	O3G-C3G-C2G	-8.56	90.63	110.99
35	AD	405	PL9	C7-C8-C9	-8.45	112.38	126.70
36	AF	101	HEM	CMA-C3A-C2A	-8.38	107.71	125.24
35	BD	5406	PL9	C7-C8-C9	-8.38	112.50	126.70
36	AV	201	HEM	CMA-C3A-C2A	-8.26	107.97	125.24
36	BV	5201	HEM	CMA-C3A-C2A	-8.23	108.03	125.24
36	BF	5101	HEM	C3C-CAC-CBC	-8.17	111.92	124.46
28	AA	411	DGD	C6D-C5D-C4D	-8.09	93.70	112.03
36	AF	101	HEM	C3C-CAC-CBC	-8.01	112.17	124.46
28	BA	5412	DGD	C6D-C5D-C4D	-7.99	93.92	112.03
27	AJ	101	BCR	C32-C1-C2	-7.72	81.14	108.79
35	AD	405	PL9	C10-C9-C8	-7.63	108.51	123.50
27	BJ	5101	BCR	C32-C1-C2	-7.59	81.62	108.79
28	BC	5519	DGD	C6D-O5D-C1E	-7.52	98.02	113.82
31	AD	407	LMG	C19-C18-C17	-7.51	75.76	114.53
31	BD	5409	LMG	C19-C18-C17	-7.48	75.90	114.53
35	BD	5406	PL9	C10-C9-C8	-7.33	109.11	123.50
35	BD	5406	PL9	C32-C33-C34	-7.15	112.22	127.76
28	AC	519	DGD	C6D-O5D-C1E	-7.06	98.99	113.82
35	AD	405	PL9	C32-C33-C34	-7.04	112.45	127.76
28	BA	5412	DGD	C6D-O5D-C1E	-6.86	99.41	113.82
28	AA	411	DGD	C6D-O5D-C1E	-6.77	99.60	113.82
31	AD	408	LMG	C13-C12-C11	-6.76	88.49	113.29
31	BD	5410	LMG	C13-C12-C11	-6.76	88.49	113.29
31	BL	5101	LMG	C7-O1-C1	-6.69	99.77	113.82
31	AB	620	LMG	C7-O1-C1	-6.58	99.99	113.82
31	AJ	102	LMG	C13-C12-C11	-6.47	89.56	113.29
31	AA	417	LMG	C7-O1-C1	-6.46	100.25	113.82
31	AB	620	LMG	C13-C12-C11	-6.43	89.70	113.29
31	BD	5408	LMG	C7-O1-C1	-6.43	100.31	113.82
25	AA	408	MST	C10-N9-C4	-6.43	120.93	128.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	BD	5408	LMG	C13-C12-C11	-6.42	89.73	113.29
31	BL	5101	LMG	C13-C12-C11	-6.38	89.90	113.29
28	AC	517	DGD	O1G-C1G-C2G	-6.32	91.68	108.69
31	BA	5402	LMG	C7-O1-C1	-6.31	100.56	113.82
31	BA	5402	LMG	C13-C12-C11	-6.30	90.20	113.29
31	AA	417	LMG	C13-C12-C11	-6.28	90.26	113.29
31	AJ	102	LMG	C7-O1-C1	-6.28	100.63	113.82
28	BC	5519	DGD	C4B-C3B-C2B	-6.20	90.56	113.29
35	AD	405	PL9	C22-C23-C24	-6.18	114.33	127.76
28	AC	518	DGD	C4A-C3A-C2A	-6.16	90.70	113.29
28	BC	5517	DGD	O1G-C1G-C2G	-6.15	92.14	108.69
25	BA	5409	MST	C10-N9-C4	-6.07	121.33	128.05
35	BD	5406	PL9	C3-C2-C1	-6.06	119.28	122.97
28	AA	411	DGD	C1D-O6D-C5D	-6.03	102.04	113.75
28	AC	519	DGD	C4B-C3B-C2B	-6.01	91.23	113.29
28	BB	5602	DGD	C3G-O3G-C1D	-6.00	101.22	113.82
31	BD	5409	LMG	C13-C12-C11	-5.99	91.32	113.29
28	AC	517	DGD	C4B-C3B-C2B	-5.98	91.35	113.29
28	BC	5518	DGD	C4A-C3A-C2A	-5.98	91.37	113.29
35	BD	5406	PL9	C22-C23-C24	-5.98	114.77	127.76
28	BC	5517	DGD	C4B-C3B-C2B	-5.97	91.39	113.29
28	BC	5517	DGD	C6D-O5D-C1E	-5.97	101.29	113.82
31	AD	407	LMG	C13-C12-C11	-5.93	91.53	113.29
28	BA	5412	DGD	C1D-O6D-C5D	-5.93	102.23	113.75
32	BC	5522	LMT	C1B-O1B-C4'	-5.91	102.55	118.01
28	AB	628	DGD	C3G-O3G-C1D	-5.91	101.39	113.82
28	AC	519	DGD	C6D-C5D-C4D	-5.86	98.75	112.03
28	AC	518	DGD	C3G-O3G-C1D	-5.79	101.66	113.82
28	BC	5518	DGD	C6D-O5D-C1E	-5.76	101.72	113.82
32	AI	103	LMT	C1B-O1B-C4'	-5.72	103.06	118.01
28	BC	5518	DGD	C3G-O3G-C1D	-5.70	101.84	113.82
28	AC	517	DGD	C6D-O5D-C1E	-5.67	101.91	113.82
31	BD	5409	LMG	C17-C16-C15	-5.67	85.27	114.53
31	AD	407	LMG	C17-C16-C15	-5.59	85.67	114.53
24	AA	405	CLA	CAA-C2A-C1A	-5.57	92.81	112.47
24	BA	5406	CLA	CAA-C2A-C1A	-5.55	92.90	112.47
35	BD	5406	PL9	C12-C13-C14	-5.53	115.73	127.76
28	AC	518	DGD	C6D-O5D-C1E	-5.47	102.33	113.82
30	BB	5625	SQD	O9-S-C6	-5.47	102.33	106.94
35	AD	405	PL9	C12-C13-C14	-5.38	116.06	127.76
24	AC	505	CLA	CAA-CBA-CGA	-5.36	97.64	113.32
28	BC	5519	DGD	C6D-C5D-C4D	-5.35	99.91	112.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	AD	405	PL9	C3-C2-C1	-5.34	119.72	122.97
24	BC	5505	CLA	CAA-CBA-CGA	-5.34	97.68	113.32
32	BD	5411	LMT	C1B-O1B-C4'	-5.34	104.06	118.01
28	AC	517	DGD	C6D-C5D-C4D	-5.29	100.05	112.03
30	BB	5601	SQD	O9-S-C6	-5.25	102.52	106.94
28	BC	5517	DGD	C6D-C5D-C4D	-5.22	100.20	112.03
24	BB	5612	CLA	CAA-C2A-C1A	-5.20	94.13	112.47
28	BH	5101	DGD	O3G-C1D-C2D	-5.20	101.48	108.04
24	AB	608	CLA	CAA-C2A-C1A	-5.18	94.20	112.47
32	AD	409	LMT	C1B-O1B-C4'	-5.16	104.52	118.01
28	AH	101	DGD	O3G-C1D-C2D	-5.10	101.60	108.04
28	BC	5519	DGD	O2G-C2G-C1G	-5.09	90.41	108.36
24	BA	5407	CLA	CAA-C2A-C1A	-5.03	94.72	112.47
28	BH	5101	DGD	C6D-O5D-C1E	-5.03	103.26	113.82
30	BF	5102	SQD	O9-S-C6	-5.01	102.72	106.94
30	AF	102	SQD	O9-S-C6	-4.97	102.75	106.94
35	AD	405	PL9	C20-C19-C18	-4.96	113.77	123.50
31	BD	5409	LMG	C9-C8-C7	-4.94	100.51	112.07
30	AB	622	SQD	O9-S-C6	-4.93	102.79	106.94
30	AB	627	SQD	O9-S-C6	-4.92	102.79	106.94
24	BB	5611	CLA	CAA-C2A-C1A	-4.91	95.14	112.47
31	AD	407	LMG	C9-C8-C7	-4.91	100.58	112.07
30	BA	5414	SQD	O9-S-C6	-4.90	102.81	106.94
30	AA	416	SQD	O9-S-C6	-4.90	102.81	106.94
28	AC	517	DGD	O3G-C1D-C2D	-4.89	101.87	108.04
35	BD	5406	PL9	C7-C3-C2	-4.88	119.37	123.42
24	AB	607	CLA	CAA-C2A-C1A	-4.85	95.36	112.47
30	BA	5401	SQD	O9-S-C6	-4.84	102.86	106.94
28	AH	101	DGD	O3G-C3G-C2G	-4.83	99.50	110.99
24	AA	406	CLA	CAA-C2A-C1A	-4.82	95.48	112.47
28	BH	5101	DGD	C6D-C5D-C4D	-4.81	101.12	112.03
28	AH	101	DGD	C6D-O5D-C1E	-4.80	103.73	113.82
31	BC	5521	LMG	C13-C12-C11	-4.80	95.69	113.29
31	AC	521	LMG	C13-C12-C11	-4.79	95.72	113.29
28	AC	519	DGD	O2G-C2G-C1G	-4.78	91.50	108.36
28	AC	518	DGD	C6D-C5D-C4D	-4.76	101.24	112.03
28	AH	101	DGD	C6D-C5D-C4D	-4.75	101.26	112.03
31	AC	521	LMG	C7-O1-C1	-4.74	103.86	113.82
31	BC	5521	LMG	C7-O1-C1	-4.72	103.90	113.82
28	BC	5519	DGD	C1D-O6D-C5D	-4.72	104.59	113.75
27	AJ	101	BCR	C1-C6-C5	-4.70	115.75	122.66
35	BD	5406	PL9	C20-C19-C18	-4.69	114.29	123.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BC	5517	DGD	C4A-C3A-C2A	-4.68	96.12	113.29
27	BJ	5101	BCR	C1-C6-C5	-4.67	115.81	122.66
28	BC	5517	DGD	O3G-C1D-C2D	-4.65	102.17	108.04
31	BE	5101	LMG	C7-O1-C1	-4.65	104.06	113.82
31	AA	414	LMG	C7-O1-C1	-4.64	104.08	113.82
28	BC	5518	DGD	C6D-C5D-C4D	-4.62	101.56	112.03
28	BH	5101	DGD	O3G-C3G-C2G	-4.61	100.01	110.99
35	AD	405	PL9	C7-C3-C2	-4.57	119.63	123.42
28	BC	5518	DGD	C1D-O6D-C5D	-4.57	104.88	113.75
24	AB	608	CLA	CAA-CBA-CGA	-4.56	99.96	113.32
28	AC	519	DGD	C1D-O6D-C5D	-4.53	104.95	113.75
27	AD	406	BCR	C38-C26-C27	-4.51	104.87	113.43
28	AC	517	DGD	C4A-C3A-C2A	-4.51	96.74	113.29
31	BD	5408	LMG	O8-C9-C8	-4.50	96.59	108.69
28	BC	5519	DGD	C1E-C2E-C3E	-4.48	101.15	109.97
28	AA	411	DGD	C1G-O1G-C1A	-4.44	104.42	116.85
28	BA	5412	DGD	C1G-O1G-C1A	-4.44	104.43	116.85
28	AC	518	DGD	C1D-O6D-C5D	-4.43	105.16	113.75
31	AJ	102	LMG	O8-C9-C8	-4.37	96.92	108.69
27	AJ	101	BCR	C38-C26-C27	-4.37	105.14	113.43
24	BB	5612	CLA	CAA-CBA-CGA	-4.35	100.59	113.32
27	AK	102	BCR	C33-C5-C4	-4.33	105.21	113.43
25	AA	408	MST	N5-C6-N1	-4.33	119.57	126.22
27	BD	5407	BCR	C38-C26-C27	-4.30	105.28	113.43
25	BA	5409	MST	N5-C6-N1	-4.30	119.61	126.22
31	AD	407	LMG	C15-C14-C13	-4.27	92.47	114.53
31	BD	5409	LMG	C15-C14-C13	-4.26	92.55	114.53
28	AH	101	DGD	C5B-C4B-C3B	-4.23	92.68	114.53
24	AC	504	CLA	CAA-C2A-C1A	-4.23	97.56	112.47
24	AB	614	CLA	C2C-C1C-NC	-4.22	107.10	110.24
24	BC	5511	CLA	C2C-C1C-NC	-4.22	107.10	110.24
28	AC	519	DGD	C1E-C2E-C3E	-4.21	101.68	109.97
27	BJ	5101	BCR	C38-C26-C27	-4.21	105.45	113.43
35	BD	5406	PL9	C35-C34-C33	-4.20	115.25	123.50
27	AB	618	BCR	C38-C26-C27	-4.20	105.47	113.43
28	BH	5101	DGD	C5B-C4B-C3B	-4.20	92.85	114.53
24	AC	511	CLA	C2C-C1C-NC	-4.17	107.14	110.24
35	AD	405	PL9	C35-C34-C33	-4.15	115.35	123.50
27	BB	5622	BCR	C38-C26-C27	-4.15	105.56	113.43
28	AB	628	DGD	C4B-C3B-C2B	-4.14	98.10	113.29
24	BC	5504	CLA	CAA-C2A-C1A	-4.13	97.90	112.47
28	AC	519	DGD	C8A-C7A-C6A	-4.13	93.20	114.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BB	5602	DGD	C4B-C3B-C2B	-4.10	98.26	113.29
27	BX	5101	BCR	C38-C26-C27	-4.10	105.66	113.43
27	BK	5102	BCR	C33-C5-C4	-4.09	105.67	113.43
31	AI	101	LMG	C9-C8-C7	-4.09	102.50	112.07
28	BC	5519	DGD	C8A-C7A-C6A	-4.09	93.40	114.53
28	BE	5102	DGD	C6D-O5D-C1E	-4.08	105.25	113.82
27	BC	5516	BCR	C33-C5-C4	-4.08	105.69	113.43
27	BB	5621	BCR	C38-C26-C27	-4.07	105.71	113.43
24	BC	5508	CLA	O1D-CGD-CBD	-4.05	118.82	124.62
24	BB	5618	CLA	C2C-C1C-NC	-4.04	107.24	110.24
27	BT	5101	BCR	C33-C5-C4	-4.03	105.79	113.43
31	BD	5410	LMG	C19-C18-C17	-4.03	93.72	114.53
27	AX	101	BCR	C38-C26-C27	-4.02	105.80	113.43
25	AA	408	MST	N5-C4-N3	-4.02	120.03	126.22
27	AT	101	BCR	C33-C5-C4	-4.02	105.81	113.43
28	BC	5518	DGD	C8A-C7A-C6A	-4.00	93.86	114.53
32	AB	629	LMT	C1-O1'-C1'	-3.99	106.96	113.94
35	BD	5406	PL9	C11-C9-C8	-3.99	113.48	121.05
31	AD	408	LMG	C19-C18-C17	-3.99	93.94	114.53
31	BA	5402	LMG	O8-C9-C8	-3.99	97.96	108.69
28	AC	518	DGD	C8A-C7A-C6A	-3.98	93.96	114.53
27	AC	514	BCR	C38-C26-C27	-3.96	105.93	113.43
28	AC	517	DGD	C1D-O6D-C5D	-3.95	106.07	113.75
27	AB	617	BCR	C38-C26-C27	-3.95	105.94	113.43
27	AC	515	BCR	C38-C26-C27	-3.94	105.96	113.43
28	AE	101	DGD	C6D-O5D-C1E	-3.93	105.56	113.82
25	BA	5409	MST	N5-C4-N3	-3.92	120.19	126.22
31	BI	5101	LMG	C9-C8-C7	-3.92	102.89	112.07
27	AC	516	BCR	C33-C5-C4	-3.92	105.99	113.43
28	BC	5517	DGD	C1D-O6D-C5D	-3.92	106.13	113.75
31	AD	408	LMG	C7-O1-C1	-3.91	105.61	113.82
27	BC	5515	BCR	C33-C5-C4	-3.91	106.02	113.43
35	BD	5406	PL9	C15-C14-C13	-3.91	115.83	123.50
27	BB	5621	BCR	C33-C5-C4	-3.90	106.04	113.43
27	AC	515	BCR	C33-C5-C4	-3.89	106.05	113.43
32	BB	5626	LMT	C1B-O1B-C4'	-3.89	107.85	118.01
28	AC	518	DGD	C3G-C2G-C1G	-3.88	103.00	112.07
31	BD	5410	LMG	C7-O1-C1	-3.88	105.68	113.82
32	BB	5603	LMT	C1-O1'-C1'	-3.87	107.17	113.94
27	BT	5101	BCR	C38-C26-C27	-3.85	106.12	113.43
28	BC	5518	DGD	C3G-C2G-C1G	-3.85	103.06	112.07
24	BB	5607	CLA	C2C-C1C-NC	-3.85	107.38	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	AA	413	SQD	O9-S-C6	-3.85	103.69	106.94
27	AJ	101	BCR	C30-C25-C26	-3.85	117.00	122.66
27	AC	516	BCR	C38-C26-C27	-3.85	106.13	113.43
24	BC	5503	CLA	O1D-CGD-CBD	-3.85	119.11	124.62
28	AC	519	DGD	C6B-C5B-C4B	-3.84	94.73	114.53
27	BJ	5101	BCR	C33-C5-C4	-3.83	106.17	113.43
35	AD	405	PL9	C11-C9-C8	-3.82	113.81	121.05
35	AD	405	PL9	C25-C24-C23	-3.81	116.01	123.50
27	AT	101	BCR	C38-C26-C27	-3.80	106.22	113.43
28	BB	5602	DGD	O1G-C1G-C2G	-3.80	98.46	108.69
24	BC	5510	CLA	O1D-CGD-CBD	-3.80	119.18	124.62
24	BC	5508	CLA	CAA-C2A-C1A	-3.79	99.09	112.47
27	AK	102	BCR	C38-C26-C27	-3.79	106.25	113.43
27	BC	5515	BCR	C38-C26-C27	-3.79	106.25	113.43
24	BC	5505	CLA	CAA-C2A-C1A	-3.78	99.12	112.47
27	BJ	5101	BCR	C30-C25-C26	-3.78	117.11	122.66
28	AH	101	DGD	C3B-C2B-C1B	-3.78	98.73	113.59
27	AJ	101	BCR	C33-C5-C4	-3.78	106.26	113.43
31	AB	621	LMG	C14-C13-C12	-3.78	95.02	114.53
36	BV	5201	HEM	CBD-CAD-C3D	-3.77	102.58	113.55
28	BC	5519	DGD	C6B-C5B-C4B	-3.76	95.10	114.53
31	BB	5624	LMG	C14-C13-C12	-3.76	95.11	114.53
31	AA	417	LMG	O8-C9-C8	-3.75	98.58	108.69
28	BH	5101	DGD	C3B-C2B-C1B	-3.75	98.84	113.59
31	BC	5520	LMG	C12-C11-C10	-3.75	98.87	113.59
31	AB	621	LMG	C37-C36-C35	-3.74	95.23	114.53
28	AB	628	DGD	O1G-C1G-C2G	-3.74	98.63	108.69
24	AC	505	CLA	CAA-C2A-C1A	-3.73	99.30	112.47
32	AB	623	LMT	C1B-O1B-C4'	-3.73	108.26	118.01
31	BB	5624	LMG	C37-C36-C35	-3.73	95.28	114.53
35	AD	405	PL9	C15-C14-C13	-3.72	116.20	123.50
27	BC	5516	BCR	C38-C26-C27	-3.71	106.40	113.43
27	BK	5102	BCR	C38-C26-C27	-3.69	106.43	113.43
24	AC	513	CLA	C2C-C1C-NC	-3.69	107.50	110.24
31	AC	520	LMG	C12-C11-C10	-3.68	99.12	113.59
24	AB	603	CLA	C2C-C1C-NC	-3.68	107.50	110.24
36	AV	201	HEM	CBD-CAD-C3D	-3.68	102.86	113.55
24	AC	508	CLA	CAA-C2A-C1A	-3.67	99.52	112.47
28	BC	5519	DGD	O1G-C1G-C2G	-3.66	98.84	108.69
27	AB	617	BCR	C33-C5-C4	-3.64	106.52	113.43
35	BD	5406	PL9	C25-C24-C23	-3.63	116.38	123.50
27	BA	5411	BCR	C38-C26-C27	-3.62	106.56	113.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AC	514	BCR	C33-C5-C4	-3.60	106.59	113.43
27	BB	5623	BCR	C38-C26-C27	-3.60	106.60	113.43
27	BC	5514	BCR	C38-C26-C27	-3.60	106.61	113.43
24	BB	5616	CLA	O1D-CGD-CBD	-3.58	119.49	124.62
24	BC	5513	CLA	C2C-C1C-NC	-3.57	107.58	110.24
27	AA	410	BCR	C38-C26-C27	-3.57	106.66	113.43
27	BA	5411	BCR	C33-C5-C4	-3.57	106.66	113.43
27	AD	406	BCR	C30-C25-C26	-3.57	117.42	122.66
27	BD	5407	BCR	C30-C25-C26	-3.56	117.43	122.66
27	AX	101	BCR	C30-C25-C26	-3.51	117.50	122.66
24	AC	501	CLA	CAA-C2A-C1A	-3.48	100.20	112.47
27	AC	516	BCR	C1-C6-C5	-3.47	117.56	122.66
24	BB	5618	CLA	CAA-CBA-CGA	-3.47	103.15	113.32
24	AB	612	CLA	O1D-CGD-CBD	-3.47	119.65	124.62
27	BT	5101	BCR	C30-C25-C26	-3.47	117.56	122.66
24	BC	5501	CLA	CAA-C2A-C1A	-3.47	100.24	112.47
27	AB	619	BCR	C38-C26-C27	-3.47	106.86	113.43
25	AA	408	MST	N3-C2-N1	-3.47	120.15	126.75
31	BB	5624	LMG	C33-C32-C31	-3.46	96.64	114.53
27	BX	5101	BCR	C33-C5-C4	-3.46	106.86	113.43
27	AK	102	BCR	C1-C6-C5	-3.46	117.58	122.66
27	BD	5407	BCR	C33-C5-C4	-3.46	106.87	113.43
27	AA	410	BCR	C33-C5-C4	-3.45	106.89	113.43
27	AT	101	BCR	C30-C25-C26	-3.45	117.59	122.66
28	AC	519	DGD	O1G-C1G-C2G	-3.44	99.42	108.69
32	BC	5522	LMT	O1'-C1-C2	-3.44	96.18	109.88
34	BD	5404	PHO	O1D-CGD-CBD	-3.43	119.71	124.62
27	BK	5102	BCR	C1-C6-C5	-3.43	117.63	122.66
32	AI	103	LMT	O1'-C1-C2	-3.42	96.26	109.88
24	AC	503	CLA	O1D-CGD-CBD	-3.42	119.72	124.62
34	AD	403	PHO	O1D-CGD-CBD	-3.42	119.73	124.62
27	AX	101	BCR	C33-C5-C4	-3.41	106.97	113.43
24	AB	614	CLA	CAA-CBA-CGA	-3.40	103.35	113.32
24	AB	611	CLA	O1D-CGD-CBD	-3.39	119.76	124.62
36	AF	101	HEM	CBD-CAD-C3D	-3.39	103.69	113.55
27	AK	102	BCR	C30-C25-C26	-3.39	117.68	122.66
28	BA	5412	DGD	O1G-C1A-O1A	-3.39	114.75	123.49
24	AA	406	CLA	O1D-CGD-CBD	-3.38	119.77	124.62
24	AC	508	CLA	O1D-CGD-CBD	-3.38	119.77	124.62
32	BB	5603	LMT	C1B-O1B-C4'	-3.38	109.18	118.01
27	BX	5101	BCR	C30-C25-C26	-3.38	117.70	122.66
31	AB	621	LMG	C33-C32-C31	-3.38	97.09	114.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	5409	MST	N3-C2-N1	-3.38	120.32	126.75
28	AA	411	DGD	O1G-C1A-O1A	-3.38	114.78	123.49
36	BF	5101	HEM	CBD-CAD-C3D	-3.37	103.74	113.55
24	AC	510	CLA	O1D-CGD-CBD	-3.37	119.79	124.62
31	AI	101	LMG	C7-O1-C1	-3.37	106.74	113.82
27	AB	618	BCR	C33-C5-C4	-3.36	107.05	113.43
24	AB	612	CLA	C2C-C1C-NC	-3.36	107.74	110.24
28	BA	5412	DGD	C3A-C2A-C1A	-3.36	100.38	113.59
27	AB	618	BCR	C30-C25-C26	-3.36	117.72	122.66
32	AB	629	LMT	C1B-O1B-C4'	-3.36	109.23	118.01
28	BC	5517	DGD	C6B-C5B-C4B	-3.36	97.20	114.53
28	AC	517	DGD	C6B-C5B-C4B	-3.35	97.22	114.53
31	BD	5409	LMG	O1-C7-C8	-3.35	103.02	110.99
24	BA	5408	CLA	O1D-CGD-CBD	-3.34	119.83	124.62
24	AC	501	CLA	CAA-CBA-CGA	-3.34	103.53	113.32
27	AD	406	BCR	C33-C5-C4	-3.34	107.09	113.43
24	BC	5511	CLA	CAA-C2A-C1A	-3.34	100.70	112.47
27	BB	5622	BCR	C30-C25-C26	-3.33	117.77	122.66
27	AB	619	BCR	C33-C5-C4	-3.33	107.12	113.43
24	AB	605	CLA	CAA-C2A-C1A	-3.33	100.74	112.47
31	BI	5101	LMG	C7-O1-C1	-3.32	106.84	113.82
28	AA	411	DGD	C3A-C2A-C1A	-3.32	100.54	113.59
27	BK	5102	BCR	C8-C9-C10	-3.31	113.64	118.98
24	BB	5611	CLA	CAA-CBA-CGA	-3.30	103.64	113.32
27	AC	516	BCR	C30-C25-C26	-3.29	117.82	122.66
24	BC	5508	CLA	C2C-C1C-NC	-3.28	107.80	110.24
24	AC	511	CLA	CAA-C2A-C1A	-3.27	100.92	112.47
24	BB	5609	CLA	CAA-C2A-C1A	-3.27	100.93	112.47
28	BH	5101	DGD	C1D-O6D-C5D	-3.27	107.40	113.75
31	AD	408	LMG	C17-C16-C15	-3.27	97.65	114.53
24	AB	610	CLA	O1D-CGD-CBD	-3.27	119.94	124.62
27	BC	5516	BCR	C1-C6-C5	-3.27	117.86	122.66
24	BC	5502	CLA	CAA-C2A-C1A	-3.26	100.97	112.47
34	BD	5403	PHO	O1D-CGD-CBD	-3.26	119.95	124.62
31	AB	621	LMG	C12-C11-C10	-3.26	100.80	113.59
24	BB	5607	CLA	O1D-CGD-CBD	-3.26	119.96	124.62
27	BC	5514	BCR	C33-C5-C4	-3.26	107.26	113.43
24	BC	5501	CLA	CAA-CBA-CGA	-3.25	103.79	113.32
24	BC	5502	CLA	O1D-CGD-CBD	-3.24	119.98	124.62
24	BB	5615	CLA	O1D-CGD-CBD	-3.24	119.98	124.62
27	BB	5623	BCR	C33-C5-C4	-3.23	107.31	113.43
27	AC	515	BCR	C30-C25-C26	-3.23	117.92	122.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BC	5504	CLA	O1D-CGD-CBD	-3.22	120.00	124.62
24	AD	401	CLA	O1D-CGD-CBD	-3.22	120.01	124.62
24	BA	5406	CLA	C3D-CAD-CBD	-3.21	103.05	107.60
27	BC	5515	BCR	C1-C6-C5	-3.21	117.94	122.66
31	AC	520	LMG	C14-C13-C12	-3.21	97.94	114.53
24	AA	405	CLA	O1D-CGD-CBD	-3.21	120.02	124.62
31	BD	5410	LMG	C17-C16-C15	-3.21	97.98	114.53
31	BB	5624	LMG	C12-C11-C10	-3.20	101.01	113.59
31	AI	101	LMG	C12-C11-C10	-3.19	101.06	113.59
24	BB	5615	CLA	CAA-C2A-C1A	-3.19	101.23	112.47
31	AD	407	LMG	O1-C7-C8	-3.19	103.41	110.99
27	BB	5621	BCR	C30-C25-C26	-3.19	117.98	122.66
31	BI	5101	LMG	C12-C11-C10	-3.18	101.09	113.59
27	AK	102	BCR	C8-C9-C10	-3.17	113.87	118.98
34	BD	5404	PHO	CBD-CHA-C4D	-3.17	104.91	108.46
28	BH	5101	DGD	C3G-C2G-C1G	-3.17	104.65	112.07
31	BD	5408	LMG	O7-C8-C9	-3.17	97.20	108.36
27	BK	5102	BCR	C30-C25-C26	-3.17	118.01	122.66
27	AC	515	BCR	C1-C6-C5	-3.16	118.01	122.66
31	BD	5408	LMG	O7-C10-C11	-3.16	104.65	111.53
24	BD	5402	CLA	O1D-CGD-CBD	-3.16	120.09	124.62
24	AA	405	CLA	CAA-CBA-CGA	-3.16	104.07	113.32
24	BB	5615	CLA	C2C-C1C-NC	-3.16	107.89	110.24
24	AB	614	CLA	CAA-C2A-C1A	-3.16	101.34	112.47
27	AC	514	BCR	C1-C6-C5	-3.15	118.03	122.66
27	BB	5622	BCR	C33-C5-C4	-3.15	107.46	113.43
31	BC	5520	LMG	C14-C13-C12	-3.15	98.27	114.53
24	BB	5619	CLA	O1D-CGD-CBD	-3.14	120.12	124.62
27	BX	5101	BCR	C1-C6-C5	-3.14	118.04	122.66
24	AA	407	CLA	O1D-CGD-CBD	-3.14	120.12	124.62
24	AB	605	CLA	O1D-CGD-CBD	-3.14	120.12	124.62
35	BD	5406	PL9	C50-C49-C48	-3.14	112.51	122.61
28	AH	101	DGD	C1D-O6D-C5D	-3.13	107.66	113.75
24	BB	5609	CLA	O1D-CGD-CBD	-3.13	120.13	124.62
31	BD	5408	LMG	C15-C14-C13	-3.13	98.37	114.53
24	BB	5618	CLA	CAA-C2A-C1A	-3.13	101.44	112.47
27	BC	5516	BCR	C30-C25-C26	-3.13	118.07	122.66
31	AJ	102	LMG	C15-C14-C13	-3.12	98.41	114.53
24	AC	508	CLA	C2C-C1C-NC	-3.12	107.92	110.24
24	AC	502	CLA	CAA-C2A-C1A	-3.12	101.47	112.47
31	AJ	102	LMG	O7-C8-C9	-3.12	97.37	108.36
24	BB	5610	CLA	C3D-CAD-CBD	-3.12	103.19	107.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AB	617	BCR	C30-C25-C26	-3.12	118.08	122.66
27	BC	5515	BCR	C30-C25-C26	-3.11	118.09	122.66
27	BK	5102	BCR	C12-C13-C14	-3.11	113.98	118.98
28	BC	5519	DGD	CBA-CAA-C9A	-3.11	98.49	114.53
24	BD	5405	CLA	O1D-CGD-CBD	-3.10	120.17	124.62
24	BC	5507	CLA	O1D-CGD-CBD	-3.10	120.18	124.62
31	AC	521	LMG	O8-C9-C8	-3.10	100.35	108.69
31	AC	520	LMG	C9-C8-C7	-3.10	104.82	112.07
24	AA	406	CLA	O2A-CGA-O1A	-3.09	115.52	123.49
24	AC	502	CLA	O1D-CGD-CBD	-3.09	120.19	124.62
24	BA	5406	CLA	CAA-CBA-CGA	-3.09	104.28	113.32
35	AD	405	PL9	C50-C49-C48	-3.07	112.74	122.61
28	AH	101	DGD	C3G-C2G-C1G	-3.06	104.91	112.07
30	AB	622	SQD	C3-C4-C5	-3.06	104.87	110.20
31	BC	5520	LMG	C9-C8-C7	-3.05	104.93	112.07
