Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:50 PM GMT

PDB ID	:	4V9G
Title	:	RC-LH1-PufX dimer complex from Rhodobacter sphaeroides
Authors	:	Qian, P.; Papiz, M.Z.; Jackson, P.J.; Brindley, A.A.; Ng, I.W.; Olsen, J.D.; Dickman, M.J.; Bullough, P.A.; Hunter, C.N.
Deposited on	:	2013-02-21
Resolution	:	7.78 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

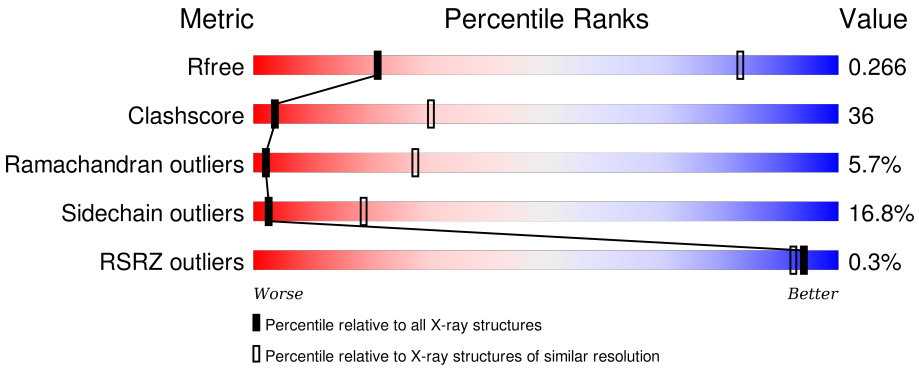
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 7.78 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	1015 (11.50-3.66)
Clashscore	102246	1064 (11.50-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

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 <=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	A1	58	33% 26% 14% 28%
1	A2	58	12% 47% 14% 28%
1	A3	58	40% 21% 12% 28%
1	A5	58	31% 31% 10% 28%
1	A7	58	2% 28% 26% 16% • 28%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	AD	58	31% 28% 12% 28%
1	AF	58	2% 38% 26% 9% 28%
1	AJ	58	34% 28% 9% 28%
1	AN	58	31% 31% 9% 28%
1	AP	58	34% 28% 9% 28%
1	AT	58	38% 28% 5% 28%
1	AV	58	36% 29% 5% 28%
1	AX	58	2% 34% 24% 10% 28%
1	AZ	58	31% 24% 16% 28%
1	B1	58	2% 22% 34% 16% 28%
1	B2	58	31% 34% 7% 28%
1	B3	58	36% 29% 7% 28%
1	B5	58	29% 34% 9% 28%
1	B7	58	22% 33% 16% 28%
1	BD	58	2% 21% 34% 17% 28%
1	BF	58	34% 31% 7% 28%
1	BJ	58	24% 36% 12% 28%
1	BN	58	34% 29% 9% 28%
1	BP	58	2% 22% 31% 19% 28%
1	BT	58	36% 33% 28%
1	BV	58	47% 14% 12% 28%
1	BX	58	5% 38% 26% 9% 28%
1	BZ	58	29% 28% 12% 28%
2	AB	82	33% 28% 7% 30%
2	BB	82	41% 20% 7% 30%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	A4	49	43% 39% 14%
3	A6	49	57% 33% 8%
3	A8	49	59% 29% 10%
3	A9	49	53% 37% 8%
3	AE	49	47% 41% 10%
3	AG	49	45% 45% 8%
3	AI	49	47% 45% 6%
3	AK	49	53% 35% 10%
3	AO	49	53% 37% 6%
3	AQ	49	61% 31% 6%
3	AS	49	69% 16% 6% 6%
3	AU	49	43% 47% 8%
3	AW	49	2% 49% 41% 8%
3	AY	49	39% 45% 12%
3	B4	49	49% 39% 10%
3	B6	49	45% 41% 12%
3	B8	49	2% 59% 33% 6%
3	B9	49	53% 41%
3	BE	49	49% 37% 12%
3	BG	49	2% 57% 35% 6%
3	BI	49	61% 33%
3	BK	49	57% 27% 14%
3	BO	49	55% 35% 8%
3	BQ	49	51% 45%
3	BS	49	2% 47% 41% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	BU	49	55% 33% 8%
3	BW	49	55% 39%
3	BY	49	2% 61% 27% 10%
4	AH	260	46% 42% 8%
4	BH	260	52% 39% 5%
5	AL	282	34% 51% 14%
5	BL	282	34% 56% 9%
6	AM	308	41% 46% 11%
6	BM	308	43% 46% 8%

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
7	BCL	A6	101	-	-	-	X
7	BCL	AL	301	-	-	X	-
7	BCL	AL	302	-	-	X	-
7	BCL	AM	401	-	-	X	-
7	BCL	AM	402	-	-	X	-
7	BCL	AO	101	-	-	-	X
7	BCL	B5	101	-	-	-	X
7	BCL	BL	302	-	-	X	-
7	BCL	BL	303	-	-	X	X
7	BCL	BM	401	-	-	X	-
7	BCL	BO	101	-	-	-	X
8	BPH	AL	303	-	-	X	-
8	BPH	BL	304	-	-	X	-
8	BPH	BM	402	-	-	X	-
9	U10	AL	304	-	-	X	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 38108 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 Light-harvesting protein B-875 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A5	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AT	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AV	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AX	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	A3	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	A7	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AD	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AF	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	A1	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AJ	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	A2	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AN	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AP	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AZ	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	B5	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	BT	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BV	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	BX	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	B3	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	B7	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	BD	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	BF	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	B1	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	BJ	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	B2	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	BN	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	BP	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	BZ	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			

- Molecule 2 is a protein called Intrinsic membrane protein PufX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	57	Total	C	N	O	S	0	0	0
			452	299	79	71	3			
2	BB	57	Total	C	N	O	S	0	0	0
			452	299	79	71	3			

- Molecule 3 is a protein called Light-harvesting protein B-875 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AS	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	A9	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	AO	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AQ	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	A6	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	AU	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	AW	48	Total	C	N	O	S	0	0	0
			387	256	60	70	1			
3	AY	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	A4	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	A8	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	AE	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	AG	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	AI	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	AK	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	BS	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	B9	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	BO	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	BQ	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	B6	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	BU	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	BW	48	Total	C	N	O	S	0	0	0
			387	256	60	70	1			
3	BY	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	B4	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	B8	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	BE	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	BG	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	BI	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	BK	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			

- Molecule 4 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AH	250	Total	C	N	O	S	0	0	0
			1901	1216	324	351	10			
4	BH	250	Total	C	N	O	S	0	0	0
			1901	1216	324	351	10			

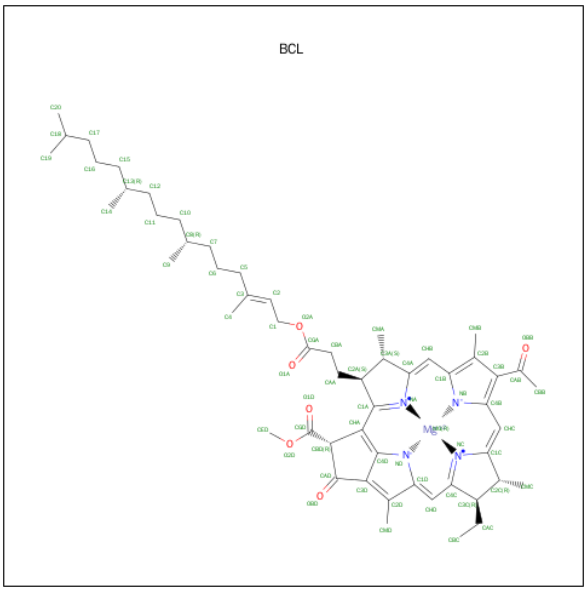
- Molecule 5 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AL	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			
5	BL	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

- Molecule 6 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AM	304	Total	C	N	O	S	0	1	0
			2427	1619	398	399	11			
6	BM	304	Total	C	N	O	S	0	1	0
			2427	1619	398	399	11			

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	AT	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AT	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AV	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	A3	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	A7	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AD	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AD	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AF	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	A1	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AJ	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	A2	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AN	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AP	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AP	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	AZ	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AS	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	A9	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AO	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	A6	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	A6	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AW	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AY	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AY	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	A4	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	A8	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AG	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AI	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AK	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AL	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	AL	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	AM	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	AM	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	B5	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BT	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BV	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		

Continued on next page...

Continued from previous page...

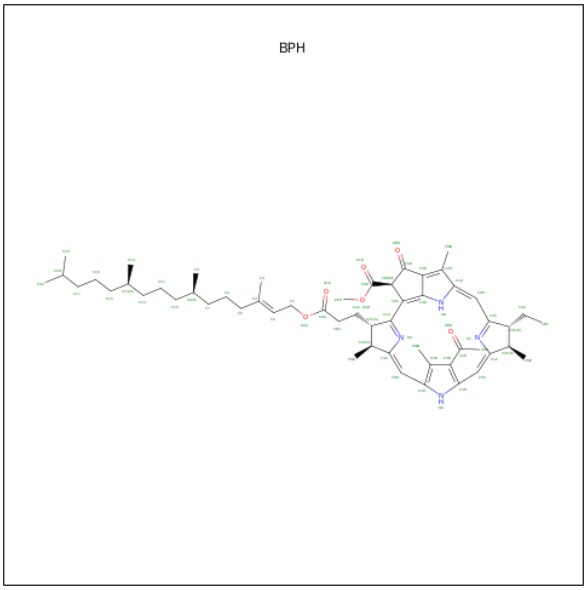
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	BV	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	B3	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	B7	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BD	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BD	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BF	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BF	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	B1	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	B2	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BP	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BP	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BZ	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BZ	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	B9	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BO	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BO	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	B6	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BU	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BY	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BY	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	B4	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B8	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BI	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BK	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BK	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BL	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	BL	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	BL	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	BM	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 8 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



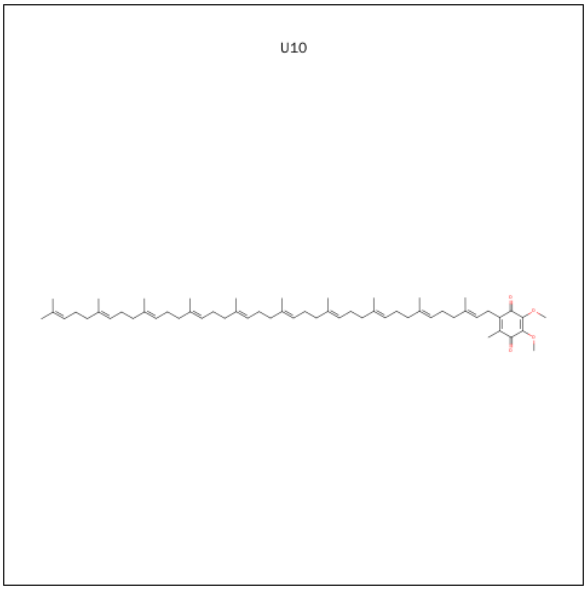
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	AL	1	Total	C	N	O	0	0
			65	55	4	6		
8	AM	1	Total	C	N	O	0	0
			65	55	4	6		
8	BL	1	Total	C	N	O	0	0
			65	55	4	6		

Continued on next page...

Continued from previous page...

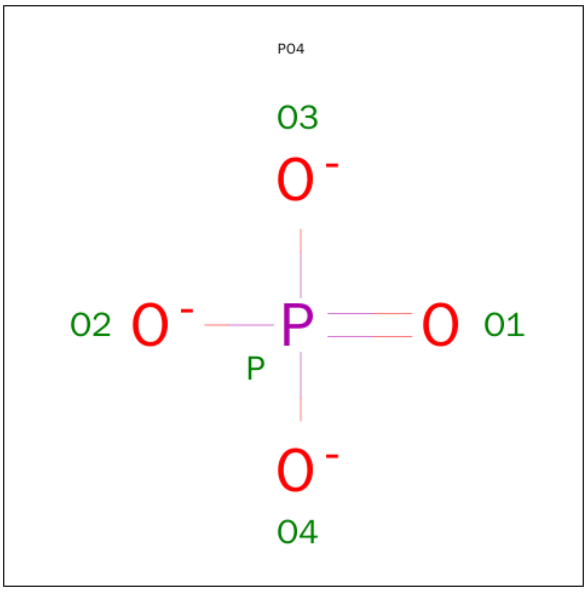
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	BM	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 9 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	AL	1	Total	C	O	0	0
			48	44	4		
9	AM	1	Total	C	O	0	0
			48	44	4		
9	BL	1	Total	C	O	0	0
			48	44	4		

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

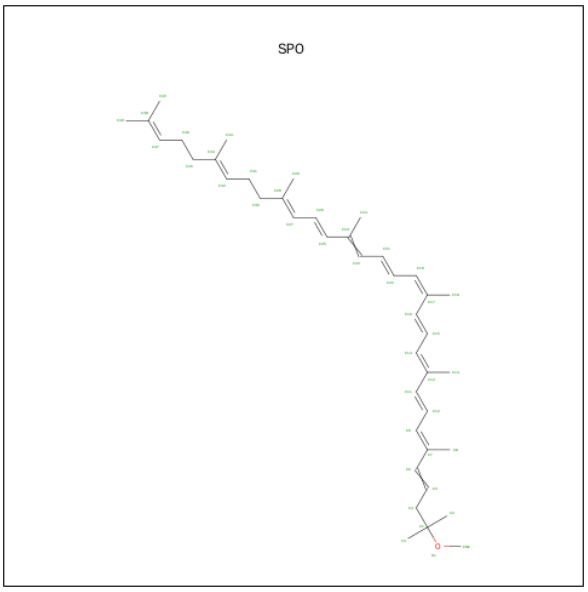


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	AL	1	Total O P 5 4 1	0	0
10	BL	1	Total O P 5 4 1	0	0

- Molecule 11 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	BL	1	Total Fe 1 1	0	0
11	AM	1	Total Fe 1 1	0	0

- Molecule 12 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



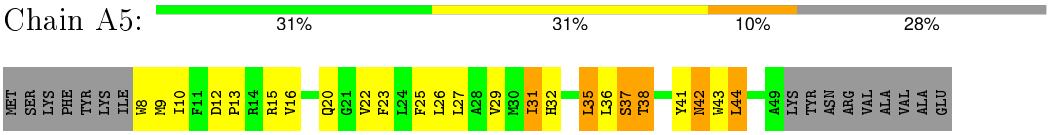
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
12	AM	1	42	41	1	0	0

3 Residue-property plots (i)

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.

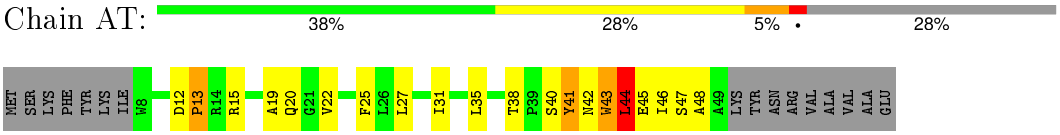
- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain A5:



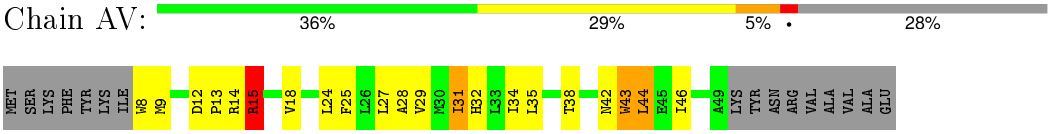
- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AT:



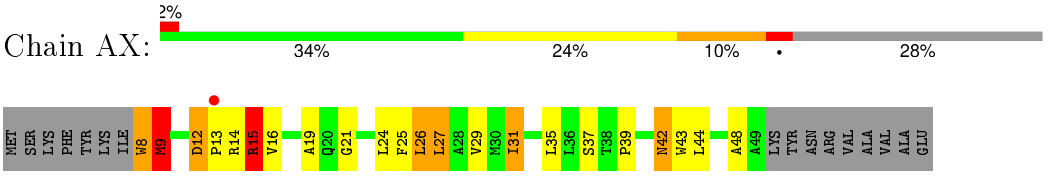
- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AV:



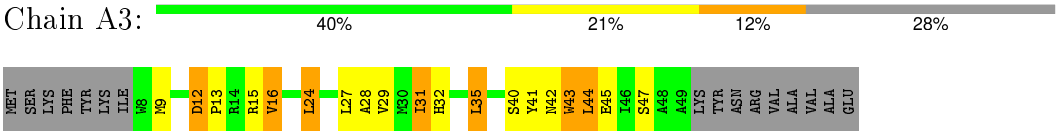
- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AX:



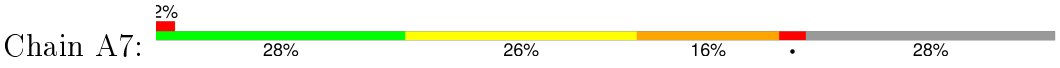
- Molecule 1: Light-harvesting protein B-875 alpha chain

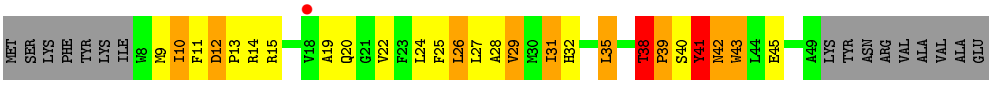
Chain A3:



- Molecule 1: Light-harvesting protein B-875 alpha chain

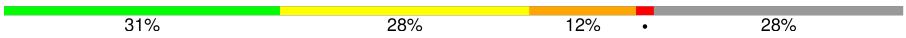
Chain A7:

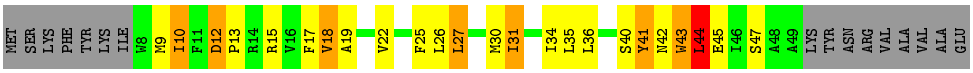




• Molecule 1: Light-harvesting protein B-875 alpha chain

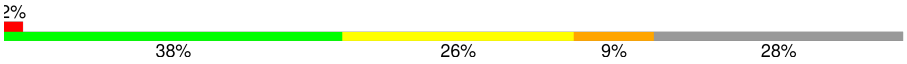
Chain AD:





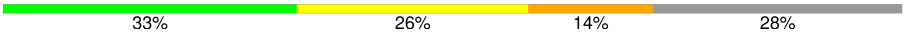
• Molecule 1: Light-harvesting protein B-875 alpha chain

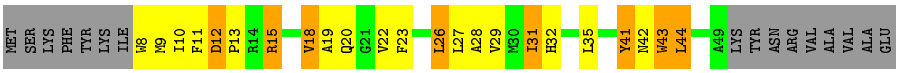
Chain AF:



• Molecule 1: Light-harvesting protein B-875 alpha chain

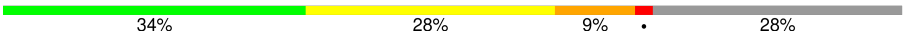
Chain A1:

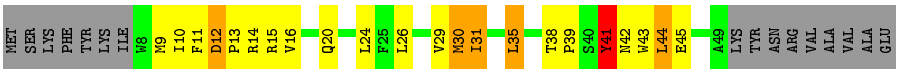




• Molecule 1: Light-harvesting protein B-875 alpha chain

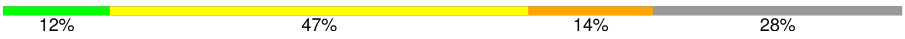
Chain AJ:

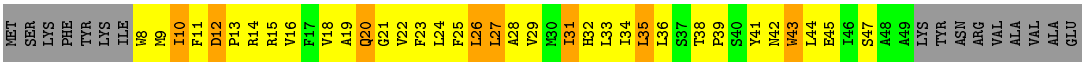




• Molecule 1: Light-harvesting protein B-875 alpha chain

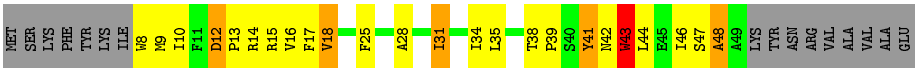
Chain A2:





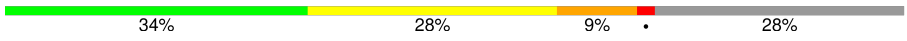
• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AN:



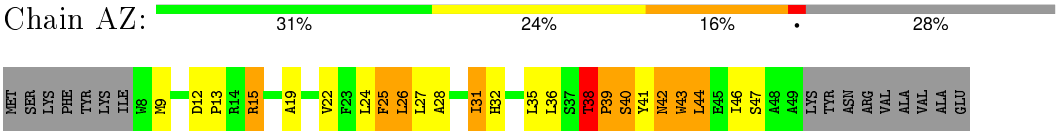
• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AP:



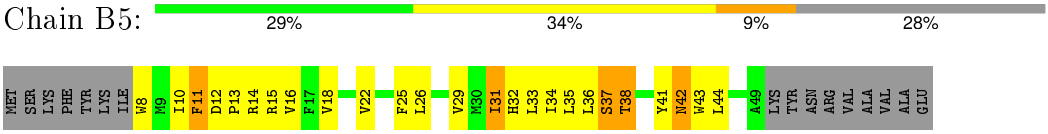
• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AZ:



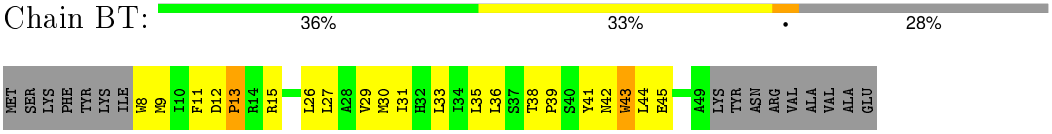
• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain B5:



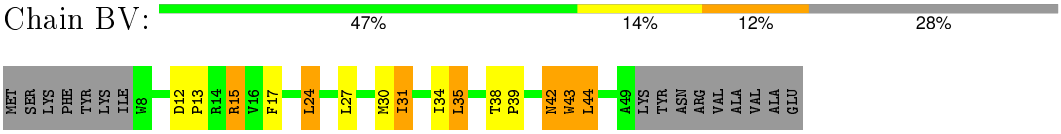
• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain BT:



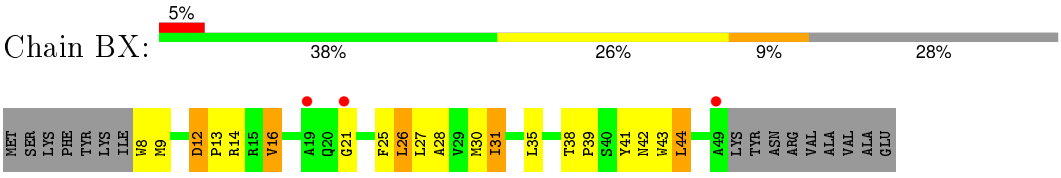
• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain BV:



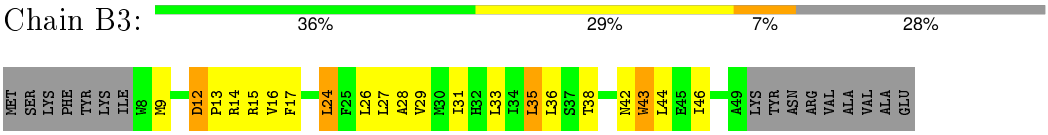
• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain BX:



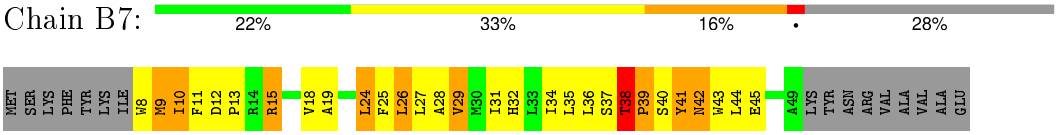
• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain B3:



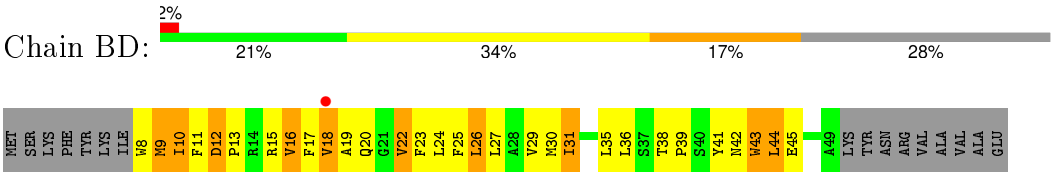
• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain B7:



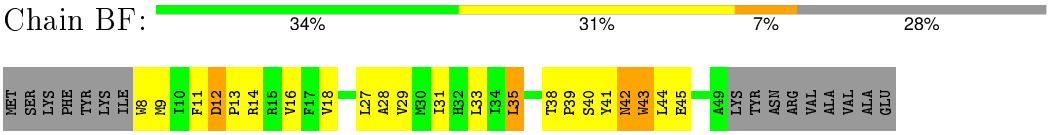
• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain BD:



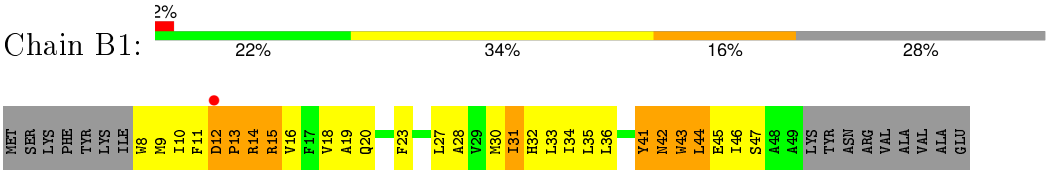
• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain BF:



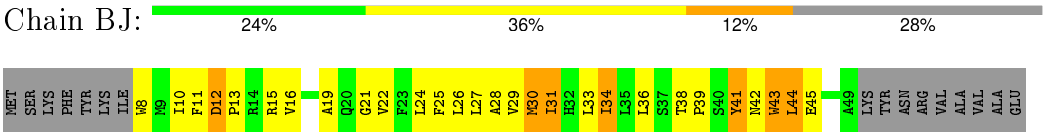
• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain B1:



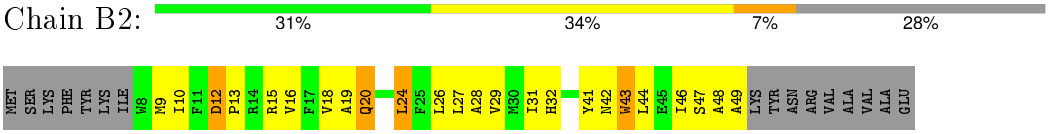
• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain BJ:



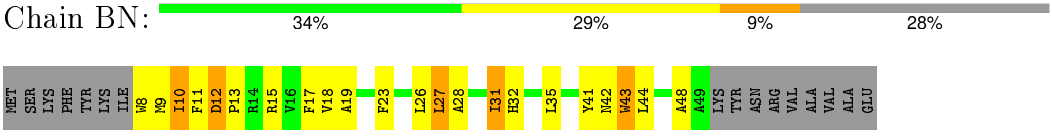
• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain B2:



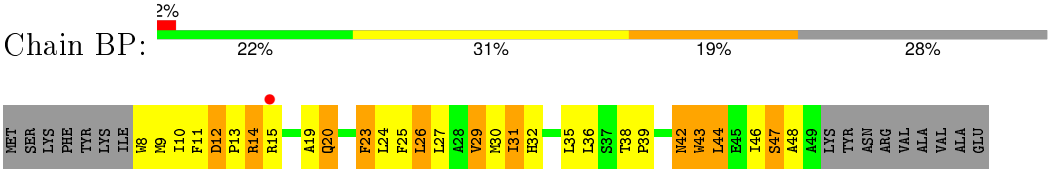
• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain BN:



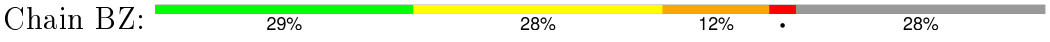
• Molecule 1: Light-harvesting protein B-875 alpha chain

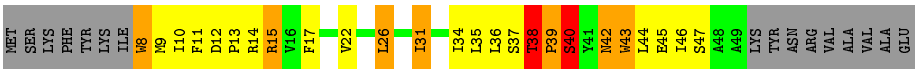
Chain BP:



• Molecule 1: Light-harvesting protein B-875 alpha chain

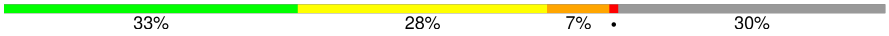
Chain BZ:

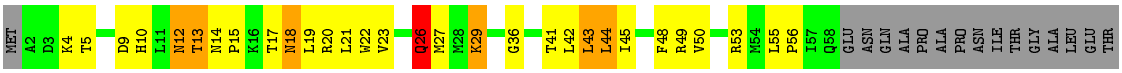




• Molecule 2: Intrinsic membrane protein PufX

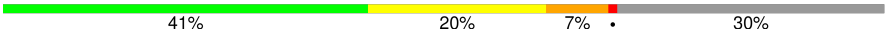
Chain AB:

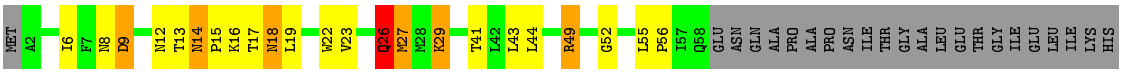




• Molecule 2: Intrinsic membrane protein PufX

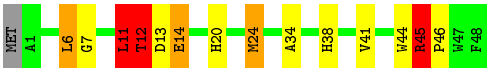
Chain BB:





• Molecule 3: Light-harvesting protein B-875 beta chain

Chain AS:

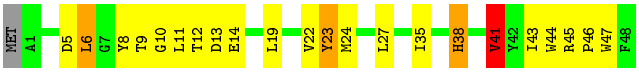


• Molecule 3: Light-harvesting protein B-875 beta chain

Chain A9:

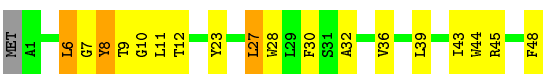
• Molecule 3: Light-harvesting protein B-875 beta chain

Chain AO:



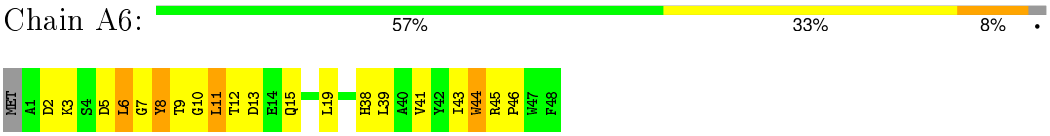
• Molecule 3: Light-harvesting protein B-875 beta chain

Chain AQ:



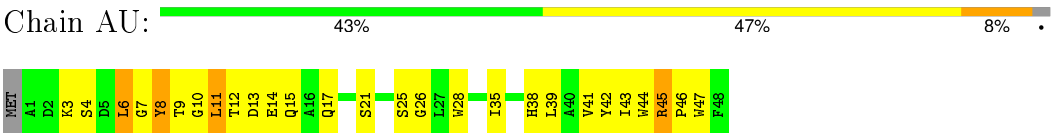
• Molecule 3: Light-harvesting protein B-875 beta chain

Chain A6:



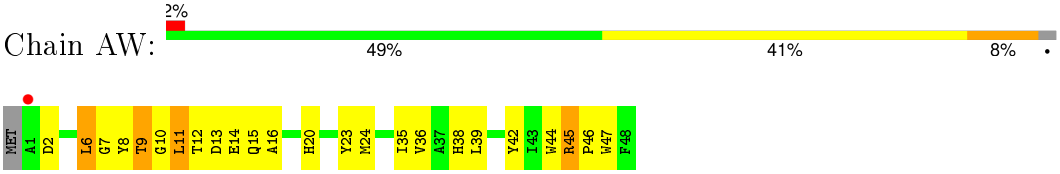
• Molecule 3: Light-harvesting protein B-875 beta chain

Chain AU:



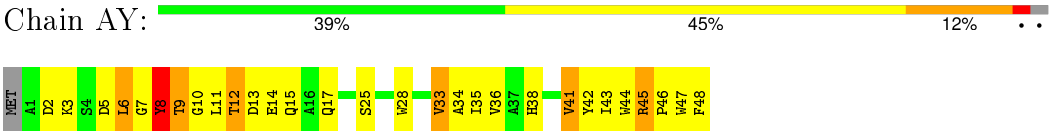
• Molecule 3: Light-harvesting protein B-875 beta chain

Chain AW:



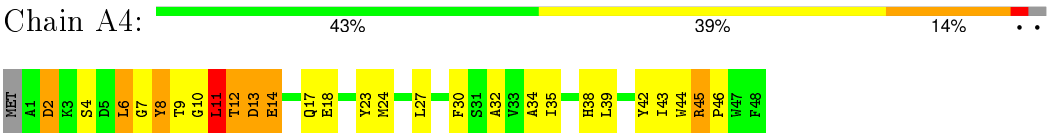
• Molecule 3: Light-harvesting protein B-875 beta chain

Chain AY:



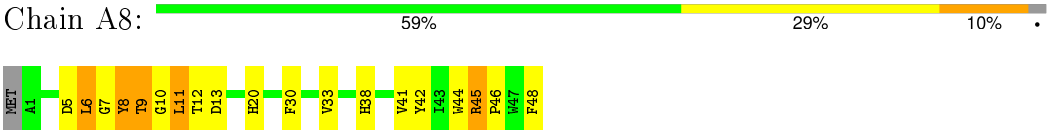
• Molecule 3: Light-harvesting protein B-875 beta chain

Chain A4:



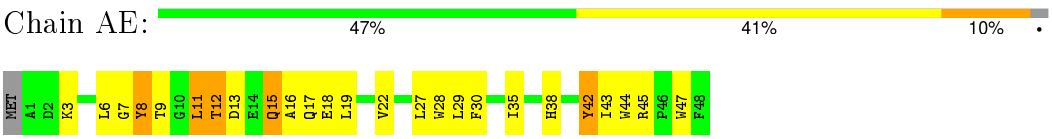
• Molecule 3: Light-harvesting protein B-875 beta chain

Chain A8:



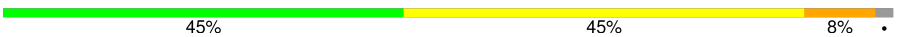
• Molecule 3: Light-harvesting protein B-875 beta chain

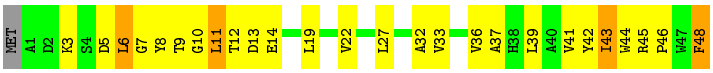
Chain AE:



• Molecule 3: Light-harvesting protein B-875 beta chain

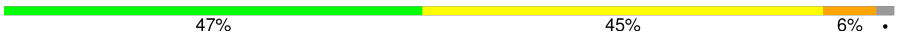
Chain AG:





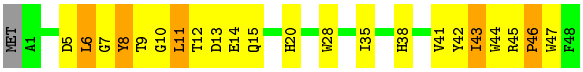
• Molecule 3: Light-harvesting protein B-875 beta chain

Chain AI:



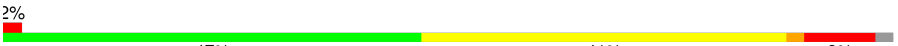
• Molecule 3: Light-harvesting protein B-875 beta chain

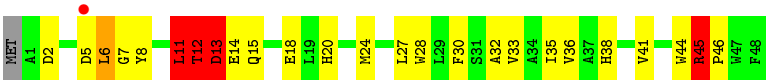
Chain AK:



• Molecule 3: Light-harvesting protein B-875 beta chain

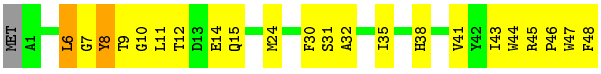
Chain BS:





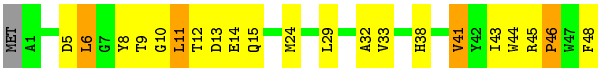
• Molecule 3: Light-harvesting protein B-875 beta chain

Chain B9:



• Molecule 3: Light-harvesting protein B-875 beta chain

Chain BO:



• Molecule 3: Light-harvesting protein B-875 beta chain

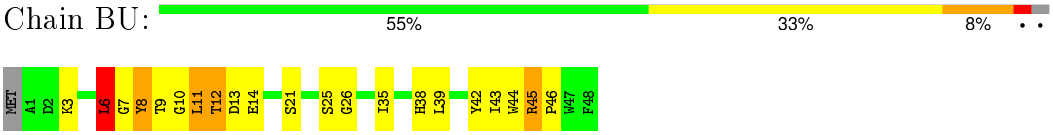
Chain BQ:

• Molecule 3: Light-harvesting protein B-875 beta chain

Chain B6:

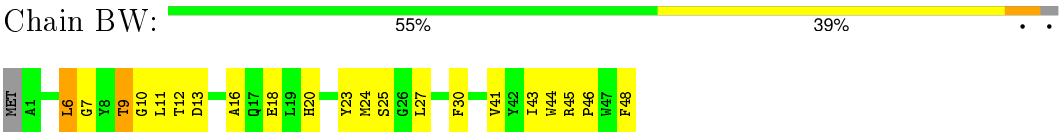
• Molecule 3: Light-harvesting protein B-875 beta chain

Chain BU:



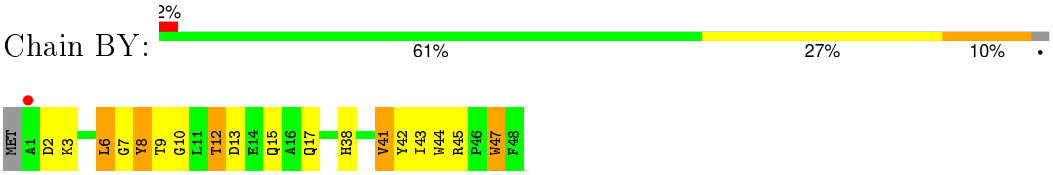
• Molecule 3: Light-harvesting protein B-875 beta chain

Chain BW:



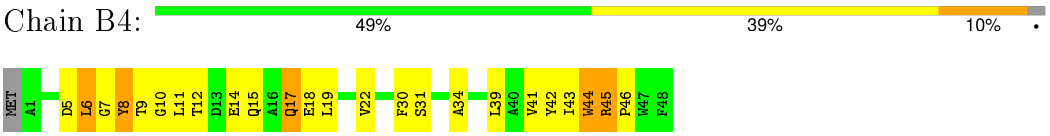
• Molecule 3: Light-harvesting protein B-875 beta chain

Chain BY:



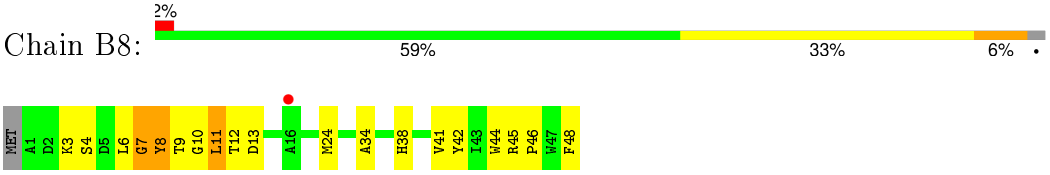
• Molecule 3: Light-harvesting protein B-875 beta chain

Chain B4:



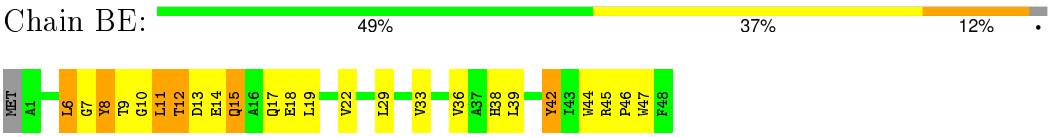
• Molecule 3: Light-harvesting protein B-875 beta chain

Chain B8:



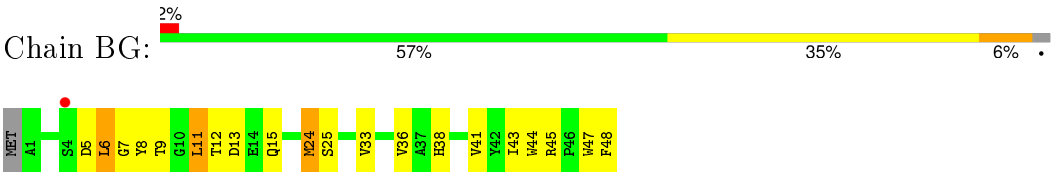
• Molecule 3: Light-harvesting protein B-875 beta chain

Chain BE:



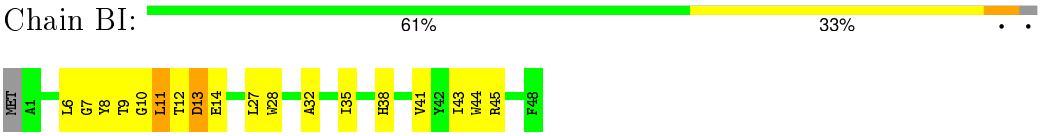
• Molecule 3: Light-harvesting protein B-875 beta chain

Chain BG:



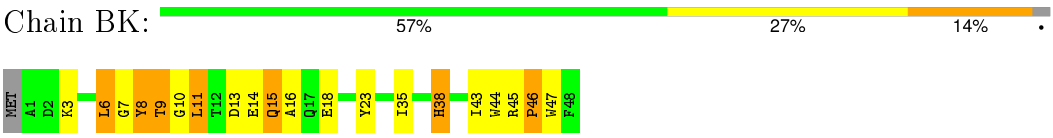
• Molecule 3: Light-harvesting protein B-875 beta chain

Chain BI:



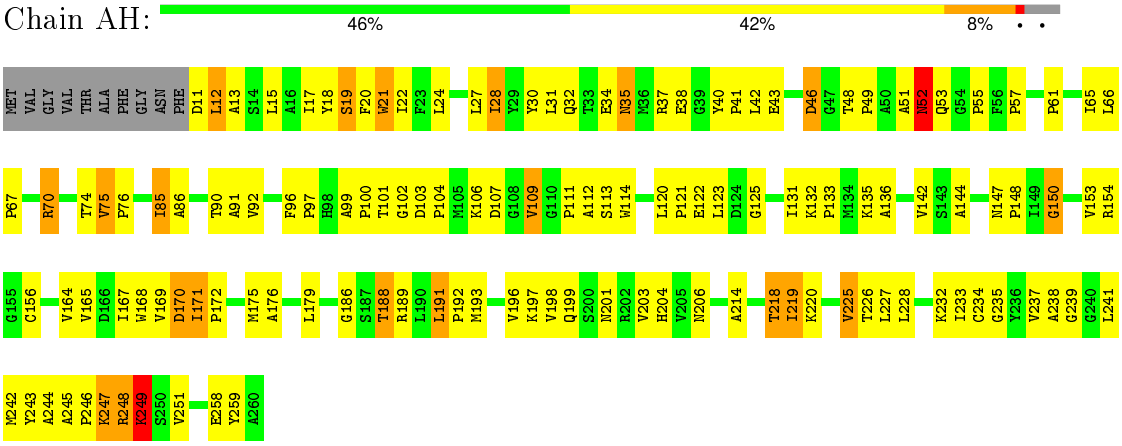
• Molecule 3: Light-harvesting protein B-875 beta chain

Chain BK:



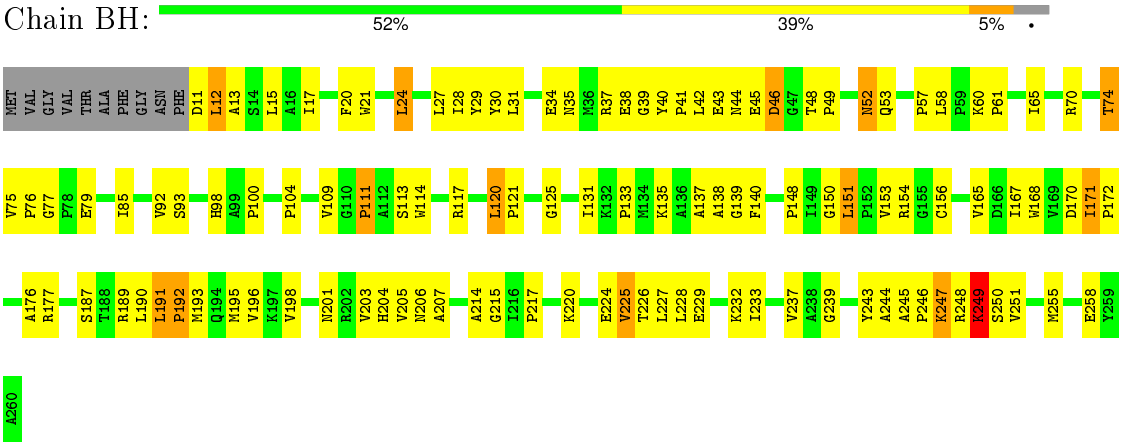
• Molecule 4: Reaction center protein H chain

Chain AH:



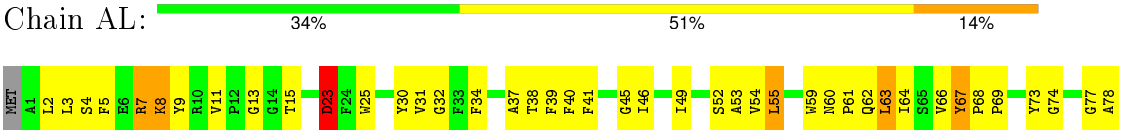
• Molecule 4: Reaction center protein H chain

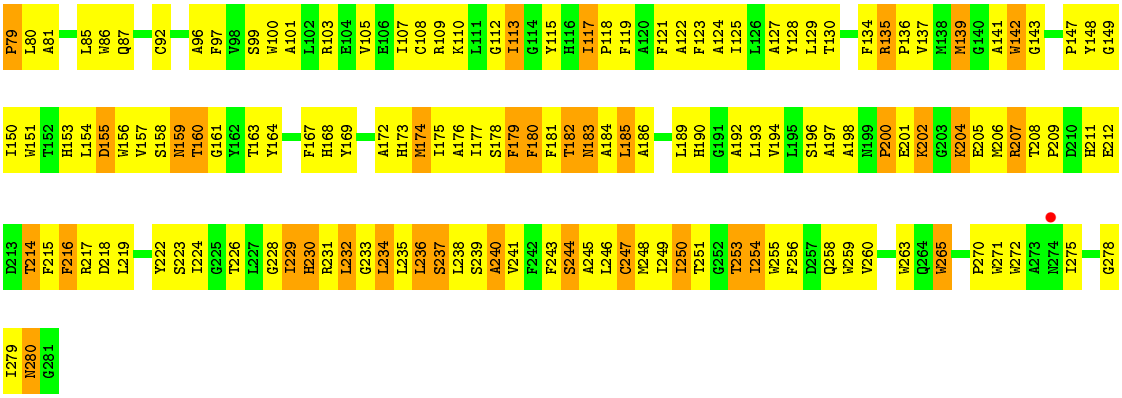
Chain BH:



• Molecule 5: Reaction center protein L chain

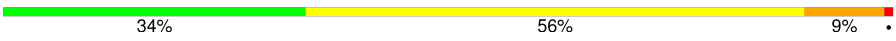
Chain AL:

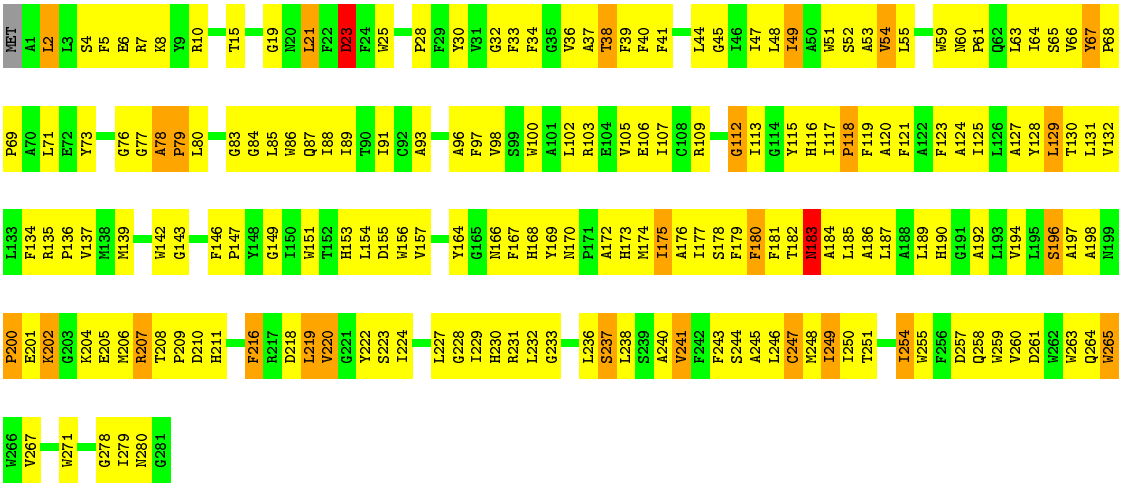




• Molecule 5: Reaction center protein L chain

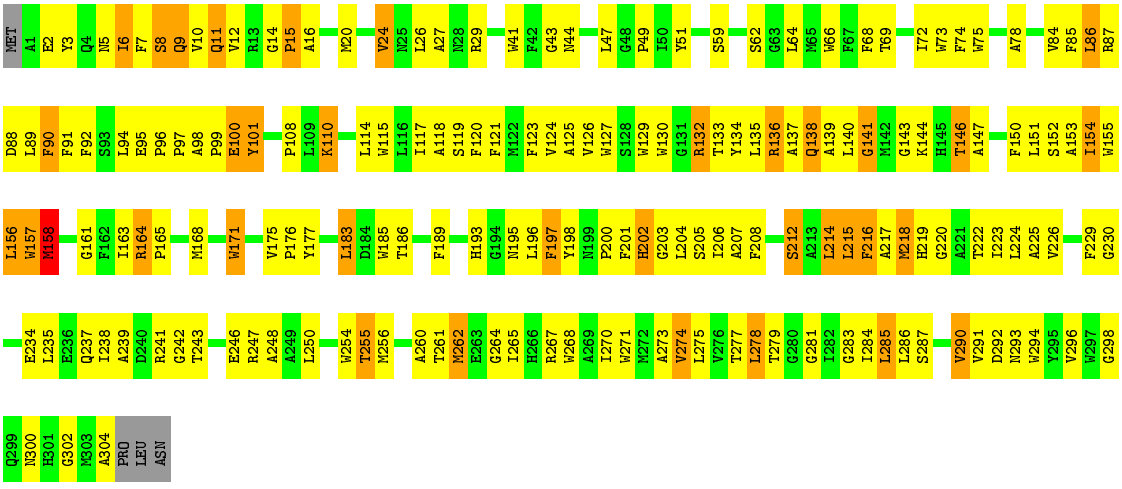
Chain BL:





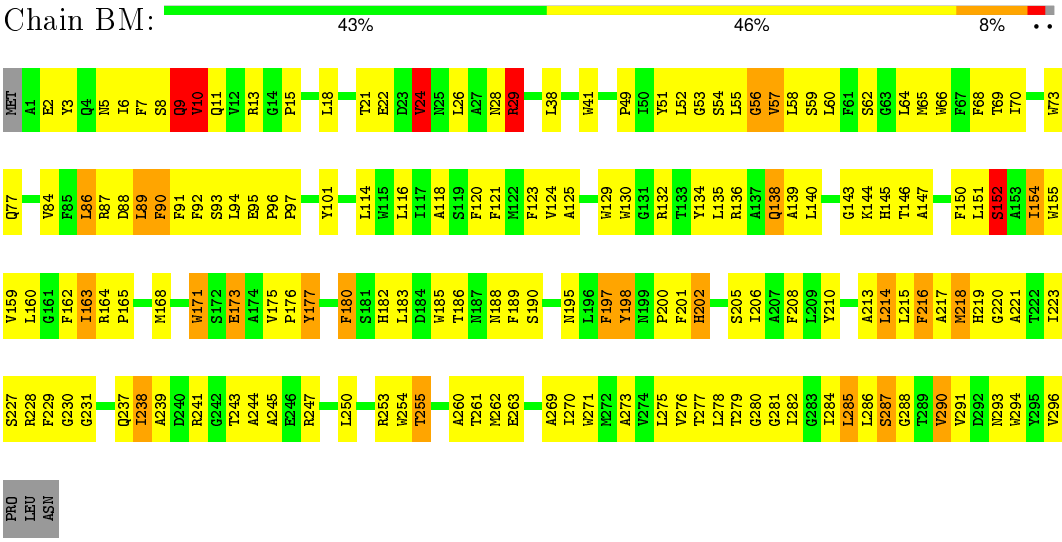
• Molecule 6: Reaction center protein M chain

Chain AM:



• Molecule 6: Reaction center protein M chain

Chain BM:


43%
46%
8%
MET A1 E2 Y3 Q4 N5 I6 F7 S8 Q9 V10 Q11 V12 R13 G14 P15 L18 T21 E22 D23 V24 M25 L26 A27 M28 R29 L38 W41 P49 I50 Y51 L52 G53 S54 L55 G56 V57 L58 S59 L60 F61 S62 G63 L64 M65 W66 F67 F68 T69 I70 W73 F74 W75 Y76
Q77 V84 F85 L86 R87 D88 L89 F90 F91 F92 S93 L94 E95 P96 P97 Y101 L114 W115 L116 I117 A118 S119 F120 F121 M122 F123 V124 A125 W129 W130 G131 R132 T133 Y134 L135 R136 A137 Q138 A139 L140 G143 K144 H145 T146 A147 F150 L151 S152 A153 I154 W155 L156 W157 M158
V159 L160 G161 F162 I163 R164 P165 M168 W171 S172 E173 A174 V175 P176 Y177 F180 S181 H182 L183 D184 W185 T186 N187 N188 F189 S190 N195 L196 F197 Y198 N199 P200 F201 H202 S205 I206 A207 F208 L209 Y210 A213 L214 L215 F216 A217 M218 H219 G220 A221 T222 I223 L224 A225 V226
S227 R228 F229 G230 G231 Q237 I238 A239 D240 R241 G242 T243 A244 A245 E246 R247 L250 R253 W254 T255 A260 T261 M262 E263 A269 I270 W271 M272 A273 V274 L275 V276 T277 L278 T279 G280 G281 I282 G283 I284 L285 L286 S287 G288 T289 V290 V291 D292 M293 W294 Y295 V296 W297 A304
PRO LEU ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.08Å 415.07Å 129.82Å 90.00° 105.75° 90.00°	Depositor
Resolution (Å)	20.39 – 7.78 20.07 – 8.00	Depositor EDS
% Data completeness (in resolution range)	73.7 (20.39-7.78) 73.6 (20.07-8.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 7.79Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.228 , 0.258 0.239 , 0.266	Depositor DCC
R_{free} test set	319 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	430.3	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.09 , 318.7	EDS
Estimated twinning fraction	0.883 for H, K, L 0.117 for -H, -K, H+L 0.178 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.883 for H, K, L 0.117 for -H, -K, H+L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.33$, $< L^2 > = 0.16$	Xtriage
Outliers	0 of 6309 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	38108	wwPDB-VP
Average B, all atoms (Å^2)	258.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, BPH, PO4, FE2, SPO, U10

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	A1	0.23	0/356	0.31	0/486
1	A2	0.24	0/356	0.31	0/486
1	A3	0.26	0/356	0.31	0/486
1	A5	0.25	0/356	0.31	0/486
1	A7	0.25	0/356	0.31	0/486
1	AD	0.25	0/356	0.31	0/486
1	AF	0.24	0/356	0.31	0/486
1	AJ	0.24	0/356	0.31	0/486
1	AN	0.25	0/356	0.31	0/486
1	AP	0.24	0/356	0.31	0/486
1	AT	0.26	0/356	0.31	0/486
1	AV	0.24	0/356	0.31	0/486
1	AX	0.25	0/356	0.31	0/486
1	AZ	0.26	0/356	0.31	0/486
1	B1	0.24	0/356	0.31	0/486
1	B2	0.25	0/356	0.31	0/486
1	B3	0.24	0/356	0.31	0/486
1	B5	0.24	0/356	0.31	0/486
1	B7	0.25	0/356	0.31	0/486
1	BD	0.26	0/356	0.31	0/486
1	BF	0.25	0/356	0.31	0/486
1	BJ	0.25	0/356	0.31	0/486
1	BN	0.24	0/356	0.31	0/486
1	BP	0.25	0/356	0.31	0/486
1	BT	0.24	0/356	0.31	0/486
1	BV	0.24	0/356	0.31	0/486
1	BX	0.26	0/356	0.31	0/486
1	BZ	0.25	0/356	0.31	0/486
2	AB	0.24	0/464	0.32	0/626
2	BB	0.24	0/464	0.32	0/626
3	A4	0.22	0/401	0.29	0/547
3	A6	0.22	0/401	0.29	0/547

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	A8	0.22	0/401	0.29	0/547
3	A9	0.22	0/401	0.29	0/547
3	AE	0.23	0/401	0.29	0/547
3	AG	0.22	0/401	0.29	0/547
3	AI	0.22	0/401	0.29	0/547
3	AK	0.22	0/401	0.29	0/547
3	AO	0.22	0/401	0.29	0/547
3	AQ	0.23	0/401	0.29	0/547
3	AS	0.24	0/401	0.29	0/547
3	AU	0.22	0/401	0.29	0/547
3	AW	0.21	0/400	0.29	0/545
3	AY	0.22	0/401	0.29	0/547
3	B4	0.23	0/401	0.29	0/547
3	B6	0.22	0/401	0.29	0/547
3	B8	0.21	0/401	0.29	0/547
3	B9	0.22	0/401	0.29	0/547
3	BE	0.23	0/401	0.29	0/547
3	BG	0.22	0/401	0.29	0/547
3	BI	0.22	0/401	0.29	0/547
3	BK	0.23	0/401	0.29	0/547
3	BO	0.22	0/401	0.29	0/547
3	BQ	0.24	0/401	0.29	0/547
3	BS	0.24	0/401	0.29	0/547
3	BU	0.22	0/401	0.29	0/547
3	BW	0.20	0/400	0.29	0/545
3	BY	0.22	0/401	0.29	0/547
4	AH	0.21	0/1950	0.34	0/2652
4	BH	0.21	0/1950	0.34	0/2652
5	AL	0.59	8/2320 (0.3%)	0.36	0/3175
5	BL	0.71	10/2320 (0.4%)	0.37	0/3175
6	AM	0.48	5/2524 (0.2%)	0.32	0/3445
6	BM	0.53	1/2524 (0.0%)	0.31	0/3445
All	All	0.36	24/35710 (0.1%)	0.32	0/48716

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	A7	0	1
1	AZ	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B1	0	1
1	B7	0	1
3	AQ	0	1
3	AS	0	2
3	BS	0	2
4	BH	0	1
5	AL	0	3
6	AM	0	3
6	BM	0	1
All	All	0	17

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	BM	152	SER	CB-OG	22.34	1.71	1.42
5	BL	196	SER	CB-OG	17.38	1.64	1.42
6	AM	212	SER	CB-OG	12.58	1.58	1.42
5	AL	212	GLU	CD-OE1	11.48	1.38	1.25
5	BL	247	CYS	CB-SG	11.36	2.01	1.82
5	AL	212	GLU	CD-OE2	9.99	1.36	1.25
5	AL	92	CYS	CB-SG	9.65	1.98	1.82
5	BL	155	ASP	CG-OD2	8.99	1.46	1.25
5	AL	159	ASN	CG-ND2	8.79	1.54	1.32
5	BL	223	SER	CB-OG	8.70	1.53	1.42
5	BL	155	ASP	CG-OD1	8.63	1.45	1.25
5	BL	183	ASN	CG-OD1	8.05	1.41	1.24
5	BL	183	ASN	CG-ND2	7.88	1.52	1.32
5	AL	155	ASP	CG-OD1	7.71	1.43	1.25
6	AM	262	MET	CB-CG	7.45	1.75	1.51
5	AL	155	ASP	CG-OD2	7.13	1.41	1.25
5	BL	219	LEU	CG-CD2	7.07	1.78	1.51
5	AL	159	ASN	CG-OD1	6.99	1.39	1.24
5	BL	219	LEU	CG-CD1	6.42	1.75	1.51
5	AL	204	LYS	CE-NZ	5.99	1.64	1.49
5	BL	237	SER	CB-OG	5.97	1.50	1.42
6	AM	168	MET	CG-SD	5.75	1.96	1.81
6	AM	158	MET	CG-SD	5.74	1.96	1.81
6	AM	158	MET	SD-CE	5.33	2.07	1.77

There are no bond angle outliers.

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A7	38	THR	Peptide
5	AL	229	ILE	Peptide
5	AL	230	HIS	Peptide
5	AL	236	LEU	Peptide
6	AM	183	LEU	Peptide
6	AM	205	SER	Peptide
6	AM	9	GLN	Peptide
3	AQ	27	LEU	Peptide
3	AS	11	LEU	Peptide
3	AS	12	THR	Peptide
1	AZ	38	THR	Peptide
1	B1	42	ASN	Peptide
1	B7	38	THR	Peptide
4	BH	249	LYS	Peptide
6	BM	9	GLN	Peptide
3	BS	11	LEU	Peptide
3	BS	12	THR	Peptide

5.2 Too-close contacts (i)

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	A1	345	0	355	25	0
1	A2	345	0	355	38	0
1	A3	345	0	355	22	0
1	A5	345	0	355	26	0
1	A7	345	0	355	33	0
1	AD	345	0	355	30	0
1	AF	345	0	355	19	0
1	AJ	345	0	355	21	0
1	AN	345	0	355	25	0
1	AP	345	0	355	25	0
1	AT	345	0	355	21	0
1	AV	345	0	355	15	0
1	AX	345	0	355	15	0
1	AZ	345	0	355	26	0
1	B1	345	0	355	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B2	345	0	355	23	0
1	B3	345	0	355	15	0
1	B5	345	0	355	21	0
1	B7	345	0	355	39	0
1	BD	345	0	355	34	0
1	BF	345	0	355	25	0
1	BJ	345	0	355	23	0
1	BN	345	0	355	23	0
1	BP	345	0	355	27	0
1	BT	345	0	355	16	0
1	BV	345	0	355	14	0
1	BX	345	0	355	15	0
1	BZ	345	0	355	35	0
2	AB	452	0	462	19	0
2	BB	452	0	462	20	0
3	A4	388	0	370	31	0
3	A6	388	0	370	23	0
3	A8	388	0	370	18	0
3	A9	388	0	370	24	0
3	AE	388	0	370	32	0
3	AG	388	0	370	22	0
3	AI	388	0	370	29	0
3	AK	388	0	370	22	0
3	AO	388	0	370	22	0
3	AQ	388	0	370	18	0
3	AS	388	0	370	31	0
3	AU	388	0	370	24	0
3	AW	387	0	363	26	0
3	AY	388	0	370	22	0
3	B4	388	0	370	16	0
3	B6	388	0	370	27	0
3	B8	388	0	370	18	0
3	B9	388	0	370	19	0
3	BE	388	0	370	38	0
3	BG	388	0	370	12	0
3	BI	388	0	370	26	0
3	BK	388	0	370	21	0
3	BO	388	0	370	23	0
3	BQ	388	0	370	27	0
3	BS	388	0	370	35	0
3	BU	388	0	370	19	0
3	BW	387	0	363	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BY	388	0	370	13	0
4	AH	1901	0	1909	120	0
4	BH	1901	0	1909	109	0
5	AL	2232	0	2187	258	0
5	BL	2232	0	2187	284	0
6	AM	2427	0	2338	241	0
6	BM	2427	0	2338	220	0
7	A1	46	0	35	2	0
7	A2	46	0	35	3	0
7	A3	46	0	35	6	0
7	A4	46	0	35	6	0
7	A6	92	0	70	14	0
7	A7	46	0	35	9	0
7	A8	46	0	35	9	0
7	A9	46	0	35	11	0
7	AD	92	0	70	21	0
7	AF	46	0	35	12	0
7	AG	46	0	35	2	0
7	AI	46	0	35	11	0
7	AJ	46	0	35	8	0
7	AK	46	0	35	6	0
7	AL	132	0	148	55	0
7	AM	132	0	148	50	0
7	AN	46	0	35	4	0
7	AO	46	0	35	16	0
7	AP	92	0	70	21	0
7	AS	46	0	35	15	0
7	AT	92	0	70	16	0
7	AV	46	0	35	6	0
7	AW	46	0	35	1	0
7	AY	92	0	70	7	0
7	AZ	46	0	35	12	0
7	B1	46	0	35	2	0
7	B2	46	0	35	9	0
7	B3	46	0	35	7	0
7	B4	46	0	35	3	0
7	B5	46	0	35	1	0
7	B6	46	0	35	5	0
7	B7	46	0	35	3	0
7	B8	46	0	35	11	0
7	B9	46	0	35	7	0
7	BD	92	0	70	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	BF	92	0	70	13	0
7	BI	46	0	35	12	0
7	BK	92	0	70	18	0
7	BL	198	0	222	87	0
7	BM	66	0	74	27	0
7	BO	92	0	70	25	0
7	BP	92	0	70	28	0
7	BT	46	0	35	7	0
7	BU	46	0	35	6	0
7	BV	92	0	70	12	0
7	BY	92	0	70	8	0
7	BZ	92	0	70	29	0
8	AL	65	0	76	27	0
8	AM	65	0	76	18	0
8	BL	65	0	76	45	0
8	BM	65	0	76	26	0
9	AL	48	0	63	21	0
9	AM	48	0	63	12	0
9	BL	48	0	63	20	0
10	AL	5	0	0	0	0
10	BL	5	0	0	0	0
11	AM	1	0	0	0	0
11	BL	1	0	0	0	0
12	AM	42	0	60	9	0
All	All	38108	0	37183	2683	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 36.