32	BC	5522	LMT	C4-C3-C2	-3.05	98.77	114.53
28	AC	517	DGD	C3G-O3G-C1D	-3.05	107.41	113.82
34	AD	402	PHO	O1D-CGD-CBD	-3.05	120.25	124.62
24	AB	607	CLA	CAA-CBA-CGA	-3.04	104.41	113.32
31	BC	5521	LMG	O8-C9-C8	-3.04	100.50	108.69
28	AC	519	DGD	C1D-C2D-C3D	-3.04	103.98	109.97
32	BC	5522	LMT	O1'-C1'-C2'	-3.04	104.20	108.04
24	AC	511	CLA	O1D-CGD-CBD	-3.03	120.27	124.62
32	AI	103	LMT	C4-C3-C2	-3.03	98.87	114.53
24	AA	405	CLA	C3D-CAD-CBD	-3.03	103.31	107.60
31	AM	101	LMG	C12-C11-C10	-3.02	101.71	113.59
24	AC	504	CLA	CAA-CBA-CGA	-3.02	104.47	113.32
24	AC	503	CLA	C7-C6-C5	-3.02	104.15	113.06
24	BA	5407	CLA	O2A-CGA-O1A	-3.02	115.70	123.49
24	BA	5406	CLA	O1D-CGD-CBD	-3.01	120.31	124.62
24	BC	5504	CLA	CAA-CBA-CGA	-3.01	104.50	113.32
32	BB	5603	LMT	C9-C8-C7	-3.01	98.99	114.53
27	AA	410	BCR	C30-C25-C26	-3.01	118.24	122.66
28	AC	519	DGD	CBA-CAA-C9A	-3.01	99.00	114.53
24	BA	5406	CLA	O2A-CGA-O1A	-3.01	115.73	123.49
24	BB	5616	CLA	C2C-C1C-NC	-3.01	108.00	110.24
27	BC	5516	BCR	C40-C30-C29	-3.01	98.02	108.79
24	AC	504	CLA	C2C-C1C-NC	-3.00	108.01	110.24
32	AB	629	LMT	C9-C8-C7	-3.00	99.06	114.53
30	BB	5625	SQD	C3-C4-C5	-2.99	104.98	110.20
24	BD	5405	CLA	CAA-C2A-C1A	-2.99	101.94	112.47
24	AC	509	CLA	O1D-CGD-CBD	-2.98	120.34	124.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	606	CLA	C3D-CAD-CBD	-2.98	103.38	107.60
24	AB	611	CLA	CAA-C2A-C1A	-2.98	101.94	112.47
32	AI	103	LMT	O1'-C1'-C2'	-2.98	104.27	108.04
24	BC	5511	CLA	O1D-CGD-CBD	-2.98	120.35	124.62
27	BC	5514	BCR	C1-C6-C5	-2.98	118.29	122.66
32	BB	5604	LMT	C4-C3-C2	-2.98	99.16	114.53
34	BD	5404	PHO	CAB-C3B-C2B	-2.97	118.44	128.41
28	BC	5517	DGD	C3G-O3G-C1D	-2.97	107.57	113.82
27	BX	5101	BCR	C12-C13-C14	-2.97	114.20	118.98
24	AD	404	CLA	CAA-C2A-C1A	-2.97	102.00	112.47
28	BC	5519	DGD	C8B-C7B-C6B	-2.97	99.21	114.53
24	AB	616	CLA	O1D-CGD-CBD	-2.96	120.38	124.62
27	BA	5411	BCR	C30-C25-C26	-2.96	118.32	122.66
32	AB	630	LMT	C4-C3-C2	-2.96	99.27	114.53
24	AB	611	CLA	C2C-C1C-NC	-2.96	108.04	110.24
28	AH	101	DGD	C7B-C6B-C5B	-2.95	99.28	114.53
24	AC	511	CLA	C6-C7-C8	-2.95	105.70	115.49
34	AD	403	PHO	CAB-C3B-C2B	-2.94	118.54	128.41
27	AC	516	BCR	C40-C30-C29	-2.94	98.25	108.79
28	AC	519	DGD	C8B-C7B-C6B	-2.94	99.34	114.53
27	BB	5623	BCR	C30-C25-C26	-2.94	118.35	122.66
34	AD	402	PHO	CAB-C3B-C2B	-2.93	118.58	128.41
27	AK	102	BCR	C12-C13-C14	-2.93	114.26	118.98
24	BC	5503	CLA	C3D-CAD-CBD	-2.93	103.46	107.60
24	AB	607	CLA	C2C-C1C-NC	-2.92	108.07	110.24
27	AB	619	BCR	C30-C25-C26	-2.92	118.37	122.66
27	BC	5515	BCR	C12-C13-C14	-2.92	114.28	118.98
27	AX	101	BCR	C12-C13-C14	-2.92	114.28	118.98
31	AJ	102	LMG	O7-C10-C11	-2.92	105.19	111.53
27	AC	514	BCR	C30-C25-C26	-2.91	118.38	122.66
24	AB	607	CLA	CAA-C2A-C3A	-2.91	104.84	113.22
24	BB	5614	CLA	O1D-CGD-CBD	-2.91	120.45	124.62
24	AC	504	CLA	O1D-CGD-CBD	-2.91	120.45	124.62
32	BB	5603	LMT	C4-C3-C2	-2.91	99.51	114.53
30	AA	416	SQD	C3-C4-C5	-2.91	105.13	110.20
28	BH	5101	DGD	C7B-C6B-C5B	-2.90	99.53	114.53
27	AT	101	BCR	C1-C6-C5	-2.90	118.40	122.66
31	BI	5101	LMG	C14-C13-C12	-2.90	99.56	114.53
31	BD	5410	LMG	C32-C31-C30	-2.90	99.56	114.53
24	AC	506	CLA	CAA-C2A-C1A	-2.90	102.26	112.47
31	BM	5102	LMG	C12-C11-C10	-2.90	102.21	113.59
34	AD	403	PHO	CBD-CHA-C4D	-2.89	105.22	108.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AX	101	BCR	C1-C6-C5	-2.89	118.42	122.66
24	AB	615	CLA	O1D-CGD-CBD	-2.89	120.49	124.62
27	BT	5101	BCR	C1-C6-C5	-2.88	118.42	122.66
30	BA	5401	SQD	C3-C4-C5	-2.88	105.17	110.20
24	BB	5611	CLA	C2C-C1C-NC	-2.88	108.10	110.24
24	BC	5511	CLA	C6-C7-C8	-2.87	105.95	115.49
31	AD	408	LMG	C32-C31-C30	-2.87	99.73	114.53
24	AB	603	CLA	CAA-C2A-C3A	-2.86	104.98	113.22
24	BC	5503	CLA	C7-C6-C5	-2.86	104.61	113.06
24	AB	603	CLA	CAA-C2A-C1A	-2.86	102.38	112.47
24	BC	5506	CLA	CAA-C2A-C1A	-2.86	102.38	112.47
24	AA	405	CLA	O2A-CGA-O1A	-2.86	116.11	123.49
27	AD	406	BCR	C12-C13-C14	-2.86	114.38	118.98
31	BB	5624	LMG	O7-C10-O9	-2.86	116.00	123.67
27	AC	515	BCR	C12-C13-C14	-2.86	114.38	118.98
24	BC	5508	CLA	C3D-CAD-CBD	-2.85	103.57	107.60
24	AA	407	CLA	CAA-C2A-C1A	-2.85	102.44	112.47
24	BA	5407	CLA	C2C-C1C-NC	-2.84	108.13	110.24
31	BB	5624	LMG	C16-C15-C14	-2.84	99.86	114.53
24	BA	5407	CLA	O1D-CGD-CBD	-2.83	120.56	124.62
24	AC	508	CLA	C3D-CAD-CBD	-2.83	103.60	107.60
34	BD	5403	PHO	CAB-C3B-C2B	-2.83	118.94	128.41
31	BL	5101	LMG	C15-C14-C13	-2.82	99.95	114.53
31	AI	101	LMG	C14-C13-C12	-2.82	99.95	114.53
24	BC	5502	CLA	C3D-CAD-CBD	-2.82	103.61	107.60
28	AA	411	DGD	O6D-C1D-C2D	-2.81	104.51	110.28
24	AC	507	CLA	O1D-CGD-CBD	-2.81	120.59	124.62
24	BC	5509	CLA	O1D-CGD-CBD	-2.81	120.59	124.62
34	BD	5404	PHO	C2A-C1A-NA	-2.81	108.48	112.08
31	AB	621	LMG	C16-C15-C14	-2.81	100.03	114.53
24	BB	5620	CLA	O1D-CGD-CBD	-2.81	120.60	124.62
24	BC	5510	CLA	C3D-CAD-CBD	-2.80	103.64	107.60
27	AD	406	BCR	C23-C22-C21	-2.80	114.48	118.98
31	AD	407	LMG	O1-C1-C2	-2.80	104.51	108.04
31	AB	621	LMG	O7-C10-O9	-2.79	116.17	123.67
24	BB	5607	CLA	CAA-C2A-C3A	-2.79	105.18	113.22
24	BB	5611	CLA	CAA-C2A-C3A	-2.79	105.19	113.22
32	AB	629	LMT	C4-C3-C2	-2.79	100.14	114.53
31	AB	620	LMG	C15-C14-C13	-2.79	100.14	114.53
24	BC	5507	CLA	C7-C6-C5	-2.78	104.84	113.06
27	BC	5514	BCR	C23-C22-C21	-2.78	114.50	118.98
24	BA	5405	CLA	C3D-CAD-CBD	-2.78	103.66	107.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5610	CLA	CAA-C2A-C1A	-2.78	102.67	112.47
24	AB	608	CLA	C2C-C1C-NC	-2.78	108.18	110.24
28	BA	5412	DGD	O6D-C1D-C2D	-2.77	104.60	110.28
24	BC	5509	CLA	C2C-C1C-NC	-2.76	108.19	110.24
24	BB	5617	CLA	C2C-C1C-NC	-2.76	108.19	110.24
24	BC	5504	CLA	C2C-C1C-NC	-2.76	108.19	110.24
24	AC	509	CLA	C2C-C1C-NC	-2.76	108.19	110.24
24	BB	5607	CLA	CAA-C2A-C1A	-2.75	102.78	112.47
24	BC	5513	CLA	O1D-CGD-CBD	-2.75	120.69	124.62
27	BB	5622	BCR	C1-C6-C5	-2.74	118.63	122.66
31	BD	5409	LMG	O1-C1-C2	-2.74	104.58	108.04
24	AC	506	CLA	O1D-CGD-CBD	-2.74	120.70	124.62
27	AD	406	BCR	C1-C6-C5	-2.73	118.65	122.66
24	AB	603	CLA	C7-C6-C5	-2.73	105.00	113.06
31	BD	5410	LMG	C15-C14-C13	-2.73	100.43	114.53
24	BB	5611	CLA	O2A-CGA-O1A	-2.73	116.45	123.49
24	BB	5610	CLA	O2A-CGA-O1A	-2.73	116.46	123.49
27	AA	410	BCR	C1-C6-C5	-2.72	118.67	122.66
34	AD	402	PHO	C3A-C4A-NA	-2.71	108.82	113.57
32	BI	5102	LMT	C4-C3-C2	-2.71	100.52	114.53
27	BD	5407	BCR	C1-C6-C5	-2.71	118.68	122.66
24	AD	404	CLA	O1D-CGD-CBD	-2.71	120.74	124.62
24	BC	5506	CLA	O1D-CGD-CBD	-2.71	120.74	124.62
27	BB	5623	BCR	C1-C6-C5	-2.70	118.69	122.66
32	AI	102	LMT	C4-C3-C2	-2.70	100.59	114.53
24	BA	5408	CLA	CAA-C2A-C1A	-2.70	102.96	112.47
34	BD	5403	PHO	C3A-C4A-NA	-2.69	108.86	113.57
27	AC	514	BCR	C23-C22-C21	-2.69	114.66	118.98
24	AC	507	CLA	C7-C6-C5	-2.68	105.14	113.06
24	AB	605	CLA	C2C-C1C-NC	-2.68	108.25	110.24
30	BA	5414	SQD	O8-S-O9	-2.68	105.38	111.61
24	AA	407	CLA	C2C-C1C-NC	-2.67	108.26	110.24
24	AB	606	CLA	CAA-C2A-C1A	-2.67	103.06	112.47
24	BB	5607	CLA	CAA-CBA-CGA	-2.67	105.51	113.32
24	BB	5617	CLA	O1D-CGD-CBD	-2.65	120.82	124.62
24	BB	5606	CLA	C3D-CAD-CBD	-2.64	103.86	107.60
27	BD	5407	BCR	C23-C22-C21	-2.64	114.72	118.98
24	BB	5612	CLA	C3D-CAD-CBD	-2.64	103.86	107.60
24	BC	5505	CLA	C3D-CAD-CBD	-2.64	103.87	107.60
24	AC	503	CLA	C3D-CAD-CBD	-2.63	103.88	107.60
28	AC	517	DGD	C8A-C7A-C6A	-2.63	100.97	114.53
24	BA	5408	CLA	C2C-C1C-NC	-2.62	108.29	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	AA	417	LMG	C15-C14-C13	-2.62	101.00	114.53
24	AC	502	CLA	C2C-C1C-NC	-2.62	108.29	110.24
30	BB	5601	SQD	C3-C4-C5	-2.62	105.63	110.20
24	BC	5501	CLA	O2A-CGA-O1A	-2.62	116.73	123.49
24	AA	404	CLA	C3D-CAD-CBD	-2.62	103.89	107.60
24	AB	601	CLA	O1D-CGD-CBD	-2.62	120.87	124.62
24	AC	513	CLA	O1D-CGD-CBD	-2.61	120.88	124.62
31	AD	408	LMG	C15-C14-C13	-2.61	101.05	114.53
27	BC	5514	BCR	C30-C25-C26	-2.61	118.83	122.66
24	BB	5615	CLA	C3D-CAD-CBD	-2.61	103.91	107.60
27	AB	618	BCR	C1-C6-C5	-2.61	118.83	122.66
27	AB	619	BCR	C1-C6-C5	-2.60	118.84	122.66
24	BC	5504	CLA	C3D-CAD-CBD	-2.60	103.92	107.60
24	AB	608	CLA	C3D-CAD-CBD	-2.60	103.92	107.60
31	BA	5402	LMG	C15-C14-C13	-2.60	101.12	114.53
24	AB	602	CLA	C3D-CAD-CBD	-2.59	103.93	107.60
31	AC	520	LMG	C32-C31-C30	-2.59	101.14	114.53
24	AA	406	CLA	C2C-C1C-NC	-2.59	108.31	110.24
27	BB	5621	BCR	C1-C6-C5	-2.59	118.86	122.66
24	AB	607	CLA	O2A-CGA-O1A	-2.58	116.82	123.49
24	AB	609	CLA	O1D-CGD-CBD	-2.58	120.92	124.62
27	BT	5101	BCR	C8-C9-C10	-2.58	114.83	118.98
24	BB	5607	CLA	C7-C6-C5	-2.58	105.45	113.06
24	AA	406	CLA	CAA-CBA-CGA	-2.58	105.77	113.32
24	BB	5615	CLA	C4-C3-C5	-2.56	111.50	115.41
24	BB	5608	CLA	C3D-CAD-CBD	-2.56	103.98	107.60
24	AB	605	CLA	CAA-CBA-CGA	-2.55	105.86	113.32
24	AB	608	CLA	C4-C3-C5	-2.54	111.53	115.41
31	AA	417	LMG	C32-C31-C30	-2.54	101.42	114.53
31	BC	5520	LMG	C32-C31-C30	-2.54	101.42	114.53
34	AD	403	PHO	C2A-C1A-NA	-2.54	108.83	112.08
29	BA	5415	LHG	C5-O7-C7	-2.53	111.81	117.89
28	BC	5519	DGD	C1D-C2D-C3D	-2.53	104.98	109.97
29	AA	415	LHG	C5-O7-C7	-2.53	111.83	117.89
27	BT	5101	BCR	C19-C18-C17	-2.52	114.92	118.98
30	AB	627	SQD	C3-C4-C5	-2.52	105.80	110.20
27	AT	101	BCR	C8-C9-C10	-2.52	114.92	118.98
27	AT	101	BCR	C19-C18-C17	-2.52	114.92	118.98
27	AT	101	BCR	C23-C22-C21	-2.52	114.92	118.98
24	AA	405	CLA	C2C-C1C-NC	-2.52	108.37	110.24
24	AB	613	CLA	C3D-CAD-CBD	-2.52	104.03	107.60
24	AB	603	CLA	O1D-CGD-CBD	-2.52	121.01	124.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	AA	411	DGD	C5A-C4A-C3A	-2.52	101.53	114.53
24	BC	5506	CLA	C3D-CAD-CBD	-2.52	104.04	107.60
27	AK	102	BCR	C32-C1-C2	-2.52	99.78	108.79
30	AB	622	SQD	O8-S-O9	-2.51	105.76	111.61
31	BA	5402	LMG	C32-C31-C30	-2.51	101.56	114.53
30	BB	5625	SQD	O8-S-O9	-2.51	105.77	111.61
24	AB	603	CLA	CAA-CBA-CGA	-2.51	105.97	113.32
31	AJ	102	LMG	C32-C31-C30	-2.51	101.58	114.53
24	BC	5508	CLA	CAA-CBA-CGA	-2.51	105.98	113.32
28	BC	5517	DGD	C8A-C7A-C6A	-2.50	101.60	114.53
27	BC	5515	BCR	C19-C18-C17	-2.50	114.95	118.98
28	BA	5412	DGD	C5A-C4A-C3A	-2.50	101.62	114.53
24	BC	5501	CLA	O1D-CGD-CBD	-2.50	121.04	124.62
27	AC	515	BCR	C19-C18-C17	-2.50	114.96	118.98
24	BB	5612	CLA	C4-C3-C5	-2.50	111.59	115.41
24	BC	5512	CLA	C3D-CAD-CBD	-2.50	104.07	107.60
24	AB	606	CLA	O2A-CGA-O1A	-2.50	117.05	123.49
24	BA	5406	CLA	C4-C3-C5	-2.49	111.60	115.41
27	AB	617	BCR	C8-C9-C10	-2.49	114.97	118.98
24	AC	512	CLA	O1D-CGD-CBD	-2.49	121.06	124.62
24	AC	504	CLA	C3D-CAD-CBD	-2.49	104.08	107.60
24	AC	503	CLA	CAA-C2A-C1A	-2.49	103.71	112.47
24	AC	505	CLA	O1D-CGD-CBD	-2.48	121.06	124.62
28	AC	517	DGD	O2G-C2G-C1G	-2.48	99.61	108.36
34	BD	5404	PHO	C3A-C4A-NA	-2.48	109.23	113.57
34	AD	403	PHO	C6-C7-C8	-2.48	107.27	115.49
24	AB	610	CLA	C3D-CAD-CBD	-2.48	104.10	107.60
24	BB	5609	CLA	C2C-C1C-NC	-2.47	108.40	110.24
31	BD	5408	LMG	C36-C35-C34	-2.47	101.78	114.53
24	BB	5609	CLA	CAA-CBA-CGA	-2.47	106.09	113.32
27	BD	5407	BCR	C12-C13-C14	-2.47	115.01	118.98
24	BB	5614	CLA	C3D-CAD-CBD	-2.46	104.11	107.60
24	AB	611	CLA	C7-C6-C5	-2.46	105.78	113.06
24	AB	605	CLA	C3D-CAD-CBD	-2.46	104.12	107.60
24	BB	5605	CLA	O1D-CGD-CBD	-2.46	121.09	124.62
27	BA	5411	BCR	C1-C6-C5	-2.46	119.05	122.66
24	BB	5608	CLA	O2A-CGA-O1A	-2.46	117.15	123.49
31	AD	408	LMG	O7-C8-C9	-2.46	99.70	108.36
24	AB	607	CLA	C3D-CAD-CBD	-2.46	104.12	107.60
24	AB	604	CLA	C3D-CAD-CBD	-2.46	104.12	107.60
24	BB	5617	CLA	C3D-CAD-CBD	-2.45	104.13	107.60
24	BC	5503	CLA	CAA-C2A-C1A	-2.45	103.82	112.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	AB	628	DGD	C4A-C3A-C2A	-2.45	104.30	113.29
27	BT	5101	BCR	C40-C30-C29	-2.45	100.02	108.79
30	BF	5102	SQD	C3-C4-C5	-2.45	105.93	110.20
24	BB	5612	CLA	C2C-C1C-NC	-2.45	108.42	110.24
28	AC	519	DGD	O6D-C1D-C2D	-2.45	105.25	110.28
24	BB	5609	CLA	C3D-CAD-CBD	-2.45	104.14	107.60
24	BB	5615	CLA	C7-C6-C5	-2.45	105.84	113.06
31	AB	621	LMG	C7-O1-C1	-2.44	108.68	113.82
31	AM	101	LMG	O7-C10-O9	-2.44	117.11	123.67
36	AF	101	HEM	CAA-C2A-C1A	-2.44	124.36	127.01
31	BD	5408	LMG	C32-C31-C30	-2.44	101.92	114.53
24	AC	508	CLA	CAA-CBA-CGA	-2.44	106.17	113.32
27	BK	5102	BCR	C32-C1-C2	-2.44	100.04	108.79
24	AB	611	CLA	CAA-CBA-CGA	-2.44	106.17	113.32
24	AC	502	CLA	C3D-CAD-CBD	-2.44	104.15	107.60
24	AD	401	CLA	O2A-CGA-O1A	-2.44	117.20	123.49
31	AC	521	LMG	C15-C14-C13	-2.44	101.95	114.53
24	AC	506	CLA	C3D-CAD-CBD	-2.44	104.15	107.60
27	BC	5514	BCR	C12-C13-C14	-2.44	115.06	118.98
24	AB	608	CLA	O1D-CGD-CBD	-2.43	121.14	124.62
32	BB	5627	LMT	C4-C3-C2	-2.43	101.98	114.53
24	AB	613	CLA	C6-C7-C8	-2.43	107.43	115.49
31	AB	620	LMG	O7-C8-C9	-2.43	99.81	108.36
24	AA	406	CLA	CMB-C2B-C1B	-2.43	124.35	128.36
34	AD	402	PHO	C4D-C3D-C2D	-2.42	104.00	106.74
24	BC	5513	CLA	C3D-CAD-CBD	-2.42	104.17	107.60
28	AC	518	DGD	CBA-CAA-C9A	-2.42	102.03	114.53
28	BC	5518	DGD	CBA-CAA-C9A	-2.42	102.05	114.53
31	BC	5521	LMG	C15-C14-C13	-2.42	102.05	114.53
27	AB	617	BCR	C1-C6-C5	-2.42	119.11	122.66
36	BF	5101	HEM	CAA-C2A-C1A	-2.42	124.39	127.01
24	BB	5616	CLA	C3D-CAD-CBD	-2.42	104.18	107.60
24	BB	5616	CLA	CAA-CBA-CGA	-2.41	106.25	113.32
24	AC	508	CLA	O2A-CGA-O1A	-2.41	117.26	123.49
24	BB	5606	CLA	O1D-CGD-CBD	-2.41	121.17	124.62
31	BB	5624	LMG	C40-C39-C38	-2.41	102.10	114.53
24	AC	512	CLA	C3D-CAD-CBD	-2.41	104.19	107.60
24	AC	513	CLA	C3D-CAD-CBD	-2.40	104.20	107.60
27	BB	5621	BCR	C12-C13-C14	-2.40	115.11	118.98
24	BA	5407	CLA	CAA-CBA-CGA	-2.40	106.29	113.32
24	AB	612	CLA	CAA-CBA-CGA	-2.40	106.29	113.32
27	BT	5101	BCR	C23-C22-C21	-2.40	115.12	118.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	AB	624	LMT	C4-C3-C2	-2.40	102.15	114.53
24	BA	5406	CLA	C2C-C1C-NC	-2.40	108.46	110.24
31	BL	5101	LMG	O7-C8-C9	-2.39	99.92	108.36
31	BM	5102	LMG	O7-C10-O9	-2.39	117.25	123.67
24	AB	613	CLA	O1D-CGD-CBD	-2.39	121.19	124.62
31	AB	621	LMG	C40-C39-C38	-2.39	102.18	114.53
24	BB	5613	CLA	O1D-CGD-CBD	-2.39	121.20	124.62
28	BC	5517	DGD	CBA-CAA-C9A	-2.39	102.21	114.53
24	AC	501	CLA	O1D-CGD-CBD	-2.39	121.20	124.62
36	AF	101	HEM	C3B-CAB-CBB	-2.38	120.80	124.46
24	BB	5612	CLA	O1D-CGD-CBD	-2.38	121.21	124.62
24	AB	612	CLA	C3D-CAD-CBD	-2.38	104.23	107.60
27	BB	5621	BCR	C19-C18-C17	-2.38	115.15	118.98
31	BD	5410	LMG	O7-C8-C9	-2.38	99.99	108.36
24	AC	501	CLA	O2A-CGA-O1A	-2.38	117.36	123.49
27	BD	5407	BCR	C8-C9-C10	-2.37	115.16	118.98
28	BB	5602	DGD	C4A-C3A-C2A	-2.37	104.59	113.29
28	AC	517	DGD	CBA-CAA-C9A	-2.37	102.29	114.53
27	BA	5411	BCR	C12-C13-C14	-2.37	115.17	118.98
28	BC	5519	DGD	O1G-C1A-O1A	-2.37	117.38	123.49
24	AA	406	CLA	C3D-CAD-CBD	-2.37	104.25	107.60
31	BM	5102	LMG	C14-C13-C12	-2.36	102.33	114.53
27	BC	5516	BCR	C23-C22-C21	-2.36	115.18	118.98
24	BB	5607	CLA	CMB-C2B-C1B	-2.36	124.46	128.36
24	BC	5508	CLA	O2A-CGA-O1A	-2.36	117.41	123.49
24	BB	5608	CLA	C6-C7-C8	-2.35	107.68	115.49
24	AC	510	CLA	O2A-CGA-O1A	-2.35	117.42	123.49
27	AC	514	BCR	C12-C13-C14	-2.35	115.19	118.98
24	BC	5511	CLA	C3D-CAD-CBD	-2.35	104.27	107.60
31	BC	5520	LMG	O1-C7-C8	-2.35	105.40	110.99
24	AC	511	CLA	C3D-CAD-CBD	-2.35	104.28	107.60
34	AD	403	PHO	C3A-C4A-NA	-2.35	109.47	113.57
28	BC	5517	DGD	O2G-C2G-C1G	-2.34	100.10	108.36
24	BA	5405	CLA	CAA-C2A-C3A	-2.34	106.48	113.22
24	BC	5509	CLA	C3D-CAD-CBD	-2.34	104.28	107.60
28	AB	628	DGD	C6B-C5B-C4B	-2.34	102.44	114.53
24	BB	5613	CLA	O2A-CGA-O1A	-2.34	117.45	123.49
31	AM	101	LMG	C14-C13-C12	-2.34	102.44	114.53
27	AT	101	BCR	C40-C30-C29	-2.34	100.41	108.79
30	BF	5102	SQD	O8-S-O9	-2.34	106.17	111.61
27	AB	617	BCR	C12-C13-C14	-2.34	115.22	118.98
31	AJ	102	LMG	C36-C35-C34	-2.34	102.47	114.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BD	5404	PHO	C4-C3-C5	-2.34	111.84	115.41
24	BB	5608	CLA	CAA-C2A-C1A	-2.33	104.24	112.47
24	AB	602	CLA	O1D-CGD-CBD	-2.33	121.28	124.62
31	AC	521	LMG	C19-C18-C17	-2.33	102.48	114.53
30	AF	102	SQD	C3-C4-C5	-2.33	106.13	110.20
24	BB	5619	CLA	C2C-C1C-NC	-2.33	108.51	110.24
24	AD	401	CLA	C6-C7-C8	-2.33	107.76	115.49
24	BB	5611	CLA	C3D-CAD-CBD	-2.33	104.30	107.60
36	BF	5101	HEM	C3B-CAB-CBB	-2.33	120.89	124.46
28	BE	5102	DGD	C5B-C4B-C3B	-2.33	102.52	114.53
24	BB	5611	CLA	OBD-CAD-CBD	-2.32	122.43	125.94
31	BB	5624	LMG	C7-O1-C1	-2.32	108.95	113.82
24	BC	5511	CLA	CAA-CBA-CGA	-2.32	106.53	113.32
24	AB	606	CLA	CAA-C2A-C3A	-2.32	106.55	113.22
24	BA	5405	CLA	C2C-C1C-NC	-2.31	108.52	110.24
24	AB	604	CLA	CAA-C2A-C1A	-2.31	104.31	112.47
24	AA	405	CLA	C4-C3-C5	-2.31	111.88	115.41
24	AA	404	CLA	CAA-C2A-C3A	-2.31	106.58	113.22
24	AA	407	CLA	C3D-CAD-CBD	-2.31	104.33	107.60
24	AC	511	CLA	CAA-CBA-CGA	-2.31	106.56	113.32
24	AA	405	CLA	CMB-C2B-C1B	-2.30	124.55	128.36
28	BB	5602	DGD	C6B-C5B-C4B	-2.30	102.64	114.53
34	AD	403	PHO	C4-C3-C5	-2.30	111.90	115.41
24	AB	603	CLA	CMB-C2B-C1B	-2.30	124.56	128.36
24	BD	5402	CLA	C6-C7-C8	-2.29	107.88	115.49
31	BD	5409	LMG	C32-C31-C30	-2.29	102.70	114.53
28	AE	101	DGD	C5B-C4B-C3B	-2.29	102.71	114.53
24	BD	5405	CLA	CAA-CBA-CGA	-2.29	106.62	113.32
24	AB	604	CLA	OBD-CAD-CBD	-2.28	122.49	125.94
27	BC	5514	BCR	C32-C1-C2	-2.28	100.62	108.79
24	BC	5502	CLA	C2C-C1C-NC	-2.28	108.55	110.24
24	AB	604	CLA	O2A-CGA-O1A	-2.28	117.62	123.49
27	AB	617	BCR	C19-C18-C17	-2.27	115.32	118.98
24	BB	5608	CLA	C2C-C1C-NC	-2.27	108.55	110.24
24	AA	407	CLA	O2A-CGA-O1A	-2.27	117.63	123.49
24	BB	5610	CLA	CAA-C2A-C3A	-2.27	106.70	113.22
31	BL	5101	LMG	C19-C18-C17	-2.27	102.83	114.53
27	BB	5621	BCR	C8-C9-C10	-2.26	115.33	118.98
24	AD	404	CLA	C3D-CAD-CBD	-2.26	104.40	107.60
24	BA	5407	CLA	C3D-CAD-CBD	-2.26	104.40	107.60
31	AC	520	LMG	O9-C10-C11	-2.26	114.69	123.72
31	BC	5520	LMG	O9-C10-C11	-2.26	114.70	123.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	604	CLA	C6-C7-C8	-2.26	108.00	115.49
31	AD	407	LMG	C32-C31-C30	-2.25	102.89	114.53
34	BD	5403	PHO	C4D-C3D-C2D	-2.25	104.19	106.74
35	BD	5406	PL9	C42-C41-C39	-2.25	105.38	112.71
24	BC	5510	CLA	C3B-CAB-CBB	-2.25	121.72	126.32
31	AC	520	LMG	O1-C7-C8	-2.25	105.64	110.99
24	AB	611	CLA	OBD-CAD-CBD	-2.24	122.56	125.94
24	AC	509	CLA	C3D-CAD-CBD	-2.24	104.43	107.60
24	AC	505	CLA	C3D-CAD-CBD	-2.24	104.43	107.60
30	AA	413	SQD	O8-S-O9	-2.24	106.40	111.61
24	BA	5406	CLA	CMB-C2B-C1B	-2.24	124.67	128.36
28	BH	5101	DGD	O2G-C1B-O1B	-2.23	117.67	123.67
24	BA	5408	CLA	O2A-CGA-O1A	-2.23	117.73	123.49
24	BC	5503	CLA	CAA-CBA-CGA	-2.23	106.78	113.32
31	AD	408	LMG	O8-C9-C8	-2.23	102.68	108.69
30	AF	102	SQD	O8-S-O9	-2.23	106.41	111.61
28	AC	518	DGD	CDB-CCB-CBB	-2.23	103.01	114.53
24	AB	611	CLA	C3D-CAD-CBD	-2.23	104.45	107.60