All (2683) 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)
3:BS:12:THR:CB	3:BS:13:ASP:HB2	1.15	1.62
5:BL:219:LEU:CG	5:BL:219:LEU:CD2	1.78	1.62
5:BL:219:LEU:CG	5:BL:219:LEU:CD1	1.75	1.58
6:AM:262:MET:CG	6:AM:262:MET:CB	1.75	1.57
5:BL:125:ILE:CG1	5:BL:125:ILE:CD1	1.75	1.57
9:AM:405:U10:C41	9:AM:405:U10:C39	1.75	1.54
3:BS:12:THR:HB	3:BS:13:ASP:CB	1.04	1.50
3:AS:12:THR:CB	3:AS:13:ASP:HB2	1.43	1.47
5:BL:247:CYS:SG	5:BL:247:CYS:CB	2.01	1.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BL:196:SER:CB	5:BL:196:SER:OG	1.64	1.43
5:BL:184:ALA:HB3	8:BM:402:BPH:CMC	1.50	1.41
6:AM:158:MET:CE	6:AM:158:MET:SD	2.07	1.41
3:AS:12:THR:HB	3:AS:13:ASP:CB	1.53	1.38
6:BM:152:SER:OG	6:BM:152:SER:CB	1.71	1.38
5:BL:184:ALA:CB	8:BM:402:BPH:HMC3	1.51	1.37
5:BL:173:HIS:CE1	5:BL:177:ILE:HD11	1.65	1.31
3:B9:38:HIS:CE1	7:B9:101:BCL:HAA1	1.67	1.30
1:AZ:38:THR:HB	1:AZ:39:PRO:CD	1.64	1.26
5:AL:45:GLY:HA3	8:AL:303:BPH:C9	1.72	1.20
5:BL:176:ALA:O	7:BL:302:BCL:HMA1	1.38	1.19
5:AL:45:GLY:CA	8:AL:303:BPH:H9C1	1.74	1.18
6:AM:10:VAL:CG1	6:AM:11:GLN:H	1.58	1.16
7:AD:102:BCL:HMB3	7:AF:101:BCL:HMA3	1.16	1.15
3:BS:12:THR:HB	3:BS:13:ASP:HB3	1.28	1.15
1:BF:12:ASP:HB2	1:BF:13:PRO:HD3	1.20	1.14
1:BZ:38:THR:HB	1:BZ:39:PRO:CD	1.75	1.12
1:AJ:12:ASP:HB3	1:AJ:13:PRO:HD3	1.32	1.11
3:A9:6:LEU:HD22	3:A9:7:GLY:HA2	1.19	1.11
6:BM:152:SER:HB3	6:BM:278:LEU:HD13	1.31	1.10
7:AP:102:BCL:HMA1	7:AZ:101:BCL:HMA1	1.14	1.10
5:BL:124:ALA:HB1	7:BL:302:BCL:H71	1.27	1.10
3:A6:41:VAL:HG12	7:A6:102:BCL:HBC1	1.34	1.10
4:AH:191:LEU:HD13	4:AH:192:PRO:HD2	1.33	1.10
5:BL:176:ALA:O	7:BL:302:BCL:CMA	2.00	1.09
3:B9:38:HIS:HE1	7:B9:101:BCL:HAA1	0.92	1.08
5:AL:184:ALA:HB3	8:AM:403:BPH:HMC3	1.35	1.08
5:AL:208:THR:HB	5:AL:209:PRO:HD2	1.34	1.08
6:AM:202:HIS:HA	7:AM:402:BCL:HED1	1.29	1.07
3:BQ:6:LEU:HD22	3:BQ:7:GLY:HA2	1.35	1.07
5:AL:183:ASN:HA	5:AL:236:LEU:HB3	1.34	1.06
7:BP:102:BCL:HAC2	3:BQ:41:VAL:CG1	1.84	1.06
3:BO:41:VAL:HG13	7:BO:102:BCL:HAC2	1.27	1.06
5:AL:229:ILE:HD12	5:AL:232:LEU:HB3	1.37	1.05
3:AS:38:HIS:CE1	7:AS:101:BCL:HAA1	1.91	1.05
7:BL:301:BCL:HMD2	7:BL:302:BCL:OBB	1.55	1.04
1:B1:14:ARG:HD3	4:BH:57:PRO:HB2	1.37	1.04
5:BL:45:GLY:HA3	8:BL:304:BPH:H9C1	1.39	1.04
1:AZ:38:THR:HB	1:AZ:39:PRO:HD3	1.36	1.04
7:BP:101:BCL:HMA3	7:BO:102:BCL:HHB	1.40	1.04
1:BZ:31:ILE:HG23	7:BZ:102:BCL:HMD3	1.39	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BL:30:TYR:HB2	6:BM:254:TRP:HB3	1.39	1.03
7:BL:303:BCL:HMD2	7:BM:401:BCL:OBB	1.54	1.03
7:B2:101:BCL:HMA3	7:BK:102:BCL:HMA3	1.35	1.03
1:BZ:31:ILE:HG23	7:BZ:102:BCL:CMD	1.89	1.03
7:BP:101:BCL:HMA3	7:BO:102:BCL:CHB	1.87	1.03
7:BL:302:BCL:HBB2	7:BM:401:BCL:HHB	1.37	1.02
1:BZ:38:THR:HB	1:BZ:39:PRO:HD3	1.05	1.02
5:AL:229:ILE:HA	5:AL:232:LEU:HB2	1.38	1.02
3:AU:45:ARG:H	3:AU:46:PRO:HD3	1.23	1.02
5:BL:181:PHE:HB2	7:BL:301:BCL:O1A	1.58	1.02
6:AM:10:VAL:CG1	6:AM:11:GLN:N	2.20	1.01
3:AO:41:VAL:HG13	7:AO:101:BCL:HAC2	1.36	1.01
7:AP:101:BCL:CMA	7:AO:101:BCL:HMA3	1.89	1.01
3:BS:12:THR:CB	3:BS:13:ASP:CB	1.95	1.01
3:BK:6:LEU:HD22	3:BK:7:GLY:HA2	1.43	1.01
1:AD:9:MET:O	1:AD:10:ILE:HG22	1.58	1.00
7:BP:102:BCL:CMA	7:BZ:101:BCL:HMA1	1.91	1.00
5:BL:183:ASN:HA	5:BL:236:LEU:HB3	1.44	1.00
3:BI:11:LEU:H	3:BI:14:GLU:HB2	1.26	0.99
3:B9:6:LEU:HD22	3:B9:7:GLY:HA2	1.42	0.99
5:AL:148:TYR:CD1	8:AL:303:BPH:H142	1.96	0.99
6:AM:10:VAL:HG12	6:AM:11:GLN:N	1.76	0.99
6:BM:62:SER:HB3	6:BM:121:PHE:O	1.62	0.99
5:AL:229:ILE:HG13	5:AL:229:ILE:O	1.63	0.98
7:AP:101:BCL:HMA3	7:AO:101:BCL:CHB	1.94	0.98
1:A7:10:ILE:HG13	1:A7:11:PHE:H	1.27	0.98
6:AM:10:VAL:HG13	6:AM:41:TRP:CZ3	1.97	0.98
3:AE:6:LEU:HD22	3:AE:7:GLY:HA2	1.41	0.98
1:A1:12:ASP:H	1:A1:13:PRO:HD2	1.29	0.97
1:BZ:38:THR:CB	1:BZ:39:PRO:HD3	1.94	0.97
7:BP:102:BCL:HMA1	7:BZ:101:BCL:CMA	1.94	0.97
7:BP:102:BCL:HAC2	3:BQ:41:VAL:HG11	1.43	0.97
3:BI:41:VAL:HG13	7:BI:101:BCL:HAC2	1.40	0.97
6:AM:10:VAL:HG13	6:AM:11:GLN:H	1.25	0.97
3:BS:12:THR:CA	3:BS:13:ASP:HB2	1.94	0.97
5:AL:229:ILE:HA	5:AL:232:LEU:CB	1.93	0.97
3:B9:38:HIS:HE1	7:B9:101:BCL:CAA	1.77	0.96
1:AD:43:TRP:CZ2	7:AD:101:BCL:HHC	2.00	0.96
7:AZ:101:BCL:HBC2	3:AS:45:ARG:HD3	1.47	0.96
1:A3:43:TRP:CD1	1:A3:43:TRP:O	2.18	0.96
7:AD:102:BCL:CMB	7:AF:101:BCL:HMA3	1.94	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AP:12:ASP:HB2	1:AP:13:PRO:HD3	1.47	0.96
7:BP:102:BCL:HMA1	7:BZ:101:BCL:HMA1	0.98	0.96
5:BL:34:PHE:HB2	5:BL:103:ARG:HB2	1.47	0.96
7:AP:102:BCL:HMA1	7:AZ:101:BCL:CMA	1.95	0.96
1:A7:29:VAL:HA	1:A7:32:HIS:CD2	2.01	0.96
7:AL:301:BCL:H141	8:AL:303:BPH:H172	1.47	0.96
7:AP:101:BCL:HMA3	7:AO:101:BCL:HHB	1.44	0.96
3:AE:43:ILE:HG23	3:AE:44:TRP:HD1	1.30	0.95
7:AL:302:BCL:HMD1	6:AM:206:ILE:HG21	1.45	0.95
7:AI:101:BCL:HMA1	7:AK:101:BCL:HMA1	1.49	0.95
1:B1:31:ILE:HG22	7:BI:101:BCL:HMD3	1.49	0.95
3:B4:6:LEU:HD22	3:B4:7:GLY:HA2	1.49	0.95
3:BY:41:VAL:HB	7:BY:102:BCL:HBC1	1.49	0.95
3:BO:10:GLY:HA3	3:BO:11:LEU:HB2	1.47	0.94
7:B2:101:BCL:HMA3	7:BK:102:BCL:CMA	1.97	0.94
1:BP:9:MET:HG2	1:BZ:14:ARG:HG3	1.47	0.94
5:AL:148:TYR:CD1	8:AL:303:BPH:C14	2.51	0.94
5:AL:168:HIS:HB3	6:AM:183:LEU:HD13	1.49	0.94
3:AU:45:ARG:N	3:AU:46:PRO:HD3	1.83	0.93
1:A2:15:ARG:HA	1:A2:19:ALA:HB3	1.51	0.93
5:BL:208:THR:HB	5:BL:209:PRO:HD2	1.51	0.93
5:BL:250:ILE:HD12	9:BL:306:U10:H402	1.50	0.93
3:BO:41:VAL:HG13	7:BO:102:BCL:CAC	1.99	0.93
4:AH:153:VAL:HG12	4:AH:154:ARG:H	1.33	0.93
5:BL:127:ALA:CB	7:BL:302:BCL:H12	1.99	0.93
5:BL:183:ASN:ND2	5:BL:237:SER:OG	2.01	0.92
5:AL:124:ALA:HB1	7:AL:301:BCL:H71	1.51	0.92
3:BS:12:THR:CG2	3:BS:13:ASP:HB2	1.98	0.92
5:AL:49:ILE:O	5:AL:64:ILE:HD13	1.70	0.92
6:AM:175:VAL:HG11	7:AM:401:BCL:CMC	1.98	0.92
3:AI:41:VAL:HG13	7:AI:101:BCL:H2C	1.51	0.92
9:AL:304:U10:H4M2	9:AL:304:U10:H3M3	1.51	0.92
3:AS:45:ARG:HB3	3:AS:46:PRO:HD3	1.49	0.92
1:A7:10:ILE:HG13	1:A7:11:PHE:N	1.85	0.92
1:BF:12:ASP:HB2	1:BF:13:PRO:CD	1.99	0.92
3:AI:43:ILE:HG23	3:AI:44:TRP:HD1	1.33	0.92
5:BL:278:GLY:HA3	6:BM:92:PHE:HE1	1.34	0.91
1:A7:26:LEU:HG	5:AL:40:PHE:HD1	1.34	0.91
5:AL:219:LEU:HD11	6:AM:133:THR:HG23	1.51	0.91
1:BF:41:TYR:O	1:BF:42:ASN:HB2	1.70	0.91
6:AM:238:ILE:HG12	6:AM:262:MET:HB3	1.51	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AI:43:ILE:HG23	3:AI:44:TRP:CD1	2.06	0.91
2:AB:14:ASN:HB3	2:AB:15:PRO:HD3	1.52	0.91
1:A1:12:ASP:H	1:A1:13:PRO:CD	1.84	0.91
5:BL:241:VAL:CG2	8:BL:304:BPH:HBC2	2.01	0.91
6:BM:10:VAL:HG12	6:BM:41:TRP:HZ3	1.35	0.90
3:AS:12:THR:CA	3:AS:13:ASP:HB2	2.00	0.90
3:A8:41:VAL:O	7:A8:101:BCL:HBC1	1.72	0.90
3:A9:38:HIS:HE1	7:A9:101:BCL:HAA1	1.37	0.90
4:BH:198:VAL:HG11	6:BM:7:PHE:HD1	1.34	0.90
3:AE:11:LEU:HD13	3:AE:11:LEU:H	1.32	0.90
5:BL:157:VAL:HG21	7:BL:303:BCL:H3C	1.52	0.90
3:A4:39:LEU:HA	3:A4:42:TYR:HD2	1.34	0.90
7:BL:303:BCL:H122	8:BL:304:BPH:H203	1.53	0.89
7:AD:102:BCL:HMB3	7:AF:101:BCL:CMA	2.00	0.89
3:AE:11:LEU:CD1	3:AE:11:LEU:N	2.35	0.89
3:BS:12:THR:N	3:BS:14:GLU:H	1.70	0.89
5:AL:244:SER:HB3	7:AL:301:BCL:H2A	1.54	0.89
1:AZ:38:THR:HB	1:AZ:39:PRO:HD2	1.52	0.89
5:AL:46:ILE:HG12	7:AL:302:BCL:H18	1.53	0.89
3:A4:6:LEU:HD22	3:A4:7:GLY:HA2	1.55	0.89
1:A3:43:TRP:HD1	1:A3:43:TRP:O	1.50	0.89
4:AH:192:PRO:HG3	4:AH:237:VAL:HG21	1.53	0.89
6:AM:62:SER:HB3	6:AM:121:PHE:O	1.73	0.89
7:AP:101:BCL:HMA2	7:AO:101:BCL:HMA3	1.51	0.88
1:B7:10:ILE:HG13	1:B7:11:PHE:H	1.37	0.88
1:AV:8:TRP:HD1	3:AW:9:THR:H	1.19	0.88
1:BP:11:PHE:HB2	1:BP:15:ARG:HB2	1.52	0.88
5:BL:173:HIS:CE1	5:BL:177:ILE:CD1	2.56	0.88
6:AM:73:TRP:CD1	6:AM:94:LEU:HB2	2.07	0.88
7:BP:102:BCL:CAC	3:BQ:41:VAL:HG11	2.03	0.88
4:BH:171:ILE:HB	4:BH:172:PRO:HD3	1.56	0.88
3:A9:6:LEU:CD2	3:A9:7:GLY:HA2	2.02	0.88
5:BL:241:VAL:HG21	8:BL:304:BPH:HBC2	1.53	0.88
1:B5:33:LEU:HD13	5:BL:87:GLN:HB3	1.54	0.88
3:B8:41:VAL:O	7:B8:101:BCL:HBC1	1.74	0.88
3:AG:43:ILE:HG23	3:AG:44:TRP:HD1	1.39	0.88
3:BY:44:TRP:HA	3:BY:45:ARG:HG2	1.56	0.88
1:A5:37:SER:HB3	5:AL:79:PRO:O	1.73	0.88
7:BL:301:BCL:HMD2	7:BL:302:BCL:CAB	2.02	0.87
1:BD:9:MET:O	1:BD:10:ILE:HG22	1.72	0.87
3:BI:8:TYR:HB3	3:BI:11:LEU:HD22	1.56	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A7:15:ARG:HH22	1:AD:17:PHE:HB3	1.39	0.87
6:AM:9:GLN:CB	6:AM:10:VAL:HA	2.04	0.87
1:A1:44:LEU:HG	1:A1:44:LEU:O	1.73	0.87
5:BL:241:VAL:HG21	8:BL:304:BPH:CBC	2.04	0.87
1:B1:12:ASP:HB3	1:B1:13:PRO:HD3	1.55	0.87
1:AJ:42:ASN:O	1:AJ:44:LEU:N	2.07	0.87
5:BL:127:ALA:HB3	7:BL:302:BCL:H12	1.57	0.87
7:AL:302:BCL:HMA1	8:AL:303:BPH:H18	1.57	0.86
1:B7:29:VAL:HA	1:B7:32:HIS:CD2	2.09	0.86
5:AL:30:TYR:HD2	5:AL:103:ARG:HH11	1.23	0.86
5:BL:78:ALA:HB1	5:BL:79:PRO:HD2	1.57	0.86
3:B8:10:GLY:HA3	3:B8:11:LEU:HB2	1.57	0.86
6:AM:156:LEU:HD12	7:AM:402:BCL:H43	1.58	0.86
7:B2:101:BCL:CMA	7:BK:102:BCL:HMA3	2.05	0.86
7:A7:101:BCL:HMA1	7:A6:102:BCL:CMA	2.06	0.86
3:AS:38:HIS:HE1	7:AS:101:BCL:HAA1	1.36	0.85
1:AF:43:TRP:CD1	1:AF:43:TRP:O	2.30	0.85
5:BL:67:TYR:HD2	5:BL:68:PRO:HD2	1.42	0.85
3:AO:10:GLY:HA3	3:AO:11:LEU:HB2	1.55	0.85
8:BL:304:BPH:HMD2	6:BM:218:MET:CG	2.06	0.85
6:BM:273:ALA:O	8:BM:402:BPH:HBC1	1.77	0.85
6:AM:9:GLN:HB3	6:AM:10:VAL:HA	1.56	0.85
3:AE:11:LEU:HD22	3:AE:12:THR:H	1.41	0.85
7:BL:303:BCL:HMB3	8:BL:304:BPH:H192	1.58	0.84
6:BM:57:VAL:O	6:BM:57:VAL:HG12	1.76	0.84
3:AE:6:LEU:HD22	3:AE:7:GLY:CA	2.07	0.84
7:BL:302:BCL:H141	8:BL:304:BPH:H172	1.59	0.84
1:AF:35:LEU:HD13	1:AF:43:TRP:CZ2	2.11	0.84
1:B2:42:ASN:O	1:B2:44:LEU:N	2.10	0.84
6:AM:73:TRP:HD1	6:AM:94:LEU:HB2	1.40	0.84
1:A2:31:ILE:CG2	7:A9:101:BCL:HMD3	2.08	0.84
3:AW:11:LEU:H	3:AW:15:GLN:N	1.75	0.84
1:A5:31:ILE:HG21	7:A6:102:BCL:HMD3	1.60	0.83
7:BL:303:BCL:HMA1	8:BL:304:BPH:H18	1.59	0.83
3:AI:44:TRP:HA	3:AI:45:ARG:HG2	1.60	0.83
5:AL:186:ALA:HB3	5:AL:236:LEU:CD1	2.09	0.83
7:AL:301:BCL:HBB2	7:AL:301:BCL:HMB1	1.58	0.83
3:BY:6:LEU:HD22	3:BY:7:GLY:HA2	1.60	0.83
5:AL:172:ALA:HB2	9:AL:304:U10:H352	1.59	0.83
1:AD:35:LEU:HB3	1:AD:43:TRP:HZ3	1.43	0.83
7:AT:102:BCL:HMA1	7:AV:101:BCL:HMA1	1.60	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BO:102:BCL:HMB1	7:BO:102:BCL:HBB2	1.61	0.83
1:BN:10:ILE:HG21	1:BP:14:ARG:HB2	1.61	0.83
6:AM:186:THR:O	7:AM:402:BCL:HMD2	1.78	0.83
3:AU:44:TRP:HA	3:AU:45:ARG:HG2	1.58	0.83
3:BE:11:LEU:HD13	3:BE:12:THR:H	1.44	0.83
1:B1:8:TRP:O	1:B1:9:MET:HB2	1.79	0.83
1:BZ:37:SER:O	1:BZ:39:PRO:HD2	1.78	0.82
6:AM:202:HIS:CA	7:AM:402:BCL:HED1	2.09	0.82
7:AP:102:BCL:CMA	7:AZ:101:BCL:HMA1	2.06	0.82
4:AH:171:ILE:HB	4:AH:172:PRO:HD3	1.59	0.82
3:BO:41:VAL:CG1	7:BO:102:BCL:HAC2	2.09	0.82
3:A6:6:LEU:HD22	3:A6:7:GLY:HA2	1.60	0.82
5:BL:2:LEU:HB2	5:BL:6:GLU:HB3	1.60	0.82
5:BL:45:GLY:CA	8:BL:304:BPH:H9C1	2.10	0.82
6:AM:126:VAL:HG22	7:AM:402:BCL:H121	1.61	0.82
7:B8:101:BCL:HBB2	7:B8:101:BCL:HMB1	1.61	0.82
3:BW:9:THR:HG22	3:BW:10:GLY:HA3	1.58	0.82
5:AL:208:THR:HB	5:AL:209:PRO:CD	2.10	0.82
7:AJ:101:BCL:HBB2	7:AJ:101:BCL:HMB1	1.62	0.82
5:AL:34:PHE:HB2	5:AL:103:ARG:HB2	1.61	0.82
5:AL:251:THR:HG23	5:AL:259:TRP:HE1	1.45	0.82
3:BO:10:GLY:HA3	3:BO:11:LEU:CB	2.08	0.81
6:AM:98:ALA:HB1	6:AM:99:PRO:HD2	1.62	0.81
1:B2:10:ILE:HD11	1:BN:15:ARG:HA	1.62	0.81
7:AL:302:BCL:HHB	8:AL:303:BPH:HMB3	1.63	0.81
5:BL:181:PHE:CB	7:BL:301:BCL:O1A	2.27	0.81
3:AE:11:LEU:HD13	3:AE:11:LEU:N	1.95	0.81
4:BH:191:LEU:HD13	4:BH:192:PRO:HD2	1.60	0.81
1:A3:9:MET:HG2	2:AB:29:LYS:HB3	1.60	0.81
6:BM:26:LEU:HA	6:BM:29:ARG:HG3	1.61	0.81
7:AP:101:BCL:HMA3	7:AO:101:BCL:HMA3	1.62	0.81
5:BL:181:PHE:CZ	7:BL:302:BCL:HBB3	2.15	0.81
2:BB:12:ASN:O	2:BB:13:THR:HG22	1.78	0.81
3:BQ:43:ILE:HG23	3:BQ:44:TRP:HD1	1.45	0.81
8:BL:304:BPH:HMD2	6:BM:218:MET:HG2	1.61	0.81
7:BM:401:BCL:H151	8:BM:402:BPH:H3A	1.63	0.81
9:AM:405:U10:H8	9:AM:405:U10:H1M1	1.63	0.81
3:A9:6:LEU:HD22	3:A9:7:GLY:CA	2.09	0.81
5:AL:9:TYR:OH	6:AM:246:GLU:HB3	1.80	0.81
5:BL:173:HIS:NE2	5:BL:177:ILE:HD11	1.95	0.80
1:A5:22:VAL:HA	1:A5:25:PHE:HB3	1.63	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B7:38:THR:O	1:B7:40:SER:N	2.14	0.80
5:BL:67:TYR:CD2	5:BL:68:PRO:HD2	2.15	0.80
3:BE:8:TYR:H	3:BE:8:TYR:HD2	1.28	0.80
5:AL:78:ALA:HB1	5:AL:79:PRO:HD2	1.64	0.80
7:BL:303:BCL:HBD	7:BL:303:BCL:HAA1	1.64	0.80
6:AM:156:LEU:CD1	7:AM:402:BCL:H43	2.11	0.80
7:AL:301:BCL:CMB	7:AM:402:BCL:HMB2	2.12	0.80
6:BM:210:TYR:HE2	7:BM:401:BCL:OBB	1.65	0.80
1:AJ:31:ILE:HG23	7:AJ:101:BCL:HMD3	1.63	0.80
1:AF:44:LEU:HG	1:AF:45:GLU:H	1.46	0.80
6:BM:154:ILE:HG12	7:BM:401:BCL:H93	1.62	0.80
5:AL:148:TYR:CE1	8:AL:303:BPH:H142	2.17	0.80
4:BH:248:ARG:O	4:BH:249:LYS:HB2	1.79	0.80
3:BS:12:THR:CA	3:BS:13:ASP:CB	2.57	0.80
3:AY:43:ILE:HG23	3:AY:44:TRP:HD1	1.47	0.80
7:AL:302:BCL:H2	8:AL:303:BPH:HMB2	1.63	0.79
7:A8:101:BCL:HMB1	7:A8:101:BCL:HBB2	1.64	0.79
4:AH:43:GLU:HB2	5:AL:4:SER:HA	1.64	0.79
6:BM:185:TRP:HA	6:BM:188:ASN:HB3	1.64	0.79
1:AF:44:LEU:HG	1:AF:45:GLU:N	1.96	0.79
2:BB:14:ASN:HB3	2:BB:15:PRO:HD3	1.65	0.79
5:BL:267:VAL:HG23	6:BM:87:ARG:HD2	1.62	0.79
1:BD:43:TRP:CZ2	7:BD:101:BCL:HHC	2.16	0.79
1:BN:12:ASP:HB2	1:BN:13:PRO:HD3	1.63	0.79
3:AE:44:TRP:HA	3:AE:45:ARG:HG2	1.65	0.79
6:BM:138:GLN:HG2	6:BM:138:GLN:O	1.83	0.79
1:AV:29:VAL:HA	1:AV:32:HIS:ND1	1.98	0.78
7:BZ:101:BCL:HBC2	3:BS:45:ARG:HD3	1.65	0.78
5:BL:117:ILE:HB	5:BL:118:PRO:HD3	1.64	0.78
5:BL:175:ILE:HD12	9:BL:306:U10:H262	1.65	0.78
7:BT:101:BCL:CMC	7:BZ:102:BCL:HMB1	2.13	0.78
5:AL:251:THR:HG23	5:AL:259:TRP:NE1	1.98	0.78
5:AL:38:THR:HG21	5:AL:100:TRP:HE3	1.49	0.78
5:BL:219:LEU:CD1	5:BL:219:LEU:CB	2.61	0.78
3:BW:20:HIS:HA	3:BW:23:TYR:HB3	1.65	0.78
3:BS:11:LEU:O	3:BS:12:THR:OG1	2.02	0.78
3:B8:10:GLY:HA3	3:B8:11:LEU:CB	2.13	0.78
5:AL:164:TYR:HB3	5:AL:259:TRP:HD1	1.48	0.78
7:BL:301:BCL:CMD	7:BL:302:BCL:OBB	2.30	0.78
6:BM:94:LEU:HD21	6:BM:114:LEU:O	1.84	0.78
3:B6:6:LEU:HD22	3:B6:7:GLY:HA2	1.64	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AL:183:ASN:HA	5:AL:236:LEU:CB	2.13	0.77
3:BG:43:ILE:HG23	3:BG:44:TRP:HD1	1.49	0.77
3:BE:6:LEU:HD22	3:BE:7:GLY:HA2	1.66	0.77
3:AS:34:ALA:HB1	7:AS:101:BCL:HBA2	1.66	0.77
4:BH:140:PHE:CZ	6:BM:13:ARG:HB3	2.19	0.77
7:BL:303:BCL:CMB	8:BL:304:BPH:H192	2.15	0.77
3:BO:38:HIS:HE1	7:BO:102:BCL:HAA2	1.49	0.77
4:AH:35:ASN:HD22	4:AH:35:ASN:N	1.81	0.77
3:BS:45:ARG:HB3	3:BS:46:PRO:HD3	1.67	0.77
5:BL:120:ALA:HB1	6:BM:217:ALA:O	1.85	0.77
6:AM:129:TRP:CD2	8:AM:403:BPH:H1C2	2.19	0.77
7:AF:101:BCL:HMD2	7:AG:101:BCL:HAC1	1.65	0.77
1:AN:31:ILE:HD12	7:AO:101:BCL:HMD3	1.64	0.77
4:AH:153:VAL:HG12	4:AH:154:ARG:N	1.99	0.77
3:B9:41:VAL:HG11	7:B9:101:BCL:HAC2	1.67	0.77
1:BZ:31:ILE:CG2	7:BZ:102:BCL:CMD	2.61	0.77
1:AZ:38:THR:CB	1:AZ:39:PRO:CD	2.53	0.77
7:AT:102:BCL:HAC2	3:AU:41:VAL:HG11	1.67	0.77
7:AP:101:BCL:HMA3	7:AO:101:BCL:C4A	2.15	0.77
5:AL:249:ILE:CG2	5:AL:250:ILE:HD13	2.15	0.77
7:BT:101:BCL:HMC3	7:BZ:102:BCL:HMB1	1.67	0.77
5:BL:184:ALA:C	8:BM:402:BPH:HMC2	2.05	0.77
4:BH:75:VAL:HA	4:BH:76:PRO:C	2.04	0.77
5:BL:233:GLY:HA2	5:BL:236:LEU:HD12	1.65	0.76
1:B1:15:ARG:HA	1:B1:19:ALA:HB3	1.67	0.76
3:B8:45:ARG:N	3:B8:46:PRO:HD3	2.00	0.76
5:BL:278:GLY:HA3	6:BM:92:PHE:CE1	2.20	0.76
1:A1:10:ILE:HG13	1:A1:11:PHE:H	1.49	0.76
5:BL:175:ILE:HG21	9:BL:306:U10:H261	1.67	0.76
1:B2:12:ASP:H	1:B2:13:PRO:CD	1.97	0.76
5:BL:184:ALA:CB	8:BM:402:BPH:CMC	2.31	0.76
1:AF:38:THR:HG1	1:AF:41:TYR:HD1	1.30	0.76
6:BM:190:SER:OG	7:BM:401:BCL:HBC3	1.85	0.76
7:BL:302:BCL:CBB	7:BL:302:BCL:HMB1	2.16	0.76
3:A4:39:LEU:HA	3:A4:42:TYR:CD2	2.19	0.76
1:A3:12:ASP:H	1:A3:13:PRO:CD	1.99	0.76
3:B6:41:VAL:HG12	7:B6:101:BCL:HBC1	1.67	0.76
4:AH:75:VAL:HA	4:AH:76:PRO:C	2.06	0.76
3:BO:43:ILE:HG23	3:BO:44:TRP:HD1	1.51	0.76
3:BS:12:THR:HB	3:BS:13:ASP:CG	2.03	0.75
1:A7:15:ARG:NH2	1:AD:17:PHE:HB3	2.01	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AL:186:ALA:HB3	5:AL:236:LEU:HD11	1.67	0.75
5:AL:214:THR:HB	6:AM:140:LEU:HD21	1.68	0.75
3:B6:45:ARG:N	3:B6:46:PRO:HD3	2.02	0.75
5:AL:117:ILE:H	5:AL:118:PRO:CD	1.99	0.75
5:AL:109:ARG:HG2	5:AL:115:TYR:OH	1.86	0.75
7:B1:101:BCL:HAA2	7:B1:101:BCL:HBD	1.67	0.75
7:AL:301:BCL:C2B	7:AM:402:BCL:HMB2	2.16	0.75
5:BL:184:ALA:HB3	8:BM:402:BPH:HMC3	0.76	0.75
1:B1:10:ILE:HG13	1:B1:11:PHE:H	1.51	0.75
3:AS:6:LEU:HD13	3:AS:7:GLY:H	1.52	0.75
7:BU:101:BCL:HMB1	7:BU:101:BCL:HBB2	1.68	0.75
5:BL:153:HIS:O	5:BL:157:VAL:HG23	1.86	0.75
7:BM:401:BCL:H143	8:BM:402:BPH:CGA	2.17	0.75
8:AL:303:BPH:HMD2	6:AM:218:MET:HG2	1.68	0.75
5:BL:279:ILE:HG13	6:BM:92:PHE:HA	1.68	0.75
3:AE:35:ILE:HA	3:AE:38:HIS:ND1	2.01	0.75
5:AL:176:ALA:HB2	5:AL:243:PHE:CB	2.17	0.75
1:BZ:31:ILE:CG2	7:BZ:102:BCL:HMD1	2.16	0.75
5:AL:53:ALA:HB1	5:AL:59:TRP:HA	1.69	0.75
6:BM:156:LEU:HB3	7:BM:401:BCL:H43	1.69	0.74
6:BM:210:TYR:CE2	7:BM:401:BCL:OBB	2.39	0.74
3:AU:45:ARG:N	3:AU:46:PRO:CD	2.49	0.74
7:A7:101:BCL:HMA1	7:A6:102:BCL:HMA1	1.66	0.74
6:BM:55:LEU:HD21	6:BM:135:LEU:HD12	1.67	0.74
5:BL:78:ALA:HB1	5:BL:79:PRO:CD	2.16	0.74
3:BK:35:ILE:HA	3:BK:38:HIS:HB2	1.68	0.74
3:AK:45:ARG:N	3:AK:46:PRO:CD	2.49	0.74
3:BO:45:ARG:N	3:BO:46:PRO:HD3	2.03	0.74
3:BW:43:ILE:HG23	3:BW:44:TRP:HD1	1.51	0.74
6:AM:73:TRP:HE3	6:AM:114:LEU:HD12	1.52	0.74
6:BM:278:LEU:O	6:BM:282:ILE:HG13	1.88	0.74
1:A5:43:TRP:O	1:A5:43:TRP:HD1	1.69	0.74
5:BL:177:ILE:HG23	7:BL:302:BCL:HMB3	1.69	0.74
7:AD:101:BCL:HMC3	7:A8:101:BCL:OBB	1.88	0.74
7:BP:101:BCL:HMA3	7:BO:102:BCL:C4A	2.17	0.74
3:AE:6:LEU:HD23	4:AH:48:THR:HG23	1.70	0.74
1:AJ:42:ASN:O	1:AJ:44:LEU:HD23	1.88	0.74
1:B3:9:MET:HG2	2:BB:29:LYS:HB3	1.69	0.74
1:BF:11:PHE:HB2	4:BH:52:ASN:HA	1.69	0.74
3:BS:6:LEU:HD13	3:BS:7:GLY:H	1.53	0.74
7:AD:101:BCL:OBD	7:AD:102:BCL:HAA2	1.88	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AM:198:TYR:HB3	6:AM:298:GLY:HA3	1.69	0.73
1:B5:12:ASP:HB2	1:B5:13:PRO:HD3	1.70	0.73
5:AL:127:ALA:HB2	5:AL:241:VAL:HG11	1.70	0.73
7:AD:101:BCL:CMC	7:A8:101:BCL:OBB	2.36	0.73
3:B8:44:TRP:HA	3:B8:45:ARG:HG2	1.70	0.73
4:BH:133:PRO:HA	4:BH:168:TRP:HA	1.70	0.73
6:AM:119:SER:HB2	12:AM:406:SPO:H342	1.69	0.73
5:BL:173:HIS:CA	5:BL:247:CYS:SG	2.76	0.73
4:AH:198:VAL:HG22	4:AH:203:VAL:HG13	1.70	0.73
1:A7:38:THR:H	1:A7:39:PRO:CD	2.01	0.73
3:A8:45:ARG:N	3:A8:46:PRO:HD3	2.04	0.73
3:BW:9:THR:CG2	3:BW:10:GLY:HA3	2.19	0.73
3:AO:8:TYR:HB3	3:AO:9:THR:OG1	1.88	0.73
6:AM:5:ASN:HA	6:AM:41:TRP:HH2	1.53	0.73
1:B7:10:ILE:HG13	1:B7:11:PHE:N	2.04	0.73
6:AM:226:VAL:HG11	6:AM:248:ALA:HB2	1.70	0.73
6:BM:151:LEU:O	6:BM:151:LEU:HD13	1.88	0.73
2:AB:12:ASN:O	2:AB:13:THR:O	2.07	0.72
5:AL:69:PRO:O	5:AL:143:GLY:HA2	1.89	0.72
6:AM:237:GLN:HB3	6:AM:262:MET:HG2	1.69	0.72
7:AY:101:BCL:HAA2	7:AY:101:BCL:HBD	1.71	0.72
6:BM:130:TRP:HD1	6:BM:150:PHE:CD2	2.07	0.72
3:AO:10:GLY:HA3	3:AO:11:LEU:CB	2.16	0.72
6:AM:152:SER:OG	6:AM:278:LEU:HB2	1.88	0.72
1:AN:43:TRP:CZ2	7:AN:101:BCL:HHC	2.25	0.72
1:A5:43:TRP:CD1	1:A5:43:TRP:O	2.42	0.72
1:A7:12:ASP:H	1:A7:13:PRO:HD2	1.53	0.72
5:BL:173:HIS:HA	5:BL:247:CYS:SG	2.28	0.72
6:BM:202:HIS:O	6:BM:206:ILE:HG13	1.89	0.72
5:AL:177:ILE:HG21	7:AM:401:BCL:OBD	1.89	0.72
1:B7:38:THR:H	1:B7:39:PRO:HD3	1.55	0.72
2:BB:55:LEU:N	2:BB:56:PRO:HD2	2.05	0.72
7:AI:101:BCL:HMA1	7:AK:101:BCL:CMA	2.20	0.72
7:BL:303:BCL:HAA1	7:BL:303:BCL:CBD	2.18	0.72
1:A2:42:ASN:O	1:A2:44:LEU:N	2.22	0.72
7:AM:401:BCL:H42	8:AM:403:BPH:HHB	1.71	0.72
7:BP:102:BCL:HMB1	7:BP:102:BCL:HBB3	1.72	0.72
4:AH:86:ALA:O	4:AH:109:VAL:HG21	1.90	0.72
3:A9:44:TRP:HA	3:A9:45:ARG:HG2	1.70	0.72
3:BO:38:HIS:CE1	7:BO:102:BCL:HAA2	2.24	0.72
7:BP:101:BCL:CMA	7:BO:102:BCL:HMA3	2.19	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AF:43:TRP:HD1	1:AF:43:TRP:O	1.73	0.72
3:A9:38:HIS:CE1	7:A9:101:BCL:HAA1	2.24	0.72
7:BL:303:BCL:H101	7:BL:303:BCL:CMA	2.20	0.71
7:AM:402:BCL:H151	8:AM:403:BPH:CGA	2.19	0.71
1:BJ:12:ASP:HB3	1:BJ:13:PRO:HD3	1.70	0.71
7:A1:101:BCL:HAA2	7:A1:101:BCL:HBD	1.72	0.71
3:BI:8:TYR:HB3	3:BI:11:LEU:CD2	2.20	0.71
5:AL:41:PHE:O	8:AL:303:BPH:H9C2	1.91	0.71
3:AI:11:LEU:H	3:AI:14:GLU:HB2	1.55	0.71
7:AM:402:BCL:H162	8:AM:403:BPH:H4C2	1.73	0.71
7:AY:101:BCL:CBD	7:AY:101:BCL:HAA2	2.21	0.71
6:BM:198:TYR:O	6:BM:200:PRO:HD3	1.90	0.71
6:AM:10:VAL:HG13	6:AM:41:TRP:HZ3	1.54	0.71
3:AS:34:ALA:HB1	7:AS:101:BCL:CBA	2.19	0.71
1:AV:31:ILE:HG12	1:AV:34:ILE:HD12	1.73	0.71
1:AD:10:ILE:HD13	1:AF:13:PRO:O	1.91	0.71
7:BY:101:BCL:HAA2	7:BY:101:BCL:HBD	1.72	0.71
5:BL:233:GLY:HA2	5:BL:236:LEU:CD1	2.21	0.71
3:AK:45:ARG:C	3:AK:47:TRP:H	1.93	0.71
1:AZ:41:TYR:O	1:AZ:42:ASN:HB2	1.89	0.71
6:BM:237:GLN:HB2	6:BM:262:MET:HG2	1.70	0.71
5:BL:173:HIS:HB2	5:BL:247:CYS:SG	2.29	0.71
7:BL:303:BCL:CMD	7:BM:401:BCL:OBB	2.37	0.71
3:BS:12:THR:H	3:BS:14:GLU:H	1.36	0.71
6:AM:5:ASN:HA	6:AM:41:TRP:CH2	2.26	0.71
7:B3:101:BCL:CBD	7:B3:101:BCL:HAA2	2.20	0.71
5:AL:164:TYR:HE1	5:AL:256:PHE:HA	1.54	0.71
3:AS:45:ARG:HB3	3:AS:46:PRO:CD	2.21	0.70
5:AL:77:GLY:HA2	5:AL:87:GLN:HE22	1.55	0.70
5:BL:15:THR:CG2	5:BL:33:PHE:HB2	2.21	0.70
3:BU:43:ILE:HG23	3:BU:44:TRP:HD1	1.56	0.70
7:B1:101:BCL:CBD	7:B1:101:BCL:HAA2	2.19	0.70
6:BM:66:TRP:CD1	6:BM:118:ALA:HB1	2.27	0.70
1:A7:38:THR:H	1:A7:39:PRO:HD3	1.55	0.70
7:BL:303:BCL:C2B	8:BL:304:BPH:H192	2.21	0.70
5:BL:96:ALA:HB1	8:BL:304:BPH:H4C2	1.72	0.70
7:AP:101:BCL:HMA3	7:AO:101:BCL:CMA	2.22	0.70
1:AF:11:PHE:HD2	4:AH:52:ASN:HA	1.56	0.70
4:AH:131:ILE:HG22	4:AH:168:TRP:HE3	1.54	0.70
1:AX:8:TRP:HE3	1:AX:9:MET:H	1.37	0.70
6:BM:73:TRP:HD1	6:BM:93:SER:O	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AL:232:LEU:O	5:AL:236:LEU:HD11	1.91	0.70
5:AL:130:THR:HA	5:AL:134:PHE:HB2	1.73	0.70
6:BM:208:PHE:O	6:BM:276:VAL:HG22	1.91	0.70
7:AL:302:BCL:HAA1	7:AL:302:BCL:HBD	1.74	0.70
7:A1:101:BCL:HAA2	7:A1:101:BCL:CBD	2.20	0.70
1:AX:8:TRP:O	1:AX:9:MET:HB2	1.91	0.70
5:AL:254:ILE:HG13	5:AL:255:TRP:N	2.06	0.70
6:BM:96:PRO:HB2	6:BM:97:PRO:HD2	1.71	0.70
3:BI:44:TRP:HA	3:BI:45:ARG:HG2	1.72	0.70
1:A3:44:LEU:HG	1:A3:45:GLU:H	1.56	0.70
7:AT:102:BCL:HMA1	7:AV:101:BCL:CMA	2.21	0.70
1:B7:38:THR:H	1:B7:39:PRO:CD	2.04	0.70
5:AL:117:ILE:H	5:AL:118:PRO:HD2	1.56	0.70
5:BL:169:TYR:HD2	5:BL:263:TRP:HD1	1.40	0.69
7:AN:101:BCL:OBB	7:A9:101:BCL:HBB2	1.92	0.69
7:A3:101:BCL:CBD	7:A3:101:BCL:HAA2	2.22	0.69
6:BM:66:TRP:HD1	6:BM:118:ALA:HB1	1.56	0.69
5:BL:109:ARG:HG2	5:BL:115:TYR:OH	1.91	0.69
5:AL:224:ILE:HG12	5:AL:228:GLY:HA3	1.73	0.69
5:AL:183:ASN:CA	5:AL:236:LEU:HB3	2.17	0.69
6:BM:10:VAL:HG12	6:BM:41:TRP:CZ3	2.25	0.69
3:BW:45:ARG:N	3:BW:46:PRO:HD3	2.07	0.69
1:A3:44:LEU:HG	1:A3:45:GLU:N	2.06	0.69
6:BM:296:VAL:HG12	6:BM:296:VAL:O	1.91	0.69
7:AP:102:BCL:HMB1	7:AP:102:BCL:HBB3	1.73	0.69
3:BE:11:LEU:O	3:BE:12:THR:HB	1.91	0.69
3:BS:44:TRP:CG	3:BS:44:TRP:O	2.44	0.69
7:BL:303:BCL:H101	7:BL:303:BCL:HMA1	1.73	0.69
6:BM:69:THR:HB	6:BM:118:ALA:HB2	1.74	0.69
3:BW:45:ARG:N	3:BW:46:PRO:CD	2.55	0.69
6:BM:226:VAL:HB	6:BM:244:ALA:HB1	1.74	0.69
3:BS:33:VAL:HA	3:BS:36:VAL:HB	1.74	0.69
7:BU:101:BCL:CBB	7:BU:101:BCL:HMB1	2.23	0.69
1:BF:28:ALA:HB2	7:BF:101:BCL:CGA	2.22	0.69
2:AB:14:ASN:HB3	2:AB:15:PRO:CD	2.21	0.69
4:BH:187:SER:HB2	4:BH:189:ARG:HH12	1.56	0.69
3:A8:10:GLY:HA3	3:A8:11:LEU:HB2	1.73	0.69
1:AD:22:VAL:HA	1:AD:25:PHE:HB3	1.74	0.69
7:BL:302:BCL:HMB1	7:BL:302:BCL:HBB3	1.75	0.69
7:AL:302:BCL:H3A	7:AL:302:BCL:H71	1.75	0.69
7:AM:401:BCL:HAA1	7:AM:401:BCL:HBD	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A5:31:ILE:HG23	1:A5:35:LEU:HD23	1.75	0.69
1:A1:35:LEU:HD11	1:A1:43:TRP:HZ3	1.58	0.69
7:B3:101:BCL:HBD	7:B3:101:BCL:HAA2	1.74	0.69
3:B8:41:VAL:HG12	7:B8:101:BCL:HAC1	1.73	0.69
6:BM:73:TRP:CD1	6:BM:94:LEU:HB2	2.28	0.69
7:BY:101:BCL:HAA2	7:BY:101:BCL:CBD	2.21	0.69
4:AH:131:ILE:HD12	4:AH:225:VAL:HG21	1.75	0.69
4:BH:187:SER:CB	4:BH:189:ARG:HH12	2.05	0.69
3:A6:45:ARG:N	3:A6:46:PRO:HD3	2.07	0.69
1:AZ:19:ALA:HA	1:AZ:22:VAL:HG22	1.74	0.69
1:A7:10:ILE:CG1	1:A7:11:PHE:H	1.98	0.69
1:A1:20:GLN:HA	1:A1:23:PHE:HB2	1.75	0.69
4:BH:24:LEU:HD11	6:BM:275:LEU:HD11	1.75	0.69
1:BP:12:ASP:HB2	1:BP:13:PRO:HD3	1.73	0.69
5:BL:124:ALA:CB	7:BL:302:BCL:H71	2.16	0.69
5:BL:184:ALA:HB1	8:BM:402:BPH:HMC3	1.71	0.69
6:AM:73:TRP:CE3	6:AM:114:LEU:HD12	2.28	0.69
6:AM:9:GLN:HB3	6:AM:10:VAL:CA	2.22	0.69
7:BI:101:BCL:HMB2	7:BK:101:BCL:HMA3	1.74	0.69
5:AL:258:GLN:HB3	5:AL:260:VAL:HG12	1.74	0.69
3:BE:8:TYR:CD2	3:BE:8:TYR:N	2.59	0.68
6:BM:229:PHE:HB3	6:BM:243:THR:HG23	1.74	0.68
5:BL:167:PHE:HB3	7:BL:302:BCL:H3C	1.75	0.68
1:AJ:12:ASP:HB3	1:AJ:13:PRO:CD	2.19	0.68
5:AL:243:PHE:CE1	9:AL:304:U10:H28	2.27	0.68
3:BO:10:GLY:CA	3:BO:11:LEU:HB2	2.23	0.68
6:AM:222:THR:HA	6:AM:225:ALA:HB3	1.76	0.68
1:AD:47:SER:HB3	3:A8:48:PHE:H	1.57	0.68
1:BD:12:ASP:H	1:BD:13:PRO:HD2	1.58	0.68
5:AL:127:ALA:HB1	7:AL:301:BCL:C2	2.24	0.68
1:A1:35:LEU:HD11	1:A1:43:TRP:CZ3	2.28	0.68
6:AM:171:TRP:CE3	6:AM:171:TRP:HA	2.26	0.68
6:BM:164:ARG:NH1	6:BM:173:GLU:HG3	2.09	0.68
7:AL:301:BCL:HBB1	7:AM:401:BCL:HMD2	1.75	0.68
6:BM:29:ARG:HB3	6:BM:49:PRO:HB2	1.75	0.68
3:AS:20:HIS:HA	3:AS:24:MET:HB2	1.75	0.68
5:BL:185:LEU:HD12	8:BM:402:BPH:NB	2.09	0.68
4:BH:42:LEU:H	4:BH:53:GLN:HE22	1.39	0.68
1:B7:15:ARG:HH22	1:BD:17:PHE:HB3	1.59	0.68
5:BL:149:GLY:O	5:BL:153:HIS:CE1	2.46	0.68
6:BM:90:PHE:O	6:BM:180:PHE:HB2	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BQ:27:LEU:O	3:BQ:31:SER:HB2	1.94	0.68
1:B7:38:THR:N	1:B7:39:PRO:CD	2.57	0.68
5:BL:216:PHE:CD1	9:BL:306:U10:H3M2	2.29	0.68
5:BL:157:VAL:CG2	7:BL:303:BCL:H3C	2.22	0.67
3:A9:11:LEU:O	3:A9:13:ASP:N	2.27	0.67
3:AE:6:LEU:CD2	4:AH:48:THR:HG23	2.23	0.67
3:BE:11:LEU:N	3:BE:11:LEU:CD1	2.56	0.67
3:B9:9:THR:HG23	3:B9:11:LEU:HB2	1.75	0.67
1:A2:12:ASP:H	1:A2:13:PRO:CD	2.08	0.67
5:AL:127:ALA:HB1	7:AL:301:BCL:C1	2.24	0.67
3:BI:35:ILE:HA	3:BI:38:HIS:ND1	2.09	0.67
5:BL:186:ALA:HB3	5:BL:236:LEU:HD11	1.76	0.67
5:BL:30:TYR:HD2	5:BL:103:ARG:HH11	1.42	0.67
1:B7:26:LEU:HG	5:BL:40:PHE:HD1	1.59	0.67
6:BM:150:PHE:HB2	8:BM:402:BPH:HMD3	1.76	0.67
4:AH:144:ALA:HB3	6:AM:2:GLU:HB2	1.77	0.67
3:A8:41:VAL:HG12	7:A8:101:BCL:HAC1	1.76	0.67
5:AL:78:ALA:HB1	5:AL:79:PRO:CD	2.25	0.67
1:A3:24:LEU:HB2	7:A3:101:BCL:O2A	1.94	0.67
4:BH:189:ARG:HE	4:BH:214:ALA:HA	1.58	0.67
3:A9:9:THR:HG23	3:A9:11:LEU:HB2	1.76	0.67
6:AM:152:SER:HB2	6:AM:274:VAL:HG23	1.74	0.67
5:BL:180:PHE:CD2	5:BL:240:ALA:HB1	2.30	0.67
7:BO:101:BCL:HAA2	7:BO:101:BCL:HBD	1.76	0.67
7:A3:101:BCL:HBD	7:A3:101:BCL:HAA2	1.76	0.67
4:AH:37:ARG:HB2	6:AM:261:THR:HG21	1.76	0.67
5:BL:181:PHE:CZ	7:BL:302:BCL:CBB	2.78	0.67
6:BM:273:ALA:O	8:BM:402:BPH:CBC	2.42	0.67
3:BO:38:HIS:CE1	7:BO:102:BCL:CAA	2.78	0.67
3:AE:11:LEU:H	3:AE:11:LEU:CD1	1.99	0.67
6:BM:73:TRP:CD1	6:BM:93:SER:O	2.47	0.67
1:AJ:10:ILE:HG13	1:AJ:11:PHE:H	1.60	0.67
3:AU:43:ILE:HG23	3:AU:44:TRP:HD1	1.60	0.67
4:AH:28:ILE:HG23	6:AM:268:TRP:HH2	1.60	0.67
6:AM:175:VAL:HG11	7:AM:401:BCL:HMC1	1.76	0.66
6:AM:175:VAL:HG11	7:AM:401:BCL:HMC3	1.77	0.66
4:AH:191:LEU:HD13	4:AH:192:PRO:CD	2.20	0.66
1:AX:42:ASN:O	1:AX:43:TRP:CG	2.48	0.66
5:BL:173:HIS:CE1	7:BL:302:BCL:HMC3	2.31	0.66
8:BL:304:BPH:HMD2	6:BM:218:MET:HG3	1.77	0.66
7:BP:101:BCL:HMA2	7:BO:102:BCL:HMA3	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AM:155:TRP:CD1	6:AM:281:GLY:HA3	2.30	0.66
3:AY:33:VAL:HA	3:AY:36:VAL:HB	1.77	0.66
4:BH:38:GLU:HB3	6:BM:241:ARG:HE	1.60	0.66
4:AH:191:LEU:CD1	4:AH:192:PRO:HD2	2.19	0.66
3:AO:41:VAL:CG1	7:AO:101:BCL:HAC2	2.17	0.66
5:BL:208:THR:HB	5:BL:209:PRO:CD	2.25	0.66
3:B6:45:ARG:N	3:B6:46:PRO:CD	2.59	0.66
3:AK:11:LEU:H	3:AK:14:GLU:HB2	1.60	0.66
9:AM:405:U10:C8	9:AM:405:U10:H1M1	2.25	0.66
3:AI:41:VAL:HG22	7:AI:101:BCL:HAC2	1.77	0.66
1:BZ:31:ILE:HG23	7:BZ:102:BCL:HMD1	1.70	0.66
7:BI:101:BCL:HHB	7:BK:101:BCL:HMA1	1.76	0.66
5:AL:249:ILE:HG22	5:AL:250:ILE:HD13	1.77	0.66
1:B3:12:ASP:H	1:B3:13:PRO:CD	2.08	0.66
1:A1:8:TRP:O	1:A1:9:MET:HB2	1.94	0.66
6:BM:164:ARG:HB3	6:BM:165:PRO:HD3	1.77	0.66
4:BH:117:ARG:HB2	4:BH:228:LEU:HA	1.77	0.66
3:BI:11:LEU:H	3:BI:14:GLU:CB	2.04	0.66
4:AH:170:ASP:HB3	4:AH:175:MET:H	1.61	0.66
7:BZ:102:BCL:HAC2	3:BS:41:VAL:HG13	1.77	0.66
1:AF:12:ASP:HB2	1:AF:13:PRO:HD3	1.77	0.66
1:AP:12:ASP:HB2	1:AP:13:PRO:CD	2.25	0.66
5:AL:239:SER:C	5:AL:241:VAL:H	1.99	0.66
7:AZ:101:BCL:CBC	3:AS:45:ARG:HD3	2.24	0.66
4:AH:175:MET:HG2	4:AH:176:ALA:H	1.58	0.66
5:BL:120:ALA:CB	6:BM:217:ALA:O	2.44	0.65
7:AL:302:BCL:HHB	8:AL:303:BPH:CMB	2.25	0.65
1:BD:16:VAL:HG11	3:BE:22:VAL:HB	1.78	0.65
6:BM:165:PRO:HB3	6:BM:173:GLU:HB3	1.78	0.65
3:AQ:43:ILE:HG23	3:AQ:44:TRP:HD1	1.61	0.65
5:AL:175:ILE:HG21	9:AL:304:U10:H261	1.77	0.65
1:AN:8:TRP:O	1:AN:9:MET:HB2	1.96	0.65
1:AN:25:PHE:HA	1:AN:28:ALA:HB3	1.78	0.65
3:AS:12:THR:HB	3:AS:13:ASP:HB2	0.69	0.65
7:AL:301:BCL:HMB2	7:AM:402:BCL:HMB2	1.77	0.65
6:BM:28:ASN:HB3	6:BM:52:LEU:HB3	1.79	0.65
7:AL:301:BCL:HMB1	7:AL:301:BCL:CBB	2.27	0.65
3:BK:38:HIS:CE1	7:BK:102:BCL:HAA1	2.32	0.65
1:AV:8:TRP:HD1	3:AW:9:THR:N	1.92	0.65
5:BL:153:HIS:HA	5:BL:156:TRP:HB3	1.78	0.65
6:AM:256:MET:HB2	9:AM:405:U10:H211	1.76	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B7:101:BCL:HMB1	7:B7:101:BCL:HBB3	1.77	0.65
5:BL:36:VAL:O	5:BL:36:VAL:HG12	1.95	0.65
5:AL:182:THR:HG22	9:AL:304:U10:H112	1.78	0.65
6:AM:10:VAL:HG12	6:AM:11:GLN:H	1.38	0.65
6:AM:7:PHE:O	6:AM:8:SER:HB3	1.95	0.65
1:B7:12:ASP:H	1:B7:13:PRO:CD	2.09	0.65
1:BJ:22:VAL:HA	1:BJ:25:PHE:HB3	1.79	0.65
5:AL:208:THR:CB	5:AL:209:PRO:HD2	2.21	0.65
5:AL:249:ILE:HG23	5:AL:250:ILE:HD13	1.79	0.65
3:A8:10:GLY:HA3	3:A8:11:LEU:CB	2.27	0.65
1:A2:8:TRP:HD1	1:AN:13:PRO:HD2	1.61	0.65
6:AM:153:ALA:HA	6:AM:277:THR:OG1	1.96	0.65
6:BM:29:ARG:HD2	6:BM:49:PRO:HB2	1.77	0.65
5:BL:200:PRO:HG2	5:BL:204:LYS:HB3	1.78	0.65
5:BL:186:ALA:HB2	9:BL:306:U10:H8	1.79	0.65
7:AL:302:BCL:CMD	6:AM:206:ILE:HG21	2.23	0.65
5:BL:241:VAL:HG23	8:BL:304:BPH:HBC2	1.79	0.64
3:AQ:6:LEU:HD22	3:AQ:7:GLY:HA2	1.79	0.64
1:BT:29:VAL:HG13	1:BT:30:MET:N	2.12	0.64
5:AL:233:GLY:HA3	6:AM:216:PHE:CE1	2.32	0.64
7:BI:101:BCL:HMA1	7:BK:101:BCL:HMA1	1.78	0.64
3:AG:44:TRP:CE3	3:AG:45:ARG:HG2	2.32	0.64
1:AT:15:ARG:HA	1:AT:19:ALA:HB3	1.78	0.64
4:AH:86:ALA:HB3	4:AH:107:ASP:HB3	1.78	0.64
1:BD:12:ASP:H	1:BD:13:PRO:CD	2.11	0.64
4:AH:31:LEU:HB3	6:AM:268:TRP:CE2	2.32	0.64
3:A9:7:GLY:O	3:A9:8:TYR:C	2.36	0.64
1:AZ:12:ASP:HB2	1:AZ:13:PRO:HD3	1.78	0.64
1:A7:20:GLN:O	1:A7:24:LEU:HD23	1.98	0.64
7:AD:102:BCL:HHB	7:AF:101:BCL:HMA1	1.80	0.64
7:AN:101:BCL:CBD	7:AN:101:BCL:HAA2	2.27	0.64
1:AV:12:ASP:N	1:AV:13:PRO:CD	2.61	0.64
1:B2:15:ARG:NH2	1:BN:17:PHE:HB2	2.13	0.64
6:AM:262:MET:CG	6:AM:262:MET:CA	2.72	0.64
3:AS:11:LEU:O	3:AS:12:THR:OG1	2.13	0.64
5:AL:127:ALA:HB1	7:AL:301:BCL:H12	1.78	0.64
5:BL:97:PHE:CD1	5:BL:121:PHE:HZ	2.15	0.64
7:BO:101:BCL:CBD	7:BO:101:BCL:HAA2	2.27	0.64
6:AM:175:VAL:HB	12:AM:406:SPO:C24	2.27	0.64
1:AV:43:TRP:CD1	1:AV:43:TRP:C	2.70	0.64
5:BL:233:GLY:HA3	6:BM:216:PHE:CZ	2.32	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AL:74:GLY:H	5:AL:141:ALA:HB2	1.62	0.64
3:BE:44:TRP:HA	3:BE:45:ARG:HG2	1.80	0.64
3:A4:12:THR:H	3:A4:14:GLU:HB2	1.61	0.64
3:AE:43:ILE:HG23	3:AE:44:TRP:CD1	2.22	0.64
5:AL:184:ALA:HB3	8:AM:403:BPH:CMC	2.21	0.63
4:AH:40:TYR:HD2	4:AH:53:GLN:OE1	1.81	0.63
3:B4:19:LEU:HA	3:B4:22:VAL:HG22	1.80	0.63
3:BS:11:LEU:HA	3:BS:15:GLN:HB2	1.78	0.63
7:BL:303:BCL:HMD2	7:BM:401:BCL:CAB	2.26	0.63
5:AL:186:ALA:HB3	5:AL:236:LEU:HD13	1.81	0.63
1:BX:42:ASN:O	1:BX:43:TRP:CG	2.51	0.63
3:AS:12:THR:HB	3:AS:13:ASP:CG	2.18	0.63
1:A2:31:ILE:HG22	7:A9:101:BCL:HMD3	1.80	0.63
3:B6:44:TRP:HA	3:B6:45:ARG:HG2	1.79	0.63
6:AM:204:LEU:HA	6:AM:207:ALA:HB3	1.81	0.63
7:AL:302:BCL:CBD	7:AL:302:BCL:HAA1	2.27	0.63
1:B2:12:ASP:H	1:B2:13:PRO:HD3	1.63	0.63
3:AK:6:LEU:HD22	3:AK:7:GLY:HA2	1.79	0.63
6:BM:24:VAL:HG13	6:BM:139:ALA:HB1	1.81	0.63
4:BH:111:PRO:HG2	4:BH:239:GLY:HA2	1.81	0.63
3:AS:44:TRP:O	3:AS:44:TRP:CG	2.51	0.63
7:AN:101:BCL:HBD	7:AN:101:BCL:HAA2	1.80	0.63
7:BD:101:BCL:HAA2	7:BD:101:BCL:HBD	1.78	0.63
6:BM:86:LEU:HA	6:BM:89:LEU:HB2	1.78	0.63
5:BL:176:ALA:HB2	5:BL:243:PHE:C	2.19	0.63
3:BI:9:THR:HG23	3:BI:11:LEU:HB2	1.80	0.63
3:B9:7:GLY:O	3:B9:8:TYR:C	2.36	0.63
1:A1:28:ALA:HA	7:AI:101:BCL:OBD	1.98	0.63
1:B7:44:LEU:HB2	3:B6:46:PRO:HB3	1.80	0.63
5:AL:157:VAL:HG21	7:AL:302:BCL:H3C	1.81	0.63
7:B8:101:BCL:HMB1	7:B8:101:BCL:CBB	2.29	0.63
7:BD:101:BCL:HAA2	7:BD:101:BCL:CBD	2.28	0.63
3:AG:44:TRP:HE3	3:AG:45:ARG:HG2	1.63	0.63
3:AU:21:SER:HA	3:AU:25:SER:HB3	1.80	0.63
7:AM:401:BCL:HAA1	7:AM:401:BCL:CBD	2.28	0.63
1:BJ:16:VAL:HG13	1:BJ:16:VAL:O	1.98	0.63
3:AE:11:LEU:HD12	3:AE:11:LEU:N	2.13	0.62
5:BL:154:LEU:HD22	6:BM:197:PHE:CE1	2.34	0.62
1:A2:45:GLU:O	1:A2:45:GLU:HG3	1.98	0.62
3:AG:39:LEU:HA	3:AG:42:TYR:CD2	2.34	0.62
3:A4:9:THR:HB	3:A4:10:GLY:O	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A7:38:THR:N	1:A7:39:PRO:CD	2.62	0.62
5:BL:53:ALA:HB1	5:BL:59:TRP:HA	1.81	0.62
4:BH:150:GLY:HA2	4:BH:165:VAL:HG12	1.81	0.62
5:AL:175:ILE:HG23	9:AL:304:U10:H23	1.81	0.62
6:AM:150:PHE:HB2	8:AM:403:BPH:HMD3	1.82	0.62
1:AF:35:LEU:HD13	1:AF:43:TRP:HZ2	1.64	0.62
3:AI:41:VAL:HG22	7:AI:101:BCL:CAC	2.29	0.62