24	BB	5615	CLA	CMB-C2B-C1B	-2.23	124.68	128.36
31	AC	520	LMG	O7-C10-O9	-2.22	117.70	123.67
24	BB	5615	CLA	CAA-CBA-CGA	-2.22	106.81	113.32
31	BD	5410	LMG	O8-C9-C8	-2.22	102.71	108.69
24	BD	5402	CLA	O2A-CGA-O1A	-2.22	117.76	123.49
24	AA	404	CLA	O1D-CGD-CBD	-2.22	121.44	124.62
31	BC	5521	LMG	C19-C18-C17	-2.22	103.07	114.53
24	AC	502	CLA	CAA-CBA-CGA	-2.22	106.82	113.32
27	BC	5516	BCR	C32-C1-C2	-2.22	100.84	108.79
31	AB	620	LMG	C19-C18-C17	-2.22	103.08	114.53
28	BC	5518	DGD	CDB-CCB-CBB	-2.22	103.09	114.53
34	BD	5404	PHO	C6-C7-C8	-2.21	108.14	115.49
27	BC	5516	BCR	C19-C18-C17	-2.21	115.42	118.98
31	BD	5409	LMG	C1-O6-C5	-2.21	109.45	113.75
24	AB	610	CLA	CMB-C2B-C1B	-2.21	124.70	128.36
24	AB	603	CLA	C3D-CAD-CBD	-2.21	104.47	107.60
28	AC	518	DGD	C8B-C7B-C6B	-2.21	103.11	114.53
24	BB	5614	CLA	CMB-C2B-C1B	-2.21	124.71	128.36
27	AA	410	BCR	C8-C9-C10	-2.21	115.42	118.98
24	BC	5507	CLA	C3D-CAD-CBD	-2.21	104.47	107.60
24	BC	5510	CLA	O2A-CGA-O1A	-2.21	117.80	123.49
31	AB	620	LMG	C17-C16-C15	-2.20	103.15	114.53
24	AB	611	CLA	C4-C3-C5	-2.20	112.04	115.41
24	AB	613	CLA	C2C-C1C-NC	-2.20	108.60	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	607	CLA	O1D-CGD-CBD	-2.20	121.47	124.62
28	BC	5518	DGD	C8B-C7B-C6B	-2.20	103.17	114.53
24	BB	5610	CLA	CMB-C2B-C1B	-2.20	124.73	128.36
24	AB	604	CLA	C2C-C1C-NC	-2.20	108.61	110.24
24	AC	505	CLA	CMB-C2B-C1B	-2.19	124.74	128.36
27	AC	516	BCR	C23-C22-C21	-2.19	115.45	118.98
24	BC	5512	CLA	O1D-CGD-CBD	-2.19	121.48	124.62
24	AB	614	CLA	O1D-CGD-CBD	-2.19	121.48	124.62
27	BA	5411	BCR	C8-C9-C10	-2.19	115.46	118.98
31	BL	5101	LMG	C17-C16-C15	-2.18	103.25	114.53
27	BK	5102	BCR	C40-C30-C29	-2.18	100.97	108.79
24	BB	5618	CLA	C3D-CAD-CBD	-2.18	104.51	107.60
24	BA	5406	CLA	C12-C11-C10	-2.18	102.16	112.99
24	BD	5402	CLA	C4-C3-C5	-2.18	112.07	115.41
27	AB	618	BCR	C23-C22-C21	-2.18	115.47	118.98
24	AD	401	CLA	CMB-C2B-C1B	-2.18	124.75	128.36
24	AC	503	CLA	CAA-CBA-CGA	-2.18	106.93	113.32
24	AB	601	CLA	CMB-C2B-C1B	-2.18	124.76	128.36
24	BB	5605	CLA	CMB-C2B-C1B	-2.18	124.76	128.36
27	AB	619	BCR	C12-C13-C14	-2.18	115.48	118.98
24	AB	614	CLA	C3D-CAD-CBD	-2.18	104.52	107.60
35	AD	405	PL9	C42-C41-C39	-2.18	105.62	112.71
35	BD	5406	PL9	C31-C29-C28	-2.17	116.93	121.05
24	AB	615	CLA	C3D-CAD-CBD	-2.17	104.53	107.60
31	BC	5521	LMG	C17-C16-C15	-2.17	103.31	114.53
27	AD	406	BCR	C8-C9-C10	-2.17	115.49	118.98
35	AD	405	PL9	C31-C29-C28	-2.17	116.94	121.05
24	BC	5505	CLA	O1D-CGD-CBD	-2.16	121.52	124.62
24	BB	5613	CLA	C3D-CAD-CBD	-2.16	104.54	107.60
24	BD	5402	CLA	CMB-C2B-C1B	-2.16	124.79	128.36
24	BB	5613	CLA	CAA-C2A-C1A	-2.16	104.85	112.47
28	AH	101	DGD	O2G-C1B-O1B	-2.16	117.87	123.67
27	AC	516	BCR	C32-C1-C2	-2.16	101.05	108.79
24	AA	406	CLA	OBD-CAD-CBD	-2.16	122.68	125.94
24	BB	5606	CLA	CAA-CBA-CGA	-2.16	107.00	113.32
31	BD	5409	LMG	C6-C5-C4	-2.16	107.70	113.02
24	AC	510	CLA	C3D-CAD-CBD	-2.15	104.55	107.60
27	AC	514	BCR	C32-C1-C2	-2.15	101.07	108.79
27	AD	406	BCR	C19-C18-C17	-2.15	115.51	118.98
24	BD	5405	CLA	C3D-CAD-CBD	-2.15	104.55	107.60
27	AA	410	BCR	C12-C13-C14	-2.15	115.52	118.98
24	BC	5505	CLA	CMB-C2B-C1B	-2.15	124.81	128.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	602	CLA	O2A-CGA-O1A	-2.15	117.94	123.49
24	AB	609	CLA	CAA-C2A-C1A	-2.15	104.90	112.47
24	BD	5402	CLA	C3D-CAD-CBD	-2.15	104.56	107.60
24	BA	5407	CLA	OBD-CAD-CBD	-2.14	122.70	125.94
34	BD	5403	PHO	C4-C3-C5	-2.14	112.13	115.41
24	BB	5617	CLA	C6-C7-C8	-2.14	108.40	115.49
24	BB	5611	CLA	O1D-CGD-CBD	-2.14	121.56	124.62
24	BB	5610	CLA	C2C-C1C-NC	-2.13	108.66	110.24
24	AC	507	CLA	C3D-CAD-CBD	-2.13	104.58	107.60
24	AB	609	CLA	C6-C7-C8	-2.13	108.43	115.49
24	BA	5407	CLA	CMB-C2B-C1B	-2.13	124.84	128.36
24	AA	407	CLA	OBD-CAD-CBD	-2.13	122.73	125.94
27	BC	5515	BCR	C32-C1-C2	-2.12	101.18	108.79
27	BD	5407	BCR	C19-C18-C17	-2.12	115.56	118.98
24	AA	404	CLA	C6-C7-C8	-2.12	108.45	115.49
24	AB	605	CLA	CAA-C2A-C3A	-2.12	107.12	113.22
31	AC	521	LMG	O7-C8-C9	-2.12	100.89	108.36
28	BA	5412	DGD	O1A-C1A-C2A	-2.12	115.25	123.72
36	BV	5201	HEM	C3B-CAB-CBB	-2.11	121.22	124.46
32	AB	624	LMT	C1'-O5'-C5'	-2.11	109.65	113.75
24	AB	606	CLA	O1D-CGD-CBD	-2.11	121.60	124.62
24	BB	5613	CLA	OBD-CAD-CBD	-2.11	122.75	125.94
30	BA	5414	SQD	C3-C4-C5	-2.11	106.52	110.20
24	AB	606	CLA	C2C-C1C-NC	-2.11	108.67	110.24
24	AA	404	CLA	C2C-C1C-NC	-2.10	108.68	110.24
24	AB	609	CLA	O2A-CGA-O1A	-2.10	118.07	123.49
24	AB	607	CLA	OBD-CAD-CBD	-2.10	122.77	125.94
24	AB	604	CLA	O1D-CGD-CBD	-2.10	121.61	124.62
24	BB	5609	CLA	CAA-C2A-C3A	-2.10	107.18	113.22
27	BK	5102	BCR	C23-C22-C21	-2.10	115.60	118.98
31	AC	521	LMG	C17-C16-C15	-2.10	103.69	114.53
24	BB	5613	CLA	CMB-C2B-C1B	-2.10	124.90	128.36
24	AB	611	CLA	O2A-CGA-O1A	-2.09	118.09	123.49
32	AI	103	LMT	C3'-C4'-C5'	-2.09	106.11	110.84
31	BD	5408	LMG	C17-C16-C15	-2.09	103.73	114.53
24	BC	5506	CLA	O2A-CGA-O1A	-2.09	118.10	123.49
24	BC	5513	CLA	O2A-CGA-O1A	-2.09	118.10	123.49
30	BB	5601	SQD	O8-S-O9	-2.09	106.75	111.61
24	BB	5613	CLA	C6-C7-C8	-2.09	108.56	115.49
24	AD	404	CLA	CAA-CBA-CGA	-2.09	107.21	113.32
24	AC	503	CLA	C4-C3-C5	-2.09	112.22	115.41
27	AB	619	BCR	C23-C22-C21	-2.08	115.62	118.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5615	CLA	O2A-CGA-O1A	-2.08	118.12	123.49
24	AC	513	CLA	O2A-CGA-O1A	-2.08	118.13	123.49
24	BC	5503	CLA	C4-C3-C5	-2.08	112.23	115.41
24	AA	405	CLA	CAA-C2A-C3A	-2.07	107.25	113.22
28	AA	411	DGD	O1A-C1A-C2A	-2.07	115.43	123.72
24	AB	609	CLA	C3D-CAD-CBD	-2.07	104.67	107.60
24	BA	5408	CLA	CMB-C2B-C1B	-2.07	124.94	128.36
27	BB	5622	BCR	C23-C22-C21	-2.07	115.64	118.98
24	AA	404	CLA	CMB-C2B-C1B	-2.07	124.94	128.36
31	BC	5521	LMG	O7-C8-C9	-2.07	101.06	108.36
30	AA	413	SQD	C3-C4-C5	-2.07	106.59	110.20
24	BC	5502	CLA	CAA-CBA-CGA	-2.07	107.26	113.32
24	AB	602	CLA	CAA-CBA-CGA	-2.07	107.26	113.32
24	BB	5608	CLA	CAA-CBA-CGA	-2.07	107.26	113.32
30	AA	413	SQD	O6-C44-C45	-2.06	106.08	110.99
31	BM	5102	LMG	C6-C5-C4	-2.06	107.93	113.02
31	BC	5520	LMG	O7-C10-O9	-2.06	118.14	123.67
24	BC	5504	CLA	CMB-C2B-C1B	-2.06	124.96	128.36
31	AM	101	LMG	C6-C5-C4	-2.06	107.94	113.02
24	AC	503	CLA	C2C-C1C-NC	-2.06	108.71	110.24
28	AE	101	DGD	C4A-C3A-C2A	-2.06	105.75	113.29
24	AA	405	CLA	C12-C11-C10	-2.05	102.80	112.99
32	BI	5102	LMT	C9-C8-C7	-2.05	103.92	114.53
27	BJ	5101	BCR	C40-C30-C29	-2.05	101.43	108.79
24	AC	506	CLA	C2C-C1C-NC	-2.05	108.71	110.24
24	AC	506	CLA	O2A-CGA-O1A	-2.05	118.20	123.49
28	BA	5412	DGD	O1B-C1B-C2B	-2.05	115.52	123.72
31	AC	520	LMG	C36-C35-C34	-2.05	103.94	114.53
24	AD	401	CLA	OBD-CAD-CBD	-2.05	122.84	125.94
34	BD	5404	PHO	O2A-CGA-O1A	-2.05	118.20	123.49
24	BA	5405	CLA	C7-C6-C5	-2.05	107.02	113.06
24	BB	5618	CLA	O1D-CGD-CBD	-2.05	121.69	124.62
27	AC	516	BCR	C19-C18-C17	-2.05	115.69	118.98
32	BB	5627	LMT	C1'-O5'-C5'	-2.04	109.78	113.75
31	AC	520	LMG	O1-C1-C2	-2.04	105.46	108.04
31	BC	5520	LMG	C6-C5-C4	-2.04	107.98	113.02
24	AB	611	CLA	CMB-C2B-C1B	-2.04	124.99	128.36
30	BB	5601	SQD	O48-C23-O10	-2.04	118.23	123.49
30	AB	627	SQD	O8-S-O9	-2.04	106.86	111.61
27	BC	5514	BCR	C8-C9-C10	-2.04	115.70	118.98
24	BC	5506	CLA	CAA-CBA-CGA	-2.04	107.35	113.32
28	AE	101	DGD	C6D-C5D-C4D	-2.04	107.41	112.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AC	515	BCR	C32-C1-C2	-2.04	101.50	108.79
31	AD	407	LMG	C1-O6-C5	-2.04	109.79	113.75
27	AD	406	BCR	C40-C30-C29	-2.04	101.50	108.79
30	BF	5102	SQD	O3-C3-C2	-2.04	105.75	110.34
24	AB	609	CLA	C2C-C1C-NC	-2.03	108.73	110.24
34	AD	402	PHO	CBD-CHA-C4D	-2.03	106.19	108.46
27	BC	5515	BCR	C8-C9-C10	-2.03	115.71	118.98
24	AA	407	CLA	CAA-CBA-CGA	-2.03	107.38	113.32
31	BC	5520	LMG	O1-C1-C2	-2.03	105.48	108.04
34	BD	5403	PHO	CBD-CHA-C4D	-2.03	106.19	108.46
28	AA	411	DGD	O1B-C1B-C2B	-2.03	115.62	123.72
30	BA	5401	SQD	O8-S-O9	-2.03	106.90	111.61
24	BB	5619	CLA	C3D-CAD-CBD	-2.02	104.73	107.60
27	AX	101	BCR	C32-C1-C2	-2.02	101.53	108.79
24	BA	5405	CLA	CAA-CBA-CGA	-2.02	107.39	113.32
36	AV	201	HEM	C3B-CAB-CBB	-2.02	121.35	124.46
24	AB	615	CLA	C2C-C1C-NC	-2.02	108.74	110.24
24	BC	5506	CLA	C2C-C1C-NC	-2.02	108.74	110.24
24	BC	5509	CLA	C3B-CAB-CBB	-2.02	122.19	126.32
24	BB	5614	CLA	O2A-CGA-O1A	-2.02	118.28	123.49
24	AB	604	CLA	CAA-CBA-CGA	-2.02	107.42	113.32
28	AC	519	DGD	C3E-C4E-C5E	-2.02	106.68	110.20
27	AC	516	BCR	C12-C13-C14	-2.01	115.74	118.98
32	AI	102	LMT	C9-C8-C7	-2.01	104.14	114.53
24	BB	5614	CLA	C3B-CAB-CBB	-2.01	122.20	126.32
24	BA	5408	CLA	CAA-CBA-CGA	-2.01	107.43	113.32
24	BB	5608	CLA	OBD-CAD-CBD	-2.01	122.90	125.94
24	BA	5405	CLA	O1D-CGD-CBD	-2.01	121.74	124.62
31	AJ	102	LMG	C17-C16-C15	-2.01	104.15	114.53
27	AA	410	BCR	C19-C18-C17	-2.01	115.74	118.98
27	AC	514	BCR	C40-C30-C29	-2.01	101.59	108.79
24	AB	616	CLA	C3D-CAD-CBD	-2.01	104.75	107.60
24	AD	401	CLA	C4-C3-C5	-2.01	112.34	115.41
27	AK	102	BCR	C40-C30-C29	-2.01	101.59	108.79
28	AC	519	DGD	O1G-C1A-O1A	-2.01	118.31	123.49
28	AH	101	DGD	O1B-C1B-C2B	-2.01	115.69	123.72
24	AC	513	CLA	CMB-C2B-C1B	-2.01	125.04	128.36
27	BB	5623	BCR	C23-C22-C21	-2.01	115.75	118.98
28	BE	5102	DGD	C6E-C5E-C4E	-2.01	108.07	113.02
24	BB	5620	CLA	C3D-CAD-CBD	-2.00	104.76	107.60
24	AD	404	CLA	O2A-CGA-O1A	-2.00	118.33	123.49
24	AB	610	CLA	C3B-CAB-CBB	-2.00	122.22	126.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AJ	101	BCR	C40-C30-C29	-2.00	101.62	108.79
30	AA	416	SQD	O8-S-O9	-2.00	106.95	111.61
28	BE	5102	DGD	C4A-C3A-C2A	-2.00	105.95	113.29
24	AB	614	CLA	OBD-CAD-C3D	2.00	132.44	128.35
30	BA	5414	SQD	O47-C7-C8	2.00	115.88	111.53
24	BB	5605	CLA	C3A-C2A-C1A	2.00	104.90	101.50
24	AC	513	CLA	C2A-C1A-CHA	2.00	127.58	123.89
28	AC	519	DGD	C4D-C3D-C2D	2.00	114.53	110.79
24	AB	606	CLA	OBD-CAD-C3D	2.00	132.45	128.35
24	BB	5615	CLA	CHC-C1C-NC	2.01	127.45	123.67
24	AC	504	CLA	C1D-CHD-C4C	2.01	125.64	122.60
27	BB	5623	BCR	C30-C25-C24	2.01	121.45	115.82
27	AC	514	BCR	C30-C25-C24	2.01	121.45	115.82
24	AC	510	CLA	C1D-CHD-C4C	2.01	125.65	122.60
27	AT	101	BCR	C34-C9-C8	2.01	121.45	118.10
24	BB	5612	CLA	C1D-CHD-C4C	2.01	125.65	122.60
30	BA	5414	SQD	C13-C12-C11	2.01	124.93	114.53
24	BC	5504	CLA	C1D-CHD-C4C	2.01	125.65	122.60
27	AC	514	BCR	C20-C21-C22	2.01	130.11	127.20
31	BM	5102	LMG	C34-C33-C32	2.01	124.93	114.53
27	AK	102	BCR	C11-C12-C13	2.01	132.25	126.32
27	AX	101	BCR	C32-C1-C6	2.01	113.46	110.30
27	BC	5514	BCR	C20-C21-C22	2.02	130.11	127.20
28	AA	411	DGD	C3G-C2G-C1G	2.02	116.79	112.07
30	BF	5102	SQD	C17-C16-C15	2.02	124.96	114.53
27	AB	618	BCR	C37-C22-C23	2.02	121.46	118.10
27	BC	5514	BCR	C36-C18-C19	2.02	121.46	118.10
27	BC	5515	BCR	C11-C10-C9	2.02	130.12	127.20
27	BB	5623	BCR	C16-C17-C18	2.02	130.12	127.20
28	BA	5412	DGD	O3D-C3D-C2D	2.02	114.89	110.34
24	AB	612	CLA	CED-O2D-CGD	2.02	120.73	115.99
24	AC	502	CLA	OBD-CAD-C3D	2.02	132.49	128.35
27	AJ	101	BCR	C30-C25-C24	2.02	121.49	115.82
24	AC	508	CLA	OBD-CAD-C3D	2.02	132.49	128.35
30	BA	5414	SQD	O47-C45-C44	2.03	115.50	108.36
24	AA	404	CLA	C1D-CHD-C4C	2.03	125.67	122.60
31	AB	621	LMG	C9-O8-C28	2.03	122.52	116.85
24	BC	5505	CLA	C1D-CHD-C4C	2.03	125.67	122.60
27	AA	410	BCR	C32-C1-C6	2.03	113.48	110.30
24	BA	5406	CLA	C5-C3-C2	2.03	124.90	121.05
28	AA	411	DGD	O3D-C3D-C2D	2.03	114.91	110.34
27	BX	5101	BCR	C34-C9-C8	2.03	121.47	118.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AC	504	CLA	CED-O2D-CGD	2.03	120.75	115.99
27	BX	5101	BCR	C37-C22-C23	2.03	121.48	118.10
28	BH	5101	DGD	O1G-C1A-C2A	2.03	118.09	111.90
27	AC	515	BCR	C11-C10-C9	2.03	130.13	127.20
24	BC	5503	CLA	C5-C3-C2	2.03	124.91	121.05
27	BC	5514	BCR	C28-C27-C26	2.04	117.10	113.87
28	AC	518	DGD	O6E-C1E-C2E	2.04	114.45	110.28
27	BT	5101	BCR	C34-C9-C8	2.04	121.49	118.10
27	BB	5621	BCR	C34-C9-C8	2.04	121.49	118.10
24	AB	608	CLA	OBD-CAD-C3D	2.04	132.52	128.35
24	AC	507	CLA	C1D-CHD-C4C	2.04	125.69	122.60
24	BB	5611	CLA	CED-O2D-CGD	2.04	120.78	115.99
27	BC	5515	BCR	C32-C1-C6	2.04	113.50	110.30
30	AB	627	SQD	C15-C14-C13	2.04	125.07	114.53
27	AD	406	BCR	C20-C21-C22	2.04	130.15	127.20
32	BM	5101	LMT	C6B-C5B-C4B	2.05	118.06	113.02
24	AB	602	CLA	OBD-CAD-C3D	2.05	132.53	128.35
27	BB	5623	BCR	C37-C22-C23	2.05	121.50	118.10
28	AE	101	DGD	C3G-C2G-C1G	2.05	116.86	112.07
34	BD	5403	PHO	C1B-NB-C4B	2.05	110.57	106.51
32	AI	103	LMT	C3-C2-C1	2.05	122.64	113.47
24	BB	5617	CLA	OBD-CAD-C3D	2.05	132.55	128.35
24	AC	511	CLA	OBD-CAD-C3D	2.05	132.55	128.35
27	AB	619	BCR	C16-C17-C18	2.05	130.16	127.20
24	BC	5507	CLA	C3A-C2A-C1A	2.05	104.98	101.50
24	AA	406	CLA	CED-O2D-CGD	2.06	120.81	115.99
30	AA	416	SQD	C17-C16-C15	2.06	125.15	114.53
30	AF	102	SQD	C17-C16-C15	2.06	125.16	114.53
27	AB	619	BCR	C30-C25-C24	2.06	121.59	115.82
31	BB	5624	LMG	C9-O8-C28	2.06	122.62	116.85
32	BC	5522	LMT	C6B-C5B-C4B	2.06	118.11	113.02
24	AC	513	CLA	OBD-CAD-C3D	2.06	132.57	128.35
27	AC	514	BCR	C36-C18-C19	2.06	121.53	118.10
32	BM	5101	LMT	O1B-C1B-C2B	2.07	113.13	108.10
30	AF	102	SQD	C32-C31-C30	2.07	129.67	113.44
24	AB	613	CLA	CED-O2D-CGD	2.07	120.84	115.99
28	AC	518	DGD	O6E-C5E-C4E	2.07	113.56	109.68
24	BC	5502	CLA	OBD-CAD-C3D	2.07	132.57	128.35
30	AA	413	SQD	C17-C16-C15	2.07	125.21	114.53
27	BA	5411	BCR	C34-C9-C8	2.07	121.54	118.10
24	BC	5509	CLA	CBA-CAA-C2A	2.07	119.57	113.73
27	AC	515	BCR	C32-C1-C6	2.07	113.55	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BC	5503	CLA	C2A-C1A-CHA	2.07	127.70	123.89
30	BB	5601	SQD	C15-C14-C13	2.07	125.23	114.53
31	AD	407	LMG	C9-O8-C28	2.07	122.65	116.85
27	BB	5621	BCR	C24-C23-C22	2.07	129.38	126.22
27	AK	102	BCR	C28-C27-C26	2.07	117.16	113.87
27	BC	5515	BCR	C7-C8-C9	2.08	129.38	126.22
24	AA	405	CLA	OBD-CAD-C3D	2.08	132.59	128.35
24	AC	510	CLA	C3A-C2A-C1A	2.08	105.02	101.50
24	BC	5512	CLA	C1D-CHD-C4C	2.08	125.75	122.60
24	AA	405	CLA	C2A-C1A-CHA	2.08	127.72	123.89
31	BD	5408	LMG	C35-C34-C33	2.08	125.28	114.53
24	AC	512	CLA	C3A-C2A-C1A	2.08	105.03	101.50
31	AC	521	LMG	O1-C7-C8	2.08	115.94	110.99
31	AJ	102	LMG	C35-C34-C33	2.08	125.29	114.53
30	BF	5102	SQD	C32-C31-C30	2.08	129.81	113.44
24	AC	509	CLA	CBA-CAA-C2A	2.09	119.62	113.73
30	AA	413	SQD	O47-C45-C44	2.09	115.72	108.36
24	BC	5506	CLA	OBD-CAD-C3D	2.09	132.62	128.35
36	BV	5201	HEM	CAD-CBD-CGD	2.09	121.54	113.02
24	AC	511	CLA	C3A-C2A-C1A	2.09	105.04	101.50
24	BB	5612	CLA	OBD-CAD-C3D	2.09	132.62	128.35
24	AC	513	CLA	C3A-C2A-C1A	2.09	105.05	101.50
27	BC	5514	BCR	C30-C25-C24	2.09	121.68	115.82
27	AA	410	BCR	C34-C9-C8	2.09	121.58	118.10
28	BC	5518	DGD	O6E-C1E-C2E	2.10	114.58	110.28
27	AC	516	BCR	C36-C18-C19	2.10	121.58	118.10
31	AC	520	LMG	O8-C28-C29	2.10	118.29	111.90
27	BD	5407	BCR	C15-C14-C13	2.10	130.23	127.20
34	AD	402	PHO	CBD-CHA-C1A	2.10	131.30	126.36
27	BC	5515	BCR	C24-C23-C22	2.10	129.42	126.22
27	BA	5411	BCR	C1-C6-C7	2.10	121.70	115.82
24	AB	614	CLA	C2A-C1A-CHA	2.10	127.75	123.89
27	BA	5411	BCR	C32-C1-C6	2.10	113.60	110.30
36	AV	201	HEM	CAD-CBD-CGD	2.10	121.59	113.02
27	BB	5622	BCR	C37-C22-C23	2.10	121.60	118.10
24	BB	5614	CLA	CED-O2D-CGD	2.10	120.93	115.99
30	AA	413	SQD	O47-C7-C8	2.11	116.11	111.53
32	AM	102	LMT	O1B-C1B-C2B	2.11	113.23	108.10
24	BC	5513	CLA	C3A-C2A-C1A	2.11	105.08	101.50
30	BA	5414	SQD	C17-C16-C15	2.11	125.44	114.53
28	BC	5519	DGD	O3G-C3G-C2G	2.11	116.02	110.99
31	AA	417	LMG	O1-C1-C2	2.12	110.71	108.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BX	5101	BCR	C36-C18-C19	2.12	121.62	118.10
24	AC	507	CLA	C3A-C2A-C1A	2.12	105.09	101.50
24	AC	506	CLA	OBD-CAD-C3D	2.12	132.68	128.35
24	BD	5402	CLA	C3A-C2A-C1A	2.12	105.09	101.50
24	AB	601	CLA	C3A-C2A-C1A	2.12	105.09	101.50
24	BB	5610	CLA	OBD-CAD-C3D	2.12	132.68	128.35
24	AD	401	CLA	C3A-C2A-C1A	2.12	105.10	101.50
24	AC	505	CLA	C1D-CHD-C4C	2.12	125.81	122.60
27	BB	5621	BCR	C8-C7-C6	2.13	133.71	127.32
24	BB	5616	CLA	OBD-CAD-C3D	2.13	132.70	128.35
36	AF	101	HEM	CAD-C3D-C4D	2.13	119.98	112.47
34	BD	5403	PHO	CBD-CHA-C1A	2.13	131.38	126.36
24	BB	5613	CLA	OBD-CAD-C3D	2.13	132.71	128.35
27	AB	619	BCR	C40-C30-C25	2.13	113.65	110.30
34	AD	402	PHO	CED-O2D-CGD	2.13	121.00	115.99
27	AX	101	BCR	C7-C8-C9	2.13	129.47	126.22
31	BD	5409	LMG	C9-O8-C28	2.13	122.82	116.85
27	AC	515	BCR	C37-C22-C23	2.14	121.65	118.10
24	AB	608	CLA	C5-C3-C2	2.14	125.11	121.05
24	BC	5511	CLA	C3A-C2A-C1A	2.14	105.13	101.50
27	AJ	101	BCR	C16-C17-C18	2.14	130.29	127.20
30	BA	5401	SQD	C17-C16-C15	2.15	125.61	114.53
24	AC	512	CLA	C1D-CHD-C4C	2.15	125.85	122.60
24	AA	406	CLA	C3A-C2A-C1A	2.15	105.14	101.50
34	BD	5404	PHO	C1B-NB-C4B	2.15	110.77	106.51
28	AC	518	DGD	C7A-C6A-C5A	2.15	125.64	114.53
30	AA	413	SQD	O8-S-O7	2.15	116.62	111.61
27	BX	5101	BCR	C1-C6-C7	2.15	121.85	115.82
31	BD	5409	LMG	C14-C13-C12	2.15	125.65	114.53
27	BT	5101	BCR	C28-C27-C26	2.16	117.29	113.87
27	AB	617	BCR	C8-C7-C6	2.16	133.80	127.32
24	BC	5501	CLA	C1D-CHD-C4C	2.16	125.87	122.60
27	AT	101	BCR	C8-C7-C6	2.16	133.82	127.32
24	AB	606	CLA	C1D-CHD-C4C	2.16	125.88	122.60
27	BX	5101	BCR	C7-C8-C9	2.17	129.52	126.22
30	BA	5401	SQD	C34-C33-C32	2.17	125.74	114.53
31	BL	5101	LMG	C34-C33-C32	2.17	125.75	114.53
24	BB	5606	CLA	CED-O2D-CGD	2.18	121.11	115.99
27	BT	5101	BCR	C8-C7-C6	2.18	133.88	127.32
36	BF	5101	HEM	C3B-C4B-CHC	2.19	126.24	123.16
34	BD	5404	PHO	CED-O2D-CGD	2.19	121.12	115.99
27	BD	5407	BCR	C36-C18-C19	2.19	121.74	118.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5612	CLA	CED-O2D-CGD	2.19	121.12	115.99
27	AB	618	BCR	C1-C6-C7	2.19	121.95	115.82
27	AB	619	BCR	C37-C22-C23	2.19	121.74	118.10
28	BC	5518	DGD	O6D-C1D-O3G	2.19	115.33	110.05
31	BC	5520	LMG	C39-C38-C37	2.19	125.84	114.53
31	AD	407	LMG	C14-C13-C12	2.19	125.84	114.53
27	AC	514	BCR	C28-C27-C26	2.19	117.34	113.87
28	AH	101	DGD	C1G-O1G-C1A	2.19	122.98	116.85
27	AA	410	BCR	C36-C18-C19	2.19	121.75	118.10
27	AT	101	BCR	C28-C27-C26	2.19	117.35	113.87
27	BC	5516	BCR	C36-C18-C19	2.19	121.75	118.10
27	AA	410	BCR	C1-C6-C7	2.20	121.97	115.82
24	AC	502	CLA	C3A-C2A-C1A	2.20	105.22	101.50
27	BB	5621	BCR	C11-C10-C9	2.20	130.37	127.20
27	AC	515	BCR	C34-C9-C8	2.20	121.76	118.10
30	BB	5601	SQD	O47-C7-C8	2.20	116.31	111.53
28	BC	5518	DGD	C7A-C6A-C5A	2.20	125.89	114.53
27	AA	410	BCR	C37-C22-C23	2.20	121.76	118.10
27	AT	101	BCR	C40-C30-C25	2.20	113.75	110.30
30	AA	416	SQD	C34-C33-C32	2.20	125.90	114.53
27	BC	5515	BCR	C37-C22-C23	2.20	121.76	118.10
28	BC	5519	DGD	O2E-C2E-C3E	2.20	115.30	110.34
34	AD	403	PHO	CED-O2D-CGD	2.21	121.16	115.99
24	BB	5617	CLA	C1D-CHD-C4C	2.21	125.94	122.60
24	AB	611	CLA	C5-C3-C2	2.21	125.24	121.05
24	AA	407	CLA	CED-O2D-CGD	2.21	121.17	115.99
27	BB	5623	BCR	C35-C13-C12	2.21	121.77	118.10
28	BC	5519	DGD	C5B-C4B-C3B	2.21	125.94	114.53
27	AB	619	BCR	C24-C23-C22	2.21	129.58	126.22
24	BB	5615	CLA	OBD-CAD-C3D	2.21	132.87	128.35
36	BF	5101	HEM	CAD-C3D-C4D	2.21	120.27	112.47
28	AC	518	DGD	O2G-C2G-C1G	2.21	116.16	108.36
30	BF	5102	SQD	C15-C14-C13	2.22	125.97	114.53
24	BA	5405	CLA	OBD-CAD-C3D	2.22	132.88	128.35
24	BA	5407	CLA	OBD-CAD-C3D	2.22	132.89	128.35
27	BC	5515	BCR	C34-C9-C8	2.22	121.80	118.10
27	AX	101	BCR	C36-C18-C19	2.22	121.80	118.10
30	AF	102	SQD	C15-C14-C13	2.22	126.01	114.53
30	AB	627	SQD	O47-C7-C8	2.22	116.36	111.53
24	BD	5402	CLA	CED-O2D-CGD	2.22	121.21	115.99
30	BA	5401	SQD	C15-C14-C13	2.23	126.02	114.53
28	BE	5102	DGD	C3G-C2G-C1G	2.23	117.28	112.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AC	508	CLA	C2A-C1A-CHA	2.23	127.99	123.89
24	AB	602	CLA	CED-O2D-CGD	2.23	121.22	115.99
27	AT	101	BCR	C37-C22-C23	2.23	121.81	118.10
27	AX	101	BCR	C1-C6-C7	2.23	122.07	115.82
24	BB	5606	CLA	C3A-C2A-C1A	2.23	105.28	101.50
31	BC	5520	LMG	O7-C8-C9	2.23	116.23	108.36
24	BB	5618	CLA	C3A-C2A-C1A	2.23	105.29	101.50
31	AB	620	LMG	C34-C33-C32	2.24	126.07	114.53
27	BA	5411	BCR	C37-C22-C23	2.24	121.82	118.10
24	AC	504	CLA	OBD-CAD-C3D	2.24	132.92	128.35
36	AF	101	HEM	C3B-C4B-CHC	2.24	126.32	123.16
24	AA	407	CLA	OBD-CAD-C3D	2.24	132.94	128.35
24	BC	5508	CLA	C2A-C1A-CHA	2.24	128.02	123.89
31	BA	5402	LMG	O1-C1-C2	2.25	110.88	108.04
24	BA	5405	CLA	C2A-C1A-CHA	2.25	128.02	123.89
24	AB	607	CLA	C11-C12-C13	2.25	122.94	115.49
24	BB	5611	CLA	C11-C12-C13	2.25	122.94	115.49
24	AB	603	CLA	CED-O2D-CGD	2.25	121.26	115.99
27	BB	5622	BCR	C16-C17-C18	2.25	130.45	127.20
27	BA	5411	BCR	C36-C18-C19	2.25	121.84	118.10
24	BA	5408	CLA	CED-O2D-CGD	2.25	121.27	115.99
31	AC	520	LMG	O7-C8-C9	2.25	116.30	108.36
24	AA	407	CLA	C1D-CHD-C4C	2.25	126.01	122.60
31	AC	521	LMG	C9-C8-C7	2.26	117.35	112.07
28	BH	5101	DGD	O2G-C2G-C3G	2.26	116.31	108.36
27	BC	5516	BCR	C16-C17-C18	2.26	130.46	127.20
27	AB	618	BCR	C16-C17-C18	2.26	130.46	127.20
28	AC	519	DGD	C5B-C4B-C3B	2.26	126.19	114.53
24	BC	5503	CLA	CED-O2D-CGD	2.26	121.29	115.99
27	AA	410	BCR	C30-C25-C24	2.26	122.14	115.82
24	AC	507	CLA	C11-C12-C13	2.26	122.98	115.49
28	AH	101	DGD	O2G-C2G-C3G	2.26	116.33	108.36
27	BA	5411	BCR	C30-C25-C24	2.26	122.15	115.82
34	AD	403	PHO	CBD-CHA-C1A	2.26	131.69	126.36
24	AB	602	CLA	C2A-C1A-CHA	2.26	128.05	123.89
28	AC	517	DGD	O2G-C2G-C3G	2.26	116.34	108.36
24	BB	5606	CLA	C2A-C1A-CHA	2.27	128.06	123.89
27	BJ	5101	BCR	C40-C30-C25	2.27	113.86	110.30
24	AB	611	CLA	OBD-CAD-C3D	2.27	132.99	128.35
31	AC	520	LMG	C39-C38-C37	2.27	126.26	114.53
24	BC	5511	CLA	CED-O2D-CGD	2.27	121.32	115.99
24	AB	607	CLA	C1D-CHD-C4C	2.27	126.04	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5619	CLA	CED-O2D-CGD	2.27	121.32	115.99
24	AA	404	CLA	OBD-CAD-C3D	2.27	133.00	128.35
24	AB	608	CLA	CED-O2D-CGD	2.27	121.32	115.99
28	BC	5518	DGD	C1G-O1G-C1A	2.28	123.21	116.85
28	AC	518	DGD	C1G-O1G-C1A	2.28	123.21	116.85
27	AD	406	BCR	C15-C14-C13	2.28	130.49	127.20
27	BT	5101	BCR	C37-C22-C23	2.28	121.89	118.10
24	BB	5619	CLA	C1D-CHD-C4C	2.28	126.05	122.60
31	AD	407	LMG	O8-C28-C29	2.28	118.86	111.90
24	AB	615	CLA	C1D-CHD-C4C	2.29	126.06	122.60
27	BJ	5101	BCR	C3-C4-C5	2.29	117.50	113.87
24	AB	613	CLA	C3A-C2A-C1A	2.29	105.39	101.50
24	BB	5610	CLA	C1D-CHD-C4C	2.29	126.07	122.60
27	BJ	5101	BCR	C28-C27-C26	2.29	117.51	113.87
27	AB	619	BCR	C1-C6-C7	2.30	122.26	115.82
24	AB	608	CLA	C2A-C1A-CHA	2.30	128.12	123.89
24	AC	501	CLA	C1D-CHD-C4C	2.30	126.09	122.60
30	AA	416	SQD	O47-C7-C8	2.30	116.53	111.53
27	AD	406	BCR	C36-C18-C19	2.30	121.93	118.10
27	AC	514	BCR	C15-C14-C13	2.30	130.53	127.20
24	BA	5405	CLA	C3A-C2A-C1A	2.30	105.41	101.50
27	BT	5101	BCR	C20-C21-C22	2.30	130.53	127.20
24	AA	406	CLA	OBD-CAD-C3D	2.31	133.06	128.35
30	AA	416	SQD	C15-C14-C13	2.31	126.44	114.53
24	BC	5505	CLA	C2A-C1A-CHA	2.31	128.13	123.89
24	AB	614	CLA	C3A-C2A-C1A	2.31	105.41	101.50
24	AC	509	CLA	C3A-C2A-C1A	2.31	105.41	101.50
27	BC	5515	BCR	C36-C18-C19	2.31	121.94	118.10
27	BD	5407	BCR	C34-C9-C8	2.31	121.94	118.10
24	BC	5504	CLA	OBD-CAD-C3D	2.31	133.07	128.35
27	AC	516	BCR	C30-C25-C24	2.31	122.30	115.82
24	AC	511	CLA	CED-O2D-CGD	2.31	121.42	115.99
24	AC	503	CLA	C2A-C1A-CHA	2.31	128.15	123.89
24	AC	503	CLA	CED-O2D-CGD	2.31	121.42	115.99
31	BC	5521	LMG	C12-C11-C10	2.31	122.69	113.59
28	BC	5518	DGD	O2G-C2G-C1G	2.32	116.53	108.36
27	AK	102	BCR	C15-C14-C13	2.32	130.55	127.20
24	AD	404	CLA	C2A-C1A-CHA	2.32	128.16	123.89
24	BB	5607	CLA	CBA-CAA-C2A	2.32	120.29	113.73
24	AB	607	CLA	OBD-CAD-C3D	2.32	133.10	128.35
24	BC	5512	CLA	C3A-C2A-C1A	2.32	105.44	101.50
27	AB	617	BCR	C37-C22-C23	2.33	121.97	118.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	AC	519	DGD	O3G-C3G-C2G	2.33	116.53	110.99
24	BB	5608	CLA	OBD-CAD-C3D	2.33	133.11	128.35
31	BC	5520	LMG	C13-C12-C11	2.33	121.84	113.29
34	BD	5403	PHO	C3A-C4A-CHB	2.33	126.17	121.84
27	AC	515	BCR	C15-C14-C13	2.33	130.57	127.20
24	AD	401	CLA	CED-O2D-CGD	2.33	121.46	115.99
27	BC	5516	BCR	C30-C25-C24	2.34	122.36	115.82
24	AB	602	CLA	C3A-C2A-C1A	2.34	105.46	101.50
24	BC	5507	CLA	C11-C12-C13	2.34	123.25	115.49
31	AC	521	LMG	C34-C33-C32	2.34	126.62	114.53
24	AB	605	CLA	C2A-C1A-CHA	2.34	128.19	123.89
31	BD	5409	LMG	O8-C28-C29	2.35	119.05	111.90
24	BD	5405	CLA	C2A-C1A-CHA	2.35	128.21	123.89
28	BC	5519	DGD	C1E-O6E-C5E	2.35	118.31	113.75
24	BB	5612	CLA	C2A-C1A-CHA	2.35	128.22	123.89
27	AC	515	BCR	C36-C18-C19	2.36	122.02	118.10
30	AA	413	SQD	C15-C14-C13	2.36	126.72	114.53
27	AC	514	BCR	C8-C7-C6	2.36	134.41	127.32
27	AJ	101	BCR	C28-C27-C26	2.36	117.61	113.87
27	AC	516	BCR	C24-C23-C22	2.36	129.82	126.22
30	BA	5401	SQD	O47-C7-C8	2.36	116.67	111.53
27	BB	5623	BCR	C1-C6-C7	2.37	122.45	115.82
34	BD	5404	PHO	CBD-CHA-C1A	2.37	131.94	126.36
31	BD	5409	LMG	C39-C38-C37	2.37	126.77	114.53
24	BB	5609	CLA	C2A-C1A-CHA	2.37	128.25	123.89
31	BC	5521	LMG	C34-C33-C32	2.37	126.78	114.53
31	AB	621	LMG	C13-C12-C11	2.37	122.00	113.29
27	AJ	101	BCR	C3-C4-C5	2.38	117.64	113.87
28	BC	5517	DGD	C3A-C2A-C1A	2.38	122.94	113.59
27	BJ	5101	BCR	C16-C17-C18	2.38	130.63	127.20
27	AC	516	BCR	C37-C22-C23	2.38	122.06	118.10
27	AJ	101	BCR	C40-C30-C25	2.38	114.04	110.30
30	BA	5414	SQD	C15-C14-C13	2.39	126.86	114.53
31	AC	521	LMG	C12-C11-C10	2.39	122.98	113.59
24	AB	615	CLA	CED-O2D-CGD	2.39	121.59	115.99
27	BT	5101	BCR	C40-C30-C25	2.39	114.05	110.30
27	AA	410	BCR	C35-C13-C12	2.39	122.08	118.10
27	BC	5514	BCR	C8-C7-C6	2.39	134.51	127.32
28	AC	518	DGD	O6D-C1D-O3G	2.39	115.82	110.05
31	AD	407	LMG	C39-C38-C37	2.40	126.90	114.53
27	BA	5411	BCR	C16-C17-C18	2.40	130.66	127.20
24	BA	5407	CLA	C3A-C2A-C1A	2.40	105.56	101.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AA	404	CLA	C3A-C2A-C1A	2.40	105.56	101.50
27	BT	5101	BCR	C36-C18-C19	2.40	122.09	118.10
24	BB	5611	CLA	OBD-CAD-C3D	2.40	133.25	128.35
27	AC	515	BCR	C24-C23-C22	2.40	129.87	126.22
32	AI	103	LMT	C1B-C2B-C3B	2.40	114.70	109.97
30	AF	102	SQD	O47-C7-C8	2.40	116.75	111.53
30	BF	5102	SQD	C45-O47-C7	2.40	123.65	117.89
31	BB	5624	LMG	C13-C12-C11	2.40	122.10	113.29
27	BK	5102	BCR	C15-C14-C13	2.41	130.67	127.20
27	BB	5622	BCR	C1-C6-C7	2.41	122.56	115.82
28	BC	5519	DGD	C3G-C2G-C1G	2.41	117.70	112.07
24	AB	603	CLA	CBA-CAA-C2A	2.41	120.53	113.73
27	BB	5623	BCR	C24-C23-C22	2.42	129.90	126.22
24	AB	610	CLA	CED-O2D-CGD	2.42	121.66	115.99
27	AB	619	BCR	C35-C13-C12	2.42	122.12	118.10
27	BT	5101	BCR	C23-C24-C25	2.42	134.59	127.32
27	BK	5102	BCR	C37-C22-C23	2.42	122.13	118.10
28	BH	5101	DGD	C1G-O1G-C1A	2.42	123.63	116.85
34	AD	402	PHO	O2A-CGA-CBA	2.43	119.30	111.90
36	BV	5201	HEM	CAA-CBA-CGA	2.43	117.20	112.75
24	AC	505	CLA	C2A-C1A-CHA	2.43	128.37	123.89
27	AK	102	BCR	C37-C22-C23	2.43	122.15	118.10
31	AC	520	LMG	C13-C12-C11	2.44	122.22	113.29
24	AB	613	CLA	C1D-CHD-C4C	2.44	126.29	122.60
32	BC	5522	LMT	C1B-C2B-C3B	2.44	114.77	109.97
24	BC	5509	CLA	C1D-CHD-C4C	2.44	126.29	122.60
32	BB	5626	LMT	O1B-C1B-C2B	2.44	114.04	108.10
28	BB	5602	DGD	O2G-C2G-C3G	2.44	116.96	108.36
24	AC	507	CLA	CED-O2D-CGD	2.44	121.72	115.99
36	AV	201	HEM	C3B-C4B-CHC	2.44	126.60	123.16
24	BA	5405	CLA	CED-O2D-CGD	2.44	121.72	115.99
30	BA	5401	SQD	C36-C35-C34	2.45	127.17	114.53
31	BC	5521	LMG	C9-C8-C7	2.45	117.80	112.07
34	BD	5403	PHO	CED-O2D-CGD	2.45	121.73	115.99
27	AC	516	BCR	C35-C13-C12	2.45	122.17	118.10
24	BC	5510	CLA	CED-O2D-CGD	2.45	121.74	115.99
24	BB	5617	CLA	CED-O2D-CGD	2.45	121.74	115.99
28	AC	517	DGD	C3A-C2A-C1A	2.46	123.25	113.59
27	BD	5407	BCR	C35-C13-C12	2.46	122.19	118.10
24	AB	604	CLA	OBD-CAD-C3D	2.46	133.38	128.35
27	AK	102	BCR	C30-C25-C24	2.46	122.71	115.82
27	BK	5102	BCR	C34-C9-C8	2.46	122.19	118.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BC	5514	BCR	C7-C8-C9	2.46	129.97	126.22
24	AB	604	CLA	C3A-C2A-C1A	2.46	105.67	101.50
27	BJ	5101	BCR	C31-C1-C2	2.46	117.60	108.79
24	AB	606	CLA	CBA-CAA-C2A	2.46	120.68	113.73
24	BC	5502	CLA	CED-O2D-CGD	2.46	121.77	115.99
24	BB	5615	CLA	C5-C3-C2	2.47	125.73	121.05
24	AB	609	CLA	C2A-C1A-CHA	2.47	128.43	123.89
24	BC	5503	CLA	C6-C5-C3	2.47	117.90	112.48
27	AJ	101	BCR	C31-C1-C2	2.47	117.62	108.79
31	AB	620	LMG	C12-C11-C10	2.47	123.29	113.59
30	AB	622	SQD	C15-C14-C13	2.47	127.27	114.53
24	AC	510	CLA	CED-O2D-CGD	2.47	121.78	115.99
27	AB	618	BCR	C32-C1-C6	2.47	114.17	110.30
36	BV	5201	HEM	C3B-C4B-CHC	2.47	126.64	123.16
27	AA	410	BCR	C24-C23-C22	2.47	129.98	126.22
28	AC	518	DGD	C3A-C2A-C1A	2.47	123.31	113.59
28	BC	5518	DGD	C5A-C4A-C3A	2.47	127.31	114.53
27	AB	617	BCR	C11-C10-C9	2.48	130.77	127.20
28	AC	518	DGD	C5A-C4A-C3A	2.48	127.32	114.53
28	BC	5518	DGD	C3A-C2A-C1A	2.48	123.33	113.59
27	BX	5101	BCR	C16-C17-C18	2.48	130.78	127.20
34	BD	5403	PHO	O2A-CGA-CBA	2.48	119.45	111.90
27	BD	5407	BCR	C37-C22-C23	2.48	122.22	118.10
30	BF	5102	SQD	O47-C7-C8	2.48	116.92	111.53
29	BA	5413	LHG	O8-C6-C5	2.48	115.37	108.69
24	BB	5615	CLA	CED-O2D-CGD	2.48	121.81	115.99
30	BB	5625	SQD	C15-C14-C13	2.48	127.36	114.53
24	BC	5502	CLA	C3A-C2A-C1A	2.48	105.71	101.50
24	AA	404	CLA	C2A-C1A-CHA	2.49	128.46	123.89
28	AC	519	DGD	C3G-C2G-C1G	2.49	117.89	112.07
34	AD	402	PHO	C3A-C4A-CHB	2.49	126.46	121.84
27	BC	5516	BCR	C37-C22-C23	2.49	122.24	118.10
27	AC	514	BCR	C1-C6-C7	2.49	122.80	115.82
24	BC	5510	CLA	C3A-C2A-C1A	2.49	105.73	101.50
36	AV	201	HEM	CAA-CBA-CGA	2.49	117.32	112.75
24	BB	5613	CLA	C3A-C2A-C1A	2.49	105.73	101.50
24	BB	5620	CLA	C3A-C2A-C1A	2.50	105.73	101.50
24	BC	5507	CLA	CED-O2D-CGD	2.50	121.84	115.99
35	AD	405	PL9	C45-C44-C46	2.50	119.22	115.41
27	BX	5101	BCR	C28-C27-C26	2.50	117.83	113.87
31	BL	5101	LMG	C12-C11-C10	2.50	123.43	113.59
27	BD	5407	BCR	C28-C27-C26	2.50	117.84	113.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AT	101	BCR	C23-C24-C25	2.50	134.84	127.32
24	AD	401	CLA	CBA-CAA-C2A	2.50	120.80	113.73
30	BB	5601	SQD	C31-C30-C29	2.51	133.12	113.44
31	AA	414	LMG	O8-C9-C8	2.51	115.44	108.69
24	AC	503	CLA	C6-C5-C3	2.51	117.99	112.48
28	AB	628	DGD	O2G-C2G-C3G	2.51	117.21	108.36
27	BK	5102	BCR	C30-C25-C24	2.51	122.85	115.82
24	BC	5506	CLA	C2A-C1A-CHA	2.51	128.51	123.89
27	AD	406	BCR	C37-C22-C23	2.51	122.28	118.10
27	AB	617	BCR	C24-C23-C22	2.52	130.05	126.22
30	AB	627	SQD	C31-C30-C29	2.52	133.21	113.44
27	AD	406	BCR	C35-C13-C12	2.52	122.28	118.10
34	AD	402	PHO	C3A-C2A-C1A	2.52	105.03	101.84
27	AC	514	BCR	C37-C22-C23	2.52	122.29	118.10
24	BA	5406	CLA	C3A-C2A-C1A	2.52	105.77	101.50
30	AA	416	SQD	C36-C35-C34	2.52	127.54	114.53
24	BB	5613	CLA	C2A-C1A-CHA	2.52	128.53	123.89
27	AJ	101	BCR	C1-C6-C7	2.52	122.88	115.82
34	AD	402	PHO	C1C-NC-C4C	2.52	111.50	106.51
28	AC	518	DGD	O6D-C5D-C4D	2.52	114.42	109.68
30	AB	622	SQD	C31-C30-C29	2.53	133.28	113.44
24	BB	5613	CLA	CED-O2D-CGD	2.53	121.91	115.99
27	BC	5514	BCR	C37-C22-C23	2.53	122.30	118.10
27	BB	5622	BCR	C32-C1-C6	2.53	114.27	110.30
24	AD	404	CLA	C3A-C2A-C1A	2.53	105.79	101.50
27	AT	101	BCR	C36-C18-C19	2.53	122.31	118.10
24	BC	5509	CLA	C3A-C2A-C1A	2.53	105.79	101.50
24	AB	611	CLA	CED-O2D-CGD	2.53	121.93	115.99
24	BC	5509	CLA	CED-O2D-CGD	2.53	121.93	115.99
34	BD	5403	PHO	C1C-NC-C4C	2.53	111.52	106.51
24	AC	512	CLA	CED-O2D-CGD	2.53	121.93	115.99
27	BJ	5101	BCR	C1-C6-C7	2.53	122.92	115.82
27	BC	5516	BCR	C24-C23-C22	2.54	130.08	126.22
30	AA	416	SQD	C45-O47-C7	2.54	123.97	117.89
32	AB	623	LMT	O1B-C1B-C2B	2.54	114.28	108.10
24	BB	5614	CLA	C3A-C2A-C1A	2.54	105.80	101.50
36	BF	5101	HEM	CMD-C2D-C3D	2.54	125.58	114.35
27	BB	5621	BCR	C36-C18-C19	2.54	122.32	118.10
27	AC	514	BCR	C32-C1-C6	2.54	114.28	110.30
24	AB	609	CLA	C3A-C2A-C1A	2.54	105.81	101.50
27	BC	5514	BCR	C32-C1-C6	2.54	114.29	110.30
24	AB	616	CLA	C3A-C2A-C1A	2.54	105.81	101.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AC	502	CLA	CED-O2D-CGD	2.55	121.96	115.99
24	AB	616	CLA	CED-O2D-CGD	2.55	121.97	115.99
24	AC	506	CLA	C2A-C1A-CHA	2.55	128.58	123.89
30	BB	5625	SQD	C31-C30-C29	2.55	133.50	113.44
27	BJ	5101	BCR	C11-C10-C9	2.56	130.89	127.20
35	AD	405	PL9	C2-C1-C6	2.56	123.84	118.27
24	BB	5608	CLA	C3A-C2A-C1A	2.57	105.85	101.50
31	BE	5101	LMG	O8-C9-C8	2.57	115.60	108.69
27	AC	516	BCR	C16-C17-C18	2.57	130.91	127.20
31	AB	620	LMG	O1-C1-C2	2.57	111.29	108.04
30	AF	102	SQD	C45-O47-C7	2.57	124.07	117.89
24	AC	501	CLA	CED-O2D-CGD	2.57	122.03	115.99
27	BC	5514	BCR	C40-C30-C25	2.58	114.34	110.30
24	BC	5501	CLA	CED-O2D-CGD	2.58	122.03	115.99
36	BV	5201	HEM	CMD-C2D-C3D	2.58	125.75	114.35
24	AB	609	CLA	CED-O2D-CGD	2.58	122.04	115.99
24	AB	610	CLA	C3A-C2A-C1A	2.58	105.87	101.50
28	AC	519	DGD	O3D-C3D-C2D	2.58	116.14	110.34
24	BD	5402	CLA	CBA-CAA-C2A	2.58	121.02	113.73
24	BB	5607	CLA	CED-O2D-CGD	2.58	122.05	115.99
35	BD	5406	PL9	C2-C1-C6	2.58	123.90	118.27
27	BB	5623	BCR	C23-C24-C25	2.58	135.08	127.32
30	BA	5401	SQD	C45-O47-C7	2.59	124.10	117.89
31	BL	5101	LMG	O1-C1-C2	2.59	111.31	108.04
24	BB	5610	CLA	CBA-CAA-C2A	2.60	121.06	113.73
24	BC	5512	CLA	CED-O2D-CGD	2.60	122.08	115.99
24	BD	5405	CLA	C3A-C2A-C1A	2.61	105.92	101.50
31	BB	5624	LMG	O8-C28-C29	2.61	119.84	111.90
27	BA	5411	BCR	C35-C13-C12	2.61	122.43	118.10
34	AD	403	PHO	C1C-NC-C4C	2.61	111.68	106.51
24	AB	604	CLA	CBA-CAA-C2A	2.61	121.11	113.73
28	AB	628	DGD	O6E-C1E-O5D	2.62	116.36	110.05
27	AC	515	BCR	C35-C13-C12	2.63	122.47	118.10
27	AC	514	BCR	C7-C8-C9	2.63	130.23	126.22
28	AC	519	DGD	O6E-C5E-C4E	2.64	114.63	109.68
27	BB	5621	BCR	C35-C13-C12	2.64	122.49	118.10
28	BC	5519	DGD	O3D-C3D-C2D	2.64	116.28	110.34
27	AX	101	BCR	C28-C27-C26	2.64	118.06	113.87
36	AF	101	HEM	CMD-C2D-C3D	2.64	126.04	114.35
27	BC	5514	BCR	C1-C6-C7	2.64	123.22	115.82
24	AA	404	CLA	O2D-CGD-CBD	2.65	114.93	111.30
24	BC	5503	CLA	CBA-CAA-C2A	2.65	121.20	113.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AB	603	CLA	C1D-CHD-C4C	2.65	126.61	122.60
24	BB	5611	CLA	C1D-CHD-C4C	2.65	126.61	122.60
24	AB	601	CLA	CED-O2D-CGD	2.65	122.20	115.99
27	AT	101	BCR	C20-C21-C22	2.65	131.03	127.20
27	BC	5516	BCR	C35-C13-C12	2.65	122.51	118.10
27	AX	101	BCR	C15-C14-C13	2.65	131.03	127.20
28	BC	5517	DGD	C3G-C2G-C1G	2.65	118.28	112.07
36	AV	201	HEM	CMD-C2D-C3D	2.65	126.09	114.35
27	AB	617	BCR	C16-C17-C18	2.66	131.04	127.20
24	AB	612	CLA	C2A-C1A-CHA	2.66	128.78	123.89
28	AC	517	DGD	C3G-C2G-C1G	2.66	118.29	112.07
27	AC	514	BCR	C35-C13-C12	2.66	122.52	118.10
27	BB	5623	BCR	C8-C7-C6	2.66	135.32	127.32
24	AB	613	CLA	O2A-CGA-CBA	2.66	120.02	111.90
27	BA	5411	BCR	C2-C1-C6	2.67	114.58	110.36
24	AA	405	CLA	C3A-C2A-C1A	2.67	106.02	101.50
27	AB	619	BCR	C8-C7-C6	2.67	135.33	127.32
27	AX	101	BCR	C16-C17-C18	2.67	131.05	127.20
27	AK	102	BCR	C34-C9-C8	2.67	122.54	118.10
28	BH	5101	DGD	O6D-C1D-O3G	2.67	116.48	110.05
24	AC	503	CLA	CBA-CAA-C2A	2.67	121.27	113.73
24	AC	510	CLA	C2A-C1A-CHA	2.68	128.82	123.89
27	AX	101	BCR	C35-C13-C12	2.68	122.56	118.10
27	AC	514	BCR	C40-C30-C25	2.68	114.51	110.30
24	BA	5408	CLA	C2A-C1A-CHA	2.69	128.83	123.89
24	BB	5610	CLA	CED-O2D-CGD	2.69	122.30	115.99
27	AA	410	BCR	C16-C17-C18	2.69	131.09	127.20
28	AE	101	DGD	O5D-C6D-C5D	2.69	113.96	109.08
28	BE	5102	DGD	O5D-C6D-C5D	2.70	113.97	109.08
28	BC	5518	DGD	O6D-C5D-C4D	2.70	114.75	109.68
27	BK	5102	BCR	C35-C13-C12	2.70	122.59	118.10
24	AC	511	CLA	C1D-CHD-C4C	2.70	126.69	122.60
27	BK	5102	BCR	C8-C7-C6	2.70	135.44	127.32
24	BB	5617	CLA	C2A-C1A-CHA	2.71	128.87	123.89
27	AB	617	BCR	C36-C18-C19	2.71	122.61	118.10
24	AC	509	CLA	CED-O2D-CGD	2.71	122.34	115.99
29	AA	415	LHG	O8-C23-C24	2.71	120.16	111.90
28	AH	101	DGD	O6D-C1D-O3G	2.71	116.58	110.05
27	BJ	5101	BCR	C16-C15-C14	2.71	129.39	123.39
35	BD	5406	PL9	C45-C44-C46	2.71	119.55	115.41
24	BB	5605	CLA	CED-O2D-CGD	2.71	122.36	115.99
24	AC	506	CLA	C3A-C2A-C1A	2.71	106.10	101.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	AB	621	LMG	O7-C8-C7	2.72	117.93	108.36
24	BC	5513	CLA	CED-O2D-CGD	2.72	122.37	115.99
28	BB	5602	DGD	O6E-C1E-O5D	2.72	116.60	110.05
24	BC	5507	CLA	C1C-NC-C4C	2.72	109.57	106.27
24	BB	5620	CLA	CED-O2D-CGD	2.72	122.37	115.99
27	AB	617	BCR	C35-C13-C12	2.72	122.63	118.10
27	BJ	5101	BCR	C8-C7-C6	2.72	135.49	127.32
32	AB	629	LMT	O1B-C1B-C2B	2.72	114.73	108.10
27	BX	5101	BCR	C11-C10-C9	2.73	131.13	127.20
24	BC	5506	CLA	C3A-C2A-C1A	2.73	106.12	101.50
29	BA	5415	LHG	O8-C23-C24	2.73	120.21	111.90
27	BB	5621	BCR	C16-C17-C18	2.73	131.14	127.20
24	AB	615	CLA	C3A-C2A-C1A	2.73	106.13	101.50
32	BB	5603	LMT	O1B-C1B-C2B	2.73	114.75	108.10
24	BB	5608	CLA	CBA-CAA-C2A	2.73	121.44	113.73
24	AD	401	CLA	C2A-C1A-CHA	2.73	128.92	123.89
27	AK	102	BCR	C35-C13-C12	2.73	122.65	118.10
24	AB	616	CLA	O2A-CGA-CBA	2.74	120.23	111.90
27	BX	5101	BCR	C15-C14-C13	2.74	131.15	127.20
28	BC	5519	DGD	O1G-C1A-C2A	2.74	120.25	111.90
31	BC	5520	LMG	O7-C8-C7	2.74	118.02	108.36
27	AJ	101	BCR	C16-C15-C14	2.74	129.46	123.39
27	AB	619	BCR	C23-C24-C25	2.75	135.57	127.32
24	AC	507	CLA	C1C-NC-C4C	2.75	109.61	106.27
27	BA	5411	BCR	C24-C23-C22	2.75	130.41	126.22
24	AB	614	CLA	CED-O2D-CGD	2.75	122.44	115.99
31	AC	520	LMG	O7-C8-C7	2.76	118.07	108.36
31	AB	621	LMG	O8-C28-C29	2.76	120.30	111.90
24	BB	5605	CLA	C2A-C1A-CHA	2.76	128.97	123.89
24	BB	5607	CLA	C1D-CHD-C4C	2.76	126.78	122.60
27	AT	101	BCR	C32-C1-C6	2.76	114.64	110.30