3:A6:3:LYS:HB2	3:A6:8:TYR:HB3	1.81	0.62
1:B7:12:ASP:H	1:B7:13:PRO:HD2	1.63	0.62
3:AW:44:TRP:CA	3:AW:45:ARG:HG2	2.30	0.62
6:BM:171:TRP:HA	6:BM:171:TRP:CE3	2.34	0.62
3:A9:38:HIS:HE1	7:A9:101:BCL:CAA	2.10	0.62
3:BK:45:ARG:N	3:BK:46:PRO:CD	2.62	0.62
1:A5:12:ASP:HB2	1:A5:13:PRO:HD3	1.81	0.62
1:A5:32:HIS:O	1:A5:36:LEU:HB2	2.00	0.62
5:BL:237:SER:HB3	6:BM:213:ALA:HA	1.81	0.62
6:AM:72:ILE:HG13	6:AM:114:LEU:HD13	1.81	0.62
3:A6:45:ARG:N	3:A6:46:PRO:CD	2.63	0.62
3:AE:11:LEU:HD22	3:AE:12:THR:N	2.13	0.62
3:B8:6:LEU:HD22	3:B8:7:GLY:CA	2.30	0.62
5:BL:176:ALA:O	7:BL:302:BCL:HMA2	1.95	0.62
8:BM:402:BPH:H141	8:BM:402:BPH:H18	1.82	0.62
5:BL:125:ILE:CD1	5:BL:125:ILE:CB	2.74	0.62
3:BW:45:ARG:H	3:BW:46:PRO:HD3	1.64	0.62
6:BM:176:PRO:HG2	6:BM:182:HIS:HA	1.80	0.62
1:B5:16:VAL:HG13	1:B5:16:VAL:O	2.00	0.62
6:AM:95:GLU:HG2	6:AM:176:PRO:HB3	1.82	0.62
1:AJ:12:ASP:CB	1:AJ:13:PRO:HD3	2.18	0.62
6:BM:9:GLN:H	6:BM:10:VAL:CA	2.13	0.62
4:AH:27:LEU:O	4:AH:31:LEU:HB2	1.99	0.62
1:B3:12:ASP:H	1:B3:13:PRO:HD2	1.64	0.62
3:A4:45:ARG:N	3:A4:46:PRO:HD3	2.15	0.62
1:BF:35:LEU:HD13	1:BF:43:TRP:HH2	1.64	0.62
8:AM:403:BPH:H18	8:AM:403:BPH:H141	1.82	0.62
7:BP:102:BCL:HMB3	7:BZ:101:BCL:NB	2.15	0.62
4:AH:153:VAL:CG1	4:AH:154:ARG:H	2.11	0.62
1:B7:10:ILE:HG23	1:B7:11:PHE:N	2.13	0.62
5:AL:164:TYR:HB3	5:AL:259:TRP:CD1	2.34	0.62
3:B8:6:LEU:HD22	3:B8:7:GLY:HA3	1.82	0.62
5:BL:181:PHE:HZ	7:BL:302:BCL:CBB	2.13	0.61
5:AL:229:ILE:O	5:AL:229:ILE:CG1	2.46	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AZ:31:ILE:HG23	7:AS:101:BCL:HMD3	1.82	0.61
7:BP:102:BCL:CAC	3:BQ:41:VAL:CG1	2.66	0.61
3:A6:7:GLY:O	3:A6:8:TYR:C	2.39	0.61
1:A7:38:THR:O	1:A7:40:SER:N	2.33	0.61
3:B9:45:ARG:N	3:B9:46:PRO:HD3	2.15	0.61
5:AL:215:PHE:CE1	6:AM:137:ALA:HB2	2.35	0.61
1:BF:42:ASN:O	1:BF:43:TRP:CG	2.53	0.61
3:BY:44:TRP:CA	3:BY:45:ARG:HG2	2.28	0.61
5:AL:30:TYR:HB2	6:AM:254:TRP:HB3	1.82	0.61
3:A6:3:LYS:HG3	3:A6:11:LEU:HD21	1.82	0.61
3:B6:11:LEU:H	3:B6:14:GLU:HB2	1.64	0.61
5:AL:107:ILE:HA	5:AL:110:LYS:HE2	1.82	0.61
5:AL:243:PHE:HE1	9:AL:304:U10:H28	1.65	0.61
7:BI:101:BCL:CMB	7:BK:101:BCL:HMA3	2.30	0.61
4:AH:35:ASN:HB3	6:AM:260:ALA:HA	1.82	0.61
7:BV:101:BCL:C1D	7:BV:102:BCL:HMD2	2.30	0.61
5:AL:151:TRP:HA	5:AL:154:LEU:HG	1.83	0.61
7:AL:301:BCL:CBB	7:AM:402:BCL:HHB	2.30	0.61
1:AN:12:ASP:HB2	1:AN:13:PRO:HD3	1.83	0.61
1:A7:12:ASP:H	1:A7:13:PRO:CD	2.13	0.61
1:AT:12:ASP:N	1:AT:13:PRO:CD	2.63	0.61
1:BV:24:LEU:HB3	3:BW:30:PHE:CE1	2.36	0.61
1:BF:12:ASP:CB	1:BF:13:PRO:HD3	2.12	0.61
4:AH:153:VAL:HG13	4:AH:203:VAL:HB	1.81	0.61
3:B8:10:GLY:CA	3:B8:11:LEU:HB2	2.28	0.61
3:AW:20:HIS:HA	3:AW:23:TYR:HB3	1.82	0.61
4:AH:150:GLY:HA2	4:AH:165:VAL:HG12	1.83	0.61
2:BB:23:VAL:O	2:BB:23:VAL:HG13	2.00	0.61
7:AL:301:BCL:CBB	7:AM:401:BCL:HMD2	2.31	0.61
1:AX:31:ILE:HD12	7:AY:102:BCL:HMD3	1.83	0.61
5:BL:49:ILE:HG22	5:BL:64:ILE:HG21	1.83	0.61
7:AD:102:BCL:HBB1	7:AF:101:BCL:HMC3	1.81	0.61
5:AL:216:PHE:HA	5:AL:219:LEU:HB2	1.83	0.61
1:AT:12:ASP:H	1:AT:13:PRO:HD3	1.65	0.61
5:BL:15:THR:HG22	5:BL:33:PHE:HB2	1.83	0.61
5:BL:227:LEU:O	5:BL:227:LEU:HG	2.01	0.61
3:AI:38:HIS:HD2	3:AI:41:VAL:HG11	1.64	0.61
4:BH:198:VAL:HG22	4:BH:203:VAL:HG13	1.81	0.61
6:BM:223:ILE:HG22	6:BM:223:ILE:O	2.00	0.61
1:BP:29:VAL:HA	1:BP:32:HIS:HD1	1.66	0.61
5:AL:278:GLY:O	5:AL:280:ASN:N	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AL:200:PRO:HB3	6:AM:141:GLY:O	2.01	0.61
5:BL:211:HIS:HD2	6:BM:140:LEU:HD13	1.65	0.61
7:BL:303:BCL:HHB	8:BL:304:BPH:HMB3	1.83	0.60
3:AS:45:ARG:CB	3:AS:46:PRO:HD3	2.24	0.60
7:BZ:101:BCL:H3A	7:BZ:101:BCL:CGA	2.30	0.60
4:AH:133:PRO:HA	4:AH:168:TRP:HA	1.83	0.60
4:AH:66:LEU:HD13	4:AH:70:ARG:HB3	1.82	0.60
3:B4:41:VAL:HG12	3:B4:41:VAL:O	2.00	0.60
5:BL:93:ALA:HB2	8:BL:304:BPH:H112	1.83	0.60
6:AM:164:ARG:N	6:AM:165:PRO:CD	2.64	0.60
6:AM:6:ILE:HG22	6:AM:7:PHE:H	1.67	0.60
3:BK:45:ARG:N	3:BK:46:PRO:HD3	2.15	0.60
1:AV:12:ASP:N	1:AV:13:PRO:HD2	2.17	0.60
1:AT:12:ASP:H	1:AT:13:PRO:CD	2.14	0.60
5:AL:196:SER:HB2	6:AM:143:GLY:HA3	1.82	0.60
3:AO:45:ARG:N	3:AO:46:PRO:HD3	2.15	0.60
5:BL:241:VAL:CG2	8:BL:304:BPH:CBC	2.71	0.60
6:AM:203:GLY:O	6:AM:206:ILE:HB	2.02	0.60
1:AJ:31:ILE:O	1:AJ:35:LEU:HD23	2.01	0.60
1:B2:44:LEU:HA	3:BK:46:PRO:HB3	1.82	0.60
6:BM:134:TYR:HD2	6:BM:147:ALA:HB3	1.65	0.60
6:BM:202:HIS:HA	7:BM:401:BCL:HED1	1.82	0.60
3:AS:12:THR:CB	3:AS:13:ASP:CB	2.39	0.60
1:AZ:38:THR:CB	1:AZ:39:PRO:HD2	2.28	0.60
5:BL:34:PHE:CB	5:BL:103:ARG:HB2	2.28	0.60
1:AF:10:ILE:HG23	1:AF:10:ILE:O	2.01	0.60
1:AN:34:ILE:HD13	1:AP:33:LEU:HD21	1.84	0.60
5:BL:190:HIS:CE1	5:BL:229:ILE:CG2	2.85	0.60
6:AM:129:TRP:CG	8:AM:403:BPH:H1C2	2.36	0.60
6:BM:88:ASP:HB2	6:BM:92:PHE:CE2	2.37	0.60
5:BL:85:LEU:O	5:BL:89:ILE:HG13	2.01	0.60
2:BB:55:LEU:N	2:BB:56:PRO:CD	2.65	0.60
3:B9:44:TRP:HA	3:B9:45:ARG:HG2	1.84	0.60
5:AL:123:PHE:HB2	5:AL:238:LEU:HD22	1.82	0.60
1:B2:20:GLN:HG2	1:B2:20:GLN:O	2.02	0.60
4:BH:17:ILE:HB	6:BM:201:PHE:HZ	1.66	0.60
5:AL:153:HIS:HD2	7:AL:302:BCL:HMC3	1.67	0.60
7:AD:101:BCL:HAA2	7:AD:101:BCL:HBD	1.83	0.60
7:B3:101:BCL:HBB3	7:BY:102:BCL:HBB2	1.84	0.60
1:BD:12:ASP:HB2	3:BE:19:LEU:HG	1.84	0.60
1:BT:8:TRP:O	1:BT:9:MET:HB2	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AL:222:TYR:HD2	9:AL:304:U10:H1M3	1.67	0.60
1:A7:15:ARG:HE	1:A7:19:ALA:HB2	1.64	0.60
4:AH:111:PRO:HG2	4:AH:239:GLY:HA2	1.83	0.60
3:BS:12:THR:H	3:BS:14:GLU:N	2.00	0.60
7:A7:101:BCL:HMA1	7:A6:102:BCL:HMA2	1.83	0.60
1:B2:43:TRP:CZ2	7:B2:101:BCL:HAC2	2.37	0.60
1:A3:43:TRP:CD1	1:A3:43:TRP:C	2.74	0.60
1:B5:8:TRP:N	3:B6:9:THR:HG1	1.99	0.60
3:A6:44:TRP:HA	3:A6:45:ARG:HG2	1.82	0.60
5:AL:198:ALA:C	5:AL:200:PRO:HD3	2.22	0.60
3:BG:33:VAL:HA	3:BG:36:VAL:HB	1.82	0.60
5:AL:185:LEU:HD13	7:AM:401:BCL:H2	1.84	0.60
2:BB:27:MET:HG2	2:BB:27:MET:O	2.00	0.60
6:BM:237:GLN:CB	6:BM:262:MET:HG2	2.32	0.60
3:BI:43:ILE:HG23	3:BI:44:TRP:CD1	2.36	0.60
4:BH:13:ALA:HA	6:BM:290:VAL:HG11	1.84	0.60
7:BF:101:BCL:HBD	7:BF:101:BCL:HAA2	1.82	0.59
5:BL:219:LEU:CD1	5:BL:219:LEU:CD2	2.80	0.59
8:BL:304:BPH:HMC2	6:BM:213:ALA:HB3	1.83	0.59
5:AL:228:GLY:O	5:AL:232:LEU:HB2	2.01	0.59
5:AL:176:ALA:HB2	5:AL:243:PHE:HB2	1.82	0.59
1:BJ:21:GLY:O	1:BJ:24:LEU:HG	2.02	0.59
5:BL:265:TRP:CG	5:BL:265:TRP:O	2.54	0.59
1:A1:31:ILE:HG22	7:AI:101:BCL:HMD3	1.85	0.59
3:AY:44:TRP:HA	3:AY:45:ARG:HG2	1.83	0.59
3:B6:7:GLY:O	3:B6:8:TYR:C	2.41	0.59
3:BI:44:TRP:HA	3:BI:45:ARG:CG	2.33	0.59
3:AQ:27:LEU:HD13	3:AQ:30:PHE:HB3	1.83	0.59
5:AL:182:THR:HA	5:AL:185:LEU:HB2	1.85	0.59
5:AL:153:HIS:CD2	7:AL:302:BCL:HMC3	2.37	0.59
7:AL:302:BCL:H51	8:AL:303:BPH:HMB1	1.83	0.59
5:BL:28:PRO:HB3	6:BM:253:ARG:NH1	2.17	0.59
3:A9:41:VAL:HG11	7:A9:101:BCL:HAC2	1.84	0.59
3:BW:43:ILE:HG23	3:BW:44:TRP:CD1	2.35	0.59
7:BL:302:BCL:HBB2	7:BM:401:BCL:CHB	2.23	0.59
7:AZ:101:BCL:HAA2	7:AZ:101:BCL:CBD	2.33	0.59
5:BL:36:VAL:O	5:BL:36:VAL:CG1	2.50	0.59
5:AL:101:ALA:HB2	5:AL:121:PHE:HD2	1.66	0.59
1:BX:28:ALA:O	1:BX:31:ILE:HG22	2.03	0.59
1:A5:20:GLN:HA	1:A5:23:PHE:HB3	1.85	0.59
9:AM:405:U10:H8	9:AM:405:U10:C1M	2.31	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AL:183:ASN:HB2	5:AL:236:LEU:O	2.02	0.59
5:AL:179:PHE:CD2	9:AL:304:U10:H211	2.38	0.59
1:AD:35:LEU:HB3	1:AD:43:TRP:CZ3	2.32	0.59
1:BD:43:TRP:CD1	1:BD:44:LEU:HB3	2.37	0.59
5:AL:248:MET:HA	5:AL:251:THR:HB	1.84	0.59
3:B8:45:ARG:N	3:B8:46:PRO:CD	2.65	0.59
6:BM:96:PRO:HB2	6:BM:97:PRO:CD	2.32	0.59
4:BH:24:LEU:HG	4:BH:27:LEU:HD22	1.85	0.59
5:AL:201:GLU:O	5:AL:202:LYS:CB	2.51	0.59
6:BM:156:LEU:HD12	7:BM:401:BCL:H12	1.85	0.59
3:AW:11:LEU:H	3:AW:14:GLU:C	2.05	0.59
6:AM:171:TRP:HE3	6:AM:171:TRP:HA	1.68	0.59
5:BL:116:HIS:O	6:BM:221:ALA:HB1	2.02	0.59
1:A2:20:GLN:HG2	1:A2:20:GLN:O	2.03	0.59
7:BL:303:BCL:H2	8:BL:304:BPH:HMB2	1.85	0.59
5:AL:124:ALA:O	7:AL:301:BCL:H92	2.02	0.59
2:BB:49:ARG:HH11	2:BB:49:ARG:HA	1.68	0.59
6:BM:202:HIS:CE1	6:BM:206:ILE:HD11	2.38	0.59
6:AM:175:VAL:CG1	7:AM:401:BCL:HMC1	2.33	0.59
1:A2:14:ARG:O	1:A2:18:VAL:HG12	2.03	0.59
1:A2:21:GLY:C	1:A2:23:PHE:H	2.07	0.59
6:AM:287:SER:HA	6:AM:294:TRP:HZ2	1.68	0.59
5:AL:185:LEU:CD1	7:AM:401:BCL:H2	2.33	0.58
7:A7:101:BCL:HMB1	7:A7:101:BCL:HBB3	1.84	0.58
7:B3:101:BCL:HMD2	7:B4:101:BCL:HAC1	1.83	0.58
6:BM:5:ASN:HA	6:BM:41:TRP:HH2	1.68	0.58
5:AL:105:VAL:HG12	5:AL:109:ARG:HG3	1.85	0.58
6:BM:284:ILE:HG22	6:BM:284:ILE:O	2.02	0.58
4:BH:65:ILE:O	5:BL:206:MET:HB2	2.02	0.58
6:AM:284:ILE:HG22	6:AM:284:ILE:O	2.03	0.58
6:AM:9:GLN:H	6:AM:10:VAL:HG23	1.67	0.58
3:BO:41:VAL:CG1	7:BO:102:BCL:CAC	2.76	0.58
1:A2:15:ARG:NH2	1:AN:17:PHE:HB2	2.17	0.58
4:AH:21:TRP:HA	4:AH:21:TRP:HE3	1.68	0.58
6:BM:88:ASP:C	6:BM:90:PHE:H	2.07	0.58
3:A4:30:PHE:HE2	7:A4:101:BCL:HBD	1.67	0.58
3:AQ:44:TRP:HA	3:AQ:45:ARG:HG2	1.85	0.58
4:AH:21:TRP:CE3	4:AH:21:TRP:HA	2.38	0.58
4:AH:103:ASP:HB2	4:AH:106:LYS:HD3	1.85	0.58
1:AP:11:PHE:HB2	1:AP:15:ARG:HB2	1.85	0.58
5:AL:224:ILE:HA	6:AM:44:ASN:HB2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:23:VAL:HG13	2:AB:23:VAL:O	2.03	0.58
3:BU:35:ILE:HA	3:BU:38:HIS:HB2	1.84	0.58
5:BL:219:LEU:CB	5:BL:219:LEU:CD2	2.76	0.58
7:A7:101:BCL:CMA	7:A6:102:BCL:HMA1	2.34	0.58
7:BO:102:BCL:HMB1	7:BO:102:BCL:CBB	2.30	0.58
1:B5:31:ILE:HG12	1:B5:34:ILE:HD12	1.86	0.58
3:AI:9:THR:HG23	3:AI:11:LEU:HD23	1.85	0.58
1:B3:43:TRP:C	1:B3:43:TRP:CD1	2.75	0.58
6:AM:203:GLY:HA2	6:AM:206:ILE:HD12	1.86	0.58
1:A1:12:ASP:N	1:A1:13:PRO:CD	2.57	0.58
6:AM:215:LEU:HD23	6:AM:215:LEU:O	2.03	0.58
5:BL:130:THR:HG21	5:BL:245:ALA:HB1	1.84	0.58
5:BL:244:SER:HB3	7:BL:302:BCL:H2A	1.85	0.58
7:AT:102:BCL:CAC	3:AU:41:VAL:HG11	2.33	0.58
1:BD:31:ILE:HG23	7:BD:102:BCL:CMD	2.33	0.58
5:AL:136:PRO:HB2	5:AL:142:TRP:HA	1.86	0.58
6:AM:265:ILE:HG13	6:AM:265:ILE:O	2.04	0.58
7:BL:301:BCL:HMC1	6:BM:175:VAL:HG21	1.85	0.58
1:A7:35:LEU:HD21	7:A8:101:BCL:HMD3	1.86	0.58
5:BL:69:PRO:O	5:BL:143:GLY:HA2	2.03	0.58
6:BM:65:MET:O	6:BM:69:THR:OG1	2.17	0.58
7:BV:101:BCL:HMA1	7:BU:101:BCL:HHB	1.85	0.58
4:AH:70:ARG:HH21	4:AH:120:LEU:HB3	1.69	0.58
6:BM:2:GLU:HG2	6:BM:3:TYR:H	1.68	0.58
6:AM:214:LEU:HD23	9:AM:405:U10:H151	1.85	0.58
5:BL:196:SER:HB2	6:BM:143:GLY:H	1.68	0.58
5:AL:127:ALA:HB2	5:AL:241:VAL:CG1	2.33	0.58
5:AL:157:VAL:HG13	7:AL:301:BCL:HMD2	1.86	0.58
5:AL:45:GLY:HA3	8:AL:303:BPH:H9C1	0.78	0.58
1:B7:39:PRO:HG2	5:BL:55:LEU:HD11	1.85	0.58
5:AL:117:ILE:N	5:AL:118:PRO:CD	2.65	0.58
4:AH:41:PRO:HA	4:AH:53:GLN:OE1	2.03	0.58
1:B7:12:ASP:N	1:B7:13:PRO:CD	2.66	0.58
1:AX:24:LEU:HA	1:AX:27:LEU:HB3	1.86	0.58
3:A9:11:LEU:HB3	3:A9:14:GLU:HG2	1.85	0.58
1:BP:36:LEU:HD11	7:BP:101:BCL:HBB2	1.86	0.58
3:AY:43:ILE:HG23	3:AY:44:TRP:CD1	2.34	0.58
3:AK:45:ARG:N	3:AK:46:PRO:HD3	2.18	0.58
3:BQ:8:TYR:HA	3:BQ:10:GLY:HA3	1.84	0.58
5:BL:97:PHE:CZ	7:BL:302:BCL:H91	2.39	0.57
5:BL:41:PHE:O	8:BL:304:BPH:H9C2	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BM:401:BCL:H121	8:BM:402:BPH:HAA1	1.86	0.57
5:AL:181:PHE:HZ	7:AL:301:BCL:CBB	2.16	0.57
7:BP:101:BCL:HBB3	7:BP:101:BCL:HMB1	1.85	0.57
5:BL:279:ILE:CG1	6:BM:92:PHE:HA	2.32	0.57
1:BF:43:TRP:HE1	7:BF:101:BCL:HHC	1.69	0.57
3:A4:11:LEU:HD22	3:A4:11:LEU:O	2.04	0.57
3:A4:12:THR:HA	3:A4:13:ASP:C	2.24	0.57
5:BL:135:ARG:N	5:BL:136:PRO:CD	2.66	0.57
6:AM:186:THR:HG21	7:AM:401:BCL:HMD3	1.86	0.57
6:AM:9:GLN:HG2	6:AM:41:TRP:HB3	1.84	0.57
3:AE:11:LEU:O	3:AE:12:THR:HB	2.04	0.57
3:BK:45:ARG:C	3:BK:47:TRP:H	2.08	0.57
1:A2:11:PHE:HE1	6:AM:135:LEU:HD22	1.68	0.57
5:BL:168:HIS:CD2	7:BL:302:BCL:HMC2	2.39	0.57
7:AD:101:BCL:HAA2	7:AD:101:BCL:CBD	2.34	0.57
6:BM:74:PHE:CD2	6:BM:92:PHE:HB2	2.38	0.57
6:BM:9:GLN:H	6:BM:10:VAL:HA	1.68	0.57
1:BZ:39:PRO:O	1:BZ:40:SER:CB	2.52	0.57
1:BD:42:ASN:OD1	1:BD:45:GLU:HB3	2.04	0.57
6:BM:64:LEU:HD22	6:BM:68:PHE:CE2	2.40	0.57
6:BM:70:ILE:HG23	6:BM:94:LEU:HD23	1.85	0.57
1:A5:16:VAL:HG22	1:A5:16:VAL:O	2.04	0.57
1:AN:48:ALA:HB1	3:A9:48:PHE:HB2	1.85	0.57
1:BJ:42:ASN:O	1:BJ:44:LEU:HD23	2.04	0.57
1:AX:48:ALA:HA	3:AW:47:TRP:HD1	1.69	0.57
7:BD:102:BCL:HHB	7:BF:101:BCL:CMA	2.35	0.57
1:A2:41:TYR:HB3	1:A2:43:TRP:CZ3	2.39	0.57
6:AM:243:THR:OG1	6:AM:247:ARG:NH1	2.37	0.57
5:BL:164:TYR:CZ	5:BL:251:THR:HG22	2.39	0.57
1:A5:29:VAL:HA	1:A5:32:HIS:CD2	2.40	0.57
5:AL:197:ALA:HB1	5:AL:207:ARG:H	1.69	0.57
5:AL:234:LEU:HB2	6:AM:220:GLY:HA3	1.87	0.57
3:BQ:20:HIS:O	3:BQ:24:MET:HB2	2.04	0.57
1:BF:8:TRP:O	1:BF:9:MET:HB2	2.05	0.57
4:BH:61:PRO:HB2	4:BH:74:THR:HG22	1.85	0.57
1:A2:11:PHE:HD1	6:AM:138:GLN:HG3	1.69	0.57
7:BL:303:BCL:H111	8:BL:304:BPH:H171	1.86	0.57
5:AL:190:HIS:CE1	5:AL:229:ILE:HG23	2.40	0.57
6:AM:119:SER:HB3	12:AM:406:SPO:H311	1.85	0.57
3:AW:7:GLY:O	3:AW:10:GLY:HA2	2.04	0.57
3:BY:3:LYS:HB3	3:BY:8:TYR:HD1	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BF:43:TRP:HD1	1:BF:43:TRP:O	1.88	0.57
6:BM:238:ILE:HG23	6:BM:263:GLU:HB2	1.86	0.57
3:AK:7:GLY:O	3:AK:8:TYR:C	2.43	0.57
5:BL:154:LEU:O	6:BM:197:PHE:CE2	2.58	0.57
3:B4:31:SER:HA	3:B4:34:ALA:HB3	1.87	0.57
1:BD:22:VAL:HA	1:BD:25:PHE:HB3	1.86	0.57
6:AM:185:TRP:HZ3	7:AM:401:BCL:HAC1	1.70	0.57
1:B3:24:LEU:HB2	7:B3:101:BCL:O2A	2.05	0.57
1:A3:12:ASP:H	1:A3:13:PRO:HD3	1.69	0.57
3:AO:10:GLY:CA	3:AO:11:LEU:HB2	2.32	0.57
4:BH:85:ILE:HB	5:BL:7:ARG:NH2	2.19	0.57
4:AH:121:PRO:HB3	4:AH:226:THR:HA	1.87	0.57
5:AL:244:SER:OG	7:AL:301:BCL:HMA2	2.05	0.56
6:AM:130:TRP:HA	6:AM:150:PHE:CD2	2.40	0.56
7:BZ:101:BCL:CBD	7:BZ:101:BCL:HAA2	2.35	0.56
5:BL:34:PHE:HB2	5:BL:103:ARG:CB	2.31	0.56
5:AL:215:PHE:HZ	6:AM:146:THR:HG21	1.68	0.56
4:BH:121:PRO:HA	4:BH:226:THR:HA	1.87	0.56
4:BH:137:ALA:O	4:BH:139:GLY:N	2.38	0.56
1:BX:21:GLY:O	1:BX:25:PHE:HB2	2.04	0.56
5:BL:169:TYR:CD2	5:BL:263:TRP:HD1	2.23	0.56
5:AL:37:ALA:O	5:AL:41:PHE:HD2	1.88	0.56
5:AL:183:ASN:HD21	6:AM:216:PHE:HB3	1.69	0.56
3:AG:39:LEU:HD23	3:AG:42:TYR:HD2	1.71	0.56
1:BD:8:TRP:O	1:BD:9:MET:HB2	2.05	0.56
1:A1:31:ILE:HG23	1:A1:35:LEU:HD23	1.86	0.56
7:AJ:101:BCL:HBB3	7:A2:101:BCL:H3C	1.86	0.56
6:BM:59:SER:HA	6:BM:125:ALA:HA	1.86	0.56
6:AM:29:ARG:HD2	6:AM:49:PRO:HB2	1.86	0.56
5:BL:169:TYR:HD2	5:BL:263:TRP:CD1	2.20	0.56
7:BP:102:BCL:HAC1	3:BQ:41:VAL:HG11	1.87	0.56
7:BT:101:BCL:CMC	7:BZ:102:BCL:CMB	2.82	0.56
5:BL:103:ARG:HH22	6:BM:255:THR:HG23	1.70	0.56
5:BL:30:TYR:CB	6:BM:254:TRP:HB3	2.25	0.56
3:AG:43:ILE:HG23	3:AG:44:TRP:CD1	2.31	0.56
5:AL:103:ARG:HH22	6:AM:255:THR:HG23	1.68	0.56
3:BE:11:LEU:HD13	3:BE:11:LEU:H	1.70	0.56
3:A6:6:LEU:HA	3:A6:7:GLY:C	2.26	0.56
5:AL:105:VAL:HA	5:AL:108:CYS:HB2	1.86	0.56
1:B7:15:ARG:HA	1:B7:18:VAL:HG12	1.87	0.56
1:BP:29:VAL:HA	1:BP:32:HIS:ND1	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BJ:42:ASN:O	1:BJ:44:LEU:N	2.30	0.56
1:BN:42:ASN:O	1:BN:44:LEU:N	2.34	0.56
6:AM:85:PHE:HD2	6:AM:86:LEU:HD12	1.70	0.56
5:BL:173:HIS:CB	5:BL:247:CYS:SG	2.94	0.56
5:BL:41:PHE:HB3	5:BL:96:ALA:HB2	1.86	0.56
5:AL:124:ALA:HB1	7:AL:301:BCL:C7	2.32	0.56
1:BF:31:ILE:O	1:BF:35:LEU:HG	2.05	0.56
6:BM:64:LEU:O	6:BM:68:PHE:N	2.38	0.56
4:AH:242:MET:HA	5:AL:109:ARG:O	2.06	0.56
3:BK:13:ASP:HB2	3:BK:16:ALA:HB3	1.87	0.56
3:B4:39:LEU:HA	3:B4:42:TYR:HD2	1.71	0.56
5:AL:148:TYR:HD1	8:AL:303:BPH:C14	2.11	0.56
1:A2:8:TRP:HE1	3:A9:6:LEU:HD23	1.71	0.56
5:AL:34:PHE:CB	5:AL:103:ARG:HB2	2.35	0.56
3:BW:11:LEU:HD23	3:BW:12:THR:N	2.20	0.56
1:AT:46:ILE:O	1:AT:46:ILE:HG22	2.05	0.56
1:AP:42:ASN:C	1:AP:44:LEU:H	2.09	0.56
6:BM:205:SER:HB2	6:BM:280:GLY:CA	2.35	0.56
7:AL:301:BCL:H203	7:AL:302:BCL:H61	1.87	0.56
1:BZ:11:PHE:HB2	1:BZ:15:ARG:HB2	1.87	0.56
2:AB:55:LEU:N	2:AB:56:PRO:HD2	2.21	0.56
6:AM:193:HIS:O	6:AM:293:ASN:HA	2.05	0.56
5:BL:220:VAL:HG21	9:BL:306:U10:H1M2	1.87	0.56
6:BM:156:LEU:HB2	6:BM:277:THR:HB	1.87	0.56
5:AL:233:GLY:HA3	6:AM:216:PHE:CZ	2.41	0.56
8:AM:403:BPH:HBB3	8:AM:403:BPH:HHC	1.88	0.56
6:AM:175:VAL:HB	12:AM:406:SPO:H241	1.87	0.56
4:AH:35:ASN:N	4:AH:35:ASN:ND2	2.54	0.56
1:AF:11:PHE:CD2	4:AH:52:ASN:HA	2.40	0.56
1:B7:15:ARG:HE	1:B7:19:ALA:HB2	1.71	0.56
1:A5:8:TRP:N	3:A6:9:THR:HG1	2.04	0.56
5:BL:45:GLY:HA2	5:BL:48:LEU:HD12	1.87	0.56
8:BM:402:BPH:HHC	8:BM:402:BPH:HBB3	1.88	0.56
1:BP:14:ARG:HH12	6:BM:53:GLY:HA3	1.70	0.56
3:A6:43:ILE:O	3:A6:45:ARG:HA	2.06	0.56
4:AH:70:ARG:NH2	4:AH:120:LEU:HB3	2.20	0.56
1:A2:9:MET:HG3	1:A2:10:ILE:HG23	1.87	0.56
1:BJ:10:ILE:HG13	1:BJ:11:PHE:H	1.71	0.56
1:B1:33:LEU:HA	1:B1:36:LEU:HB2	1.88	0.56
5:BL:175:ILE:HA	5:BL:178:SER:HB2	1.88	0.56
5:AL:173:HIS:CD2	7:AL:301:BCL:HMA3	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BE:18:GLU:O	3:BE:22:VAL:HG22	2.06	0.56
1:AT:15:ARG:HD2	1:AV:18:VAL:HB	1.88	0.56
3:AG:3:LYS:HD2	3:AG:8:TYR:HB3	1.86	0.56
5:AL:67:TYR:CD2	5:AL:68:PRO:HD2	2.40	0.56
3:AO:38:HIS:CE1	7:AO:101:BCL:HAA1	2.41	0.56
1:A5:22:VAL:HA	1:A5:25:PHE:CB	2.35	0.56
2:BB:17:THR:HG22	2:BB:18:ASN:N	2.21	0.56
3:AE:18:GLU:O	3:AE:22:VAL:HG22	2.06	0.56
1:B1:14:ARG:NH1	4:BH:29:TYR:OH	2.39	0.55
1:A1:12:ASP:HA	1:A1:15:ARG:HB2	1.88	0.55
7:BV:102:BCL:HMC1	1:BX:44:LEU:HD11	1.88	0.55
1:BD:13:PRO:HD3	3:BE:19:LEU:HG	1.88	0.55
5:AL:231:ARG:HG3	6:AM:224:LEU:HD11	1.88	0.55
3:BK:43:ILE:C	3:BK:46:PRO:HD2	2.25	0.55
4:AH:38:GLU:OE1	4:AH:76:PRO:HA	2.07	0.55
3:BE:15:GLN:HE21	3:BE:19:LEU:HD13	1.71	0.55
3:B9:44:TRP:CA	3:B9:45:ARG:HG2	2.37	0.55
4:BH:13:ALA:HA	6:BM:290:VAL:CG1	2.37	0.55
6:AM:201:PHE:HB3	6:AM:283:GLY:CA	2.36	0.55
6:BM:273:ALA:HA	6:BM:276:VAL:HG23	1.89	0.55
1:A3:28:ALA:O	1:A3:32:HIS:CD2	2.60	0.55
7:B9:101:BCL:HMA1	7:BO:101:BCL:HMA1	1.88	0.55
7:AL:301:BCL:CBB	7:AM:401:BCL:CMD	2.84	0.55
7:BI:101:BCL:CHB	7:BK:101:BCL:HMA1	2.37	0.55
1:AP:24:LEU:HA	7:AP:101:BCL:O2A	2.07	0.55
1:BJ:19:ALA:O	1:BJ:22:VAL:HG22	2.06	0.55
4:AH:66:LEU:HB3	4:AH:67:PRO:HD2	1.89	0.55
6:AM:130:TRP:HA	6:AM:150:PHE:CE2	2.41	0.55
1:A2:43:TRP:CE2	7:A2:101:BCL:HAC2	2.41	0.55
3:AK:43:ILE:HG13	3:AK:46:PRO:HB2	1.87	0.55
5:BL:123:PHE:O	5:BL:241:VAL:HG11	2.07	0.55
5:BL:238:LEU:HA	8:BL:304:BPH:HBC3	1.89	0.55
6:BM:214:LEU:O	6:BM:218:MET:SD	2.65	0.55
6:AM:154:ILE:HG23	6:AM:157:TRP:HB3	1.89	0.55
6:AM:156:LEU:HB2	6:AM:277:THR:HB	1.89	0.55
5:AL:184:ALA:CB	8:AM:403:BPH:HMC3	2.22	0.55
1:AN:31:ILE:HD13	1:AN:31:ILE:O	2.06	0.55
5:BL:278:GLY:H	6:BM:84:VAL:HG11	1.71	0.55
6:BM:238:ILE:HA	6:BM:262:MET:HB3	1.88	0.55
4:AH:31:LEU:HB3	6:AM:268:TRP:NE1	2.21	0.55
5:BL:134:PHE:HD1	5:BL:249:ILE:HD11	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BL:302:BCL:H141	8:BL:304:BPH:C17	2.34	0.55
5:BL:237:SER:O	8:BL:304:BPH:HBC3	2.07	0.55
1:BD:10:ILE:HD13	1:BF:13:PRO:O	2.07	0.55
1:BD:43:TRP:C	1:BD:43:TRP:CD1	2.80	0.55
5:AL:34:PHE:HB2	5:AL:103:ARG:CB	2.36	0.55
4:BH:65:ILE:H	4:BH:65:ILE:HD12	1.70	0.55
1:BP:31:ILE:O	1:BP:31:ILE:HG23	2.06	0.55
7:AL:301:BCL:H141	8:AL:303:BPH:C17	2.29	0.55
3:A6:41:VAL:CG1	7:A6:102:BCL:HBC1	2.21	0.55
1:AN:42:ASN:C	1:AN:44:LEU:H	2.10	0.55
4:AH:38:GLU:HB3	6:AM:241:ARG:HE	1.71	0.55
1:BF:11:PHE:HE2	4:BH:53:GLN:HE21	1.52	0.55
5:AL:97:PHE:O	5:AL:121:PHE:HE2	1.89	0.55
3:BI:11:LEU:N	3:BI:14:GLU:HB2	2.10	0.55
3:AY:38:HIS:HA	7:AY:101:BCL:HMD3	1.88	0.55
1:AP:11:PHE:HB3	1:AP:14:ARG:HB3	1.89	0.55
5:AL:122:ALA:HA	5:AL:125:ILE:HB	1.88	0.55
7:BL:303:BCL:C12	8:BL:304:BPH:H203	2.33	0.55
6:BM:90:PHE:HB2	6:BM:180:PHE:HD2	1.72	0.55
7:B5:101:BCL:HMD2	7:B6:101:BCL:C2D	2.37	0.55
5:BL:153:HIS:CD2	7:BL:303:BCL:HMC3	2.42	0.54
7:BL:301:BCL:HMB2	8:BM:402:BPH:HMB3	1.88	0.54
1:BF:35:LEU:HD13	1:BF:43:TRP:CH2	2.42	0.54
3:BE:11:LEU:HD13	3:BE:11:LEU:N	2.22	0.54
4:AH:144:ALA:HB3	6:AM:2:GLU:CB	2.37	0.54
4:BH:12:LEU:HB3	4:BH:15:LEU:HB2	1.87	0.54
3:BK:9:THR:HG22	3:BK:10:GLY:HA3	1.90	0.54
5:AL:181:PHE:CZ	7:AL:301:BCL:CBB	2.89	0.54
6:AM:161:GLY:HA2	6:AM:165:PRO:HG2	1.88	0.54
7:AM:402:BCL:H141	8:AM:403:BPH:H4C2	1.89	0.54
3:AE:6:LEU:HD13	3:AE:7:GLY:N	2.21	0.54
3:AI:38:HIS:HA	3:AI:41:VAL:HB	1.89	0.54
4:AH:171:ILE:CB	4:AH:172:PRO:HD3	2.34	0.54
1:B1:15:ARG:HA	1:B1:19:ALA:CB	2.35	0.54
1:AT:46:ILE:C	1:AT:48:ALA:H	2.11	0.54
3:B6:15:GLN:HG3	3:B6:15:GLN:O	2.06	0.54
5:AL:233:GLY:HA2	6:AM:216:PHE:CE2	2.43	0.54
6:BM:88:ASP:HB3	6:BM:91:PHE:HB2	1.89	0.54
1:BN:10:ILE:CG2	1:BP:14:ARG:HB2	2.36	0.54
3:A9:44:TRP:CA	3:A9:45:ARG:HG2	2.38	0.54
4:AH:31:LEU:HD13	6:AM:268:TRP:CD2	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BM:24:VAL:HG22	6:BM:139:ALA:O	2.06	0.54
5:BL:190:HIS:CE1	5:BL:229:ILE:HG21	2.42	0.54
6:BM:281:GLY:O	6:BM:285:LEU:HB2	2.07	0.54
5:BL:124:ALA:HB1	7:BL:302:BCL:C7	2.20	0.54
1:BZ:31:ILE:HD12	7:BZ:102:BCL:HMD3	1.89	0.54
1:A2:36:LEU:HD23	1:A2:43:TRP:HE1	1.71	0.54
5:AL:164:TYR:CE1	5:AL:256:PHE:HA	2.40	0.54
4:BH:140:PHE:CE1	6:BM:13:ARG:HB3	2.42	0.54
3:AI:14:GLU:O	3:AI:18:GLU:N	2.40	0.54
6:BM:238:ILE:HG12	6:BM:262:MET:O	2.07	0.54
1:B2:15:ARG:CZ	1:BN:17:PHE:HB2	2.38	0.54
5:BL:190:HIS:CE1	5:BL:229:ILE:HG23	2.42	0.54
1:B3:42:ASN:HB3	1:B3:46:ILE:HG12	1.87	0.54
5:AL:66:VAL:O	5:AL:86:TRP:HD1	1.90	0.54
1:AZ:35:LEU:HD12	1:AZ:36:LEU:HG	1.90	0.54
5:BL:222:TYR:O	9:BL:306:U10:O2	2.26	0.54
5:AL:278:GLY:HA3	6:AM:92:PHE:HE1	1.71	0.54
4:BH:39:GLY:HA2	5:BL:5:PHE:CE2	2.42	0.54
3:BO:29:LEU:HA	3:BO:32:ALA:HB3	1.89	0.54
5:BL:175:ILE:CG2	9:BL:306:U10:H23	2.37	0.54
1:AT:35:LEU:HD21	7:AT:102:BCL:HMD3	1.89	0.54
5:BL:69:PRO:HB3	5:BL:78:ALA:HB2	1.89	0.54
6:BM:57:VAL:O	6:BM:57:VAL:CG1	2.49	0.54
4:BH:85:ILE:HB	5:BL:7:ARG:HH21	1.72	0.54
1:A3:28:ALA:HA	7:A4:101:BCL:HMD1	1.90	0.54
3:AW:44:TRP:HA	3:AW:45:ARG:HG2	1.90	0.54
3:AI:25:SER:O	3:AI:29:LEU:HG	2.08	0.54
5:BL:45:GLY:HA3	8:BL:304:BPH:C9	2.25	0.54
6:AM:59:SER:HB3	6:AM:129:TRP:HE3	1.72	0.54
3:A6:38:HIS:HE1	7:A6:102:BCL:HAA1	1.73	0.54
1:AD:9:MET:O	1:AD:10:ILE:CG2	2.43	0.54
7:AK:101:BCL:HBD	7:AK:101:BCL:HAA2	1.90	0.54
4:AH:38:GLU:H	6:AM:261:THR:HG22	1.72	0.54
4:AH:197:LYS:HG2	4:AH:197:LYS:O	2.07	0.54
4:AH:188:THR:O	4:AH:218:THR:HA	2.08	0.54
5:BL:127:ALA:HB1	7:BL:302:BCL:H12	1.89	0.54
5:BL:125:ILE:O	5:BL:125:ILE:HG22	2.07	0.54
1:BZ:39:PRO:O	1:BZ:40:SER:HB2	2.07	0.54
4:BH:176:ALA:HB3	6:BM:10:VAL:HB	1.90	0.54
6:AM:62:SER:HB2	6:AM:125:ALA:HB2	1.89	0.54
1:B5:31:ILE:HG21	7:B6:101:BCL:HMD3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:27:MET:HA	2:BB:29:LYS:HE3	1.89	0.54
1:BV:24:LEU:HB3	3:BW:30:PHE:HE1	1.73	0.54
4:AH:188:THR:HB	4:AH:219:ILE:HG13	1.90	0.54
1:BV:43:TRP:CD1	1:BV:43:TRP:C	2.81	0.54
1:BP:26:LEU:O	1:BP:30:MET:HG2	2.08	0.54
5:BL:216:PHE:CE2	5:BL:219:LEU:HD23	2.42	0.54
1:AX:21:GLY:O	1:AX:25:PHE:HB2	2.08	0.54
4:AH:245:ALA:HB3	4:AH:251:VAL:HG11	1.90	0.54
4:AH:248:ARG:O	4:AH:249:LYS:HB2	2.07	0.54
5:BL:52:SER:HB2	5:BL:66:VAL:HG22	1.89	0.54
7:BL:302:BCL:HBD	7:BL:302:BCL:HAA2	1.90	0.54
5:BL:233:GLY:HA3	6:BM:216:PHE:CE1	2.43	0.54
3:A6:15:GLN:O	3:A6:19:LEU:HB2	2.08	0.54
5:BL:134:PHE:HD1	5:BL:249:ILE:CD1	2.21	0.53
7:BL:301:BCL:H2C	6:BM:160:LEU:HD13	1.90	0.53
7:AZ:101:BCL:HAA2	7:AZ:101:BCL:HBD	1.90	0.53
1:A7:10:ILE:HG23	1:A7:11:PHE:N	2.22	0.53
4:AH:70:ARG:HH22	4:AH:123:LEU:HD12	1.72	0.53
5:BL:224:ILE:HG23	5:BL:228:GLY:HA3	1.90	0.53
4:AH:100:PRO:HG2	4:AH:104:PRO:HB3	1.90	0.53
4:AH:238:ALA:HA	4:AH:241:LEU:HD12	1.90	0.53
5:AL:149:GLY:O	5:AL:153:HIS:CE1	2.61	0.53
1:BD:42:ASN:O	1:BD:43:TRP:CG	2.61	0.53
6:BM:231:GLY:HA3	6:BM:244:ALA:HB3	1.89	0.53
3:AQ:8:TYR:HA	3:AQ:10:GLY:HA3	1.89	0.53
5:BL:245:ALA:O	5:BL:249:ILE:N	2.41	0.53
5:AL:229:ILE:HA	5:AL:232:LEU:HB3	1.83	0.53
7:AL:301:BCL:HBB2	7:AM:402:BCL:HHB	1.90	0.53
5:AL:49:ILE:HD11	7:AL:302:BCL:H171	1.91	0.53
6:AM:189:PHE:HB3	7:AM:402:BCL:CMD	2.38	0.53
7:AD:102:BCL:HHB	7:AF:101:BCL:CMA	2.37	0.53
3:AS:34:ALA:CB	7:AS:101:BCL:HBA2	2.38	0.53
6:BM:90:PHE:HB2	6:BM:180:PHE:CD2	2.43	0.53
7:BL:302:BCL:C14	8:BL:304:BPH:H172	2.35	0.53
7:AL:301:BCL:H141	8:AL:303:BPH:H152	1.91	0.53
3:BK:6:LEU:CD2	3:BK:7:GLY:HA2	2.28	0.53
3:A4:27:LEU:HD13	3:A4:30:PHE:HB3	1.90	0.53
5:AL:135:ARG:H	5:AL:136:PRO:CD	2.21	0.53
6:AM:201:PHE:HB3	6:AM:283:GLY:HA3	1.90	0.53
5:BL:23:ASP:HA	5:BL:32:GLY:HA2	1.90	0.53
5:AL:229:ILE:CD1	5:AL:232:LEU:HB3	2.26	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:22:TRP:CG	2:AB:23:VAL:N	2.75	0.53
5:AL:52:SER:HB2	5:AL:66:VAL:HG22	1.91	0.53
4:AH:91:ALA:CB	4:AH:96:PHE:HB2	2.38	0.53
3:AG:11:LEU:HB3	3:AG:14:GLU:HB2	1.90	0.53
6:AM:156:LEU:HD13	7:AM:402:BCL:H43	1.90	0.53
1:B1:28:ALA:O	1:B1:32:HIS:ND1	2.40	0.53
1:B7:24:LEU:HD12	1:B7:25:PHE:N	2.24	0.53
5:AL:5:PHE:CE1	6:AM:246:GLU:HG2	2.43	0.53
3:BI:43:ILE:HG23	3:BI:44:TRP:HD1	1.74	0.53
5:AL:197:ALA:O	5:AL:200:PRO:HG3	2.08	0.53
1:B1:16:VAL:HA	1:B1:20:GLN:HB2	1.90	0.53
8:BM:402:BPH:HBC3	8:BM:402:BPH:HHD	1.90	0.53
7:AT:101:BCL:HBC1	7:AT:102:BCL:HBC1	1.90	0.53
3:AU:41:VAL:HA	3:AU:44:TRP:O	2.08	0.53
5:AL:209:PRO:HB3	6:AM:235:LEU:HD13	1.90	0.53
4:AH:198:VAL:HG23	6:AM:8:SER:HB2	1.90	0.53
1:BF:43:TRP:CD1	1:BF:43:TRP:O	2.61	0.53
3:AW:9:THR:CG2	3:AW:10:GLY:HA3	2.38	0.53
1:BN:19:ALA:O	1:BN:23:PHE:HB3	2.08	0.53
1:AZ:26:LEU:HD11	6:AM:64:LEU:HD13	1.91	0.53
7:BL:302:BCL:C2B	7:BM:401:BCL:HMB2	2.39	0.53
5:AL:244:SER:CB	7:AL:301:BCL:HMA2	2.39	0.53
6:AM:164:ARG:H	6:AM:165:PRO:HD3	1.73	0.53
1:A7:10:ILE:CG1	1:A7:11:PHE:N	2.58	0.53
7:BV:102:BCL:HED3	7:BV:102:BCL:HAA2	1.90	0.53
6:AM:96:PRO:HB2	6:AM:171:TRP:HB3	1.91	0.53
1:AX:42:ASN:O	1:AX:43:TRP:CD2	2.62	0.53
3:BE:45:ARG:N	3:BE:46:PRO:HD3	2.24	0.53
1:BT:12:ASP:N	1:BT:13:PRO:CD	2.72	0.53
3:AE:3:LYS:HG3	3:AE:9:THR:HG23	1.90	0.53
1:BZ:37:SER:O	1:BZ:39:PRO:CD	2.54	0.53
6:BM:70:ILE:CG2	6:BM:177:TYR:HB3	2.39	0.53
4:AH:61:PRO:HB3	4:AH:76:PRO:HD2	1.91	0.53
4:BH:131:ILE:HB	4:BH:225:VAL:HG11	1.91	0.53
1:B5:10:ILE:HG13	1:B5:11:PHE:H	1.73	0.53
6:AM:9:GLN:CB	6:AM:10:VAL:CA	2.84	0.53
4:BH:205:VAL:HG12	4:BH:207:ALA:H	1.74	0.53
1:B2:26:LEU:HA	1:B2:29:VAL:HG12	1.91	0.53
3:AS:12:THR:CA	3:AS:13:ASP:CB	2.76	0.52
5:AL:148:TYR:HD1	8:AL:303:BPH:H141	1.74	0.52
8:AM:403:BPH:HHD	8:AM:403:BPH:HBC3	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AD:31:ILE:O	7:AD:102:BCL:HMD3	2.09	0.52
7:AT:102:BCL:CBC	3:AU:41:VAL:HG11	2.39	0.52
1:B1:12:ASP:C	1:B1:14:ARG:H	2.12	0.52
1:BN:12:ASP:CB	1:BN:13:PRO:HD3	2.36	0.52
3:AK:45:ARG:C	3:AK:47:TRP:N	2.60	0.52
5:AL:217:ARG:NH1	5:AL:223:SER:HB3	2.23	0.52
5:BL:196:SER:CB	5:BL:196:SER:HG	2.08	0.52
7:AD:101:BCL:HMC2	7:A8:101:BCL:OBB	2.06	0.52
3:BI:41:VAL:CG1	7:BI:101:BCL:HAC2	2.26	0.52
1:A1:15:ARG:HA	1:A1:19:ALA:HB3	1.91	0.52
2:BB:14:ASN:HB3	2:BB:15:PRO:CD	2.38	0.52
1:B5:35:LEU:HD12	1:B5:36:LEU:N	2.24	0.52
1:B7:26:LEU:HD13	5:BL:39:PHE:CD2	2.44	0.52
1:BV:42:ASN:C	1:BV:44:LEU:H	2.12	0.52
3:AE:28:TRP:C	3:AE:30:PHE:H	2.11	0.52
5:AL:218:ASP:HB3	6:AM:136:ARG:CG	2.39	0.52
7:BL:303:BCL:HBA1	7:BL:303:BCL:H71	1.91	0.52
1:AX:8:TRP:HB3	1:AX:9:MET:CE	2.39	0.52
6:AM:85:PHE:CD2	6:AM:86:LEU:HD12	2.44	0.52
3:BG:6:LEU:HD22	3:BG:7:GLY:HA2	1.91	0.52
1:AZ:28:ALA:O	1:AZ:32:HIS:ND1	2.42	0.52
3:BK:38:HIS:CE1	7:BK:101:BCL:HMD1	2.44	0.52
1:AN:42:ASN:O	1:AN:44:LEU:N	2.39	0.52
1:A7:12:ASP:HB2	1:A7:13:PRO:HD3	1.90	0.52
3:AQ:8:TYR:N	3:AQ:8:TYR:CD2	2.75	0.52
1:BT:11:PHE:HB2	1:BT:15:ARG:HB2	1.91	0.52
5:BL:169:TYR:HB3	5:BL:259:TRP:O	2.09	0.52
7:BM:401:BCL:H143	8:BM:402:BPH:HAA1	1.90	0.52
5:AL:233:GLY:HA2	5:AL:236:LEU:HD12	1.92	0.52
7:AL:302:BCL:HMA2	7:AL:302:BCL:H93	1.91	0.52
6:AM:153:ALA:HA	6:AM:277:THR:HG1	1.73	0.52
1:BZ:38:THR:CB	1:BZ:39:PRO:CD	2.57	0.52
1:BP:24:LEU:HA	7:BP:101:BCL:O2A	2.09	0.52
5:BL:33:PHE:HB3	5:BL:106:GLU:OE2	2.09	0.52
3:AS:12:THR:N	3:AS:13:ASP:CB	2.73	0.52
6:AM:208:PHE:CZ	6:AM:275:LEU:HD13	2.45	0.52
7:AT:101:BCL:CAC	7:AT:102:BCL:HBC1	2.40	0.52
7:AZ:101:BCL:HMD2	7:AS:101:BCL:C1D	2.39	0.52
5:BL:149:GLY:O	5:BL:153:HIS:HE1	1.90	0.52
3:BY:41:VAL:HB	7:BY:102:BCL:CBC	2.32	0.52
1:BF:43:TRP:CD1	1:BF:43:TRP:C	2.82	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AW:11:LEU:CB	3:AW:14:GLU:HB2	2.40	0.52
6:AM:281:GLY:O	6:AM:285:LEU:HB2	2.10	0.52
1:BT:29:VAL:HG13	1:BT:30:MET:H	1.72	0.52
1:BN:42:ASN:C	1:BN:44:LEU:H	2.13	0.52
4:BH:100:PRO:HG2	4:BH:104:PRO:HB3	1.91	0.52
4:BH:215:GLY:O	4:BH:217:PRO:HD3	2.09	0.52
5:AL:224:ILE:CG1	5:AL:224:ILE:O	2.57	0.52
7:BZ:101:BCL:HBD	7:BZ:101:BCL:HAA2	1.91	0.52
1:B7:24:LEU:HD12	1:B7:25:PHE:H	1.74	0.52
3:BE:11:LEU:HD13	3:BE:12:THR:N	2.20	0.52
1:A3:32:HIS:HA	1:A3:35:LEU:HD11	1.92	0.52
3:AO:45:ARG:N	3:AO:46:PRO:CD	2.73	0.52
5:BL:168:HIS:CD2	6:BM:183:LEU:HD22	2.45	0.52
7:BL:302:BCL:H122	8:BL:304:BPH:CHB	2.39	0.52
7:AT:101:BCL:O1D	7:AT:101:BCL:H2A	2.09	0.52
7:A7:101:BCL:HHB	7:A6:102:BCL:HMA1	1.91	0.52
7:BF:101:BCL:CBD	7:BF:101:BCL:HAA2	2.38	0.52
4:BH:198:VAL:HG11	6:BM:7:PHE:CD1	2.27	0.52
3:AQ:23:TYR:O	3:AQ:27:LEU:HB2	2.09	0.52
5:BL:244:SER:OG	7:BL:302:BCL:HMA2	2.10	0.52
6:AM:256:MET:O	9:AM:405:U10:H23	2.09	0.52
7:A7:101:BCL:HHB	7:A6:102:BCL:CMA	2.39	0.52
3:BO:38:HIS:CE1	7:BO:102:BCL:HAA1	2.44	0.52
1:B7:10:ILE:CG1	1:B7:11:PHE:H	2.07	0.52
3:BQ:43:ILE:HG23	3:BQ:44:TRP:CD1	2.37	0.52
3:BE:6:LEU:HD22	3:BE:7:GLY:CA	2.37	0.52
4:AH:150:GLY:HA2	4:AH:165:VAL:HA	1.91	0.52
3:BS:27:LEU:HD13	3:BS:30:PHE:HB3	1.91	0.52
6:AM:78:ALA:HB1	6:AM:84:VAL:HB	1.90	0.52
3:BS:12:THR:N	3:BS:14:GLU:N	2.51	0.51
1:BD:11:PHE:HD1	1:BD:15:ARG:HB2	1.75	0.51
1:BD:35:LEU:HB3	1:BD:43:TRP:HZ3	1.75	0.51
3:BO:45:ARG:N	3:BO:46:PRO:CD	2.71	0.51
3:AI:11:LEU:HD13	3:AI:12:THR:H	1.75	0.51
5:AL:154:LEU:C	5:AL:156:TRP:H	2.13	0.51
3:AY:6:LEU:HD22	3:AY:7:GLY:HA2	1.92	0.51
5:BL:176:ALA:HB1	5:BL:244:SER:OG	2.09	0.51
5:AL:97:PHE:HE2	5:AL:128:TYR:CD2	2.28	0.51
1:BN:31:ILE:HD12	7:BO:102:BCL:HMD3	1.92	0.51
7:BD:101:BCL:HMC2	7:B8:101:BCL:OBB	2.10	0.51
7:BL:302:BCL:H172	8:BL:304:BPH:HMA3	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BL:185:LEU:HD12	8:BM:402:BPH:HB	1.73	0.51
1:AZ:31:ILE:O	1:AZ:31:ILE:HD13	2.09	0.51
1:BZ:12:ASP:N	1:BZ:13:PRO:CD	2.73	0.51
1:B5:37:SER:HB3	5:BL:79:PRO:O	2.11	0.51
4:AH:31:LEU:HD21	6:AM:271:TRP:HD1	1.74	0.51
3:AY:11:LEU:HB3	3:AY:14:GLU:HB2	1.93	0.51
4:AH:12:LEU:HD13	4:AH:13:ALA:H	1.74	0.51
1:BP:10:ILE:HD13	1:BZ:17:PHE:HB3	1.91	0.51
5:BL:134:PHE:CD1	5:BL:249:ILE:HD11	2.44	0.51
3:AS:41:VAL:HG11	7:AS:101:BCL:HAC2	1.91	0.51
7:BP:101:BCL:HMA3	7:BO:102:BCL:HMA3	1.89	0.51
1:A2:29:VAL:HA	1:A2:32:HIS:ND1	2.25	0.51
3:AI:9:THR:CG2	3:AI:10:GLY:HA3	2.40	0.51
6:BM:164:ARG:NH2	6:BM:189:PHE:HE2	2.08	0.51
6:BM:270:ILE:HG12	6:BM:270:ILE:O	2.10	0.51
3:BS:12:THR:HB	3:BS:13:ASP:HB2	0.57	0.51
5:BL:186:ALA:HB3	5:BL:236:LEU:CD1	2.38	0.51
7:AD:101:BCL:OBB	7:A8:101:BCL:HMC3	2.11	0.51
1:B1:12:ASP:HB3	1:B1:13:PRO:CD	2.35	0.51
7:BT:101:BCL:HMC3	7:BZ:102:BCL:CMB	2.38	0.51
3:BI:38:HIS:HD2	3:BI:41:VAL:HG11	1.75	0.51
3:AE:44:TRP:CA	3:AE:45:ARG:HG2	2.39	0.51
1:BP:12:ASP:H	1:BP:13:PRO:HD2	1.75	0.51
5:BL:216:PHE:CG	9:BL:306:U10:H3M2	2.46	0.51
5:AL:224:ILE:HG12	5:AL:224:ILE:O	2.10	0.51
3:AO:38:HIS:HE1	7:AO:101:BCL:CAA	2.23	0.51
5:AL:60:ASN:C	5:AL:62:GLN:H	2.14	0.51
6:AM:88:ASP:C	6:AM:90:PHE:H	2.13	0.51
3:BS:12:THR:CB	3:BS:13:ASP:HB3	2.05	0.51
1:AP:24:LEU:HB2	7:AP:101:BCL:O1A	2.11	0.51
4:AH:38:GLU:H	6:AM:261:THR:CG2	2.24	0.51
4:BH:117:ARG:HE	4:BH:227:LEU:HB3	1.75	0.51
1:AD:12:ASP:H	1:AD:13:PRO:HD2	1.73	0.51
1:AD:26:LEU:O	1:AD:30:MET:HG2	2.11	0.51
3:B9:30:PHE:C	3:B9:32:ALA:H	2.13	0.51
5:BL:179:PHE:O	5:BL:236:LEU:O	2.29	0.51
4:BH:171:ILE:CB	4:BH:172:PRO:HD3	2.32	0.51
5:AL:34:PHE:HB3	5:AL:99:SER:O	2.11	0.51
2:BB:15:PRO:O	2:BB:16:LYS:HB2	2.10	0.51
5:BL:194:VAL:HG12	6:BM:238:ILE:HD11	1.93	0.51
1:A7:28:ALA:O	1:A7:31:ILE:HG22	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AV:42:ASN:C	1:AV:44:LEU:H	2.14	0.51
3:AG:32:ALA:O	3:AG:36:VAL:N	2.39	0.51
5:BL:250:ILE:O	5:BL:254:ILE:HG12	2.11	0.51
1:B5:37:SER:O	1:B5:38:THR:OG1	2.26	0.51
4:AH:35:ASN:HB3	6:AM:260:ALA:CB	2.41	0.51
4:BH:43:GLU:HB2	5:BL:4:SER:HA	1.92	0.51
7:BM:401:BCL:HAA2	7:BM:401:BCL:CBD	2.41	0.51
5:AL:177:ILE:HG12	7:AL:301:BCL:HMB3	1.93	0.51
7:BP:102:BCL:HAC2	3:BQ:41:VAL:HG13	1.84	0.51
5:AL:250:ILE:HD13	5:AL:250:ILE:N	2.26	0.51
3:BW:41:VAL:O	3:BW:46:PRO:HD2	2.09	0.51
4:BH:42:LEU:H	4:BH:53:GLN:NE2	2.08	0.51
1:A2:25:PHE:C	1:A2:27:LEU:H	2.14	0.51
7:AT:101:BCL:HAC1	7:AT:102:BCL:HBC1	1.92	0.50
1:AT:35:LEU:HD22	7:AT:102:BCL:HHD	1.92	0.50
1:BZ:43:TRP:CD1	1:BZ:43:TRP:C	2.84	0.50
5:AL:176:ALA:HB2	5:AL:243:PHE:HB3	1.90	0.50
6:AM:164:ARG:N	6:AM:165:PRO:HD3	2.25	0.50
5:BL:77:GLY:HA2	5:BL:87:GLN:HE22	1.76	0.50
3:A4:30:PHE:CE2	7:A4:101:BCL:HBD	2.46	0.50
3:AK:43:ILE:HG12	3:AK:47:TRP:HB2	1.93	0.50
3:A4:45:ARG:N	3:A4:46:PRO:CD	2.74	0.50
1:BP:8:TRP:C	1:BP:10:ILE:H	2.13	0.50
1:A1:22:VAL:O	1:A1:26:LEU:HB3	2.12	0.50
7:BL:302:BCL:HMB2	7:BM:401:BCL:HMB2	1.93	0.50
8:BL:304:BPH:HMC2	6:BM:213:ALA:CB	2.40	0.50
1:AD:27:LEU:HD22	7:AD:102:BCL:HED2	1.93	0.50
6:BM:241:ARG:HG2	6:BM:245:ALA:HB3	1.93	0.50
5:AL:184:ALA:HB2	6:AM:212:SER:OG	2.12	0.50
1:AT:43:TRP:HD1	7:AS:101:BCL:HBB1	1.77	0.50
7:BD:101:BCL:HMA3	7:B8:101:BCL:HMB3	1.94	0.50
1:BD:36:LEU:HD11	1:BD:44:LEU:CD2	2.41	0.50
4:BH:31:LEU:HD11	6:BM:271:TRP:CD1	2.47	0.50
6:AM:96:PRO:HB3	6:AM:115:TRP:CD2	2.46	0.50
3:AO:43:ILE:HG23	3:AO:44:TRP:HD1	1.76	0.50