24	BC	5503	CLA	C3A-C2A-C1A	2.77	106.19	101.50
24	BC	5511	CLA	C1D-CHD-C4C	2.77	126.79	122.60
24	BB	5619	CLA	C3A-C2A-C1A	2.77	106.20	101.50
27	AJ	101	BCR	C21-C20-C19	2.77	131.58	123.13
24	BB	5618	CLA	O2A-CGA-CBA	2.77	120.35	111.90
31	BB	5624	LMG	O7-C8-C7	2.77	118.13	108.36
27	AA	410	BCR	C23-C24-C25	2.78	135.66	127.32
24	AC	509	CLA	C1D-CHD-C4C	2.78	126.81	122.60
24	BB	5617	CLA	O2D-CGD-CBD	2.78	115.11	111.30
31	BE	5101	LMG	C34-C33-C32	2.78	128.90	114.53
34	BD	5403	PHO	C4A-NA-C1A	2.78	110.70	108.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BA	5405	CLA	O2D-CGD-CBD	2.79	115.12	111.30
27	AJ	101	BCR	C11-C10-C9	2.79	131.23	127.20
34	BD	5403	PHO	C3A-C2A-C1A	2.79	105.38	101.84
24	BB	5612	CLA	C11-C12-C13	2.79	124.74	115.49
27	BX	5101	BCR	C35-C13-C12	2.79	122.74	118.10
24	BC	5510	CLA	C2A-C1A-CHA	2.79	129.03	123.89
28	AC	519	DGD	O1G-C1A-C2A	2.79	120.42	111.90
27	BC	5515	BCR	C8-C7-C6	2.80	135.71	127.32
27	AX	101	BCR	C11-C10-C9	2.80	131.24	127.20
31	BE	5101	LMG	O8-C28-C29	2.80	120.43	111.90
24	AB	612	CLA	C1D-CHD-C4C	2.80	126.84	122.60
27	BA	5411	BCR	C23-C24-C25	2.80	135.74	127.32
31	AA	414	LMG	O8-C28-C29	2.80	120.44	111.90
24	BB	5616	CLA	C2A-C1A-CHA	2.80	129.05	123.89
28	BH	5101	DGD	C3G-O3G-C1D	2.80	119.71	113.82
27	AD	406	BCR	C7-C8-C9	2.81	130.49	126.22
34	AD	402	PHO	C4A-NA-C1A	2.81	110.72	108.21
27	AC	515	BCR	C8-C7-C6	2.81	135.75	127.32
30	AB	622	SQD	C45-O47-C7	2.81	124.63	117.89
24	AB	611	CLA	C3A-C2A-C1A	2.81	106.26	101.50
24	AB	601	CLA	C1C-NC-C4C	2.81	109.68	106.27
29	AA	412	LHG	O7-C7-C8	2.81	117.64	111.53
27	AJ	101	BCR	C8-C7-C6	2.81	135.76	127.32
24	AB	616	CLA	C1C-NC-C4C	2.81	109.69	106.27
31	AA	414	LMG	C34-C33-C32	2.81	129.06	114.53
24	BB	5617	CLA	O2A-CGA-CBA	2.81	120.47	111.90
24	BB	5620	CLA	C1C-NC-C4C	2.81	109.69	106.27
24	BB	5620	CLA	O2A-CGA-CBA	2.82	120.48	111.90
24	AD	401	CLA	C1C-NC-C4C	2.82	109.69	106.27
28	AC	517	DGD	O6D-C1D-O3G	2.82	116.84	110.05
24	BC	5503	CLA	C1C-NC-C4C	2.82	109.69	106.27
24	AA	407	CLA	C2A-C1A-CHA	2.82	129.08	123.89
24	AA	407	CLA	C3A-C2A-C1A	2.82	106.28	101.50
24	AB	608	CLA	C11-C12-C13	2.82	124.84	115.49
28	AH	101	DGD	C3G-O3G-C1D	2.82	119.75	113.82
29	BA	5413	LHG	O7-C7-C8	2.82	117.66	111.53
24	AC	506	CLA	CED-O2D-CGD	2.82	122.61	115.99
27	BC	5514	BCR	C35-C13-C12	2.82	122.80	118.10
27	AK	102	BCR	C8-C7-C6	2.82	135.80	127.32
24	BC	5510	CLA	C1C-NC-C4C	2.83	109.71	106.27
24	AA	404	CLA	CED-O2D-CGD	2.83	122.63	115.99
27	BC	5515	BCR	C16-C17-C18	2.84	131.29	127.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BC	5506	CLA	CED-O2D-CGD	2.84	122.64	115.99
24	BB	5618	CLA	CED-O2D-CGD	2.84	122.64	115.99
24	BB	5614	CLA	C2A-C1A-CHA	2.84	129.11	123.89
24	AB	613	CLA	C2A-C1A-CHA	2.84	129.12	123.89
34	BD	5404	PHO	C1C-NC-C4C	2.85	112.15	106.51
28	BC	5519	DGD	O6E-C1E-C2E	2.85	116.13	110.28
28	BC	5517	DGD	O6D-C1D-O3G	2.85	116.92	110.05
24	AB	606	CLA	CED-O2D-CGD	2.85	122.68	115.99
29	AA	412	LHG	O8-C6-C5	2.86	116.38	108.69
28	AB	628	DGD	O5D-C1E-C2E	2.86	111.65	108.04
31	AA	417	LMG	C12-C11-C10	2.86	124.84	113.59
24	AB	610	CLA	C2A-C1A-CHA	2.87	129.16	123.89
27	BT	5101	BCR	C7-C8-C9	2.87	130.58	126.22
24	BB	5605	CLA	C1C-NC-C4C	2.87	109.75	106.27
27	AX	101	BCR	C8-C7-C6	2.87	135.93	127.32
24	AC	510	CLA	C1C-NC-C4C	2.87	109.76	106.27
27	BX	5101	BCR	C8-C7-C6	2.87	135.95	127.32
24	BD	5402	CLA	C2A-C1A-CHA	2.87	129.18	123.89
31	BD	5410	LMG	O7-C8-C7	2.87	118.49	108.36
24	AC	503	CLA	C3A-C2A-C1A	2.87	106.37	101.50
27	BJ	5101	BCR	C21-C20-C19	2.88	131.90	123.13
24	AC	513	CLA	C1D-CHD-C4C	2.88	126.97	122.60
24	AC	506	CLA	C1C-NC-C4C	2.88	109.77	106.27
24	BC	5507	CLA	C2A-C1A-CHA	2.89	129.20	123.89
24	AB	601	CLA	C2A-C1A-CHA	2.89	129.20	123.89
36	BV	5201	HEM	CAD-C3D-C4D	2.89	122.66	112.47
24	BC	5506	CLA	C1C-NC-C4C	2.89	109.78	106.27
28	BC	5519	DGD	O6E-C5E-C4E	2.89	115.11	109.68
24	BD	5402	CLA	C1C-NC-C4C	2.89	109.78	106.27
24	AC	508	CLA	CED-O2D-CGD	2.89	122.78	115.99
27	AK	102	BCR	C16-C17-C18	2.89	131.38	127.20
24	BC	5508	CLA	CED-O2D-CGD	2.90	122.78	115.99
31	AA	414	LMG	O7-C10-C11	2.90	117.82	111.53
24	BB	5616	CLA	C1D-CHD-C4C	2.90	126.99	122.60
24	AB	614	CLA	O2A-CGA-CBA	2.91	120.76	111.90
31	BD	5409	LMG	C12-C11-C10	2.91	125.03	113.59
27	BT	5101	BCR	C2-C1-C6	2.91	114.97	110.36
24	AC	513	CLA	CED-O2D-CGD	2.91	122.82	115.99
24	BC	5504	CLA	C3A-C2A-C1A	2.91	106.44	101.50
31	BA	5402	LMG	C12-C11-C10	2.91	125.05	113.59
24	AC	507	CLA	C2A-C1A-CHA	2.92	129.26	123.89
24	AB	605	CLA	CED-O2D-CGD	2.92	122.84	115.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AC	504	CLA	C3A-C2A-C1A	2.92	106.45	101.50
24	BB	5611	CLA	C2A-C1A-CHA	2.92	129.27	123.89
24	AC	508	CLA	C3A-C2A-C1A	2.93	106.47	101.50
27	AT	101	BCR	C2-C1-C6	2.93	115.01	110.36
31	AD	407	LMG	C12-C11-C10	2.93	125.13	113.59
24	BD	5405	CLA	O2A-CGA-CBA	2.93	120.84	111.90
24	BC	5512	CLA	C1C-NC-C4C	2.93	109.83	106.27
31	AD	408	LMG	O7-C8-C7	2.94	118.71	108.36
27	BT	5101	BCR	C32-C1-C6	2.94	114.91	110.30
27	BK	5102	BCR	C16-C17-C18	2.94	131.44	127.20
28	AA	411	DGD	C4A-C3A-C2A	2.94	124.07	113.29
31	BE	5101	LMG	O7-C10-C11	2.94	117.92	111.53
24	BC	5505	CLA	C1C-NC-C4C	2.94	109.84	106.27
24	AB	612	CLA	O2A-CGA-CBA	2.95	120.87	111.90
24	BC	5513	CLA	C1D-CHD-C4C	2.95	127.06	122.60
36	AV	201	HEM	CAD-C3D-C4D	2.95	122.86	112.47
28	BB	5602	DGD	C3B-C2B-C1B	2.95	125.18	113.59
28	AB	628	DGD	C3B-C2B-C1B	2.95	125.19	113.59
24	AB	615	CLA	O2A-CGA-CBA	2.95	120.90	111.90
28	AC	519	DGD	O6E-C1E-C2E	2.95	116.33	110.28
27	BC	5515	BCR	C35-C13-C12	2.97	123.03	118.10
24	BA	5408	CLA	C3A-C2A-C1A	2.97	106.53	101.50
28	BA	5412	DGD	C4A-C3A-C2A	2.97	124.19	113.29
27	AD	406	BCR	C11-C10-C9	2.97	131.49	127.20
27	BD	5407	BCR	C11-C10-C9	2.97	131.49	127.20
27	AB	618	BCR	C8-C7-C6	2.98	136.26	127.32
24	BB	5619	CLA	O2A-CGA-CBA	2.98	120.97	111.90
30	BB	5601	SQD	C44-O6-C1	2.98	120.08	113.82
24	AA	407	CLA	CBA-CAA-C2A	2.98	122.14	113.73
30	AB	627	SQD	C44-O6-C1	2.98	120.08	113.82
24	AA	405	CLA	C1C-NC-C4C	2.99	109.89	106.27
24	AB	607	CLA	C2A-C1A-CHA	2.99	129.39	123.89
24	AB	602	CLA	C1C-NC-C4C	2.99	109.91	106.27
27	AA	410	BCR	C2-C1-C6	3.00	115.11	110.36
31	AC	520	LMG	O8-C9-C8	3.00	116.76	108.69
24	BB	5615	CLA	C3A-C2A-C1A	3.00	106.58	101.50
24	AB	605	CLA	C3A-C2A-C1A	3.00	106.59	101.50
24	BB	5609	CLA	CED-O2D-CGD	3.00	123.03	115.99
24	BB	5610	CLA	O2D-CGD-CBD	3.01	115.42	111.30
30	AA	413	SQD	C32-C31-C30	3.01	130.06	114.53
27	AB	618	BCR	C23-C24-C25	3.01	136.35	127.32
24	BB	5614	CLA	C1C-NC-C4C	3.01	109.93	106.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AC	512	CLA	C1C-NC-C4C	3.01	109.93	106.27
28	AC	517	DGD	C3B-C2B-C1B	3.02	125.45	113.59
24	BB	5616	CLA	C3A-C2A-C1A	3.02	106.61	101.50
28	BB	5602	DGD	O5D-C1E-C2E	3.02	111.85	108.04
24	BB	5618	CLA	C1D-CHD-C4C	3.02	127.17	122.60
31	BD	5409	LMG	C16-C15-C14	3.02	130.13	114.53
28	AC	519	DGD	C3B-C2B-C1B	3.02	125.48	113.59
24	BC	5508	CLA	C3A-C2A-C1A	3.03	106.63	101.50
35	BD	5406	PL9	C51-C49-C50	3.03	122.08	114.64
27	BB	5621	BCR	C2-C1-C6	3.03	115.15	110.36
31	BC	5520	LMG	O8-C9-C8	3.03	116.85	108.69
24	BB	5615	CLA	C6-C5-C3	3.04	119.14	112.48
27	AB	619	BCR	C2-C1-C6	3.04	115.18	110.36
27	AB	617	BCR	C2-C1-C6	3.05	115.19	110.36
27	BB	5622	BCR	C8-C7-C6	3.05	136.47	127.32
27	BB	5622	BCR	C24-C23-C22	3.05	130.87	126.22
24	AB	611	CLA	CBA-CAA-C2A	3.05	122.35	113.73
31	AD	407	LMG	C16-C15-C14	3.06	130.31	114.53
27	BD	5407	BCR	C16-C17-C18	3.06	131.61	127.20
27	AC	515	BCR	C16-C17-C18	3.06	131.62	127.20
24	BC	5501	CLA	C1C-NC-C4C	3.06	109.98	106.27
35	BD	5406	PL9	C30-C29-C31	3.06	120.09	115.41
27	AX	101	BCR	C23-C24-C25	3.08	136.56	127.32
27	BX	5101	BCR	C23-C24-C25	3.08	136.58	127.32
24	AB	612	CLA	C3A-C2A-C1A	3.08	106.73	101.50
27	BD	5407	BCR	C7-C8-C9	3.08	130.91	126.22
30	BA	5414	SQD	C32-C31-C30	3.08	130.46	114.53
24	BB	5606	CLA	C1C-NC-C4C	3.09	110.02	106.27
27	AT	101	BCR	C16-C17-C18	3.09	131.66	127.20
27	BC	5516	BCR	C8-C7-C6	3.10	136.61	127.32
35	AD	405	PL9	C30-C29-C31	3.10	120.14	115.41
27	AC	514	BCR	C2-C1-C6	3.10	115.28	110.36
24	BC	5505	CLA	O2A-CGA-CBA	3.10	121.36	111.90
27	BD	5407	BCR	C8-C7-C6	3.10	136.64	127.32
24	AC	505	CLA	C1C-NC-C4C	3.11	110.04	106.27
24	BC	5512	CLA	O2D-CGD-CBD	3.11	115.56	111.30
27	AD	406	BCR	C8-C7-C6	3.12	136.68	127.32
24	AB	607	CLA	C3A-C2A-C1A	3.12	106.78	101.50
35	AD	405	PL9	C51-C49-C50	3.12	122.30	114.64
24	AB	613	CLA	O2D-CGD-CBD	3.12	115.58	111.30
24	AB	614	CLA	C1D-CHD-C4C	3.12	127.32	122.60
31	BA	5402	LMG	O1-C7-C8	3.12	118.41	110.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5615	CLA	CBA-CAA-C2A	3.12	122.54	113.73
27	AB	618	BCR	C24-C23-C22	3.13	130.98	126.22
24	BB	5610	CLA	C2A-C1A-CHA	3.13	129.65	123.89
31	BC	5520	LMG	C8-O7-C10	3.13	125.41	117.89
24	AB	606	CLA	C2A-C1A-CHA	3.13	129.66	123.89
24	AD	404	CLA	O2A-CGA-CBA	3.14	121.45	111.90
30	BB	5625	SQD	C45-O47-C7	3.14	125.43	117.89
24	AB	611	CLA	C6-C5-C3	3.14	119.38	112.48
27	AT	101	BCR	C7-C8-C9	3.14	131.01	126.22
28	AH	101	DGD	C4B-C3B-C2B	3.15	124.84	113.29
27	BK	5102	BCR	C24-C23-C22	3.15	131.02	126.22
24	BC	5505	CLA	C3A-C2A-C1A	3.15	106.85	101.50
27	AK	102	BCR	C24-C23-C22	3.15	131.02	126.22
27	BB	5622	BCR	C23-C24-C25	3.16	136.80	127.32
24	AB	615	CLA	C1C-NC-C4C	3.16	110.11	106.27
24	AB	608	CLA	O2A-CGA-CBA	3.16	121.53	111.90
24	AB	606	CLA	O2D-CGD-CBD	3.16	115.63	111.30
27	BT	5101	BCR	C24-C23-C22	3.16	131.03	126.22
24	BA	5406	CLA	C1C-NC-C4C	3.17	110.11	106.27
24	BB	5616	CLA	O2A-CGA-CBA	3.17	121.55	111.90
24	AC	505	CLA	O2A-CGA-CBA	3.17	121.56	111.90
27	AD	406	BCR	C16-C17-C18	3.18	131.78	127.20
24	BB	5617	CLA	C1C-NC-C4C	3.18	110.13	106.27
24	BB	5609	CLA	C3A-C2A-C1A	3.18	106.88	101.50
28	BB	5602	DGD	O6D-C5D-C6D	3.18	113.10	106.61
24	BB	5611	CLA	C3A-C2A-C1A	3.18	106.89	101.50
27	BD	5407	BCR	C2-C1-C6	3.18	115.40	110.36
24	BC	5508	CLA	C1C-NC-C4C	3.18	110.13	106.27
31	AM	101	LMG	O7-C8-C7	3.19	119.61	108.36
24	AC	501	CLA	C1C-NC-C4C	3.19	110.15	106.27
24	AB	616	CLA	C2A-C1A-CHA	3.19	129.76	123.89
31	BD	5410	LMG	C12-C11-C10	3.19	126.15	113.59
24	BB	5612	CLA	O2A-CGA-CBA	3.19	121.63	111.90
28	BC	5517	DGD	C3B-C2B-C1B	3.20	126.16	113.59
29	BA	5413	LHG	O8-C23-C24	3.20	121.64	111.90
24	AC	505	CLA	C3A-C2A-C1A	3.20	106.92	101.50
28	BA	5412	DGD	O2G-C2G-C3G	3.20	119.64	108.36
36	BF	5101	HEM	CAA-CBA-CGA	3.20	118.61	112.75
27	AC	516	BCR	C8-C7-C6	3.20	136.94	127.32
24	BB	5607	CLA	C6-C5-C3	3.21	119.52	112.48
24	AB	609	CLA	C1C-NC-C4C	3.21	110.17	106.27
27	BC	5516	BCR	C23-C24-C25	3.21	136.96	127.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5620	CLA	C2A-C1A-CHA	3.21	129.80	123.89
24	BA	5408	CLA	CBA-CAA-C2A	3.22	122.81	113.73
27	BC	5514	BCR	C29-C30-C25	3.22	115.47	110.36
24	BC	5504	CLA	O2A-CGA-CBA	3.22	121.72	111.90
28	AA	411	DGD	O2G-C2G-C3G	3.22	119.72	108.36
28	BB	5602	DGD	O3G-C3G-C2G	3.23	118.66	110.99
28	BH	5101	DGD	C4B-C3B-C2B	3.23	125.12	113.29
31	AC	520	LMG	C8-O7-C10	3.23	125.64	117.89
28	AB	628	DGD	O6D-C5D-C6D	3.23	113.22	106.61
24	AC	508	CLA	C1C-NC-C4C	3.23	110.19	106.27
24	AC	503	CLA	C1C-NC-C4C	3.23	110.20	106.27
31	AI	101	LMG	C8-O7-C10	3.24	125.65	117.89
27	AX	101	BCR	C24-C23-C22	3.24	131.15	126.22
31	BM	5102	LMG	O7-C8-C7	3.24	119.78	108.36
31	AD	408	LMG	C12-C11-C10	3.24	126.33	113.59
24	AB	610	CLA	C1C-NC-C4C	3.24	110.21	106.27
31	AA	417	LMG	O1-C7-C8	3.25	118.72	110.99
28	AC	518	DGD	O6E-C1E-O5D	3.25	117.88	110.05
24	BC	5501	CLA	C3A-C2A-C1A	3.26	107.02	101.50
28	BC	5519	DGD	C3B-C2B-C1B	3.26	126.39	113.59
24	AB	611	CLA	C1C-NC-C4C	3.26	110.23	106.27
27	BD	5407	BCR	C23-C24-C25	3.26	137.11	127.32
27	AT	101	BCR	C24-C23-C22	3.26	131.19	126.22
27	BB	5621	BCR	C23-C24-C25	3.26	137.12	127.32
24	BA	5408	CLA	C1C-NC-C4C	3.27	110.24	106.27
28	BC	5518	DGD	O2G-C2G-C3G	3.27	119.88	108.36
27	BC	5514	BCR	C2-C1-C6	3.27	115.54	110.36
24	AB	604	CLA	C1C-NC-C4C	3.27	110.24	106.27
27	AC	516	BCR	C23-C24-C25	3.27	137.14	127.32
30	BA	5401	SQD	C32-C31-C30	3.27	131.44	114.53
24	BB	5615	CLA	C1C-NC-C4C	3.28	110.25	106.27
24	BB	5610	CLA	C3A-C2A-C1A	3.28	107.06	101.50
24	AB	610	CLA	O2A-CGA-CBA	3.28	121.89	111.90
28	AC	518	DGD	O2G-C2G-C3G	3.28	119.92	108.36
24	AC	502	CLA	C1C-NC-C4C	3.28	110.26	106.27
24	BB	5613	CLA	C1C-NC-C4C	3.29	110.26	106.27
24	AB	608	CLA	C1C-NC-C4C	3.29	110.27	106.27
24	AC	512	CLA	O2D-CGD-CBD	3.29	115.81	111.30
24	AC	501	CLA	C2A-C1A-CHA	3.30	129.97	123.89
24	BB	5605	CLA	O2A-CGA-CBA	3.31	121.98	111.90
27	AD	406	BCR	C2-C1-C6	3.31	115.61	110.36
24	AB	608	CLA	C3A-C2A-C1A	3.31	107.11	101.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	AA	416	SQD	C32-C31-C30	3.31	131.63	114.53
24	BC	5501	CLA	C2A-C1A-CHA	3.31	129.98	123.89
36	AF	101	HEM	CAA-CBA-CGA	3.31	118.82	112.75
24	AB	609	CLA	CBA-CAA-C2A	3.31	123.08	113.73
27	AK	102	BCR	C23-C24-C25	3.32	137.28	127.32
27	AD	406	BCR	C23-C24-C25	3.32	137.29	127.32
27	BK	5102	BCR	C23-C24-C25	3.32	137.30	127.32
27	BX	5101	BCR	C24-C23-C22	3.32	131.28	126.22
24	AB	603	CLA	C6-C5-C3	3.33	119.79	112.48
34	AD	403	PHO	C4A-NA-C1A	3.33	111.19	108.21
24	BB	5614	CLA	O2A-CGA-CBA	3.33	122.05	111.90
31	AB	621	LMG	C39-C38-C37	3.33	131.74	114.53
24	BB	5608	CLA	C1C-NC-C4C	3.33	110.32	106.27
28	BC	5518	DGD	O6E-C1E-O5D	3.33	118.08	110.05
24	BD	5405	CLA	C1C-NC-C4C	3.33	110.32	106.27
31	BL	5101	LMG	C9-O8-C28	3.33	126.17	116.85
24	BB	5608	CLA	O2D-CGD-CBD	3.34	115.88	111.30
24	BC	5512	CLA	O2A-CGA-CBA	3.34	122.08	111.90
27	AA	410	BCR	C29-C30-C25	3.34	115.65	110.36
24	BB	5613	CLA	CBA-CAA-C2A	3.35	123.17	113.73
31	BD	5408	LMG	C12-C11-C10	3.35	126.75	113.59
24	AB	606	CLA	C3A-C2A-C1A	3.35	107.18	101.50
28	BE	5102	DGD	C2G-O2G-C1B	3.35	125.93	117.89
31	BI	5101	LMG	C8-O7-C10	3.35	125.93	117.89
27	BT	5101	BCR	C16-C17-C18	3.35	132.04	127.20
27	BB	5623	BCR	C2-C1-C6	3.36	115.69	110.36
24	BB	5609	CLA	O2A-CGA-CBA	3.37	122.16	111.90
31	AB	620	LMG	C9-O8-C28	3.37	126.27	116.85
24	BC	5510	CLA	O2A-CGA-CBA	3.37	122.16	111.90
27	AB	618	BCR	C2-C1-C6	3.37	115.70	110.36
24	BB	5612	CLA	C3A-C2A-C1A	3.37	107.22	101.50
24	AD	404	CLA	C1C-NC-C4C	3.38	110.37	106.27
24	AB	605	CLA	C1C-NC-C4C	3.38	110.38	106.27
24	BB	5619	CLA	C1C-NC-C4C	3.39	110.38	106.27
28	AE	101	DGD	C2G-O2G-C1B	3.39	126.02	117.89
31	BB	5624	LMG	C39-C38-C37	3.39	132.03	114.53
24	BC	5509	CLA	C2A-C1A-CHA	3.39	130.13	123.89
24	AC	511	CLA	O2A-CGA-CBA	3.39	122.23	111.90
27	AC	514	BCR	C29-C30-C25	3.39	115.73	110.36
24	AB	601	CLA	O2A-CGA-CBA	3.39	122.24	111.90
24	AC	501	CLA	O2A-CGA-CBA	3.41	122.28	111.90
27	BB	5622	BCR	C29-C30-C25	3.41	115.76	110.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AC	506	CLA	O2D-CGD-CBD	3.41	115.97	111.30
24	AC	501	CLA	C3A-C2A-C1A	3.41	107.29	101.50
34	AD	403	PHO	C3A-C2A-C1A	3.42	106.17	101.84
24	AA	407	CLA	C1C-NC-C4C	3.42	110.42	106.27
27	AB	617	BCR	C23-C24-C25	3.42	137.59	127.32
27	BB	5623	BCR	C29-C30-C25	3.43	115.79	110.36
28	AB	628	DGD	O3G-C3G-C2G	3.43	119.14	110.99
27	BB	5622	BCR	C2-C1-C6	3.43	115.79	110.36
24	AC	512	CLA	C2A-C1A-CHA	3.43	130.20	123.89
24	BB	5612	CLA	C1C-NC-C4C	3.43	110.44	106.27
27	AC	515	BCR	C29-C30-C25	3.43	115.80	110.36
24	AB	613	CLA	C1C-NC-C4C	3.44	110.44	106.27
24	BC	5511	CLA	O2A-CGA-CBA	3.44	122.37	111.90
24	AA	404	CLA	O2A-CGA-CBA	3.44	122.38	111.90
31	AJ	102	LMG	C12-C11-C10	3.44	127.11	113.59
24	AB	604	CLA	O2D-CGD-CBD	3.44	116.02	111.30
27	AB	618	BCR	C29-C30-C25	3.44	115.81	110.36
24	BB	5611	CLA	O2D-CGD-CBD	3.45	116.03	111.30
24	BC	5509	CLA	O2A-CGA-CBA	3.45	122.40	111.90
24	BA	5405	CLA	O2A-CGA-CBA	3.45	122.40	111.90
24	AC	504	CLA	O2A-CGA-CBA	3.45	122.41	111.90
29	AA	412	LHG	O8-C23-C24	3.45	122.42	111.90
24	BB	5609	CLA	C1C-NC-C4C	3.46	110.47	106.27
24	AB	605	CLA	O2A-CGA-CBA	3.46	122.45	111.90
24	AC	501	CLA	CBA-CAA-C2A	3.47	123.52	113.73
27	BC	5515	BCR	C2-C1-C6	3.47	115.86	110.36
30	AA	413	SQD	O48-C23-C24	3.48	122.49	111.90
24	BC	5512	CLA	C2A-C1A-CHA	3.48	130.29	123.89
24	AC	509	CLA	C2A-C1A-CHA	3.48	130.30	123.89
27	BA	5411	BCR	C29-C30-C25	3.48	115.88	110.36
24	AA	407	CLA	O2A-CGA-CBA	3.49	122.52	111.90
34	BD	5404	PHO	O2A-CGA-CBA	3.49	122.52	111.90
34	BD	5404	PHO	C4A-NA-C1A	3.49	111.33	108.21
27	BC	5516	BCR	C2-C1-C6	3.49	115.89	110.36
30	BA	5414	SQD	O48-C23-C24	3.49	122.54	111.90
24	AB	607	CLA	O2D-CGD-CBD	3.49	116.09	111.30
27	BK	5102	BCR	C29-C30-C25	3.50	115.90	110.36
31	AJ	102	LMG	C9-C8-C7	3.50	120.25	112.07
31	BD	5408	LMG	C9-C8-C7	3.50	120.26	112.07
24	BC	5502	CLA	O2A-CGA-CBA	3.50	122.58	111.90
24	AB	615	CLA	C2A-C1A-CHA	3.51	130.34	123.89
24	BC	5502	CLA	C1C-NC-C4C	3.51	110.54	106.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AC	510	CLA	O2A-CGA-CBA	3.51	122.61	111.90
24	AC	512	CLA	O2A-CGA-CBA	3.52	122.61	111.90
27	AC	515	BCR	C23-C24-C25	3.52	137.89	127.32
24	AC	502	CLA	O2A-CGA-CBA	3.53	122.66	111.90
34	AD	403	PHO	O2A-CGA-CBA	3.53	122.66	111.90
24	BA	5405	CLA	C1C-NC-C4C	3.54	110.56	106.27
24	BA	5408	CLA	O2A-CGA-CBA	3.54	122.67	111.90
31	BC	5520	LMG	C9-O8-C28	3.54	126.74	116.85
27	AC	515	BCR	C2-C1-C6	3.54	115.97	110.36
27	BC	5515	BCR	C23-C24-C25	3.54	137.95	127.32
24	BB	5619	CLA	C2A-C1A-CHA	3.54	130.40	123.89
24	BC	5508	CLA	O2A-CGA-CBA	3.54	122.69	111.90
27	BJ	5101	BCR	C23-C24-C25	3.55	137.97	127.32
24	AC	509	CLA	O2D-CGD-CBD	3.55	116.17	111.30
27	AK	102	BCR	C29-C30-C25	3.55	115.99	110.36
24	AB	606	CLA	C1C-NC-C4C	3.56	110.59	106.27
34	AD	402	PHO	C4D-C3D-CAD	3.57	111.92	105.51
27	AB	619	BCR	C29-C30-C25	3.57	116.02	110.36
24	BB	5607	CLA	C3A-C2A-C1A	3.57	107.55	101.50
31	AC	520	LMG	C9-O8-C28	3.57	126.84	116.85
30	AB	627	SQD	C11-C10-C9	3.57	132.99	114.53
27	BJ	5101	BCR	C7-C8-C9	3.58	131.68	126.22
27	AX	101	BCR	C2-C1-C6	3.59	116.04	110.36
24	BB	5607	CLA	O2A-CGA-CBA	3.59	122.84	111.90
24	BC	5503	CLA	O2A-CGA-CBA	3.59	122.85	111.90
30	BB	5625	SQD	C44-O6-C1	3.60	121.37	113.82
27	BC	5515	BCR	C29-C30-C25	3.60	116.06	110.36
27	AB	617	BCR	C29-C30-C25	3.60	116.06	110.36
24	AC	506	CLA	O2A-CGA-CBA	3.60	122.88	111.90
24	AB	603	CLA	C3A-C2A-C1A	3.61	107.61	101.50
24	BC	5506	CLA	O2D-CGD-CBD	3.61	116.25	111.30
34	BD	5404	PHO	C4D-C3D-CAD	3.61	112.00	105.51
34	BD	5403	PHO	C4D-C3D-CAD	3.61	112.01	105.51
24	BC	5509	CLA	O2D-CGD-CBD	3.61	116.26	111.30
24	BD	5405	CLA	CBA-CAA-C2A	3.62	123.94	113.73
34	AD	403	PHO	C4D-C3D-CAD	3.62	112.02	105.51
24	BC	5513	CLA	O2A-CGA-CBA	3.62	122.94	111.90
24	AC	507	CLA	O2A-CGA-CBA	3.63	122.95	111.90
27	BJ	5101	BCR	C29-C30-C25	3.63	116.11	110.36
24	BC	5501	CLA	CBA-CAA-C2A	3.63	123.97	113.73
30	BB	5601	SQD	C11-C10-C9	3.63	133.29	114.53