5:AL:218:ASP:HB3	6:AM:136:ARG:HG3	1.93	0.50
1:AP:27:LEU:HG	1:AZ:25:PHE:HZ	1.76	0.50
4:BH:98:HIS:HE1	5:BL:10:ARG:HD3	1.76	0.50
5:AL:230:HIS:CE1	6:AM:223:ILE:HG21	2.46	0.50
6:AM:94:LEU:HD21	6:AM:114:LEU:O	2.11	0.50
1:B1:31:ILE:HA	1:B1:34:ILE:HB	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BI:41:VAL:HG13	7:BI:101:BCL:H2C	1.93	0.50
7:AK:101:BCL:HAA2	7:AK:101:BCL:CBD	2.41	0.50
5:AL:69:PRO:HG2	5:AL:142:TRP:HB2	1.94	0.50
3:BE:38:HIS:HB3	3:BE:42:TYR:HD2	1.76	0.50
1:BD:18:VAL:HG13	1:BD:18:VAL:O	2.11	0.50
5:AL:237:SER:O	8:AL:303:BPH:HBC3	2.12	0.50
1:BZ:13:PRO:HG3	3:BQ:6:LEU:HD11	1.94	0.50
7:AJ:101:BCL:CBB	7:AJ:101:BCL:HMB1	2.38	0.50
6:BM:118:ALA:HB3	6:BM:177:TYR:CE2	2.47	0.50
1:BX:43:TRP:CD1	1:BX:44:LEU:HB3	2.46	0.50
1:B7:8:TRP:HB2	3:BE:18:GLU:CD	2.31	0.50
4:AH:150:GLY:CA	4:AH:165:VAL:HG12	2.41	0.50
2:AB:22:TRP:O	2:AB:26:GLN:HG2	2.12	0.50
5:BL:127:ALA:HB2	5:BL:241:VAL:HG13	1.93	0.50
5:AL:190:HIS:CG	5:AL:229:ILE:HG12	2.46	0.50
3:AK:7:GLY:O	3:AK:8:TYR:O	2.29	0.50
6:BM:152:SER:HB3	6:BM:278:LEU:CD1	2.22	0.50
5:AL:190:HIS:NE2	5:AL:230:HIS:CE1	2.80	0.50
1:B1:28:ALA:HA	7:BI:101:BCL:OBD	2.12	0.50
6:BM:88:ASP:C	6:BM:90:PHE:N	2.64	0.50
6:BM:88:ASP:HA	6:BM:91:PHE:HD2	1.77	0.50
1:AJ:31:ILE:HG23	7:AJ:101:BCL:CMD	2.37	0.50
1:A5:37:SER:O	1:A5:38:THR:O	2.30	0.50
1:BN:10:ILE:HG21	1:BP:14:ARG:CB	2.38	0.50
7:BV:101:BCL:HMC3	7:BU:101:BCL:CBB	2.42	0.50
7:BV:102:BCL:CMC	1:BX:44:LEU:HD11	2.42	0.50
3:A8:44:TRP:HA	3:A8:45:ARG:HG2	1.94	0.50
3:BE:44:TRP:CA	3:BE:45:ARG:HG2	2.41	0.50
7:BL:303:BCL:HMA1	8:BL:304:BPH:C18	2.38	0.50
6:BM:202:HIS:HA	6:BM:205:SER:HB3	1.93	0.50
5:AL:189:LEU:HB2	9:AL:304:U10:H4M3	1.94	0.50
7:AL:302:BCL:H51	8:AL:303:BPH:CMB	2.41	0.50
6:BM:9:GLN:N	6:BM:10:VAL:HA	2.25	0.50
7:BD:101:BCL:CMC	7:B8:101:BCL:OBB	2.59	0.50
3:A4:23:TYR:HA	3:A4:27:LEU:HD23	1.93	0.50
3:B6:8:TYR:CZ	3:B6:12:THR:HB	2.47	0.50
1:B1:15:ARG:CA	1:B1:19:ALA:HB3	2.40	0.50
1:B3:42:ASN:O	1:B3:43:TRP:CG	2.64	0.50
1:AZ:47:SER:HB3	3:AQ:48:PHE:HB2	1.93	0.50
3:A9:15:GLN:O	3:A9:19:LEU:HB2	2.11	0.50
7:BT:101:BCL:HMC2	7:BZ:102:BCL:CMB	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AI:13:ASP:HB2	3:AI:16:ALA:HB3	1.94	0.49
1:A5:10:ILE:HG22	3:A6:19:LEU:HD21	1.94	0.49
1:BF:44:LEU:HG	1:BF:45:GLU:N	2.26	0.49
8:BL:304:BPH:HED1	6:BM:214:LEU:HD23	1.94	0.49
5:AL:174:MET:HG2	7:AM:401:BCL:O1D	2.12	0.49
5:AL:179:PHE:CE2	9:AL:304:U10:H211	2.48	0.49
6:AM:6:ILE:HG22	6:AM:7:PHE:N	2.27	0.49
1:BT:30:MET:HA	1:BT:33:LEU:HD12	1.92	0.49
6:AM:84:VAL:HG13	6:AM:87:ARG:CZ	2.41	0.49
5:AL:23:ASP:HA	5:AL:32:GLY:HA2	1.94	0.49
1:AX:12:ASP:N	1:AX:13:PRO:HD2	2.27	0.49
3:AQ:12:THR:O	3:AQ:12:THR:HG23	2.12	0.49
6:AM:238:ILE:CG1	6:AM:262:MET:HB3	2.34	0.49
1:BJ:27:LEU:HD22	7:BK:102:BCL:HED3	1.93	0.49
6:BM:88:ASP:O	6:BM:90:PHE:N	2.45	0.49
6:AM:133:THR:HG22	6:AM:146:THR:HB	1.93	0.49
4:BH:198:VAL:CG1	6:BM:7:PHE:HD1	2.16	0.49
5:BL:192:ALA:HB1	6:BM:145:HIS:CB	2.42	0.49
1:BP:20:GLN:HA	1:BP:23:PHE:HB2	1.93	0.49
5:BL:103:ARG:HH12	5:BL:107:ILE:HD11	1.78	0.49
3:BU:45:ARG:N	3:BU:46:PRO:CD	2.76	0.49
3:AQ:43:ILE:HG23	3:AQ:44:TRP:CD1	2.46	0.49
1:BZ:46:ILE:O	1:BZ:47:SER:C	2.50	0.49
4:AH:169:VAL:HG12	6:AM:12:VAL:HG21	1.94	0.49
1:AV:8:TRP:O	1:AV:9:MET:HB2	2.11	0.49
3:AY:41:VAL:CG1	7:AY:102:BCL:HBC1	2.42	0.49
3:A8:45:ARG:N	3:A8:46:PRO:CD	2.74	0.49
3:BY:38:HIS:HA	7:BY:101:BCL:HMD3	1.95	0.49
5:BL:102:LEU:HD13	5:BL:105:VAL:HG21	1.95	0.49
6:BM:129:TRP:CD2	8:BM:402:BPH:H1C2	2.47	0.49
1:AD:41:TYR:O	1:AD:43:TRP:N	2.46	0.49
7:AZ:101:BCL:CGD	7:AZ:101:BCL:HAA2	2.42	0.49
1:BZ:31:ILE:CG2	7:BZ:102:BCL:HMD3	2.26	0.49
6:AM:7:PHE:O	6:AM:8:SER:CB	2.61	0.49
6:BM:55:LEU:HD21	6:BM:135:LEU:CD1	2.41	0.49
4:BH:42:LEU:N	4:BH:53:GLN:HE22	2.10	0.49
3:A4:12:THR:HA	3:A4:13:ASP:O	2.13	0.49
4:BH:12:LEU:HD13	4:BH:13:ALA:H	1.77	0.49
4:AH:12:LEU:CD1	4:AH:13:ALA:H	2.26	0.49
5:BL:192:ALA:CB	6:BM:145:HIS:HB3	2.43	0.49
1:BP:38:THR:HB	1:BZ:45:GLU:OE1	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AL:139:MET:HG3	5:AL:253:THR:HG22	1.95	0.49
3:AW:38:HIS:HB3	3:AW:42:TYR:CE2	2.47	0.49
6:AM:216:PHE:HD1	6:AM:219:HIS:HB3	1.77	0.49
6:AM:43:GLY:C	6:AM:44:ASN:HD22	2.16	0.49
7:AT:102:BCL:HHB	7:AV:101:BCL:HMA1	1.93	0.49
7:AZ:101:BCL:H3A	7:AZ:101:BCL:CGA	2.43	0.49
7:BP:101:BCL:CMA	7:BO:102:BCL:HHB	2.28	0.49
3:AY:41:VAL:HA	3:AY:44:TRP:O	2.13	0.49
3:BU:45:ARG:N	3:BU:46:PRO:HD3	2.28	0.49
4:BH:31:LEU:HD21	6:BM:271:TRP:CD1	2.48	0.49
1:BZ:35:LEU:HD12	1:BZ:36:LEU:HG	1.94	0.49
3:AU:35:ILE:HA	3:AU:38:HIS:HB2	1.95	0.49
6:AM:270:ILE:O	6:AM:270:ILE:HG12	2.13	0.49
3:A4:34:ALA:O	3:A4:38:HIS:ND1	2.45	0.49
5:AL:148:TYR:CD1	8:AL:303:BPH:H141	2.45	0.49
5:AL:49:ILE:CD1	7:AL:302:BCL:H171	2.43	0.49
7:AF:101:BCL:HAA2	7:AF:101:BCL:HBD	1.95	0.49
1:AP:35:LEU:CD2	7:AP:102:BCL:HHD	2.43	0.49
7:BK:101:BCL:HAA2	7:BK:101:BCL:HBD	1.95	0.49
3:A9:38:HIS:HB3	3:A9:42:TYR:CE2	2.47	0.49
1:B2:9:MET:HG3	1:B2:10:ILE:HG23	1.94	0.49
1:B5:41:TYR:O	1:B5:43:TRP:N	2.46	0.49
3:A8:7:GLY:O	3:A8:8:TYR:HB2	2.13	0.49
5:AL:272:TRP:HA	5:AL:275:ILE:HD13	1.95	0.49
6:BM:162:PHE:CD2	6:BM:163:ILE:HG13	2.48	0.49
5:AL:239:SER:C	5:AL:241:VAL:N	2.65	0.49
1:A3:12:ASP:N	1:A3:13:PRO:CD	2.67	0.49
1:B5:38:THR:HA	5:BL:80:LEU:HG	1.95	0.49
5:BL:117:ILE:C	5:BL:119:PHE:H	2.17	0.49
1:B5:32:HIS:O	1:B5:36:LEU:HB2	2.13	0.49
1:AF:24:LEU:HD12	1:AF:25:PHE:N	2.28	0.49
4:BH:243:TYR:O	4:BH:246:PRO:HD3	2.13	0.49
1:BP:43:TRP:CD1	1:BP:43:TRP:C	2.85	0.49
5:BL:175:ILE:HG21	9:BL:306:U10:C26	2.42	0.49
6:AM:185:TRP:CZ3	7:AM:401:BCL:HAC1	2.48	0.49
5:BL:278:GLY:HA2	6:BM:77:GLN:O	2.13	0.49
1:A2:28:ALA:HB2	7:A9:101:BCL:OBD	2.13	0.49
4:AH:35:ASN:HB3	6:AM:260:ALA:CA	2.43	0.49
5:BL:113:ILE:HG22	6:BM:229:PHE:CE1	2.47	0.49
1:BD:13:PRO:HB2	4:BH:93:SER:HB3	1.95	0.49
1:BT:12:ASP:HB2	1:BT:13:PRO:HD3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BH:98:HIS:CE1	5:BL:10:ARG:HD3	2.48	0.49
1:BV:12:ASP:N	1:BV:13:PRO:CD	2.76	0.49
1:AD:43:TRP:C	1:AD:43:TRP:CD1	2.85	0.48
1:BD:10:ILE:HG13	1:BD:11:PHE:H	1.78	0.48
1:AT:43:TRP:O	1:AT:43:TRP:CD1	2.66	0.48
7:BZ:102:BCL:HAC2	3:BS:41:VAL:CG1	2.42	0.48
1:A1:41:TYR:O	1:A1:42:ASN:HB2	2.12	0.48
1:B3:29:VAL:HG23	7:B3:101:BCL:HMB2	1.95	0.48
3:AW:6:LEU:HA	3:AW:7:GLY:HA2	1.60	0.48
1:BD:39:PRO:HA	1:BD:42:ASN:HD21	1.78	0.48
4:BH:46:ASP:HA	5:BL:7:ARG:NH1	2.28	0.48
1:A2:12:ASP:N	1:A2:13:PRO:CD	2.74	0.48
1:B3:12:ASP:N	1:B3:13:PRO:CD	2.73	0.48
2:AB:55:LEU:H	2:AB:56:PRO:HD2	1.78	0.48
4:AH:18:TYR:C	4:AH:20:PHE:H	2.15	0.48
1:B1:47:SER:O	3:BG:48:PHE:HB3	2.13	0.48
5:BL:246:LEU:O	5:BL:250:ILE:HG12	2.12	0.48
5:AL:175:ILE:CG2	9:AL:304:U10:H23	2.43	0.48
6:AM:161:GLY:O	12:AM:406:SPO:H301	2.12	0.48
1:A7:22:VAL:O	1:A7:26:LEU:HB2	2.12	0.48
1:B2:41:TYR:O	1:B2:42:ASN:HB2	2.12	0.48
3:AY:45:ARG:N	3:AY:46:PRO:HD3	2.28	0.48
3:BG:44:TRP:HA	3:BG:45:ARG:HA	1.51	0.48
6:BM:164:ARG:CB	6:BM:165:PRO:HD3	2.42	0.48
1:A2:13:PRO:O	1:A2:16:VAL:HG12	2.13	0.48
1:AJ:29:VAL:HG13	1:AJ:30:MET:N	2.28	0.48
5:AL:233:GLY:C	5:AL:235:LEU:H	2.16	0.48
7:AZ:101:BCL:HBC2	3:AS:45:ARG:CD	2.33	0.48
1:BV:42:ASN:O	1:BV:43:TRP:CG	2.66	0.48
1:AD:12:ASP:H	1:AD:13:PRO:CD	2.26	0.48
3:BU:3:LYS:HG3	3:BU:11:LEU:HD21	1.96	0.48
6:AM:290:VAL:HG12	6:AM:291:VAL:N	2.27	0.48
1:AZ:43:TRP:C	1:AZ:43:TRP:CD1	2.86	0.48
7:BL:301:BCL:HBC1	7:BM:401:BCL:OBD	2.13	0.48
3:AS:11:LEU:HG	3:AS:11:LEU:O	2.12	0.48
3:BO:8:TYR:HA	3:BO:9:THR:HA	1.63	0.48
7:BF:101:BCL:HBA1	7:BF:101:BCL:O1D	2.13	0.48
3:B6:3:LYS:HG3	3:B6:11:LEU:HD21	1.95	0.48
7:BV:101:BCL:HBD	7:BV:101:BCL:HAA2	1.94	0.48
3:BU:44:TRP:HA	3:BU:45:ARG:HG2	1.95	0.48
4:BH:111:PRO:CG	4:BH:239:GLY:HA2	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AO:43:ILE:HG13	3:AO:47:TRP:HB3	1.95	0.48
1:BT:15:ARG:NH1	1:BV:17:PHE:HB3	2.27	0.48
1:AT:43:TRP:O	1:AT:43:TRP:HD1	1.96	0.48
7:A6:102:BCL:H2A	7:A6:102:BCL:HED3	1.96	0.48
7:A9:101:BCL:HHC	7:A9:101:BCL:HBB3	1.95	0.48
6:BM:238:ILE:CG2	6:BM:263:GLU:HB2	2.42	0.48
6:BM:223:ILE:HA	6:BM:226:VAL:HG22	1.94	0.48
1:BP:46:ILE:O	1:BP:47:SER:C	2.51	0.48
4:BH:41:PRO:HD2	4:BH:79:GLU:HG3	1.96	0.48
3:BO:12:THR:HA	3:BO:13:ASP:HA	1.55	0.48
4:BH:190:LEU:HD12	4:BH:233:ILE:HD13	1.95	0.48
3:AQ:32:ALA:O	3:AQ:36:VAL:N	2.46	0.48
5:BL:164:TYR:HB3	5:BL:259:TRP:HD1	1.78	0.48
6:BM:205:SER:HB2	6:BM:280:GLY:N	2.29	0.48
6:AM:175:VAL:HG21	7:AM:401:BCL:HMC1	1.95	0.48
1:AD:42:ASN:O	1:AD:43:TRP:CD2	2.67	0.48
3:AS:38:HIS:NE2	7:AS:101:BCL:HAA1	2.27	0.48
1:A1:12:ASP:HA	1:A1:15:ARG:CB	2.44	0.48
1:A3:41:TYR:O	1:A3:42:ASN:HB2	2.14	0.48
5:BL:278:GLY:N	6:BM:84:VAL:HG11	2.28	0.48
3:AW:8:TYR:HA	3:AW:9:THR:HA	1.55	0.48
3:BE:10:GLY:HA3	3:BE:11:LEU:HB3	1.96	0.48
3:AY:35:ILE:HA	3:AY:38:HIS:HD1	1.78	0.48
1:B7:12:ASP:N	1:B7:13:PRO:HD2	2.27	0.48
5:AL:207:ARG:HG3	5:AL:211:HIS:CG	2.49	0.48
3:AY:9:THR:CG2	3:AY:10:GLY:HA3	2.43	0.48
4:AH:42:LEU:HD23	5:AL:3:LEU:HD23	1.96	0.48
4:BH:11:ASP:OD1	4:BH:11:ASP:N	2.45	0.48
5:BL:173:HIS:N	5:BL:247:CYS:SG	2.86	0.48
6:AM:10:VAL:HG13	6:AM:11:GLN:N	2.05	0.48
1:BD:42:ASN:O	1:BD:43:TRP:CD2	2.66	0.48
3:BW:12:THR:HA	3:BW:13:ASP:HA	1.53	0.48
1:B2:12:ASP:N	1:B2:13:PRO:CD	2.65	0.48
3:A9:45:ARG:N	3:A9:46:PRO:HD3	2.29	0.48
3:BQ:8:TYR:N	3:BQ:8:TYR:CD2	2.82	0.48
1:BF:29:VAL:O	1:BF:33:LEU:HB2	2.14	0.48
5:BL:146:PHE:CE2	7:BL:303:BCL:HHC	2.48	0.48
7:BL:302:BCL:HBB2	7:BL:302:BCL:HMB1	1.93	0.48
3:AS:12:THR:N	3:AS:13:ASP:HB2	2.26	0.48
5:AL:101:ALA:HB2	5:AL:121:PHE:CD2	2.47	0.48
5:AL:181:PHE:CZ	7:AL:301:BCL:HBB2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BD:15:ARG:O	1:BD:20:GLN:HB2	2.13	0.48
1:AN:41:TYR:O	1:AN:42:ASN:HB2	2.13	0.48
5:AL:80:LEU:HD22	5:AL:85:LEU:HG	1.96	0.48
1:A2:12:ASP:H	1:A2:13:PRO:HD2	1.78	0.48
4:AH:170:ASP:CB	4:AH:175:MET:H	2.25	0.48
5:BL:224:ILE:CG2	5:BL:228:GLY:O	2.62	0.48
4:AH:20:PHE:C	4:AH:22:ILE:H	2.16	0.48
3:BU:9:THR:HG23	3:BU:11:LEU:HD23	1.96	0.48
1:B7:42:ASN:HB3	1:B7:45:GLU:HB2	1.96	0.48
3:AG:33:VAL:HG13	3:AG:37:ALA:HB3	1.96	0.48
1:AV:25:PHE:HA	1:AV:28:ALA:HB3	1.96	0.48
5:BL:93:ALA:HA	8:BL:304:BPH:H7C2	1.95	0.48
7:BL:302:BCL:CBB	7:BM:401:BCL:HHB	2.26	0.48
7:AP:102:BCL:HBA1	7:AP:102:BCL:H3A	1.57	0.48
1:A7:26:LEU:HD21	5:AL:39:PHE:O	2.13	0.48
4:BH:38:GLU:H	6:BM:261:THR:HG21	1.78	0.48
3:BQ:8:TYR:HD2	3:BQ:8:TYR:N	2.11	0.48
3:BK:3:LYS:HB2	3:BK:8:TYR:HB3	1.96	0.48
9:AL:304:U10:H4M2	9:AL:304:U10:C3M	2.36	0.48
5:AL:37:ALA:O	5:AL:41:PHE:CD2	2.67	0.48
3:AW:9:THR:HG22	3:AW:10:GLY:HA3	1.96	0.48
3:AU:12:THR:N	3:AU:14:GLU:H	2.12	0.48
3:BG:24:MET:HG3	3:BG:25:SER:N	2.27	0.48
5:BL:247:CYS:HA	5:BL:250:ILE:HG12	1.96	0.47
6:AM:175:VAL:HG21	7:AM:401:BCL:CMC	2.44	0.47
1:AD:36:LEU:HD21	1:AD:44:LEU:CD2	2.43	0.47
3:A6:41:VAL:HG12	7:A6:102:BCL:CBC	2.25	0.47
6:BM:73:TRP:HB2	6:BM:114:LEU:HD12	1.96	0.47
6:BM:229:PHE:CE2	6:BM:247:ARG:NE	2.81	0.47
6:AM:97:PRO:HG2	6:AM:171:TRP:HD1	1.79	0.47
1:B7:36:LEU:HD11	7:B7:101:BCL:HBB1	1.95	0.47
4:AH:112:ALA:HB2	4:AH:239:GLY:HA3	1.96	0.47
1:A5:20:GLN:HA	1:A5:23:PHE:CB	2.43	0.47
1:B7:34:ILE:HG12	5:BL:47:ILE:HG21	1.96	0.47
5:AL:233:GLY:CA	6:AM:216:PHE:CE2	2.98	0.47
1:B1:31:ILE:HG23	1:B1:35:LEU:HD23	1.95	0.47
1:A2:31:ILE:HA	1:A2:34:ILE:HD12	1.95	0.47
1:BD:36:LEU:CD2	1:BD:45:GLU:HB2	2.44	0.47
3:BK:45:ARG:C	3:BK:47:TRP:N	2.68	0.47
5:AL:38:THR:HG21	5:AL:100:TRP:CE3	2.39	0.47
1:AF:41:TYR:O	1:AF:42:ASN:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B6:34:ALA:HB1	7:B6:101:BCL:HAA2	1.95	0.47
1:BT:33:LEU:HD13	6:BM:75:TRP:CH2	2.49	0.47
5:AL:55:LEU:HD13	5:AL:81:ALA:HB2	1.96	0.47
8:BL:304:BPH:CED	6:BM:214:LEU:CD2	2.92	0.47
5:BL:48:LEU:HB3	5:BL:89:ILE:HG12	1.95	0.47
6:AM:256:MET:HE2	9:AM:405:U10:H71	1.96	0.47
8:AL:303:BPH:H161	8:AL:303:BPH:H141	1.59	0.47
5:AL:215:PHE:CZ	6:AM:146:THR:HG21	2.47	0.47
1:BJ:42:ASN:HB3	1:BJ:45:GLU:HB2	1.96	0.47
1:BJ:30:MET:O	1:BJ:33:LEU:HB2	2.15	0.47
3:AU:3:LYS:HB2	3:AU:8:TYR:HB3	1.96	0.47
5:BL:249:ILE:HG22	5:BL:250:ILE:HG23	1.96	0.47
7:BM:401:BCL:HBD	7:BM:401:BCL:HAA2	1.96	0.47
6:AM:130:TRP:HD1	6:AM:150:PHE:CD2	2.32	0.47
1:AD:43:TRP:NE1	1:AD:44:LEU:HD22	2.29	0.47
7:AT:102:BCL:HBA1	7:AT:102:BCL:H3A	1.41	0.47
7:AT:101:BCL:CBC	7:AT:102:BCL:HBC1	2.45	0.47
3:B4:30:PHE:CE2	7:B4:101:BCL:HBD	2.50	0.47
3:AI:43:ILE:CG2	3:AI:44:TRP:HD1	2.17	0.47
1:B7:25:PHE:O	1:B7:29:VAL:HG12	2.15	0.47
3:BQ:44:TRP:HA	3:BQ:45:ARG:HA	1.61	0.47
3:AK:44:TRP:HA	3:AK:45:ARG:HA	1.52	0.47
3:BS:20:HIS:HA	3:BS:24:MET:HB3	1.97	0.47
1:BT:43:TRP:O	1:BT:43:TRP:HD1	1.98	0.47
6:BM:130:TRP:CD1	6:BM:150:PHE:CD2	2.96	0.47
1:BZ:31:ILE:HD13	1:BZ:34:ILE:HD12	1.95	0.47
3:BI:38:HIS:HA	3:BI:41:VAL:HB	1.95	0.47
1:B5:29:VAL:HA	1:B5:32:HIS:CD2	2.49	0.47
7:BV:101:BCL:HMC3	7:BU:101:BCL:HBB3	1.97	0.47
1:BJ:12:ASP:CB	1:BJ:13:PRO:HD3	2.38	0.47
1:AX:37:SER:HB2	5:AL:270:PRO:HB3	1.95	0.47
4:BH:245:ALA:HB3	4:BH:251:VAL:HG11	1.96	0.47
5:BL:166:ASN:O	5:BL:169:TYR:HB2	2.15	0.47
5:AL:232:LEU:HD21	9:AL:304:U10:H122	1.96	0.47
7:A2:101:BCL:HMD2	7:A9:101:BCL:HAC1	1.96	0.47
3:AK:45:ARG:O	3:AK:47:TRP:N	2.47	0.47
6:AM:193:HIS:C	6:AM:293:ASN:HA	2.34	0.47
3:BU:12:THR:H	3:BU:14:GLU:H	1.61	0.47
6:AM:290:VAL:HG12	6:AM:291:VAL:HG23	1.97	0.47
1:B2:46:ILE:O	1:B2:48:ALA:N	2.48	0.47
3:BS:11:LEU:HA	3:BS:15:GLN:N	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BL:49:ILE:HD12	7:BL:303:BCL:H203	1.97	0.47
6:AM:206:ILE:HA	7:AM:402:BCL:CMA	2.44	0.47
1:AV:32:HIS:CE1	7:AV:101:BCL:CHB	2.98	0.47
7:B2:101:BCL:CMA	7:BK:102:BCL:CMA	2.76	0.47
4:AH:153:VAL:CG1	4:AH:154:ARG:N	2.70	0.47
6:BM:88:ASP:HB2	6:BM:92:PHE:CZ	2.48	0.47
3:A4:11:LEU:HD22	3:A4:11:LEU:C	2.35	0.47
5:BL:69:PRO:HD3	5:BL:86:TRP:CD2	2.50	0.47
3:BQ:45:ARG:N	3:BQ:46:PRO:HD3	2.30	0.47
3:BS:6:LEU:CD1	3:BS:7:GLY:H	2.25	0.47
4:AH:52:ASN:CG	4:AH:53:GLN:H	2.18	0.47
1:A2:21:GLY:O	1:A2:23:PHE:N	2.48	0.47
1:BV:42:ASN:O	1:BV:44:LEU:N	2.46	0.47
1:BX:26:LEU:O	1:BX:30:MET:HG2	2.15	0.47
5:BL:187:LEU:HD11	6:BM:269:ALA:HB1	1.97	0.47
3:AO:41:VAL:HG22	7:AO:101:BCL:HBC1	1.96	0.47
3:AW:10:GLY:HA2	3:AW:11:LEU:HA	1.68	0.47
4:BH:20:PHE:CE2	4:BH:24:LEU:HD22	2.50	0.47
1:A5:16:VAL:HA	1:A5:20:GLN:HB2	1.97	0.47
3:A8:30:PHE:HA	3:A8:33:VAL:HB	1.96	0.47
3:AO:19:LEU:HA	3:AO:23:TYR:HB2	1.95	0.47
3:AQ:28:TRP:O	3:AQ:28:TRP:HD1	1.98	0.47
3:BQ:12:THR:HG23	3:BQ:12:THR:O	2.15	0.47
5:AL:158:SER:O	5:AL:161:GLY:N	2.45	0.47
5:BL:241:VAL:HG21	8:BL:304:BPH:HBC1	1.92	0.47
5:BL:97:PHE:CE2	7:BL:302:BCL:H91	2.50	0.47
7:B2:101:BCL:HAA2	7:B2:101:BCL:HBD	1.97	0.47
1:B5:12:ASP:CB	1:B5:13:PRO:HD3	2.40	0.47
3:AI:11:LEU:HD13	3:AI:12:THR:N	2.30	0.47
6:BM:95:GLU:HB3	6:BM:96:PRO:HD2	1.97	0.47
5:BL:129:LEU:HA	5:BL:132:VAL:HG22	1.97	0.47
5:BL:183:ASN:HD21	5:BL:237:SER:HG	1.54	0.46
7:BL:302:BCL:H141	8:BL:304:BPH:H152	1.97	0.46
8:BL:304:BPH:CMD	6:BM:218:MET:HG3	2.43	0.46
1:AD:42:ASN:O	1:AD:43:TRP:CG	2.68	0.46
7:AD:102:BCL:HMB3	7:AF:101:BCL:C4A	2.45	0.46
1:A7:26:LEU:HD13	5:AL:39:PHE:CD2	2.50	0.46
4:BH:193:MET:O	4:BH:196:VAL:HG22	2.16	0.46
3:B6:11:LEU:HB3	3:B6:14:GLU:HB2	1.98	0.46
1:AZ:15:ARG:HG2	1:AZ:19:ALA:HB2	1.96	0.46
1:BP:12:ASP:H	1:BP:13:PRO:CD	2.28	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BM:171:TRP:HA	6:BM:171:TRP:HE3	1.80	0.46
3:A6:39:LEU:HD22	2:BB:49:ARG:HB3	1.96	0.46
2:AB:26:GLN:HG2	2:AB:26:GLN:H	1.45	0.46
3:AU:7:GLY:O	3:AU:8:TYR:C	2.52	0.46
5:BL:181:PHE:HE2	7:BL:301:BCL:C3D	2.28	0.46
6:AM:157:TRP:HD1	7:AM:401:BCL:HBB1	1.79	0.46
1:BZ:31:ILE:HG21	7:BZ:102:BCL:HMD1	1.94	0.46
3:AI:39:LEU:O	3:AI:43:ILE:HG22	2.14	0.46
4:BH:45:GLU:HG3	5:BL:2:LEU:HD11	1.97	0.46
3:B6:11:LEU:O	3:B6:12:THR:C	2.54	0.46
1:A1:10:ILE:HG13	1:A1:11:PHE:N	2.22	0.46
3:B6:45:ARG:H	3:B6:46:PRO:HD3	1.76	0.46
3:B9:9:THR:HA	3:B9:10:GLY:HA3	1.56	0.46
6:AM:88:ASP:C	6:AM:90:PHE:N	2.68	0.46
4:BH:244:ALA:HA	4:BH:245:ALA:HA	1.68	0.46
3:AI:6:LEU:HA	3:AI:7:GLY:HA2	1.49	0.46
3:AO:12:THR:HA	3:AO:13:ASP:HA	1.49	0.46
7:BM:401:BCL:H151	8:BM:402:BPH:C3A	2.40	0.46
5:AL:229:ILE:HD13	9:AL:304:U10:C4	2.45	0.46
6:AM:154:ILE:HG22	6:AM:154:ILE:O	2.16	0.46
8:AM:403:BPH:H9C3	8:AM:403:BPH:H6C1	1.68	0.46
7:BP:101:BCL:HHD	3:BQ:41:VAL:HG21	1.97	0.46
1:A7:26:LEU:HG	5:AL:40:PHE:CD1	2.27	0.46
1:BD:31:ILE:HD13	7:BD:102:BCL:HMD3	1.97	0.46
3:BE:11:LEU:HD12	3:BE:11:LEU:N	2.29	0.46
3:BE:8:TYR:HA	3:BE:9:THR:HA	1.52	0.46
7:A3:101:BCL:HBB3	7:AY:102:BCL:HBB2	1.97	0.46
3:BW:41:VAL:O	3:BW:46:PRO:CD	2.63	0.46
5:AL:196:SER:CB	6:AM:143:GLY:HA3	2.45	0.46
5:BL:229:ILE:HG13	5:BL:229:ILE:O	2.15	0.46