24	BC	5501	CLA	O2D-CGD-CBD	3.64	116.29	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BC	5507	CLA	O2A-CGA-CBA	3.64	122.98	111.90
24	BC	5501	CLA	O2A-CGA-CBA	3.64	122.98	111.90
24	AC	503	CLA	O2A-CGA-CBA	3.64	122.98	111.90
24	BB	5606	CLA	O2A-CGA-CBA	3.64	122.99	111.90
24	AA	404	CLA	C4A-NA-C1A	3.64	111.07	106.36
32	AD	409	LMT	O1B-C1B-C2B	3.65	116.97	108.10
24	AC	509	CLA	O2A-CGA-CBA	3.65	123.01	111.90
30	BA	5414	SQD	C11-C10-C9	3.65	133.37	114.53
30	AA	413	SQD	C11-C10-C9	3.65	133.38	114.53
31	AJ	102	LMG	O1-C7-C8	3.65	119.67	110.99
27	BD	5407	BCR	C24-C23-C22	3.66	131.79	126.22
30	BF	5102	SQD	C11-C10-C9	3.67	133.46	114.53
24	AC	508	CLA	O2A-CGA-CBA	3.67	123.08	111.90
24	BB	5610	CLA	C1C-NC-C4C	3.67	110.73	106.27
32	BD	5411	LMT	O1B-C1B-C2B	3.67	117.04	108.10
30	AF	102	SQD	C11-C10-C9	3.68	133.51	114.53
27	AJ	101	BCR	C23-C24-C25	3.68	138.36	127.32
24	AB	603	CLA	O2A-CGA-CBA	3.69	123.14	111.90
30	BA	5414	SQD	C31-C30-C29	3.69	133.59	114.53
24	BA	5405	CLA	C4A-NA-C1A	3.69	111.13	106.36
27	AJ	101	BCR	C29-C30-C25	3.69	116.21	110.36
34	BD	5404	PHO	C3A-C2A-C1A	3.70	106.53	101.84
30	BB	5625	SQD	C11-C10-C9	3.70	133.64	114.53
24	BC	5506	CLA	O2A-CGA-CBA	3.70	123.18	111.90
24	AD	401	CLA	O2A-CGA-CBA	3.70	123.18	111.90
24	AC	506	CLA	CBA-CAA-C2A	3.71	124.20	113.73
30	AA	413	SQD	C31-C30-C29	3.71	133.70	114.53
24	BB	5611	CLA	C1C-NC-C4C	3.71	110.78	106.27
30	AB	622	SQD	C11-C10-C9	3.72	133.75	114.53
27	AA	410	BCR	C7-C8-C9	3.72	131.89	126.22
35	AD	405	PL9	C26-C27-C28	3.72	121.44	111.69
24	AA	406	CLA	C4A-NA-C1A	3.75	111.21	106.36
30	BA	5414	SQD	C45-O47-C7	3.75	126.89	117.89
27	BB	5621	BCR	C29-C30-C25	3.75	116.31	110.36
28	AA	411	DGD	O6E-C1E-O5D	3.76	119.10	110.05
30	BB	5625	SQD	O48-C23-C24	3.76	123.35	111.90
28	BA	5412	DGD	O6E-C1E-O5D	3.76	119.11	110.05
30	AA	413	SQD	C45-O47-C7	3.76	126.92	117.89
24	AB	612	CLA	C4A-NA-C1A	3.76	111.22	106.36
24	AB	602	CLA	O2A-CGA-CBA	3.76	123.37	111.90
24	AC	513	CLA	O2A-CGA-CBA	3.77	123.37	111.90
24	AB	607	CLA	C1C-NC-C4C	3.77	110.85	106.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	BD	5408	LMG	O1-C7-C8	3.77	119.96	110.99
24	BB	5607	CLA	C4A-NA-C1A	3.77	111.24	106.36
24	AA	406	CLA	C1C-NC-C4C	3.78	110.86	106.27
30	AB	622	SQD	C44-O6-C1	3.79	121.78	113.82
24	BC	5504	CLA	C1C-NC-C4C	3.79	110.87	106.27
30	BF	5102	SQD	O48-C23-C24	3.79	123.45	111.90
30	AA	416	SQD	C11-C10-C9	3.79	134.12	114.53
31	BB	5624	LMG	C34-C33-C32	3.79	134.12	114.53
24	BC	5506	CLA	CBA-CAA-C2A	3.79	124.44	113.73
30	BA	5401	SQD	C11-C10-C9	3.80	134.14	114.53
30	AB	627	SQD	O48-C23-C24	3.80	123.47	111.90
24	AB	611	CLA	O2A-CGA-CBA	3.80	123.48	111.90
24	AD	404	CLA	CBA-CAA-C2A	3.80	124.45	113.73
24	BB	5609	CLA	O2D-CGD-CBD	3.81	116.52	111.30
24	AC	513	CLA	C4A-NA-C1A	3.81	111.29	106.36
30	AF	102	SQD	O48-C23-C24	3.82	123.53	111.90
31	AB	621	LMG	C34-C33-C32	3.82	134.27	114.53
27	AJ	101	BCR	C7-C8-C9	3.83	132.05	126.22
24	BD	5402	CLA	O2A-CGA-CBA	3.83	123.56	111.90
30	BB	5601	SQD	O48-C23-C24	3.83	123.57	111.90
28	AH	101	DGD	O6D-C5D-C6D	3.83	114.44	106.61
24	BB	5615	CLA	O2A-CGA-CBA	3.83	123.58	111.90
27	BX	5101	BCR	C2-C1-C6	3.83	116.43	110.36
24	AB	603	CLA	C4A-NA-C1A	3.84	111.32	106.36
24	BB	5607	CLA	C2A-C1A-CHA	3.85	130.97	123.89
31	BD	5409	LMG	C21-C20-C19	3.85	134.40	114.53
27	AD	406	BCR	C24-C23-C22	3.85	132.08	126.22
27	AD	406	BCR	C29-C30-C25	3.85	116.46	110.36
24	AB	614	CLA	O2D-CGD-CBD	3.87	116.61	111.30
24	AB	609	CLA	O2D-CGD-CBD	3.88	116.62	111.30
24	AC	504	CLA	C1C-NC-C4C	3.88	110.98	106.27
28	BH	5101	DGD	O6D-C5D-C6D	3.89	114.56	106.61
24	AB	603	CLA	C2A-C1A-CHA	3.89	131.05	123.89
30	AA	416	SQD	C31-C30-C29	3.89	134.63	114.53
35	BD	5406	PL9	C26-C27-C28	3.89	121.89	111.69
35	BD	5406	PL9	C25-C24-C26	3.89	121.36	115.41
24	AB	609	CLA	O2A-CGA-CBA	3.90	123.77	111.90
24	AC	501	CLA	O2D-CGD-CBD	3.90	116.64	111.30
30	BA	5401	SQD	C31-C30-C29	3.90	134.68	114.53
24	AA	404	CLA	C1C-NC-C4C	3.90	111.01	106.27
24	AA	405	CLA	C4A-NA-C1A	3.91	111.41	106.36
31	BA	5402	LMG	O7-C8-C7	3.93	122.22	108.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5608	CLA	O2A-CGA-CBA	3.94	123.89	111.90
24	BC	5502	CLA	CBA-CAA-C2A	3.94	124.85	113.73
24	AB	604	CLA	O2A-CGA-CBA	3.94	123.91	111.90
27	BA	5411	BCR	C7-C8-C9	3.94	132.22	126.22
31	BL	5101	LMG	C8-O7-C10	3.94	127.36	117.89
24	BC	5513	CLA	C4A-NA-C1A	3.95	111.46	106.36
27	BT	5101	BCR	C29-C30-C25	3.95	116.61	110.36
27	AX	101	BCR	C29-C30-C25	3.95	116.62	110.36
24	BC	5508	CLA	CBA-CAA-C2A	3.96	124.90	113.73
24	BB	5613	CLA	O2A-CGA-CBA	3.96	123.96	111.90
31	BC	5521	LMG	O7-C8-C7	3.96	122.32	108.36
29	BA	5415	LHG	O7-C7-C8	3.97	120.15	111.53
29	AA	415	LHG	O7-C7-C8	3.97	120.16	111.53
24	BA	5407	CLA	C1C-NC-C4C	3.98	111.11	106.27
30	AA	416	SQD	O48-C23-C24	3.98	124.04	111.90
30	BA	5401	SQD	O48-C23-C24	3.99	124.05	111.90
31	AD	407	LMG	C21-C20-C19	3.99	135.14	114.53
24	BB	5616	CLA	C4A-NA-C1A	3.99	111.52	106.36
31	AC	521	LMG	O7-C8-C7	4.00	122.46	108.36
24	AB	605	CLA	C4A-NA-C1A	4.00	111.53	106.36
24	BB	5615	CLA	O2D-CGD-CBD	4.01	116.81	111.30
24	BB	5609	CLA	C4A-NA-C1A	4.02	111.56	106.36
31	BL	5101	LMG	O1-C7-C8	4.02	120.56	110.99
27	BX	5101	BCR	C29-C30-C25	4.02	116.73	110.36
27	BK	5102	BCR	C7-C8-C9	4.03	132.36	126.22
27	BK	5102	BCR	C2-C1-C6	4.04	116.76	110.36
24	AC	511	CLA	C4A-NA-C1A	4.05	111.59	106.36
30	AA	416	SQD	C44-O6-C1	4.06	122.34	113.82
31	AA	417	LMG	O7-C8-C7	4.06	122.67	108.36
24	AC	502	CLA	CBA-CAA-C2A	4.06	125.19	113.73
24	BA	5406	CLA	C4A-NA-C1A	4.06	111.61	106.36
35	AD	405	PL9	C25-C24-C26	4.07	121.62	115.41
30	AB	622	SQD	O48-C23-C24	4.07	124.29	111.90
27	AC	514	BCR	C24-C23-C22	4.07	132.41	126.22
24	BA	5407	CLA	C4A-NA-C1A	4.07	111.62	106.36
24	AB	609	CLA	C4A-NA-C1A	4.07	111.62	106.36
24	BB	5613	CLA	C4A-NA-C1A	4.07	111.62	106.36
27	AT	101	BCR	C29-C30-C25	4.08	116.82	110.36
35	AD	405	PL9	C15-C14-C16	4.09	121.66	115.41
24	AC	508	CLA	CBA-CAA-C2A	4.09	125.28	113.73
24	BB	5613	CLA	O2D-CGD-CBD	4.11	116.94	111.30
24	AB	607	CLA	C4A-NA-C1A	4.11	111.67	106.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BC	5505	CLA	O2D-CGD-CBD	4.11	116.94	111.30
24	BC	5504	CLA	C4A-NA-C1A	4.12	111.68	106.36
24	BB	5618	CLA	C4A-NA-C1A	4.12	111.68	106.36
24	AB	605	CLA	CBA-CAA-C2A	4.12	125.35	113.73
27	BD	5407	BCR	C29-C30-C25	4.12	116.89	110.36
24	AB	602	CLA	O2D-CGD-CBD	4.13	116.96	111.30
36	AV	201	HEM	CMC-C2C-C3C	4.13	126.83	116.53
24	AC	504	CLA	C4A-NA-C1A	4.13	111.70	106.36
24	AA	406	CLA	O2A-CGA-CBA	4.13	124.48	111.90
32	BC	5522	LMT	C1-O1'-C1'	4.13	121.17	113.94
31	AB	620	LMG	C8-O7-C10	4.13	127.81	117.89
28	BE	5102	DGD	O5D-C1E-C2E	4.14	113.27	108.04
24	BC	5511	CLA	C4A-NA-C1A	4.14	111.71	106.36
30	BA	5401	SQD	C44-O6-C1	4.15	122.53	113.82
27	AC	516	BCR	C2-C1-C6	4.16	116.94	110.36
24	AB	604	CLA	C4A-NA-C1A	4.16	111.73	106.36
27	AK	102	BCR	C7-C8-C9	4.16	132.55	126.22
24	BC	5502	CLA	O2D-CGD-CBD	4.16	117.01	111.30
24	AA	405	CLA	O2A-CGA-CBA	4.16	124.59	111.90
31	AB	620	LMG	O1-C7-C8	4.16	120.90	110.99
24	BB	5611	CLA	C4A-NA-C1A	4.17	111.75	106.36
24	BB	5619	CLA	O2D-CGD-CBD	4.17	117.02	111.30
24	BA	5407	CLA	O2A-CGA-CBA	4.17	124.62	111.90
27	BC	5516	BCR	C29-C30-C25	4.18	116.97	110.36
24	BB	5609	CLA	CBA-CAA-C2A	4.18	125.53	113.73
24	AD	401	CLA	O2D-CGD-CBD	4.20	117.06	111.30
28	BE	5102	DGD	O2G-C1B-C2B	4.20	120.66	111.53
24	AC	513	CLA	O2D-CGD-CBD	4.21	117.08	111.30
24	AB	614	CLA	C4A-NA-C1A	4.22	111.81	106.36
28	AE	101	DGD	O2G-C1B-C2B	4.22	120.70	111.53
24	AC	502	CLA	O2D-CGD-CBD	4.22	117.09	111.30
24	AB	603	CLA	O2D-CGD-CBD	4.23	117.10	111.30
27	BC	5514	BCR	C24-C23-C22	4.23	132.67	126.22
30	BA	5414	SQD	C44-O6-C1	4.23	122.71	113.82
27	AK	102	BCR	C2-C1-C6	4.24	117.07	110.36
24	AB	605	CLA	O2D-CGD-CBD	4.24	117.11	111.30
24	BB	5617	CLA	C4A-NA-C1A	4.24	111.85	106.36
31	BA	5402	LMG	C9-C8-C7	4.24	122.00	112.07
31	AA	417	LMG	C9-C8-C7	4.25	122.00	112.07
35	BD	5406	PL9	C15-C14-C16	4.25	121.90	115.41
24	AB	613	CLA	C4A-NA-C1A	4.26	111.86	106.36
32	AI	103	LMT	C1-O1'-C1'	4.26	121.39	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5607	CLA	O2D-CGD-CBD	4.26	117.14	111.30
24	BA	5408	CLA	C4A-NA-C1A	4.27	111.88	106.36
28	BE	5102	DGD	C1G-O1G-C1A	4.27	128.80	116.85
25	BA	5409	MST	C6-N5-C4	4.27	120.26	113.99
24	BD	5402	CLA	C4A-NA-C1A	4.28	111.89	106.36
24	AB	607	CLA	O2A-CGA-CBA	4.28	124.95	111.90
24	BB	5614	CLA	C4A-NA-C1A	4.29	111.91	106.36
24	AD	401	CLA	C4A-NA-C1A	4.29	111.91	106.36
24	BB	5618	CLA	O2D-CGD-CBD	4.29	117.19	111.30
24	AB	610	CLA	C4A-NA-C1A	4.31	111.93	106.36
24	AB	606	CLA	C4A-NA-C1A	4.31	111.93	106.36
30	AA	413	SQD	C44-O6-C1	4.32	122.89	113.82
28	AE	101	DGD	C1G-O1G-C1A	4.32	128.93	116.85
24	AB	608	CLA	C4A-NA-C1A	4.32	111.95	106.36
24	BA	5406	CLA	O2A-CGA-CBA	4.33	125.08	111.90
25	AA	408	MST	C6-N5-C4	4.33	120.34	113.99
36	BV	5201	HEM	CMC-C2C-C3C	4.33	127.34	116.53
24	BB	5615	CLA	C4A-NA-C1A	4.33	111.96	106.36
24	AC	511	CLA	CBA-CAA-C2A	4.34	125.98	113.73
24	BB	5612	CLA	C4A-NA-C1A	4.34	111.97	106.36
24	AB	602	CLA	C4A-NA-C1A	4.35	111.98	106.36
24	BC	5513	CLA	O2D-CGD-CBD	4.35	117.27	111.30
24	AB	611	CLA	C4A-NA-C1A	4.35	111.99	106.36
24	BB	5608	CLA	C4A-NA-C1A	4.35	111.99	106.36
24	AC	506	CLA	C4A-NA-C1A	4.36	111.99	106.36
24	BB	5610	CLA	C4A-NA-C1A	4.36	112.00	106.36
24	AB	606	CLA	O2A-CGA-CBA	4.37	125.20	111.90
24	BB	5611	CLA	O2A-CGA-CBA	4.37	125.20	111.90
24	AC	509	CLA	C4A-NA-C1A	4.38	112.02	106.36
31	AD	407	LMG	C18-C17-C16	4.38	137.13	114.53
24	BC	5511	CLA	CBA-CAA-C2A	4.38	126.10	113.73
28	AE	101	DGD	O5D-C1E-C2E	4.38	113.58	108.04
24	AC	508	CLA	O2D-CGD-CBD	4.39	117.32	111.30
24	AB	611	CLA	O2D-CGD-CBD	4.40	117.33	111.30
32	BC	5522	LMT	O1B-C1B-C2B	4.41	118.83	108.10
27	BK	5102	BCR	C11-C10-C9	4.41	133.57	127.20
24	AC	508	CLA	C4A-NA-C1A	4.41	112.07	106.36
27	AC	516	BCR	C29-C30-C25	4.42	117.36	110.36
24	AC	502	CLA	C4A-NA-C1A	4.42	112.08	106.36
24	BC	5509	CLA	C1C-NC-C4C	4.43	111.65	106.27
24	BC	5506	CLA	C4A-NA-C1A	4.43	112.08	106.36
24	BC	5503	CLA	C4A-NA-C1A	4.43	112.09	106.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	AF	101	HEM	CMC-C2C-C3C	4.44	127.61	116.53
24	BC	5509	CLA	C4A-NA-C1A	4.44	112.10	106.36
24	AB	615	CLA	O2D-CGD-CBD	4.44	117.39	111.30
24	BB	5606	CLA	O2D-CGD-CBD	4.44	117.39	111.30
24	AC	510	CLA	C4A-NA-C1A	4.44	112.11	106.36
31	BD	5409	LMG	C18-C17-C16	4.46	137.54	114.53
24	BC	5510	CLA	C4A-NA-C1A	4.46	112.13	106.36
24	BB	5610	CLA	O2A-CGA-CBA	4.46	125.50	111.90
24	BB	5606	CLA	C4A-NA-C1A	4.47	112.13	106.36
24	AC	505	CLA	C4A-NA-C1A	4.48	112.15	106.36
24	AB	616	CLA	O2D-CGD-CBD	4.49	117.46	111.30
24	AB	608	CLA	O2D-CGD-CBD	4.50	117.47	111.30
31	BD	5408	LMG	C9-O8-C28	4.50	129.43	116.85
24	AA	407	CLA	C4A-NA-C1A	4.53	112.21	106.36
31	AA	414	LMG	C8-O7-C10	4.53	128.76	117.89
28	BC	5519	DGD	O6E-C1E-O5D	4.55	121.00	110.05
28	AC	519	DGD	O6E-C1E-O5D	4.55	121.00	110.05
28	AC	519	DGD	O6D-C5D-C4D	4.55	118.22	109.68
24	BC	5505	CLA	C4A-NA-C1A	4.55	112.24	106.36
31	BE	5101	LMG	C8-O7-C10	4.57	128.86	117.89
24	BC	5507	CLA	C4A-NA-C1A	4.57	112.27	106.36
24	BC	5511	CLA	O2D-CGD-CBD	4.58	117.58	111.30
24	BB	5612	CLA	O2D-CGD-CBD	4.58	117.58	111.30
24	BD	5402	CLA	O2D-CGD-CBD	4.59	117.59	111.30
24	BB	5605	CLA	O2D-CGD-CBD	4.59	117.60	111.30
24	AC	504	CLA	CBA-CAA-C2A	4.60	126.70	113.73
24	AB	610	CLA	O2D-CGD-CBD	4.61	117.63	111.30
24	AC	509	CLA	C1C-NC-C4C	4.62	111.89	106.27
34	AD	403	PHO	O2D-CGD-CBD	4.63	117.65	111.30
28	BH	5101	DGD	O5D-C6D-C5D	4.63	117.47	109.08
24	BC	5504	CLA	CBA-CAA-C2A	4.63	126.81	113.73
32	AI	103	LMT	O1B-C1B-C2B	4.63	119.38	108.10
24	BB	5620	CLA	C4A-NA-C1A	4.64	112.35	106.36
24	AC	507	CLA	C4A-NA-C1A	4.64	112.36	106.36
31	AD	408	LMG	C9-O8-C28	4.64	129.82	116.85
24	AD	404	CLA	C4A-NA-C1A	4.64	112.36	106.36
24	AB	616	CLA	C4A-NA-C1A	4.64	112.37	106.36
31	BD	5410	LMG	C9-O8-C28	4.64	129.84	116.85
27	AK	102	BCR	C11-C10-C9	4.65	133.91	127.20
24	BC	5508	CLA	O2D-CGD-CBD	4.65	117.68	111.30
31	AJ	102	LMG	C9-O8-C28	4.65	129.86	116.85
36	BV	5201	HEM	CMB-C2B-C3B	4.66	128.16	116.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BF	5101	HEM	CMC-C2C-C3C	4.66	128.17	116.53
24	AC	503	CLA	C4A-NA-C1A	4.67	112.40	106.36
24	BB	5620	CLA	O2D-CGD-CBD	4.68	117.72	111.30
31	AD	407	LMG	C20-C19-C18	4.69	138.73	114.53
24	BB	5614	CLA	O2D-CGD-CBD	4.69	117.74	111.30
24	BD	5405	CLA	C4A-NA-C1A	4.70	112.44	106.36
24	AC	501	CLA	C4A-NA-C1A	4.70	112.44	106.36
24	AC	507	CLA	O2D-CGD-CBD	4.70	117.75	111.30
36	AF	101	HEM	CMB-C2B-C3B	4.72	128.30	116.53
34	AD	402	PHO	O2D-CGD-CBD	4.73	117.79	111.30
34	BD	5403	PHO	O2D-CGD-CBD	4.74	117.80	111.30
24	AB	601	CLA	O2D-CGD-CBD	4.74	117.80	111.30
31	BD	5409	LMG	C20-C19-C18	4.74	139.00	114.53
24	AB	615	CLA	C4A-NA-C1A	4.74	112.50	106.36
24	AC	505	CLA	CBA-CAA-C2A	4.75	127.12	113.73
28	AH	101	DGD	O5D-C6D-C5D	4.76	117.70	109.08
35	AD	405	PL9	C35-C34-C36	4.76	122.68	115.41
24	BC	5510	CLA	O2D-CGD-CBD	4.78	117.86	111.30
34	BD	5404	PHO	O2D-CGD-CBD	4.79	117.87	111.30
36	BF	5101	HEM	CMB-C2B-C3B	4.80	128.51	116.53
30	AF	102	SQD	C44-O6-C1	4.82	123.94	113.82
24	BC	5502	CLA	C4A-NA-C1A	4.82	112.59	106.36
24	BC	5508	CLA	C4A-NA-C1A	4.82	112.59	106.36
24	AB	612	CLA	C1C-NC-C4C	4.83	112.14	106.27
24	BC	5507	CLA	O2D-CGD-CBD	4.85	117.96	111.30
27	BC	5514	BCR	C33-C5-C6	4.85	129.37	124.61
24	BC	5501	CLA	C4A-NA-C1A	4.86	112.65	106.36
24	BC	5505	CLA	CBA-CAA-C2A	4.87	127.48	113.73
35	BD	5406	PL9	C35-C34-C36	4.88	122.86	115.41
24	BC	5503	CLA	O2D-CGD-CBD	4.89	118.01	111.30
24	AC	505	CLA	O2D-CGD-CBD	4.89	118.01	111.30
24	AB	614	CLA	C1C-NC-C4C	4.90	112.22	106.27
24	AC	503	CLA	O2D-CGD-CBD	4.90	118.03	111.30
27	BB	5622	BCR	C33-C5-C6	4.91	129.42	124.61
24	AC	510	CLA	O2D-CGD-CBD	4.92	118.05	111.30
24	BB	5619	CLA	C4A-NA-C1A	4.93	112.74	106.36
31	AA	417	LMG	C9-O8-C28	4.95	130.69	116.85
24	AB	614	CLA	CBA-CAA-C2A	4.95	127.70	113.73
24	BC	5512	CLA	C4A-NA-C1A	4.96	112.78	106.36
30	BF	5102	SQD	C44-O6-C1	4.97	124.26	113.82
24	AC	512	CLA	C4A-NA-C1A	4.97	112.78	106.36
28	BC	5519	DGD	O6D-C5D-C4D	4.98	119.03	109.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	5618	CLA	CBA-CAA-C2A	4.99	127.82	113.73
24	BB	5618	CLA	C1C-NC-C4C	5.00	112.34	106.27
36	AV	201	HEM	CMB-C2B-C3B	5.01	129.03	116.53
30	BB	5625	SQD	C25-C24-C23	5.03	133.35	113.59
30	AB	622	SQD	C25-C24-C23	5.04	133.39	113.59
31	BI	5101	LMG	C9-O8-C28	5.06	131.01	116.85
31	BA	5402	LMG	C9-O8-C28	5.07	131.02	116.85
24	BB	5616	CLA	C1C-NC-C4C	5.07	112.43	106.27
24	AC	504	CLA	O2D-CGD-CBD	5.08	118.27	111.30
24	BB	5605	CLA	C4A-NA-C1A	5.09	112.94	106.36
35	BD	5406	PL9	C20-C19-C21	5.10	123.19	115.41
31	AI	101	LMG	C9-O8-C28	5.11	131.14	116.85
24	BD	5405	CLA	O2D-CGD-CBD	5.13	118.34	111.30
24	AC	511	CLA	O2D-CGD-CBD	5.14	118.34	111.30
24	BA	5408	CLA	O2D-CGD-CBD	5.15	118.36	111.30
24	AB	603	CLA	C1C-NC-C4C	5.15	112.52	106.27
27	AC	514	BCR	C33-C5-C6	5.20	129.71	124.61
24	BA	5407	CLA	O2D-CGD-CBD	5.21	118.45	111.30
30	AA	416	SQD	C25-C24-C23	5.22	134.10	113.59
24	BB	5616	CLA	O2D-CGD-CBD	5.23	118.48	111.30
24	AA	407	CLA	O2D-CGD-CBD	5.24	118.48	111.30
24	AB	601	CLA	C4A-NA-C1A	5.25	113.14	106.36
30	BA	5401	SQD	C25-C24-C23	5.25	134.22	113.59
28	AA	411	DGD	O2G-C1B-C2B	5.26	122.96	111.53
24	BC	5513	CLA	C1C-NC-C4C	5.28	112.68	106.27
35	AD	405	PL9	C20-C19-C21	5.28	123.47	115.41
28	BA	5412	DGD	O2G-C1B-C2B	5.29	123.02	111.53
24	BC	5504	CLA	O2D-CGD-CBD	5.29	118.55	111.30
24	AC	513	CLA	C1C-NC-C4C	5.30	112.71	106.27
24	BB	5607	CLA	C1C-NC-C4C	5.33	112.75	106.27
24	AD	404	CLA	O2D-CGD-CBD	5.35	118.64	111.30
24	BB	5611	CLA	CBA-CAA-C2A	5.35	128.83	113.73
30	AB	627	SQD	C25-C24-C23	5.36	134.67	113.59
31	AB	620	LMG	O7-C8-C7	5.36	127.26	108.36
30	BB	5601	SQD	C25-C24-C23	5.38	134.76	113.59
24	AC	511	CLA	C1C-NC-C4C	5.39	112.82	106.27
31	BL	5101	LMG	O7-C8-C7	5.39	127.36	108.36
24	BC	5511	CLA	C1C-NC-C4C	5.40	112.83	106.27
24	AA	406	CLA	O2D-CGD-CBD	5.41	118.72	111.30
27	AB	618	BCR	C33-C5-C6	5.43	129.94	124.61
24	BA	5406	CLA	O2D-CGD-CBD	5.44	118.76	111.30
24	AA	405	CLA	O2D-CGD-CBD	5.44	118.77	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BB	5623	BCR	C33-C5-C6	5.45	129.96	124.61
30	AA	413	SQD	C25-C24-C23	5.46	135.05	113.59
24	AB	608	CLA	CBA-CAA-C2A	5.47	129.16	113.73
30	BA	5414	SQD	C25-C24-C23	5.49	135.16	113.59
24	AB	612	CLA	O2D-CGD-CBD	5.51	118.85	111.30
27	AD	406	BCR	C33-C5-C6	5.52	130.02	124.61
30	AF	102	SQD	C25-C24-C23	5.53	135.35	113.59
24	AB	607	CLA	CBA-CAA-C2A	5.57	129.45	113.73
30	BF	5102	SQD	C25-C24-C23	5.58	135.51	113.59
31	AM	101	LMG	C9-O8-C28	5.58	132.46	116.85
31	AC	521	LMG	C9-O8-C28	5.59	132.49	116.85
24	BB	5612	CLA	CBA-CAA-C2A	5.60	129.52	113.73
31	BM	5102	LMG	C9-O8-C28	5.61	132.54	116.85
27	AX	101	BCR	C33-C5-C6	5.62	130.13	124.61
28	AA	411	DGD	O6D-C1D-O3G	5.64	123.63	110.05
27	BX	5101	BCR	C33-C5-C6	5.67	130.17	124.61
27	BB	5623	BCR	C38-C26-C25	5.68	130.18	124.61
27	AB	619	BCR	C38-C26-C25	5.68	130.18	124.61
31	BC	5521	LMG	C9-O8-C28	5.70	132.78	116.85
31	BI	5101	LMG	O7-C10-C11	5.72	123.95	111.53
27	BD	5407	BCR	C33-C5-C6	5.72	130.22	124.61
31	BD	5408	LMG	O7-C8-C7	5.75	128.61	108.36
28	BA	5412	DGD	O6D-C1D-O3G	5.76	123.91	110.05
27	AB	619	BCR	C33-C5-C6	5.77	130.27	124.61
31	AI	101	LMG	O7-C10-C11	5.80	124.13	111.53
31	AJ	102	LMG	O7-C8-C7	5.80	128.79	108.36
29	BA	5413	LHG	C25-C24-C23	5.80	136.39	113.59
28	AC	517	DGD	O5D-C1E-C2E	5.80	115.36	108.04
28	AC	518	DGD	O2G-C1B-C2B	5.82	124.18	111.53
27	AJ	101	BCR	C31-C1-C6	5.83	119.44	110.30
28	BC	5518	DGD	O2G-C1B-C2B	5.83	124.20	111.53
28	AA	411	DGD	O1G-C1A-C2A	5.86	129.76	111.90
31	BD	5409	LMG	O7-C8-C7	5.86	129.03	108.36
30	AB	622	SQD	C10-C9-C8	5.87	134.82	113.29
30	BF	5102	SQD	C10-C9-C8	5.88	134.84	113.29
30	AF	102	SQD	C10-C9-C8	5.88	134.85	113.29
28	BC	5517	DGD	O5D-C1E-C2E	5.90	115.49	108.04
29	AA	412	LHG	C25-C24-C23	5.90	136.79	113.59
27	AA	410	BCR	C38-C26-C25	5.92	130.42	124.61
27	AJ	101	BCR	C33-C5-C6	5.92	130.42	124.61
27	AA	410	BCR	C33-C5-C6	5.93	130.42	124.61
30	BB	5625	SQD	C10-C9-C8	5.93	135.04	113.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BA	5412	DGD	O1G-C1A-C2A	5.93	129.97	111.90
31	AD	407	LMG	O7-C8-C7	5.93	129.26	108.36
27	BJ	5101	BCR	C33-C5-C6	5.94	130.43	124.61
27	AB	617	BCR	C33-C5-C6	5.94	130.44	124.61
30	AB	627	SQD	C10-C9-C8	5.95	135.12	113.29
27	BJ	5101	BCR	C31-C1-C6	5.96	119.65	110.30
27	BB	5621	BCR	C33-C5-C6	5.98	130.48	124.61
27	BC	5514	BCR	C38-C26-C25	5.99	130.48	124.61
30	BA	5414	SQD	C10-C9-C8	6.01	135.31	113.29
30	AA	416	SQD	C10-C9-C8	6.02	135.38	113.29
30	AA	413	SQD	C10-C9-C8	6.05	135.49	113.29
28	AB	628	DGD	C1G-O1G-C1A	6.06	133.79	116.85
27	BA	5411	BCR	C38-C26-C25	6.06	130.55	124.61
28	BB	5602	DGD	C1G-O1G-C1A	6.06	133.80	116.85
27	BA	5411	BCR	C33-C5-C6	6.08	130.57	124.61
30	BA	5401	SQD	C10-C9-C8	6.08	135.57	113.29
27	AT	101	BCR	C38-C26-C25	6.09	130.58	124.61
30	BB	5601	SQD	C10-C9-C8	6.09	135.62	113.29
25	BA	5409	MST	C8-S7-C2	6.11	106.17	102.26
25	AA	408	MST	C8-S7-C2	6.12	106.18	102.26
28	BC	5517	DGD	O6D-C5D-C6D	6.12	119.12	106.61
27	BC	5516	BCR	C38-C26-C25	6.18	130.68	124.61
27	AC	514	BCR	C38-C26-C25	6.21	130.70	124.61
27	BT	5101	BCR	C38-C26-C25	6.31	130.80	124.61
27	AK	102	BCR	C38-C26-C25	6.34	130.83	124.61
24	BA	5407	CLA	CBA-CAA-C2A	6.37	131.72	113.73
27	BK	5102	BCR	C38-C26-C25	6.38	130.87	124.61
28	AA	411	DGD	C3G-O3G-C1D	6.39	127.24	113.82
28	BA	5412	DGD	C3G-O3G-C1D	6.40	127.27	113.82
27	AC	516	BCR	C38-C26-C25	6.41	130.90	124.61
28	AC	517	DGD	O6D-C5D-C6D	6.43	119.75	106.61
28	BC	5517	DGD	O5D-C6D-C5D	6.46	120.78	109.08
31	BC	5521	LMG	C8-O7-C10	6.47	133.41	117.89
28	AC	517	DGD	O5D-C6D-C5D	6.48	120.81	109.08
27	BJ	5101	BCR	C2-C1-C6	6.49	120.64	110.36
31	AB	621	LMG	O7-C10-C11	6.53	125.72	111.53
31	AC	521	LMG	C8-O7-C10	6.54	133.57	117.89
31	BB	5624	LMG	O7-C10-C11	6.55	125.77	111.53
27	AJ	101	BCR	C2-C1-C6	6.56	120.75	110.36
31	AM	101	LMG	O7-C10-C11	6.58	125.83	111.53
24	AA	406	CLA	CBA-CAA-C2A	6.62	132.42	113.73
27	AB	617	BCR	C38-C26-C25	6.64	131.12	124.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	BM	5102	LMG	O7-C10-C11	6.65	125.98	111.53
27	AX	101	BCR	C38-C26-C25	6.65	131.14	124.61
27	BB	5621	BCR	C38-C26-C25	6.65	131.14	124.61
27	BC	5515	BCR	C38-C26-C25	6.68	131.16	124.61
27	AC	515	BCR	C33-C5-C6	6.71	131.19	124.61
27	BT	5101	BCR	C33-C5-C6	6.71	131.20	124.61
27	BJ	5101	BCR	C38-C26-C25	6.72	131.21	124.61
27	AT	101	BCR	C33-C5-C6	6.77	131.25	124.61
28	BH	5101	DGD	O2G-C1B-C2B	6.79	126.30	111.53
27	AC	515	BCR	C38-C26-C25	6.81	131.29	124.61
28	AH	101	DGD	O2G-C1B-C2B	6.82	126.36	111.53
27	AJ	101	BCR	C38-C26-C25	6.83	131.31	124.61
27	BC	5515	BCR	C33-C5-C6	6.87	131.35	124.61
27	BX	5101	BCR	C38-C26-C25	6.89	131.37	124.61
31	BD	5410	LMG	C8-O7-C10	6.91	134.47	117.89
31	AD	408	LMG	C8-O7-C10	6.94	134.55	117.89
27	BC	5516	BCR	C33-C5-C6	7.03	131.50	124.61
27	BB	5622	BCR	C38-C26-C25	7.03	131.51	124.61
27	AC	516	BCR	C33-C5-C6	7.05	131.53	124.61
27	BK	5102	BCR	C33-C5-C6	7.07	131.54	124.61
24	AA	405	CLA	CBA-CAA-C2A	7.12	133.82	113.73
31	BC	5520	LMG	O7-C10-C11	7.19	127.16	111.53
24	BA	5406	CLA	CBA-CAA-C2A	7.20	134.05	113.73
27	AB	618	BCR	C38-C26-C25	7.21	131.69	124.61
36	BV	5201	HEM	CAD-C3D-C2D	7.22	133.98	113.22
28	AC	517	DGD	C1G-O1G-C1A	7.26	137.16	116.85
36	AV	201	HEM	CAD-C3D-C2D	7.28	134.13	113.22
28	BC	5518	DGD	O6D-C5D-C6D	7.28	121.48	106.61
36	BV	5201	HEM	CMA-C3A-C4A	7.33	140.50	128.36
36	AV	201	HEM	CMA-C3A-C4A	7.35	140.52	128.36
27	AK	102	BCR	C33-C5-C6	7.35	131.82	124.61
28	BC	5517	DGD	C1G-O1G-C1A	7.39	137.50	116.85
31	AC	520	LMG	O7-C10-C11	7.40	127.60	111.53
28	AC	518	DGD	O6D-C5D-C6D	7.48	121.89	106.61
31	BD	5409	LMG	C8-O7-C10	7.50	135.90	117.89
31	AA	417	LMG	C8-O7-C10	7.55	136.00	117.89
31	AD	407	LMG	C8-O7-C10	7.56	136.04	117.89
27	BD	5407	BCR	C38-C26-C25	7.69	132.16	124.61
31	BA	5402	LMG	C8-O7-C10	7.73	136.44	117.89
36	AF	101	HEM	CMA-C3A-C4A	7.75	141.18	128.36
36	BF	5101	HEM	CMA-C3A-C4A	7.86	141.36	128.36
30	BA	5414	SQD	O6-C1-C2	7.88	117.99	108.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BC	5519	DGD	O6D-C5D-C6D	7.93	122.82	106.61
30	AA	413	SQD	O6-C1-C2	7.94	118.06	108.04
30	BB	5625	SQD	O5-C1-O6	7.97	129.25	110.05
30	AB	627	SQD	O5-C1-O6	8.01	129.33	110.05
27	AD	406	BCR	C38-C26-C25	8.01	132.47	124.61
30	BB	5601	SQD	O5-C1-O6	8.04	129.41	110.05
30	AB	622	SQD	O5-C1-O6	8.10	129.55	110.05
36	BF	5101	HEM	CAD-C3D-C2D	8.10	136.50	113.22
28	BC	5519	DGD	C2G-O2G-C1B	8.14	137.41	117.89
36	AF	101	HEM	CAD-C3D-C2D	8.14	136.62	113.22
30	AA	416	SQD	O6-C1-C2	8.24	118.44	108.04
28	AC	519	DGD	C2G-O2G-C1B	8.36	137.95	117.89
28	BC	5518	DGD	O5D-C6D-C5D	8.37	124.25	109.08
28	AC	518	DGD	O5D-C6D-C5D	8.42	124.33	109.08
28	AA	411	DGD	O6D-C5D-C6D	8.42	123.81	106.61
30	BA	5401	SQD	O6-C1-C2	8.43	118.68	108.04
28	BA	5412	DGD	O6D-C5D-C6D	8.46	123.89	106.61
28	AC	519	DGD	O6D-C5D-C6D	8.51	124.01	106.61
30	AF	102	SQD	O5-C1-O6	8.56	130.67	110.05
30	BF	5102	SQD	O5-C1-O6	8.60	130.76	110.05
30	BA	5414	SQD	O5-C1-O6	8.79	131.22	110.05
30	BA	5401	SQD	O5-C1-O6	8.82	131.28	110.05
30	AA	416	SQD	O5-C1-O6	8.86	131.39	110.05
30	AA	413	SQD	O5-C1-O6	8.91	131.51	110.05
28	AC	517	DGD	C2G-O2G-C1B	9.03	139.56	117.89
25	BA	5409	MST	C2-N3-C4	9.06	119.56	113.69
30	AF	102	SQD	O6-C1-C2	9.19	119.64	108.04
30	BF	5102	SQD	O6-C1-C2	9.25	119.72	108.04
28	BC	5517	DGD	C2G-O2G-C1B	9.25	140.10	117.89
30	AB	627	SQD	O6-C1-C2	9.37	119.87	108.04
25	AA	408	MST	C2-N3-C4	9.39	119.78	113.69
31	BD	5408	LMG	C8-O7-C10	9.41	140.46	117.89
30	AB	622	SQD	O6-C1-C2	9.48	120.01	108.04
28	AB	628	DGD	C2G-O2G-C1B	9.50	140.68	117.89
30	BB	5625	SQD	O6-C1-C2	9.51	120.05	108.04
30	BB	5601	SQD	O6-C1-C2	9.54	120.09	108.04
31	AJ	102	LMG	C8-O7-C10	9.63	140.99	117.89
28	BB	5602	DGD	C2G-O2G-C1B	9.73	141.23	117.89
28	AA	411	DGD	O1G-C1G-C2G	9.74	134.92	108.69
28	BA	5412	DGD	O1G-C1G-C2G	9.76	134.96	108.69
25	BA	5409	MST	C2-N1-C6	9.82	120.06	113.69
25	AA	408	MST	C2-N1-C6	9.93	120.12	113.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	BB	5601	SQD	O7-S-C6	10.55	115.83	106.94
28	AA	411	DGD	O5D-C1E-C2E	10.61	121.44	108.04
28	BA	5412	DGD	O5D-C1E-C2E	10.84	121.73	108.04
30	AB	627	SQD	O7-S-C6	11.03	116.23	106.94
28	BA	5412	DGD	O5D-C6D-C5D	11.07	129.13	109.08
28	AA	411	DGD	O5D-C6D-C5D	11.10	129.19	109.08
30	AB	622	SQD	O7-S-C6	11.35	116.51	106.94
28	AC	519	DGD	O5D-C1E-C2E	11.42	122.46	108.04
30	BA	5401	SQD	O7-S-C6	11.43	116.58	106.94
28	BC	5519	DGD	O5D-C1E-C2E	11.61	122.70	108.04
30	AA	416	SQD	O7-S-C6	11.72	116.82	106.94
30	BA	5414	SQD	O7-S-C6	11.82	116.91	106.94
30	BB	5625	SQD	O7-S-C6	11.92	116.99	106.94
30	AA	413	SQD	O7-S-C6	12.17	117.20	106.94
28	BC	5519	DGD	O5D-C6D-C5D	12.26	131.30	109.08
28	AC	519	DGD	O5D-C6D-C5D	12.34	131.44	109.08
30	AF	102	SQD	O7-S-C6	13.13	118.01	106.94
30	BF	5102	SQD	O7-S-C6	13.21	118.07	106.94
28	BC	5518	DGD	O5D-C1E-C2E	13.77	125.43	108.04
28	AC	518	DGD	O5D-C1E-C2E	14.02	125.75	108.04

All (288) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	BC	5502	CLA	C8
24	BC	5502	CLA	NC
24	BC	5502	CLA	ND
24	BC	5502	CLA	NA
24	BC	5511	CLA	C8
24	BC	5511	CLA	NC
24	BC	5511	CLA	ND
24	BC	5511	CLA	NA
24	AC	507	CLA	C8
24	AC	507	CLA	NC
24	AC	507	CLA	ND
24	AC	507	CLA	NA
24	BB	5617	CLA	C8
24	BB	5617	CLA	NC
24	BB	5617	CLA	ND
24	BB	5617	CLA	NA
34	BD	5403	PHO	C8
24	BB	5612	CLA	C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
24	BB	5612	CLA	NC
24	BB	5612	CLA	ND
24	BB	5612	CLA	NA
24	AC	504	CLA	C8
24	AC	504	CLA	NC
24	AC	504	CLA	ND
24	AC	504	CLA	NA
24	BC	5512	CLA	C8
24	BC	5512	CLA	NC
24	BC	5512	CLA	ND
24	BC	5512	CLA	NA
34	AD	402	PHO	C8
24	AC	506	CLA	C8
24	AC	506	CLA	NC
24	AC	506	CLA	ND
24	AC	506	CLA	NA
24	BB	5619	CLA	C8
24	BB	5619	CLA	NC
24	BB	5619	CLA	ND
24	BB	5619	CLA	NA
24	BB	5614	CLA	C8
24	BB	5614	CLA	NC
24	BB	5614	CLA	ND
24	BB	5614	CLA	NA
24	AA	405	CLA	C8
24	AA	405	CLA	NC
24	AA	405	CLA	ND
24	AA	405	CLA	NA
24	BC	5507	CLA	C8
24	BC	5507	CLA	NC
24	BC	5507	CLA	ND
24	BC	5507	CLA	NA
24	AB	612	CLA	C8
24	AB	612	CLA	NC
24	AB	612	CLA	ND
24	AB	612	CLA	NA
24	BC	5508	CLA	C8
24	BC	5508	CLA	NC
24	BC	5508	CLA	ND
24	BC	5508	CLA	NA
24	BB	5608	CLA	C8
24	BB	5608	CLA	NC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
24	BB	5608	CLA	ND
24	BB	5608	CLA	NA
24	BC	5501	CLA	C8
24	BC	5501	CLA	NC
24	BC	5501	CLA	ND
24	BC	5501	CLA	NA
24	BD	5402	CLA	C8
24	BD	5402	CLA	NC
24	BD	5402	CLA	ND
24	BD	5402	CLA	NA
24	BB	5610	CLA	C8
24	BB	5610	CLA	NC
24	BB	5610	CLA	ND
24	BB	5610	CLA	NA
24	AB	606	CLA	C8
24	AB	606	CLA	NC
24	AB	606	CLA	ND
24	AB	606	CLA	NA
24	BD	5405	CLA	C8
24	BD	5405	CLA	NC
24	BD	5405	CLA	ND
24	BD	5405	CLA	NA
24	AD	401	CLA	C8
24	AD	401	CLA	NC
24	AD	401	CLA	ND
24	AD	401	CLA	NA
24	AD	404	CLA	C8
24	AD	404	CLA	NC
24	AD	404	CLA	ND
24	AD	404	CLA	NA
34	AD	403	PHO	C8
28	AC	518	DGD	C1E
24	AB	602	CLA	C8
24	AB	602	CLA	NC
24	AB	602	CLA	ND
24	AB	602	CLA	NA
24	AC	511	CLA	C8
24	AC	511	CLA	NC
24	AC	511	CLA	ND
24	AC	511	CLA	NA
24	AC	503	CLA	C8
24	AC	503	CLA	NC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
24	AC	503	CLA	ND
24	AC	503	CLA	NA
24	AA	404	CLA	C8
24	AA	404	CLA	NC
24	AA	404	CLA	ND
24	AA	404	CLA	NA
24	BC	5503	CLA	C8
24	BC	5503	CLA	NC
24	BC	5503	CLA	ND
24	BC	5503	CLA	NA
24	AB	615	CLA	C8
24	AB	615	CLA	NC
24	AB	615	CLA	ND
24	AB	615	CLA	NA
24	BB	5620	CLA	C8
24	BB	5620	CLA	NC
24	BB	5620	CLA	ND
24	BB	5620	CLA	NA
24	AB	610	CLA	C8
24	AB	610	CLA	NC
24	AB	610	CLA	ND
24	AB	610	CLA	NA
24	BB	5606	CLA	C8
24	BB	5606	CLA	NC
24	BB	5606	CLA	ND
24	BB	5606	CLA	NA
24	AB	616	CLA	C8
24	AB	616	CLA	NC
24	AB	616	CLA	ND
24	AB	616	CLA	NA
24	AB	614	CLA	C8
24	AB	614	CLA	NC
24	AB	614	CLA	ND
24	AB	614	CLA	NA
24	AB	611	CLA	C8
24	AB	611	CLA	NC
24	AB	611	CLA	ND
24	AB	611	CLA	NA
24	AB	613	CLA	C8
24	AB	613	CLA	NC
24	AB	613	CLA	ND
24	AB	613	CLA	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
24	AC	509	CLA	C8
24	AC	509	CLA	NC
24	AC	509	CLA	ND
24	AC	509	CLA	NA
24	AA	407	CLA	C8
24	AA	407	CLA	NC
24	AA	407	CLA	ND
24	AA	407	CLA	NA
24	BC	5510	CLA	C8
24	BC	5510	CLA	NC
24	BC	5510	CLA	ND
24	BC	5510	CLA	NA
24	AC	501	CLA	C8
24	AC	501	CLA	NC
24	AC	501	CLA	ND
24	AC	501	CLA	NA
24	BB	5616	CLA	C8
24	BB	5616	CLA	NC
24	BB	5616	CLA	ND
24	BB	5616	CLA	NA
24	BA	5405	CLA	C8
24	BA	5405	CLA	NC
24	BA	5405	CLA	ND
24	BA	5405	CLA	NA
24	AA	406	CLA	C8
24	AA	406	CLA	NC
24	AA	406	CLA	ND
24	AA	406	CLA	NA
24	BC	5504	CLA	C8
24	BC	5504	CLA	NC
24	BC	5504	CLA	ND
24	BC	5504	CLA	NA
24	AB	609	CLA	C8
24	AB	609	CLA	NC
24	AB	609	CLA	ND
24	AB	609	CLA	NA
24	AC	502	CLA	C8
24	AC	502	CLA	NC
24	AC	502	CLA	ND
24	AC	502	CLA	NA
24	BC	5509	CLA	C8
24	BC	5509	CLA	NC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
24	BC	5509	CLA	ND
24	BC	5509	CLA	NA
24	AB	607	CLA	C8
24	AB	607	CLA	NC
24	AB	607	CLA	ND
24	AB	607	CLA	NA
28	AC	519	DGD	C1E
24	BC	5506	CLA	C8
24	BC	5506	CLA	NC
24	BC	5506	CLA	ND
24	BC	5506	CLA	NA
24	AC	505	CLA	C8
24	AC	505	CLA	NC
24	AC	505	CLA	ND
24	AC	505	CLA	NA
24	AC	508	CLA	C8
24	AC	508	CLA	NC
24	AC	508	CLA	ND
24	AC	508	CLA	NA
24	AC	513	CLA	C8
24	AC	513	CLA	NC
24	AC	513	CLA	ND
24	AC	513	CLA	NA
24	BB	5609	CLA	C8
24	BB	5609	CLA	NC
24	BB	5609	CLA	ND
24	BB	5609	CLA	NA
24	BC	5505	CLA	C8
24	BC	5505	CLA	NC
24	BC	5505	CLA	ND
24	BC	5505	CLA	NA
34	BD	5404	PHO	C8
24	AB	603	CLA	C8
24	AB	603	CLA	NC
24	AB	603	CLA	ND
24	AB	603	CLA	NA
24	BB	5615	CLA	C8
24	BB	5615	CLA	NC
24	BB	5615	CLA	ND
24	BB	5615	CLA	NA
24	BA	5407	CLA	C8
24	BA	5407	CLA	NC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
24	BA	5407	CLA	ND
24	BA	5407	CLA	NA
24	AB	601	CLA	C8
24	AB	601	CLA	NC
24	AB	601	CLA	ND
24	AB	601	CLA	NA
24	AC	512	CLA	C8
24	AC	512	CLA	NC
24	AC	512	CLA	ND
24	AC	512	CLA	NA
24	BB	5613	CLA	C8
24	BB	5613	CLA	NC
24	BB	5613	CLA	ND
24	BB	5613	CLA	NA
24	BB	5607	CLA	C8
24	BB	5607	CLA	NC
24	BB	5607	CLA	ND
24	BB	5607	CLA	NA
24	AB	608	CLA	C8
24	AB	608	CLA	NC
24	AB	608	CLA	ND
24	AB	608	CLA	NA
24	AC	510	CLA	C8
24	AC	510	CLA	NC
24	AC	510	CLA	ND
24	AC	510	CLA	NA
28	BC	5519	DGD	C1E
24	BB	5605	CLA	C8
24	BB	5605	CLA	NC
24	BB	5605	CLA	ND
24	BB	5605	CLA	NA
24	AB	605	CLA	C8
24	AB	605	CLA	NC
24	AB	605	CLA	ND
24	AB	605	CLA	NA
24	AB	604	CLA	C8
24	AB	604	CLA	NC
24	AB	604	CLA	ND
24	AB	604	CLA	NA
24	BA	5408	CLA	C8
24	BA	5408	CLA	NC
24	BA	5408	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
24	BA	5408	CLA	NA
24	BC	5513	CLA	C8
24	BC	5513	CLA	NC
24	BC	5513	CLA	ND
24	BC	5513	CLA	NA
28	BC	5518	DGD	C1E
24	BA	5406	CLA	C8
24	BA	5406	CLA	NC
24	BA	5406	CLA	ND
24	BA	5406	CLA	NA
24	BB	5611	CLA	C8
24	BB	5611	CLA	NC
24	BB	5611	CLA	ND
24	BB	5611	CLA	NA
24	BB	5618	CLA	C8
24	BB	5618	CLA	NC
24	BB	5618	CLA	ND
24	BB	5618	CLA	NA

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	AD	405	PL9	C29-C28-C27-C26
35	BD	5406	PL9	C49-C48-C47-C46
35	AD	405	PL9	C49-C48-C47-C46

There are no ring outliers.

167 monomers are involved in 1068 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AA	404	CLA	12	0
24	AA	405	CLA	20	0
24	AA	406	CLA	1	0
24	AA	407	CLA	9	0
25	AA	408	MST	9	0
27	AA	410	BCR	4	0
28	AA	411	DGD	9	0
29	AA	412	LHG	5	0
31	AA	414	LMG	11	0
29	AA	415	LHG	2	0
30	AA	416	SQD	2	0
31	AA	417	LMG	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AB	601	CLA	5	0
24	AB	602	CLA	7	0
24	AB	603	CLA	15	0
24	AB	604	CLA	12	0
24	AB	605	CLA	10	0
24	AB	606	CLA	9	0
24	AB	607	CLA	10	0
24	AB	608	CLA	15	0
24	AB	609	CLA	7	0
24	AB	610	CLA	8	0
24	AB	611	CLA	15	0
24	AB	612	CLA	12	0
24	AB	613	CLA	9	0
24	AB	614	CLA	10	0
24	AB	615	CLA	8	0
24	AB	616	CLA	4	0
27	AB	617	BCR	3	0
27	AB	618	BCR	2	0
27	AB	619	BCR	3	0
31	AB	620	LMG	17	0
31	AB	621	LMG	4	0
30	AB	622	SQD	6	0
32	AB	624	LMT	9	0
30	AB	627	SQD	3	0
32	AB	629	LMT	4	0
32	AB	630	LMT	2	0
24	AC	501	CLA	5	0
24	AC	502	CLA	6	0
24	AC	503	CLA	6	0
24	AC	504	CLA	10	0
24	AC	505	CLA	9	0
24	AC	506	CLA	5	0
24	AC	507	CLA	5	0
24	AC	508	CLA	10	0
24	AC	509	CLA	6	0
24	AC	510	CLA	6	0
24	AC	511	CLA	22	0
24	AC	512	CLA	4	0
24	AC	513	CLA	3	0
27	AC	514	BCR	6	0
27	AC	515	BCR	6	0
27	AC	516	BCR	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	AC	517	DGD	10	0
28	AC	518	DGD	12	0
28	AC	519	DGD	42	0
31	AC	520	LMG	4	0
31	AC	521	LMG	7	0
24	AD	401	CLA	9	0
34	AD	402	PHO	11	0
34	AD	403	PHO	3	0
24	AD	404	CLA	8	0
35	AD	405	PL9	15	0
27	AD	406	BCR	2	0
31	AD	407	LMG	4	0
31	AD	408	LMG	11	0
28	AE	101	DGD	1	0
36	AF	101	HEM	8	0
30	AF	102	SQD	1	0
28	AH	101	DGD	9	0
31	AI	101	LMG	3	0
32	AI	102	LMT	5	0
32	AI	103	LMT	4	0
27	AJ	101	BCR	4	0
31	AJ	102	LMG	2	0
27	AK	102	BCR	5	0
31	AM	101	LMG	6	0
32	AM	102	LMT	1	0
27	AT	101	BCR	10	0
36	AV	201	HEM	4	0
27	AX	101	BCR	8	0
30	BA	5401	SQD	3	0
31	BA	5402	LMG	3	0
24	BA	5405	CLA	11	0
24	BA	5406	CLA	22	0
24	BA	5407	CLA	1	0
24	BA	5408	CLA	11	0
25	BA	5409	MST	9	0
27	BA	5411	BCR	3	0
28	BA	5412	DGD	9	0
29	BA	5413	LHG	6	0
29	BA	5415	LHG	3	0
30	BB	5601	SQD	5	0
28	BB	5602	DGD	5	0
32	BB	5603	LMT	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	BB	5604	LMT	2	0
24	BB	5605	CLA	5	0
24	BB	5606	CLA	7	0
24	BB	5607	CLA	15	0
24	BB	5608	CLA	12	0
24	BB	5609	CLA	12	0
24	BB	5610	CLA	9	0
24	BB	5611	CLA	10	0
24	BB	5612	CLA	14	0
24	BB	5613	CLA	7	0
24	BB	5614	CLA	9	0
24	BB	5615	CLA	19	0
24	BB	5616	CLA	12	0
24	BB	5617	CLA	8	0
24	BB	5618	CLA	14	0
24	BB	5619	CLA	8	0
24	BB	5620	CLA	4	0
27	BB	5621	BCR	3	0
27	BB	5622	BCR	1	0
27	BB	5623	BCR	4	0
31	BB	5624	LMG	4	0
30	BB	5625	SQD	6	0
32	BB	5626	LMT	2	0
32	BB	5627	LMT	10	0
24	BC	5501	CLA	6	0
24	BC	5502	CLA	6	0
24	BC	5503	CLA	5	0
24	BC	5504	CLA	8	0
24	BC	5505	CLA	9	0
24	BC	5506	CLA	4	0
24	BC	5507	CLA	7	0
24	BC	5508	CLA	9	0
24	BC	5509	CLA	8	0
24	BC	5510	CLA	6	0
24	BC	5511	CLA	23	0
24	BC	5512	CLA	5	0
24	BC	5513	CLA	5	0
27	BC	5514	BCR	6	0
27	BC	5515	BCR	6	0
27	BC	5516	BCR	13	0
28	BC	5517	DGD	10	0
28	BC	5518	DGD	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	BC	5519	DGD	45	0
31	BC	5520	LMG	3	0
31	BC	5521	LMG	7	0
32	BC	5522	LMT	3	0
24	BD	5402	CLA	10	0
34	BD	5403	PHO	12	0
34	BD	5404	PHO	3	0
24	BD	5405	CLA	8	0
35	BD	5406	PL9	16	0
27	BD	5407	BCR	2	0
31	BD	5408	LMG	1	0
31	BD	5409	LMG	4	0
31	BD	5410	LMG	10	0
32	BD	5411	LMT	1	0
31	BE	5101	LMG	4	0
28	BE	5102	DGD	1	0
36	BF	5101	HEM	7	0
30	BF	5102	SQD	1	0
28	BH	5101	DGD	8	0
31	BI	5101	LMG	4	0
32	BI	5102	LMT	5	0
27	BJ	5101	BCR	3	0
27	BK	5102	BCR	5	0
31	BL	5101	LMG	18	0
32	BM	5101	LMT	2	0
31	BM	5102	LMG	4	0
27	BT	5101	BCR	6	0
36	BV	5201	HEM	6	0
27	BX	5101	BCR	4	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	335/344 (97%)	0.05	9 (2%) 58 44	82, 104, 147, 160	0
1	BA	335/344 (97%)	0.04	17 (5%) 32 18	86, 106, 148, 160	0
2	AB	490/510 (96%)	0.07	16 (3%) 50 35	81, 103, 136, 152	0
2	BB	490/510 (96%)	0.16	25 (5%) 32 18	81, 103, 137, 152	0
3	AC	447/461 (96%)	0.36	25 (5%) 28 16	88, 122, 148, 158	0
3	BC	447/461 (96%)	0.32	36 (8%) 15 8	91, 124, 149, 159	0
4	AD	341/352 (96%)	0.05	8 (2%) 64 49	81, 105, 139, 153	0
4	BD	341/352 (96%)	0.04	12 (3%) 48 32	84, 106, 140, 154	0
5	AE	82/84 (97%)	0.58	9 (10%) 7 4	104, 126, 151, 155	0
5	BE	82/84 (97%)	1.39	26 (31%) 1 0	106, 127, 152, 156	0
6	AF	35/45 (77%)	0.48	6 (17%) 2 1	107, 122, 157, 160	0
6	BF	35/45 (77%)	0.31	4 (11%) 7 4	110, 123, 157, 160	0
7	AH	65/66 (98%)	0.59	13 (20%) 1 1	113, 124, 140, 147	0
7	BH	65/66 (98%)	0.63	8 (12%) 5 3	114, 124, 140, 148	0
8	AI	35/38 (92%)	0.18	3 (8%) 13 7	108, 115, 141, 147	0
8	BI	35/38 (92%)	0.84	8 (22%) 1 1	108, 116, 142, 147	0
9	AJ	38/40 (95%)	0.10	3 (7%) 15 9	109, 122, 157, 159	0
9	BJ	38/40 (95%)	0.57	7 (18%) 2 1	111, 125, 158, 159	0
10	AK	37/37 (100%)	-0.02	1 (2%) 58 44	121, 135, 145, 147	0
10	BK	37/37 (100%)	0.18	1 (2%) 58 44	123, 136, 147, 148	0
11	AL	37/37 (100%)	0.29	3 (8%) 15 8	88, 104, 159, 160	0
11	BL	37/37 (100%)	0.54	6 (16%) 3 2	90, 104, 158, 160	0
12	AM	34/36 (94%)	0.29	3 (8%) 12 7	89, 99, 142, 153	0
12	BM	34/36 (94%)	-0.07	2 (5%) 26 14	90, 99, 140, 153	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AO	243/247 (98%)	0.43	22 (9%) 11 6	83, 116, 148, 160	0
13	BO	243/247 (98%)	0.38	25 (10%) 9 5	85, 117, 147, 160	0
14	AT	32/32 (100%)	0.41	3 (9%) 11 6	92, 106, 158, 160	0
14	BT	32/32 (100%)	0.04	1 (3%) 52 38	93, 106, 158, 160	0
15	AU	97/104 (93%)	0.34	6 (6%) 24 13	93, 105, 116, 125	0
15	BU	97/104 (93%)	0.21	2 (2%) 67 52	94, 106, 116, 127	0
16	AV	137/137 (100%)	0.19	3 (2%) 65 50	96, 112, 128, 132	0
16	BV	137/137 (100%)	0.54	15 (10%) 7 4	99, 114, 130, 134	0
17	Ay	28/46 (60%)	0.72	4 (14%) 4 2	141, 154, 160, 160	0
17	By	28/46 (60%)	0.93	7 (25%) 1 1	143, 154, 160, 160	0
18	AX	37/41 (90%)	0.51	7 (18%) 2 1	121, 129, 147, 150	0
18	BX	37/41 (90%)	0.53	6 (16%) 3 2	120, 130, 146, 149	0
19	AY	0/28	-	-	-	-
19	BY	0/28	-	-	-	-
20	AZ	62/62 (100%)	0.78	11 (17%) 2 1	134, 148, 160, 160	0
20	BZ	62/62 (100%)	1.61	21 (33%) 0 0	135, 150, 160, 160	0
All	All	5224/5494 (95%)	0.28	384 (7%) 17 10	81, 113, 149, 160	0

All (384) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	BZ	5062	VAL	10.1
20	BZ	5061	VAL	8.2
13	BO	5084	ASN	7.8
7	BH	5066	GLY	7.0
20	BZ	5001	MET	7.0
9	AJ	3	SER	6.7
7	BH	5065	LEU	6.2
17	By	5046	LEU	6.2
11	BL	5001	MET	6.1
20	AZ	34	ASP	6.1
5	BE	5008	ARG	5.8
1	BA	5011	ALA	5.8
8	BI	5032	PRO	5.6
2	BB	5491	VAL	5.5
18	AX	47	GLN	5.5
1	BA	5010	SER	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	BI	5033	LYS	5.1
20	BZ	5033	TRP	5.1
20	AZ	62	VAL	4.9
9	BJ	5004	GLU	4.7
20	BZ	5060	PHE	4.6
10	AK	46	ARG	4.6
4	BD	5099	GLY	4.6
20	AZ	30	PRO	4.5
3	AC	145	SER	4.5
13	BO	5051	THR	4.5
3	BC	5144	SER	4.4
8	BI	5034	ARG	4.4
13	BO	5052	ALA	4.4
20	AZ	61	VAL	4.4
20	AZ	33	TRP	4.3
11	BL	5005	PRO	4.3
11	AL	1	MET	4.3
18	AX	45	LYS	4.3
20	AZ	60	PHE	4.3
2	BB	5002	GLY	4.2
11	BL	5002	GLU	4.2
5	AE	83	LEU	4.2
5	BE	5007	GLU	4.2
17	By	5041	VAL	4.2
4	AD	13	GLY	4.1
3	AC	27	ASP	4.1
5	AE	12	ASP	4.1
6	AF	12	SER	4.1
3	BC	5183	GLY	4.1
17	Ay	45	ASN	4.1
2	AB	129	GLY	4.1
9	BJ	5005	GLY	4.1
13	BO	5050	ASP	4.1
12	BM	5034	LYS	4.1
3	BC	5255	THR	4.0
6	BF	5012	SER	4.0
3	BC	5204	LEU	4.0
3	AC	137	PRO	3.9
8	BI	5002	GLU	3.9
7	BH	5027	THR	3.9
5	BE	5021	VAL	3.8
9	AJ	4	GLU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	BE	5017	VAL	3.8
20	AZ	57	LEU	3.8
9	BJ	5003	SER	3.8
3	BC	5203	THR	3.8
4	AD	241	GLU	3.8
6	AF	11	VAL	3.8
14	AT	30	THR	3.8
11	BL	5003	PRO	3.8
7	AH	26	GLY	3.8
20	AZ	31	GLN	3.7
5	BE	5016	SER	3.7
13	BO	5049	ASP	3.7
13	AO	51	THR	3.7
2	AB	379	ALA	3.7
20	BZ	5002	THR	3.7
13	AO	114	ASN	3.7
13	AO	88	GLU	3.7
2	BB	5490	GLN	3.6
7	AH	16	SER	3.6
3	BC	5184	GLY	3.6
5	BE	5006	GLY	3.6
13	BO	5062	GLN	3.6
3	AC	138	GLU	3.6
20	BZ	5004	LEU	3.6
18	AX	46	VAL	3.6
4	BD	5239	GLN	3.6
5	BE	5013	ILE	3.6
5	BE	5073	LYS	3.5
4	BD	5233	ARG	3.5
5	BE	5082	GLN	3.5
6	AF	13	TYR	3.5
7	AH	27	THR	3.5
6	BF	5011	VAL	3.5
1	BA	5032	TRP	3.5
2	BB	5128	THR	3.5
12	AM	31	SER	3.5
13	BO	5048	LEU	3.5
9	BJ	5008	ILE	3.5
16	BV	5132	ASN	3.4
3	AC	141	GLU	3.4
12	BM	5033	GLN	3.4
2	BB	5120	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	BC	5030	SER	3.4
9	BJ	5006	GLY	3.4
5	AE	17	VAL	3.4
13	BO	5064	TYR	3.4
3	AC	78	GLU	3.3
13	BO	5112	LYS	3.3
7	AH	23	PRO	3.3
13	BO	5060	SER	3.3
3	BC	5135	ARG	3.3
13	BO	5063	THR	3.3
2	AB	125	ASP	3.3
1	BA	5015	GLU	3.3
2	BB	5121	GLU	3.3
12	AM	33	GLN	3.3
4	AD	24	ARG	3.3
3	AC	198	VAL	3.3
3	AC	255	THR	3.3
18	BX	5043	ILE	3.3
20	BZ	5036	SER	3.3
2	AB	378	LYS	3.2
2	BB	5123	PHE	3.2
14	AT	31	LYS	3.2
17	Ay	42	ARG	3.2
4	BD	5012	ARG	3.2
7	AH	25	TRP	3.2
13	AO	230	VAL	3.2
13	AO	52	ALA	3.2
3	BC	5207	ARG	3.2
3	BC	5256	PRO	3.2
4	AD	98	GLN	3.2
3	BC	5143	TYR	3.2
2	AB	130	GLU	3.1
5	BE	5059	GLU	3.1
3	AC	140	LEU	3.1
3	BC	5057	ALA	3.1
5	AE	21	VAL	3.1
3	AC	199	ILE	3.1
17	By	5045	ASN	3.1
17	Ay	21	GLN	3.1
4	BD	5226	GLY	3.1
2	BB	5219	VAL	3.1
18	BX	5011	THR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	AA	242	GLU	3.1
20	BZ	5005	PHE	3.0
2	BB	5162	PHE	3.0
6	BF	5013	TYR	3.0
20	AZ	32	ASP	3.0
3	AC	203	THR	3.0
13	BO	5167	ASP	3.0
4	BD	5098	GLN	3.0
2	BB	5161	LEU	3.0
20	BZ	5029	SER	3.0
13	AO	84	ASN	3.0
16	BV	5047	LEU	3.0
2	AB	118	TRP	2.9
3	AC	144	SER	2.9
5	BE	5083	LEU	2.9
13	BO	5091	PHE	2.9
5	BE	5018	ARG	2.9
20	AZ	35	ARG	2.9
2	AB	126	PRO	2.9
3	BC	5202	PRO	2.9
13	AO	120	THR	2.9
11	AL	4	ASN	2.9
2	AB	120	LEU	2.9
2	AB	407	ASN	2.9
1	BA	5018	CYS	2.9
1	BA	5233	ALA	2.8
1	BA	5012	ASN	2.8
2	BB	5352	GLU	2.8
13	AO	48	LEU	2.8
5	BE	5005	THR	2.8
10	BK	5014	ALA	2.8
7	AH	4	ARG	2.8
3	BC	5131	TYR	2.8
13	AO	163	THR	2.8
6	BF	5015	ILE	2.8
3	BC	5198	VAL	2.8
1	BA	5019	ASN	2.8
16	BV	5043	LYS	2.8
16	BV	5121	LEU	2.8
17	Ay	41	VAL	2.8
16	AV	116	GLU	2.8
3	BC	5200	THR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	BA	5268	SER	2.8
16	AV	43	LYS	2.7
1	AA	11	ALA	2.7
3	BC	5137	PRO	2.7
14	AT	32	LYS	2.7
13	BO	5160	THR	2.7
5	AE	84	LYS	2.7
8	AI	6	ILE	2.7
15	AU	69	ARG	2.7
11	BL	5004	ASN	2.7
1	BA	5227	THR	2.7
16	BV	5111	GLU	2.7
8	BI	5030	ARG	2.7
3	BC	5142	GLU	2.7
3	AC	48	LYS	2.7
15	AU	58	ASN	2.7
18	AX	42	GLN	2.7
3	BC	5249	ILE	2.7
1	BA	5232	SER	2.6
5	AE	18	ARG	2.6
20	AZ	38	GLN	2.6
3	AC	204	LEU	2.6
2	BB	5374	ASN	2.6
16	BV	5042	GLY	2.6
2	BB	5124	ARG	2.6
4	BD	5097	ALA	2.6
5	BE	5061	ARG	2.6
9	BJ	5013	VAL	2.6
3	BC	5033	PHE	2.6
5	BE	5010	PHE	2.6
11	BL	5010	VAL	2.6
3	AC	253	LEU	2.6
4	AD	227	GLU	2.6
3	AC	202	PRO	2.6
1	AA	10	SER	2.6
2	BB	5294	SER	2.6
13	AO	61	SER	2.6
20	BZ	5034	ASP	2.6
8	AI	2	GLU	2.6
12	AM	34	LYS	2.6
3	BC	5209	ILE	2.6
5	BE	5015	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	BE	5057	ALA	2.6
18	AX	44	ASP	2.6
20	BZ	5042	LEU	2.6
16	BV	5027	ALA	2.6
16	BV	5031	PRO	2.6
3	BC	5195	ASP	2.6
20	BZ	5039	LEU	2.6
18	BX	5045	LYS	2.5
20	BZ	5031	GLN	2.5
9	BJ	5007	ARG	2.5
2	BB	5125	ASP	2.5
20	BZ	5058	ASN	2.5
2	AB	480	SER	2.5
3	BC	5180	MET	2.5
2	BB	5117	TYR	2.5
2	BB	5482	ILE	2.5
11	AL	7	ARG	2.5
13	BO	5231	ASP	2.5
3	BC	5034	ALA	2.5
2	AB	119	ASP	2.5
13	AO	62	GLN	2.5
20	BZ	5038	GLN	2.5
13	BO	5113	VAL	2.5
2	BB	5293	ALA	2.5
16	BV	5044	THR	2.5
16	BV	5133	LEU	2.5
3	BC	5186	TYR	2.5
4	BD	5059	TYR	2.5
8	BI	5031	ASN	2.5
13	AO	232	GLY	2.5
14	BT	5030	THR	2.5
5	BE	5026	THR	2.5
5	BE	5030	LEU	2.5
15	AU	97	LEU	2.5
13	BO	5092	VAL	2.4
13	BO	5217	SER	2.4
13	AO	162	ILE	2.4
20	BZ	5003	ILE	2.4
3	BC	5230	LEU	2.4
13	BO	5030	THR	2.4
5	AE	3	GLY	2.4
4	BD	5013	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	AC	143	TYR	2.4
7	BH	5003	ARG	2.4
2	BB	5126	PRO	2.4
8	BI	5023	PHE	2.4
7	AH	2	ALA	2.4
3	BC	5185	LEU	2.4
4	BD	5024	ARG	2.4
4	AD	234	ALA	2.4
3	AC	149	TYR	2.4
3	BC	5205	ASP	2.4
8	BI	5024	LEU	2.4
1	BA	5230	THR	2.4
3	AC	212	TYR	2.4
4	BD	5025	ASP	2.3
17	By	5033	PRO	2.3
3	AC	45	LEU	2.3
1	BA	5309	ALA	2.3
1	AA	243	GLU	2.3
2	BB	5296	ALA	2.3
5	BE	5022	ILE	2.3
2	BB	5118	TRP	2.3
7	BH	5018	TYR	2.3
17	By	5021	GLN	2.3
13	BO	5230	VAL	2.3
1	BA	5013	LEU	2.3
2	BB	5119	ASP	2.3
2	AB	128	THR	2.3
13	AO	87	GLN	2.3
1	BA	5017	PHE	2.3
3	AC	148	GLY	2.3
7	AH	24	GLY	2.3
1	AA	18	CYS	2.3
18	BX	5046	VAL	2.3
5	BE	5084	LYS	2.3
13	BO	5058	ILE	2.3
13	AO	64	TYR	2.3
13	AO	58	ILE	2.3
5	BE	5071	GLU	2.3
1	AA	17	PHE	2.2
6	AF	42	PHE	2.2
3	BC	5199	ILE	2.2
3	BC	5208	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
17	By	5038	LEU	2.2
7	AH	3	ARG	2.2
18	AX	11	THR	2.2
17	By	5042	ARG	2.2
18	BX	5047	GLN	2.2
13	BO	5232	GLY	2.2
3	AC	256	PRO	2.2
13	AO	113	VAL	2.2
1	BA	5240	GLY	2.2
15	AU	71	LEU	2.2
5	BE	5025	ILE	2.2
6	AF	14	PRO	2.2
20	BZ	5030	PRO	2.2
9	AJ	7	ARG	2.2
2	AB	117	TYR	2.2
1	BA	5229	GLU	2.2
3	BC	5138	GLU	2.2
6	AF	15	ILE	2.2
16	BV	5113	GLU	2.2
13	AO	160	THR	2.2
18	AX	12	ILE	2.2
13	BO	5250	ASP	2.2
3	AC	122	SER	2.2
2	BB	5412	THR	2.1
3	BC	5364	PRO	2.1
8	AI	34	ARG	2.1
15	AU	94	ILE	2.1
7	AH	22	ALA	2.1
20	BZ	5035	ARG	2.1
2	BB	5159	THR	2.1
5	BE	5036	LEU	2.1
7	BH	5022	ALA	2.1
13	AO	55	ALA	2.1
3	BC	5100	GLY	2.1
13	AO	164	THR	2.1
7	AH	66	GLY	2.1
7	AH	21	VAL	2.1
2	AB	131	PRO	2.1
20	BZ	5007	LEU	2.1
3	AC	277	GLY	2.1
13	AO	118	SER	2.1
13	AO	117	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	AE	57	ALA	2.1
16	BV	5106	THR	2.1
20	BZ	5028	ALA	2.1
1	AA	14	TRP	2.1
2	BB	5127	ARG	2.1
16	BV	5045	ILE	2.1
16	BV	5146	LEU	2.1
4	AD	16	ASP	2.1
7	AH	5	THR	2.1
15	AU	53	GLU	2.1
15	BU	5047	LEU	2.1
5	AE	82	GLN	2.1
16	BV	5104	ASN	2.1
1	AA	16	ARG	2.1
7	BH	5004	ARG	2.1
5	BE	5060	GLN	2.1
3	BC	5253	LEU	2.1
3	BC	5338	GLY	2.1
4	AD	99	GLY	2.1
1	AA	235	TYR	2.0
3	AC	61	VAL	2.0
13	BO	5114	ASN	2.0
18	BX	5042	GLN	2.0
3	BC	5227	VAL	2.0
15	BU	5085	TYR	2.0
4	BD	5085	MET	2.0
2	AB	162	PHE	2.0
2	AB	401	PHE	2.0
16	AV	44	THR	2.0
13	BO	5225	LEU	2.0
5	BE	5074	GLN	2.0
7	BH	5010	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
28	DGD	AE	101	63/66	0.35	0.72	13.63	146,160,160,160	0
27	BCR	AJ	101	40/40	0.53	0.65	13.18	158,160,160,160	0
27	BCR	BJ	5101	40/40	0.64	0.51	7.31	160,160,160,160	0
31	LMG	BA	5402	42/55	0.61	0.50	7.22	144,157,160,160	0
31	LMG	AD	407	49/55	0.77	0.48	7.10	126,133,143,145	0
28	DGD	BB	5602	52/66	0.46	0.55	6.46	152,160,160,160	0
33	DMS	AV	202	4/4	0.83	0.66	6.16	148,148,148,149	0
33	DMS	BV	5203	4/4	0.92	0.69	5.97	160,160,160,160	0
28	DGD	BC	5518	62/66	0.69	0.50	5.90	147,156,160,160	0
32	LMT	AB	629	35/35	0.67	0.48	5.03	133,160,160,160	0
28	DGD	AC	518	62/66	0.76	0.41	5.03	146,155,160,160	0
31	LMG	BD	5410	48/55	0.65	0.58	5.01	126,131,141,141	0
32	LMT	BB	5603	35/35	0.64	0.46	4.94	132,160,160,160	0
31	LMG	AA	417	42/55	0.68	0.45	4.72	145,157,160,160	0
33	DMS	BB	5628	4/4	0.86	0.60	4.64	156,157,157,157	0
29	LHG	BA	5415	37/49	0.45	0.63	4.63	151,160,160,160	0
27	BCR	AT	101	40/40	0.83	0.40	4.43	126,140,146,147	0
31	LMG	AB	620	51/55	0.72	0.50	4.29	125,139,150,151	0
28	DGD	AB	628	52/66	0.53	0.60	4.14	154,160,160,160	0
31	LMG	AB	621	49/55	0.67	0.45	4.09	145,150,157,160	0
31	LMG	BB	5624	49/55	0.74	0.41	4.06	145,150,157,160	0
27	BCR	BT	5101	40/40	0.77	0.40	4.03	124,143,147,147	0
28	DGD	BE	5102	63/66	0.42	0.70	4.01	145,160,160,160	0
31	LMG	AD	408	48/55	0.75	0.48	3.98	121,130,139,139	0
31	LMG	BC	5520	48/55	0.55	0.56	3.87	138,159,160,160	0
31	LMG	BD	5408	46/55	0.68	0.49	3.72	139,145,160,160	0
31	LMG	BL	5101	51/55	0.79	0.48	3.63	122,138,151,152	0
27	BCR	BB	5622	40/40	0.92	0.36	3.63	110,117,120,121	0
33	DMS	BB	5629	4/4	0.93	0.29	3.55	125,126,127,127	0
23	CL	BA	5404[A]	1/1	0.72	0.33	3.54	29,29,29,29	1
33	DMS	AB	625	4/4	0.89	0.45	3.51	156,157,157,157	0
31	LMG	AJ	102	46/55	0.72	0.44	3.36	139,144,160,160	0
28	DGD	BC	5519	66/66	0.79	0.37	3.31	112,121,158,159	0
27	BCR	BD	5407	40/40	0.88	0.31	3.30	112,127,132,132	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	LMG	AC	520	48/55	0.57	0.59	3.27	136,157,160,160	0
24	CLA	BB	5617	65/65	0.91	0.33	3.24	98,102,138,141	0
32	LMT	BI	5102	35/35	0.62	0.85	3.17	151,160,160,160	0
24	CLA	BC	5504	65/65	0.88	0.34	3.14	132,135,160,160	0
28	DGD	AC	519	66/66	0.84	0.36	3.13	110,120,157,158	0
24	CLA	AB	608	65/65	0.88	0.41	3.13	123,127,135,140	0
32	LMT	BB	5604	35/35	0.70	0.53	3.12	131,160,160,160	0
32	LMT	AB	624	35/35	0.69	0.62	3.11	156,160,160,160	0
27	BCR	AK	102	40/40	0.80	0.39	3.06	133,139,151,152	0
31	LMG	AA	414	44/55	0.61	0.46	3.05	140,160,160,160	0
28	DGD	BH	5101	58/66	0.82	0.39	3.01	107,118,156,160	0
28	DGD	BA	5412	56/66	0.50	0.61	2.97	150,160,160,160	0
24	CLA	BB	5609	65/65	0.91	0.34	2.95	103,110,124,124	0
24	CLA	AB	601	65/65	0.70	0.56	2.95	146,159,160,160	0
31	LMG	BD	5409	49/55	0.79	0.42	2.93	128,133,144,146	0
24	CLA	AA	406	65/65	0.86	0.35	2.93	105,112,138,139	0
28	DGD	AC	517	53/66	0.81	0.40	2.92	121,128,135,140	0
30	SQD	BB	5625	43/54	0.57	0.48	2.89	132,148,160,160	0
28	DGD	AA	411	56/66	0.54	0.55	2.83	148,158,160,160	0
32	LMT	AM	102	35/35	0.79	0.42	2.81	126,149,154,154	0
24	CLA	AA	407	65/65	0.91	0.34	2.80	93,101,150,151	0
24	CLA	AD	404	65/65	0.87	0.36	2.70	126,130,148,149	0
24	CLA	AC	505	65/65	0.87	0.41	2.67	121,146,150,151	0
24	CLA	BB	5612	65/65	0.91	0.40	2.65	122,127,136,139	0
24	CLA	AC	504	65/65	0.89	0.34	2.60	129,134,160,160	0
32	LMT	BB	5627	35/35	0.74	0.45	2.53	156,160,160,160	0
30	SQD	BA	5401	54/54	0.64	0.47	2.53	136,160,160,160	0
35	PL9	AD	405	55/55	0.90	0.36	2.53	99,109,113,113	0
24	CLA	AC	503	65/65	0.88	0.49	2.50	137,144,147,152	0
24	CLA	AB	605	65/65	0.89	0.29	2.36	105,113,122,124	0
27	BCR	BB	5621	40/40	0.88	0.32	2.34	112,120,124,125	0
32	LMT	AI	103	35/35	0.71	0.49	2.28	156,158,160,160	0
24	CLA	AC	508	65/65	0.89	0.36	2.28	140,144,157,158	0
27	BCR	AX	101	40/40	0.60	0.50	2.24	135,143,158,159	0
27	BCR	AC	515	40/40	0.71	0.45	2.24	149,152,155,155	0
32	LMT	BM	5101	35/35	0.73	0.38	2.20	126,149,154,155	0
32	LMT	AB	630	35/35	0.73	0.50	2.19	132,160,160,160	0
24	CLA	BB	5605	65/65	0.71	0.59	2.13	146,159,160,160	0
24	CLA	AC	502	65/65	0.91	0.36	2.12	103,109,142,143	0
32	LMT	AI	102	35/35	0.70	0.60	2.07	149,158,160,160	0
27	BCR	BX	5101	40/40	0.61	0.50	2.06	136,143,157,158	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
27	BCR	AB	617	40/40	0.86	0.31	2.05	112,121,125,125	0
31	LMG	BE	5101	44/55	0.65	0.46	2.02	140,160,160,160	0
32	LMT	BC	5522	35/35	0.75	0.67	2.00	157,160,160,160	0
24	CLA	BA	5408	65/65	0.89	0.31	1.99	95,103,150,150	0
24	CLA	BB	5608	65/65	0.94	0.32	1.96	96,103,124,125	0
27	BCR	AC	516	40/40	0.69	0.48	1.94	135,138,143,143	0
24	CLA	BB	5614	65/65	0.89	0.33	1.93	117,123,124,128	0
24	CLA	AB	609	65/65	0.70	0.41	1.92	126,136,141,143	0
33	DMS	AU	201	4/4	0.75	0.40	1.89	160,160,160,160	0
28	DGD	AH	101	58/66	0.86	0.31	1.87	108,120,155,157	0
24	CLA	AC	507	65/65	0.88	0.38	1.86	137,149,152,153	0
24	CLA	BC	5502	65/65	0.89	0.33	1.85	108,111,143,144	0
24	CLA	AC	501	65/65	0.88	0.38	1.84	133,136,139,143	0
24	CLA	BD	5405	65/65	0.84	0.34	1.79	125,131,148,149	0
30	SQD	AB	622	43/54	0.62	0.43	1.78	133,149,160,160	0
24	CLA	AB	610	65/65	0.90	0.34	1.78	117,121,123,127	0
24	CLA	BB	5616	65/65	0.91	0.31	1.77	108,110,120,122	0
24	CLA	BB	5611	65/65	0.90	0.28	1.77	95,102,132,136	0
24	CLA	AB	611	65/65	0.94	0.30	1.73	99,113,116,122	0
34	PHO	BD	5403	64/64	0.88	0.34	1.72	102,109,118,118	0
27	BCR	BC	5514	40/40	0.80	0.41	1.72	123,126,129,129	0
27	BCR	AD	406	40/40	0.87	0.32	1.72	110,126,131,131	0
34	PHO	AD	403	64/64	0.93	0.28	1.72	119,123,128,129	0
31	LMG	AC	521	45/55	0.41	0.62	1.70	154,160,160,160	0
24	CLA	BC	5508	65/65	0.83	0.34	1.69	142,146,157,159	0
35	PL9	BD	5406	55/55	0.85	0.35	1.68	103,110,115,116	0
24	CLA	BA	5406	65/65	0.89	0.28	1.65	89,94,108,112	0
24	CLA	AD	401	65/65	0.92	0.28	1.63	93,100,115,119	0
33	DMS	AB	626	4/4	0.89	0.26	1.63	129,130,130,130	0
23	CL	BA	5404[B]	1/1	0.72	0.33	1.61	115,115,115,115	1
24	CLA	AB	603	65/65	0.88	0.38	1.59	107,109,119,121	0
30	SQD	BF	5102	45/54	0.67	0.56	1.56	154,160,160,160	0
24	CLA	AB	607	65/65	0.91	0.27	1.53	94,100,132,135	0
34	PHO	AD	402	64/64	0.92	0.31	1.52	99,109,116,117	0
27	BCR	BK	5102	40/40	0.79	0.37	1.52	136,140,152,152	0
27	BCR	BB	5623	40/40	0.82	0.37	1.47	111,116,131,131	0
24	CLA	BA	5407	65/65	0.87	0.30	1.47	110,114,138,139	0
27	BCR	AB	618	40/40	0.86	0.28	1.45	109,117,122,122	0
24	CLA	AC	509	65/65	0.88	0.39	1.42	115,128,135,137	0
24	CLA	AB	606	65/65	0.82	0.33	1.36	120,133,140,141	0
24	CLA	BC	5510	65/65	0.91	0.33	1.36	113,116,130,131	0
27	BCR	BC	5515	40/40	0.70	0.43	1.35	150,152,155,156	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
30	SQD	AF	102	45/54	0.73	0.46	1.34	154,160,160,160	0
24	CLA	AB	602	65/65	0.85	0.34	1.32	124,127,129,132	0
24	CLA	BC	5503	65/65	0.83	0.36	1.31	137,147,148,152	0
23	CL	AA	403[A]	1/1	0.87	0.32	1.30	33,33,33,33	1
23	CL	AA	403[B]	1/1	0.87	0.32	1.29	108,108,108,108	1
33	DMS	BV	5202	4/4	0.91	0.29	1.29	148,149,149,150	0
24	CLA	BC	5507	65/65	0.83	0.36	1.23	136,150,153,154	0
31	LMG	AM	101	42/55	0.66	0.53	1.21	136,158,160,160	0
29	LHG	AA	415	37/49	0.75	0.36	1.20	149,160,160,160	0
24	CLA	BB	5615	65/65	0.92	0.26	1.19	101,113,117,120	0
24	CLA	BC	5505	65/65	0.81	0.36	1.17	123,148,152,153	0
30	SQD	AA	416	54/54	0.75	0.33	1.16	136,160,160,160	0
24	CLA	BB	5613	65/65	0.73	0.39	1.16	127,135,140,142	0
24	CLA	AB	613	65/65	0.92	0.27	1.16	99,102,136,140	0
24	CLA	AB	614	65/65	0.83	0.38	1.14	129,133,160,160	0
32	LMT	AD	409	31/35	0.71	0.43	1.12	139,154,160,160	0
24	CLA	AB	604	65/65	0.93	0.30	1.12	96,104,125,127	0
24	CLA	AC	512	65/65	0.79	0.45	1.12	154,158,160,160	0
24	CLA	BB	5607	65/65	0.89	0.29	1.08	108,111,120,123	0
24	CLA	AB	612	65/65	0.93	0.29	1.06	107,111,120,121	0
24	CLA	AB	615	65/65	0.88	0.32	1.05	134,139,155,157	0
24	CLA	AB	616	65/65	0.85	0.41	1.04	143,147,160,160	0
24	CLA	BA	5405	65/65	0.86	0.31	1.03	90,101,105,109	0
32	LMT	BD	5411	31/35	0.66	0.51	0.99	140,152,160,160	0
27	BCR	BC	5516	40/40	0.63	0.48	0.98	136,140,145,145	0
24	CLA	AC	506	65/65	0.73	0.39	0.97	136,143,160,160	0
24	CLA	BC	5513	65/65	0.71	0.51	0.95	158,160,160,160	0
27	BCR	AC	514	40/40	0.88	0.34	0.93	120,123,127,128	0
24	CLA	BB	5619	65/65	0.90	0.35	0.92	135,137,155,157	0
31	LMG	BM	5102	42/55	0.72	0.47	0.88	136,160,160,160	0
30	SQD	AB	627	47/54	0.77	0.36	0.85	138,157,160,160	0
24	CLA	AA	404	65/65	0.91	0.27	0.83	89,99,106,108	0
27	BCR	BA	5411	40/40	0.90	0.29	0.83	94,122,132,132	0
28	DGD	BC	5517	53/66	0.86	0.28	0.82	124,130,136,139	0
24	CLA	AA	405	65/65	0.94	0.27	0.81	88,93,108,111	0
36	HEM	AF	101	43/43	0.94	0.40	0.80	148,152,159,160	0
24	CLA	BB	5606	65/65	0.84	0.31	0.79	124,127,130,131	0
24	CLA	BC	5511	65/65	0.80	0.42	0.79	154,158,159,160	0
34	PHO	BD	5404	64/64	0.90	0.28	0.78	123,125,129,130	0
24	CLA	AC	510	65/65	0.92	0.33	0.75	110,113,129,130	0
27	BCR	AB	619	40/40	0.84	0.30	0.75	111,117,131,131	0
24	CLA	BD	5402	65/65	0.90	0.27	0.72	97,101,117,119	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
29	LHG	AA	412	39/49	0.89	0.29	0.71	110,118,128,132	0
24	CLA	BC	5506	65/65	0.74	0.40	0.70	136,143,160,160	0
24	CLA	BC	5509	65/65	0.89	0.30	0.66	116,128,138,138	0
30	SQD	BA	5414	51/54	0.72	0.37	0.65	145,150,160,160	0
24	CLA	BC	5501	65/65	0.89	0.31	0.65	134,137,141,144	0
30	SQD	BB	5601	47/54	0.73	0.38	0.65	137,156,160,160	0
31	LMG	BC	5521	45/55	0.62	0.56	0.64	154,160,160,160	0
24	CLA	AC	513	65/65	0.72	0.44	0.60	158,160,160,160	0
30	SQD	AA	413	51/54	0.84	0.32	0.58	143,150,160,160	0
27	BCR	AA	410	40/40	0.91	0.27	0.52	91,122,130,130	0
24	CLA	BB	5610	65/65	0.82	0.31	0.47	121,132,140,141	0
24	CLA	BC	5512	65/65	0.81	0.36	0.47	157,160,160,160	0
24	CLA	BB	5618	65/65	0.87	0.32	0.46	128,133,160,160	0
29	LHG	BA	5413	39/49	0.87	0.28	0.42	113,122,128,129	0
36	HEM	BV	5201	43/43	0.92	0.28	0.38	97,102,106,109	0
36	HEM	AV	201	43/43	0.96	0.27	0.36	94,100,102,103	0
25	MST	AA	408	16/16	0.93	0.26	0.31	123,126,129,130	0
26	OEC	AA	409	5/9	0.95	0.28	0.29	82,83,90,110	0
36	HEM	BF	5101	43/43	0.91	0.46	0.22	148,152,160,160	0
24	CLA	AC	511	65/65	0.87	0.33	0.13	152,155,157,158	0
25	MST	BA	5409	16/16	0.92	0.23	0.08	124,129,131,132	0
24	CLA	BB	5620	65/65	0.83	0.30	-0.04	143,147,160,160	0
26	OEC	BA	5410	5/9	0.73	0.22	-0.53	23,88,99,134	0
22	BCT	AA	402	4/4	0.99	0.20	-0.79	135,136,137,137	0
21	FE2	AA	401	1/1	0.98	0.18	-0.91	115,115,115,115	0
22	BCT	BA	5403	4/4	0.97	0.16	-1.22	135,136,136,137	0
21	FE2	BD	5401	1/1	0.94	0.12	-2.42	119,119,119,119	0
32	LMT	AB	623	35/35	0.53	0.74	-	135,160,160,160	0
31	LMG	AI	101	43/55	0.35	0.80	-	159,160,160,160	0
32	LMT	BB	5626	35/35	0.38	0.63	-	131,160,160,160	0
37	CA	AK	101	1/1	0.84	0.12	-	146,146,146,146	0
37	CA	BO	5301	1/1	0.65	0.30	-	160,160,160,160	0
31	LMG	BI	5101	43/55	0.55	0.70	-	160,160,160,160	0
37	CA	BF	5103	1/1	0.14	0.16	-	146,146,146,146	0
37	CA	AO	301	1/1	0.50	0.21	-	152,152,152,152	0
37	CA	AF	103	1/1	0.36	0.23	-	150,150,150,150	0
37	CA	BK	5101	1/1	0.62	0.22	-	145,145,145,145	0

6.5 Other polymers ⓘ

There are no such residues in this entry.