3:BQ:9:THR:HA	3:BQ:10:GLY:HA3	1.54	0.46
6:AM:256:MET:CE	9:AM:405:U10:H71	2.45	0.46
5:AL:177:ILE:C	5:AL:179:PHE:H	2.18	0.46
3:A8:38:HIS:HA	3:A8:41:VAL:HB	1.97	0.46
3:AU:41:VAL:HG12	3:AU:41:VAL:O	2.14	0.46
3:AW:11:LEU:N	3:AW:15:GLN:N	2.56	0.46
7:AY:102:BCL:HBA1	7:AY:102:BCL:H3A	1.47	0.46
3:B8:44:TRP:HA	3:B8:45:ARG:HA	1.68	0.46
1:B2:12:ASP:H	1:B2:13:PRO:HD2	1.80	0.46
5:BL:194:VAL:CG1	6:BM:238:ILE:HD11	2.46	0.46
3:A8:10:GLY:CA	3:A8:11:LEU:HB2	2.41	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AP:42:ASN:O	1:AP:44:LEU:HD23	2.16	0.46
6:AM:264:GLY:HA2	6:AM:267:ARG:HG3	1.97	0.46
1:A5:26:LEU:HD22	1:A7:25:PHE:HE2	1.80	0.46
3:B4:44:TRP:HA	3:B4:45:ARG:HA	1.55	0.46
5:BL:130:THR:HG21	5:BL:245:ALA:CB	2.46	0.46
1:AD:31:ILE:HG23	7:AD:102:BCL:CMD	2.46	0.46
3:AE:6:LEU:HA	3:AE:7:GLY:HA2	1.56	0.46
3:BO:8:TYR:HA	3:BO:10:GLY:HA2	1.97	0.46
3:AG:44:TRP:HE3	3:AG:45:ARG:CG	2.27	0.46
3:B4:11:LEU:HB3	3:B4:14:GLU:HG2	1.97	0.46
5:BL:175:ILE:HD12	9:BL:306:U10:C26	2.40	0.46
7:AP:101:BCL:CMA	7:AO:101:BCL:HHB	2.30	0.46
7:AI:101:BCL:HHB	7:AK:101:BCL:HMA1	1.97	0.46
1:BD:41:TYR:O	1:BD:43:TRP:N	2.49	0.46
1:A5:22:VAL:CA	1:A5:25:PHE:HB3	2.42	0.46
3:BU:12:THR:N	3:BU:14:GLU:H	2.14	0.46
3:B4:10:GLY:HA2	3:B4:11:LEU:HA	1.71	0.46
5:BL:98:VAL:HG12	5:BL:98:VAL:O	2.16	0.46
7:BT:101:BCL:HMB3	7:BZ:102:BCL:HMA3	1.98	0.46
3:BI:9:THR:HA	3:BI:10:GLY:HA3	1.57	0.46
3:AG:44:TRP:HA	3:AG:46:PRO:HD2	1.97	0.46
1:A3:28:ALA:O	1:A3:31:ILE:HG22	2.16	0.46
1:B2:15:ARG:HH11	1:BN:18:VAL:HB	1.80	0.46
3:AW:44:TRP:C	3:AW:45:ARG:HG2	2.36	0.46
3:A4:44:TRP:HA	3:A4:45:ARG:HA	1.47	0.46
3:A4:43:ILE:C	3:A4:46:PRO:HD2	2.36	0.46
2:BB:18:ASN:ND2	2:BB:18:ASN:O	2.48	0.46
1:BP:42:ASN:C	1:BP:44:LEU:H	2.18	0.46
3:AK:35:ILE:HA	3:AK:38:HIS:HB2	1.97	0.46
1:BZ:8:TRP:C	1:BZ:10:ILE:H	2.18	0.46
5:AL:194:VAL:HG21	6:AM:234:GLU:HB3	1.97	0.46
4:AH:142:VAL:CG1	4:AH:147:ASN:HB3	2.45	0.46
1:B1:42:ASN:O	1:B1:44:LEU:N	2.48	0.46
9:BL:306:U10:H372	9:BL:306:U10:H351	1.73	0.46
7:AL:302:BCL:CHB	8:AL:303:BPH:HMB3	2.41	0.46
7:AP:102:BCL:OBB	7:AZ:101:BCL:HMC2	2.16	0.46
1:AP:36:LEU:HD11	7:AP:101:BCL:HBB1	1.96	0.46
7:BV:102:BCL:H3A	7:BV:102:BCL:HBA1	1.28	0.46
3:AW:45:ARG:N	3:AW:46:PRO:HD3	2.31	0.46
3:B8:6:LEU:HA	3:B8:7:GLY:HA2	1.54	0.46
1:B3:43:TRP:O	1:B3:43:TRP:HD1	1.99	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AH:189:ARG:NE	4:AH:214:ALA:HA	2.30	0.46
3:AU:38:HIS:O	3:AU:42:TYR:N	2.49	0.46
1:AP:10:ILE:O	1:AP:10:ILE:HG23	2.15	0.46
4:BH:114:TRP:CD1	4:BH:232:LYS:HE2	2.51	0.46
4:BH:28:ILE:O	4:BH:28:ILE:HG22	2.15	0.46
6:AM:237:GLN:HE22	6:AM:242:GLY:HA3	1.80	0.46
7:AM:402:BCL:H3A	7:AM:402:BCL:HBA2	1.52	0.46
4:AH:148:PRO:HG2	6:AM:5:ASN:O	2.15	0.46
1:AD:42:ASN:CG	1:AD:45:GLU:HB3	2.36	0.46
1:AF:43:TRP:HE1	7:AF:101:BCL:HHC	1.81	0.46
7:BD:102:BCL:HHB	7:BF:101:BCL:HMA3	1.98	0.46
3:A4:8:TYR:HA	3:A4:9:THR:HA	1.62	0.46
6:BM:293:ASN:HB2	6:BM:296:VAL:HB	1.97	0.46
1:BT:29:VAL:CG1	1:BT:30:MET:N	2.79	0.46
1:AP:40:SER:HB3	1:AZ:47:SER:HB2	1.98	0.46
9:AM:405:U10:C8	9:AM:405:U10:C1M	2.94	0.46
7:AL:301:BCL:HBA1	7:AL:301:BCL:HED3	1.98	0.46
3:AG:44:TRP:HA	3:AG:45:ARG:HA	1.55	0.46
3:BW:9:THR:HG22	3:BW:10:GLY:CA	2.37	0.46
6:BM:73:TRP:CG	6:BM:94:LEU:HD13	2.51	0.46
1:AZ:42:ASN:O	1:AZ:44:LEU:N	2.46	0.46
6:BM:96:PRO:CB	6:BM:97:PRO:CD	2.94	0.46
1:A2:12:ASP:HB2	1:A2:13:PRO:HD3	1.98	0.46
3:BK:9:THR:CG2	3:BK:10:GLY:HA3	2.45	0.46
1:BT:43:TRP:CD1	1:BT:43:TRP:O	2.69	0.46
1:AT:41:TYR:O	1:AT:42:ASN:HB2	2.15	0.46
6:AM:300:ASN:HA	6:AM:304:ALA:HB3	1.98	0.46
1:B3:33:LEU:HA	1:B3:36:LEU:HD12	1.97	0.46
3:BY:12:THR:HA	3:BY:13:ASP:HA	1.55	0.46
6:AM:123:PHE:O	6:AM:127:TRP:HB2	2.16	0.46
7:BL:302:BCL:H161	7:BL:303:BCL:H72	1.98	0.45
1:AJ:11:PHE:HB3	1:AJ:14:ARG:HB3	1.98	0.45
7:B2:101:BCL:HBA2	7:B2:101:BCL:O1D	2.16	0.45
7:BV:101:BCL:HHD	7:BV:101:BCL:HAC1	1.89	0.45
3:BW:44:TRP:HA	3:BW:45:ARG:HA	1.63	0.45
3:A8:9:THR:HA	3:A8:10:GLY:HA2	1.65	0.45
5:BL:198:ALA:HA	5:BL:206:MET:HG3	1.98	0.45
1:AN:10:ILE:HG21	1:AP:14:ARG:HB2	1.99	0.45
5:BL:52:SER:HB3	5:BL:65:SER:O	2.16	0.45
3:AE:8:TYR:HA	3:AE:9:THR:HA	1.53	0.45
5:BL:181:PHE:HZ	7:BL:302:BCL:HBB1	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BZ:37:SER:C	1:BZ:38:THR:OG1	2.54	0.45
3:AI:38:HIS:HE1	7:AI:101:BCL:HAA1	1.81	0.45
6:BM:5:ASN:HA	6:BM:41:TRP:CH2	2.51	0.45
1:A2:31:ILE:O	1:A2:35:LEU:HG	2.16	0.45
4:BH:154:ARG:HH21	4:BH:204:HIS:CG	2.34	0.45
3:AG:44:TRP:CA	3:AG:46:PRO:HD2	2.45	0.45
2:AB:29:LYS:HD3	4:AH:259:TYR:CE2	2.51	0.45
1:B7:38:THR:C	1:B7:40:SER:N	2.70	0.45
1:A3:29:VAL:HG23	7:A3:101:BCL:HMB2	1.98	0.45
1:AP:42:ASN:O	1:AP:44:LEU:N	2.49	0.45
1:B1:46:ILE:HG22	1:B1:46:ILE:O	2.17	0.45
1:AZ:38:THR:O	1:AZ:39:PRO:C	2.54	0.45
5:AL:240:ALA:O	5:AL:244:SER:OG	2.31	0.45
9:AL:304:U10:H1M1	9:AL:304:U10:H72	1.75	0.45
5:AL:141:ALA:C	5:AL:143:GLY:H	2.20	0.45
6:BM:296:VAL:O	6:BM:296:VAL:CG1	2.62	0.45
5:BL:135:ARG:HB3	5:BL:136:PRO:HD3	1.98	0.45
1:A2:10:ILE:HD11	1:AN:15:ARG:HA	1.99	0.45
1:BJ:15:ARG:HH12	1:B2:18:VAL:HB	1.80	0.45
1:AV:14:ARG:O	1:AV:15:ARG:HB2	2.15	0.45
7:AM:401:BCL:HBA1	7:AM:401:BCL:H3A	1.63	0.45
7:BZ:101:BCL:CGD	7:BZ:101:BCL:HAA2	2.47	0.45
3:B4:5:ASP:CG	3:B4:6:LEU:N	2.69	0.45
1:AN:42:ASN:O	1:AN:43:TRP:CD2	2.68	0.45
1:AJ:41:TYR:O	1:AJ:42:ASN:HB2	2.16	0.45
4:AH:244:ALA:HA	4:AH:245:ALA:HA	1.69	0.45
1:BZ:47:SER:HB3	3:BQ:48:PHE:CD1	2.52	0.45
9:BL:306:U10:H272	9:BL:306:U10:H251	1.46	0.45
5:BL:48:LEU:HD22	5:BL:89:ILE:HG12	1.98	0.45
1:AD:34:ILE:C	1:AD:36:LEU:H	2.19	0.45
3:A9:8:TYR:HA	3:A9:9:THR:HA	1.63	0.45
3:AS:34:ALA:HB1	7:AS:101:BCL:HBA1	1.96	0.45
1:BD:13:PRO:HB2	4:BH:93:SER:CB	2.47	0.45
3:BK:10:GLY:HA2	3:BK:11:LEU:HA	1.59	0.45
6:AM:286:LEU:HD22	6:AM:290:VAL:HG21	1.98	0.45
6:BM:56:GLY:C	6:BM:58:LEU:H	2.19	0.45
6:AM:69:THR:HG21	6:AM:117:ILE:HB	1.99	0.45
3:BE:36:VAL:HG13	3:BE:39:LEU:HD12	1.97	0.45
2:BB:26:GLN:HG2	2:BB:26:GLN:H	1.41	0.45
7:AL:301:BCL:C14	8:AL:303:BPH:H152	2.46	0.45
6:AM:68:PHE:O	6:AM:72:ILE:HG12	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AU:44:TRP:CA	3:AU:45:ARG:HG2	2.40	0.45
3:BI:11:LEU:O	3:BI:12:THR:C	2.55	0.45
1:A7:10:ILE:HG23	1:A7:11:PHE:H	1.81	0.45
1:AJ:44:LEU:O	1:AJ:44:LEU:HG	2.17	0.45
1:A3:31:ILE:CG2	7:A4:101:BCL:HMD3	2.46	0.45
4:BH:111:PRO:HB2	4:BH:239:GLY:HA2	1.97	0.45
5:AL:234:LEU:CD1	6:AM:217:ALA:O	2.64	0.45
3:BU:12:THR:HA	3:BU:13:ASP:HA	1.56	0.45
3:AK:12:THR:HA	3:AK:13:ASP:HA	1.49	0.45
3:BK:14:GLU:O	3:BK:18:GLU:HB2	2.17	0.45
4:AH:122:GLU:HB2	4:AH:227:LEU:HD21	1.99	0.45
1:AF:14:ARG:HG3	4:AH:51:ALA:HB1	1.99	0.45
5:BL:260:VAL:O	5:BL:260:VAL:HG22	2.17	0.45
5:BL:168:HIS:NE2	7:BL:301:BCL:HMD3	2.32	0.45
9:BL:306:U10:H72	9:BL:306:U10:H1M1	1.77	0.45
6:BM:202:HIS:HB2	7:BM:401:BCL:HED1	1.97	0.45
3:AO:38:HIS:HE1	7:AO:101:BCL:HAA2	1.81	0.45
4:BH:75:VAL:HG11	6:BM:239:ALA:HA	1.99	0.45
1:B1:10:ILE:HG13	1:B1:11:PHE:N	2.25	0.45
3:BW:43:ILE:HG12	3:BW:44:TRP:CD1	2.52	0.45
1:BX:43:TRP:C	1:BX:43:TRP:CD1	2.90	0.45
4:BH:31:LEU:HD11	6:BM:271:TRP:CG	2.52	0.45
4:BH:35:ASN:O	6:BM:261:THR:HG23	2.17	0.45
3:B9:45:ARG:N	3:B9:46:PRO:CD	2.79	0.45
1:BD:22:VAL:CA	1:BD:25:PHE:HB3	2.46	0.45
1:BN:42:ASN:O	1:BN:43:TRP:CG	2.70	0.45
5:AL:125:ILE:O	5:AL:129:LEU:HD13	2.16	0.45
5:AL:62:GLN:O	5:AL:63:LEU:HD13	2.17	0.45
1:BV:12:ASP:H	1:BV:13:PRO:CD	2.29	0.45
5:AL:13:GLY:O	5:AL:15:THR:N	2.44	0.45
6:AM:129:TRP:CE3	8:AM:403:BPH:H1C2	2.49	0.45
1:BN:31:ILE:HD13	1:BN:31:ILE:O	2.17	0.45
3:BS:45:ARG:CB	3:BS:46:PRO:HD3	2.41	0.45
3:BY:41:VAL:CB	7:BY:102:BCL:HBC1	2.32	0.45
7:A4:101:BCL:HED3	7:A4:101:BCL:H2A	1.99	0.45
3:B6:9:THR:HA	3:B6:10:GLY:HA3	1.56	0.45
3:BO:44:TRP:HA	3:BO:45:ARG:HA	1.56	0.45
3:AY:34:ALA:O	3:AY:38:HIS:ND1	2.50	0.45
3:AI:12:THR:HA	3:AI:13:ASP:HA	1.47	0.45
5:AL:206:MET:HG2	5:AL:207:ARG:N	2.32	0.45
3:AU:9:THR:CG2	3:AU:10:GLY:HA3	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:34:ALA:O	3:B8:38:HIS:HB2	2.17	0.45
5:BL:127:ALA:HB3	7:BL:302:BCL:C1	2.40	0.45
5:BL:219:LEU:HD23	5:BL:220:VAL:HG22	1.99	0.45
1:AJ:12:ASP:CB	1:AJ:13:PRO:CD	2.89	0.45
3:AU:45:ARG:H	3:AU:46:PRO:CD	2.03	0.45
7:BP:101:BCL:HED3	3:BQ:34:ALA:HA	1.99	0.45
3:AE:44:TRP:HA	3:AE:45:ARG:HA	1.71	0.45
4:BH:193:MET:SD	6:BM:10:VAL:HG23	2.57	0.45
3:BK:44:TRP:HA	3:BK:45:ARG:HA	1.53	0.45
3:BE:12:THR:HA	3:BE:13:ASP:HA	1.58	0.45
6:BM:21:THR:HG23	6:BM:26:LEU:HD13	1.98	0.45
5:AL:113:ILE:HG22	6:AM:247:ARG:HB3	1.99	0.45
3:B6:3:LYS:HB2	3:B6:8:TYR:HB3	1.98	0.45
1:A5:43:TRP:CD1	1:A5:43:TRP:C	2.90	0.45
3:B9:11:LEU:H	3:B9:14:GLU:HB2	1.82	0.45
5:BL:151:TRP:O	5:BL:154:LEU:HB2	2.17	0.45
3:AW:16:ALA:HA	3:AW:20:HIS:CG	2.51	0.45
4:BH:12:LEU:HA	4:BH:12:LEU:HD22	1.83	0.45
6:AM:284:ILE:O	6:AM:284:ILE:CG2	2.65	0.45
1:AN:46:ILE:O	1:AN:48:ALA:N	2.50	0.45
3:BU:11:LEU:H	3:BU:14:GLU:HB2	1.82	0.45
3:B4:9:THR:HA	3:B4:10:GLY:HA3	1.68	0.45
5:BL:91:ILE:O	5:BL:91:ILE:HG22	2.16	0.45
5:BL:238:LEU:O	5:BL:241:VAL:HB	2.16	0.45
3:A9:9:THR:HA	3:A9:10:GLY:HA3	1.55	0.45
7:BP:101:BCL:HAA2	7:BP:101:BCL:HBD	1.99	0.45
7:AJ:101:BCL:HAC2	3:AK:41:VAL:HB	1.99	0.45
3:BK:43:ILE:HG23	3:BK:43:ILE:O	2.15	0.45
3:B6:8:TYR:HA	3:B6:9:THR:HA	1.72	0.45
3:AK:43:ILE:C	3:AK:46:PRO:HD2	2.37	0.45
3:AY:3:LYS:HE3	3:AY:11:LEU:HD21	1.99	0.45
6:BM:54:SER:C	6:BM:56:GLY:H	2.21	0.45
3:BU:21:SER:HA	3:BU:25:SER:HB3	1.99	0.45
3:BY:9:THR:HA	3:BY:10:GLY:HA3	1.66	0.45
7:BL:301:BCL:HBB1	6:BM:157:TRP:HD1	1.83	0.44
7:B9:101:BCL:HBB2	7:BO:101:BCL:OBB	2.17	0.44
1:AJ:12:ASP:C	1:AJ:14:ARG:H	2.20	0.44
1:A1:31:ILE:HD13	1:A1:35:LEU:HB3	1.99	0.44
1:A1:43:TRP:NE1	1:A1:44:LEU:HD22	2.32	0.44
3:B8:41:VAL:HG12	7:B8:101:BCL:CAC	2.43	0.44
3:BE:9:THR:HA	3:BE:10:GLY:HA3	1.71	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BW:9:THR:HG23	3:BW:11:LEU:HD12	1.99	0.44
1:B7:38:THR:O	1:B7:39:PRO:C	2.55	0.44
3:BU:8:TYR:HA	3:BU:9:THR:HA	1.60	0.44
2:AB:45:ILE:O	2:AB:48:PHE:HB3	2.17	0.44
7:BL:302:BCL:CBD	7:BL:302:BCL:HAA2	2.47	0.44
5:AL:147:PRO:HG2	5:AL:153:HIS:HB3	1.99	0.44
5:AL:173:HIS:O	5:AL:177:ILE:HG13	2.16	0.44
6:AM:157:TRP:CD1	7:AM:401:BCL:HBB1	2.52	0.44
6:AM:198:TYR:C	6:AM:200:PRO:HD3	2.38	0.44
3:AK:9:THR:HA	3:AK:10:GLY:HA3	1.66	0.44
3:AY:6:LEU:HA	3:AY:7:GLY:HA2	1.58	0.44
3:A8:6:LEU:HD22	3:A8:6:LEU:C	2.37	0.44
4:AH:101:THR:OG1	4:AH:102:GLY:N	2.50	0.44
1:B7:37:SER:HA	5:BL:51:TRP:NE1	2.32	0.44
3:BW:6:LEU:HA	3:BW:7:GLY:HA2	1.54	0.44
5:AL:173:HIS:CE1	5:AL:177:ILE:HD11	2.52	0.44
5:AL:175:ILE:HG23	9:AL:304:U10:C23	2.47	0.44
5:AL:189:LEU:O	5:AL:193:LEU:HB2	2.17	0.44
6:AM:273:ALA:C	6:AM:275:LEU:H	2.21	0.44
12:AM:406:SPO:H10	12:AM:406:SPO:H81	1.81	0.44
1:B7:9:MET:HB3	1:B7:10:ILE:H	1.50	0.44
2:BB:9:ASP:CB	4:BH:249:LYS:HD3	2.48	0.44
5:BL:54:VAL:HG13	5:BL:59:TRP:CZ2	2.52	0.44
7:AW:101:BCL:CGA	7:AW:101:BCL:H3A	2.47	0.44
7:BL:303:BCL:H3A	7:BL:303:BCL:HBA1	1.63	0.44
5:BL:49:ILE:O	5:BL:64:ILE:HG21	2.18	0.44
6:AM:68:PHE:HE1	12:AM:406:SPO:H21A	1.82	0.44
1:AF:35:LEU:HD12	1:AF:36:LEU:N	2.31	0.44
1:BF:12:ASP:CB	1:BF:13:PRO:CD	2.77	0.44
7:AP:101:BCL:HHD	7:AP:101:BCL:HAC1	1.86	0.44
3:AI:45:ARG:N	3:AI:46:PRO:HD3	2.32	0.44
3:B6:11:LEU:C	3:B6:11:LEU:HD22	2.37	0.44
1:AZ:42:ASN:C	1:AZ:44:LEU:H	2.19	0.44
5:BL:151:TRP:HA	5:BL:154:LEU:HG	1.99	0.44
2:AB:21:LEU:HB3	2:AB:22:TRP:H	1.66	0.44
3:AU:39:LEU:HA	3:AU:42:TYR:HD2	1.83	0.44
4:BH:246:PRO:HB3	4:BH:247:LYS:HD2	2.00	0.44
3:AU:8:TYR:HA	3:AU:9:THR:HA	1.62	0.44
4:AH:193:MET:O	4:AH:196:VAL:HG22	2.17	0.44
1:BJ:38:THR:HA	1:BJ:39:PRO:HD3	1.88	0.44
3:BG:12:THR:HA	3:BG:13:ASP:HA	1.54	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AM:129:TRP:CD1	6:AM:129:TRP:O	2.70	0.44
7:BZ:101:BCL:HBC2	3:BS:45:ARG:CD	2.42	0.44
4:BH:154:ARG:HB3	4:BH:204:HIS:HA	1.99	0.44
1:B7:38:THR:C	1:B7:40:SER:H	2.20	0.44
1:A3:35:LEU:HD12	1:A3:35:LEU:O	2.18	0.44
3:AK:45:ARG:H	3:AK:46:PRO:HD3	1.82	0.44
1:AN:9:MET:HG3	6:AM:27:ALA:HB3	1.99	0.44
6:AM:204:LEU:HA	6:AM:207:ALA:CB	2.47	0.44
3:B4:8:TYR:HA	3:B4:9:THR:HA	1.59	0.44
1:BV:38:THR:HA	1:BV:39:PRO:HD3	1.85	0.44
5:BL:170:ASN:OD1	5:BL:247:CYS:HB3	2.17	0.44
7:BL:301:BCL:OBB	7:BM:401:BCL:H8	2.17	0.44
5:AL:127:ALA:CB	7:AL:301:BCL:C2	2.95	0.44
5:AL:128:TYR:CE1	7:AL:302:BCL:HBB1	2.53	0.44
3:AS:45:ARG:CB	3:AS:46:PRO:CD	2.91	0.44
7:AT:101:BCL:HMB3	7:AS:101:BCL:HHB	1.99	0.44
1:A1:44:LEU:CG	1:A1:44:LEU:O	2.52	0.44
1:BF:28:ALA:HB2	7:BF:101:BCL:O1A	2.16	0.44
3:A4:6:LEU:HA	3:A4:6:LEU:HD22	1.90	0.44
5:BL:84:GLY:O	5:BL:88:ILE:HG13	2.17	0.44
1:AP:43:TRP:C	1:AP:43:TRP:CD1	2.90	0.44
6:AM:136:ARG:HH21	6:AM:139:ALA:HB2	1.82	0.44
5:BL:157:VAL:HG13	7:BL:302:BCL:HMD2	1.98	0.44
7:AL:302:BCL:H2	8:AL:303:BPH:CMB	2.40	0.44
6:AM:175:VAL:CG2	7:AM:401:BCL:HMC1	2.48	0.44
7:AM:401:BCL:H91	7:AM:401:BCL:H172	1.99	0.44
3:BO:9:THR:HA	3:BO:10:GLY:HA2	1.70	0.44
1:A2:28:ALA:O	1:A2:32:HIS:N	2.46	0.44
1:BP:15:ARG:HG2	1:BP:19:ALA:HB3	1.99	0.44
6:AM:98:ALA:C	6:AM:100:GLU:H	2.21	0.44
6:BM:64:LEU:HD22	6:BM:68:PHE:HE2	1.82	0.44
3:B9:43:ILE:O	3:B9:45:ARG:HA	2.17	0.44
4:BH:39:GLY:HA2	5:BL:5:PHE:HE2	1.83	0.44
4:BH:77:GLY:O	4:BH:79:GLU:HG2	2.17	0.44
4:AH:85:ILE:HD12	5:AL:8:LYS:HD2	2.00	0.44
5:BL:123:PHE:HB3	5:BL:241:VAL:HG11	1.99	0.44
7:AM:401:BCL:HBC3	7:AM:401:BCL:H2C	1.73	0.44
3:B4:30:PHE:HE2	7:B4:101:BCL:HBD	1.83	0.44
5:AL:5:PHE:C	5:AL:7:ARG:H	2.22	0.44
6:BM:97:PRO:HD3	6:BM:116:LEU:HD21	2.00	0.44
7:B7:101:BCL:HHD	7:B7:101:BCL:HAC1	1.89	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A7:24:LEU:O	1:A7:28:ALA:N	2.51	0.44
1:AP:18:VAL:HG13	1:AP:19:ALA:N	2.32	0.44
1:AN:15:ARG:HG2	1:AN:18:VAL:HG12	1.99	0.44
1:BN:42:ASN:O	1:BN:43:TRP:CD2	2.71	0.44
1:BJ:11:PHE:HB2	1:BJ:15:ARG:HB2	1.99	0.44
3:AK:15:GLN:O	3:AK:20:HIS:HB2	2.18	0.44
3:BS:11:LEU:N	3:BS:14:GLU:HB2	2.33	0.44
6:BM:129:TRP:CG	8:BM:402:BPH:H1C2	2.53	0.44
5:AL:182:THR:O	5:AL:236:LEU:HD22	2.17	0.44
3:AG:39:LEU:HA	3:AG:42:TYR:HD2	1.83	0.44
1:BD:15:ARG:HA	1:BD:19:ALA:HB3	2.00	0.44
7:BP:101:BCL:HMA3	7:BO:102:BCL:CMA	2.48	0.44
4:BH:37:ARG:O	4:BH:76:PRO:HB3	2.18	0.44
2:BB:29:LYS:H	2:BB:29:LYS:HG3	1.63	0.44
5:AL:135:ARG:N	5:AL:136:PRO:CD	2.81	0.44
3:AQ:44:TRP:CA	3:AQ:45:ARG:HG2	2.47	0.44
3:AQ:8:TYR:N	3:AQ:8:TYR:HD2	2.14	0.44
6:AM:88:ASP:HB3	6:AM:91:PHE:HB2	2.00	0.44
6:AM:134:TYR:HD2	6:AM:147:ALA:HB3	1.83	0.44
1:AT:22:VAL:HA	1:AT:25:PHE:HB3	1.99	0.44
1:BX:38:THR:HA	1:BX:39:PRO:HD3	1.76	0.44
1:AP:29:VAL:HG13	6:AM:120:PHE:HZ	1.81	0.44
1:BD:9:MET:O	1:BD:10:ILE:CG2	2.55	0.43
1:B1:12:ASP:H	1:B1:13:PRO:HD2	1.83	0.43
5:BL:103:ARG:NH2	6:BM:255:THR:HG23	2.31	0.43
7:BK:101:BCL:CBD	7:BK:101:BCL:HAA2	2.48	0.43
3:BY:43:ILE:HG23	3:BY:44:TRP:HD1	1.82	0.43
3:BW:16:ALA:HA	3:BW:20:HIS:CG	2.53	0.43
1:B7:15:ARG:NE	1:B7:19:ALA:HB2	2.33	0.43
1:A7:24:LEU:C	1:A7:24:LEU:HD12	2.38	0.43
1:AX:12:ASP:H	1:AX:13:PRO:HD2	1.82	0.43
3:AW:12:THR:HA	3:AW:13:ASP:HA	1.55	0.43
3:AY:12:THR:HA	3:AY:13:ASP:HA	1.53	0.43
3:AG:43:ILE:C	3:AG:46:PRO:HD2	2.39	0.43
6:BM:70:ILE:HG12	6:BM:177:TYR:CD2	2.54	0.43
1:AZ:41:TYR:O	1:AZ:42:ASN:CB	2.61	0.43
3:BE:19:LEU:HA	3:BE:22:VAL:HG22	2.01	0.43
4:AH:27:LEU:HD21	6:AM:271:TRP:CE3	2.53	0.43
4:AH:31:LEU:HD21	6:AM:271:TRP:CD1	2.52	0.43
6:BM:24:VAL:HG12	6:BM:51:TYR:CD2	2.52	0.43
3:AO:44:TRP:HA	3:AO:45:ARG:HA	1.55	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AL:201:GLU:O	5:AL:202:LYS:HB2	2.18	0.43
6:AM:196:LEU:HG	6:AM:294:TRP:CD1	2.53	0.43
3:BI:28:TRP:O	3:BI:32:ALA:HB3	2.17	0.43
5:AL:169:TYR:HD2	5:AL:263:TRP:CD1	2.36	0.43
6:AM:15:PRO:HB2	6:AM:16:ALA:H	1.56	0.43
1:BD:26:LEU:O	1:BD:30:MET:HG2	2.17	0.43
1:BX:12:ASP:N	1:BX:13:PRO:HD2	2.33	0.43
4:BH:21:TRP:HA	4:BH:21:TRP:CE3	2.53	0.43
7:BL:301:BCL:HBC1	7:BM:401:BCL:CBD	2.48	0.43
5:AL:233:GLY:HA3	6:AM:216:PHE:CD1	2.52	0.43
1:BJ:31:ILE:HG13	7:B2:101:BCL:HMB1	2.00	0.43
7:BD:102:BCL:HMB3	7:BF:101:BCL:HMA3	2.00	0.43
3:A9:42:TYR:HE1	7:A9:101:BCL:HHC	1.83	0.43
1:AN:42:ASN:O	1:AN:43:TRP:CG	2.71	0.43
6:AM:62:SER:CB	6:AM:125:ALA:HB2	2.48	0.43
7:A3:101:BCL:HHD	7:A4:101:BCL:HBC1	1.99	0.43
4:AH:37:ARG:CB	6:AM:261:THR:HG21	2.45	0.43
6:BM:164:ARG:O	6:BM:168:MET:HB2	2.18	0.43
3:B4:44:TRP:CG	3:B4:45:ARG:HG2	2.53	0.43
1:AT:38:THR:O	1:AT:40:SER:N	2.51	0.43
1:A2:38:THR:HA	1:A2:39:PRO:HD3	1.90	0.43
4:BH:195:MET:HE2	4:BH:237:VAL:HB	2.00	0.43
7:A7:101:BCL:HBD	7:A7:101:BCL:HAA2	1.99	0.43
3:BS:45:ARG:HB3	3:BS:46:PRO:CD	2.37	0.43
1:AN:42:ASN:O	1:AN:44:LEU:HG	2.18	0.43
1:BN:10:ILE:HG23	1:BN:11:PHE:O	2.18	0.43
1:B5:34:ILE:HG12	5:BL:88:ILE:HD11	2.01	0.43
3:AO:8:TYR:HA	3:AO:9:THR:HA	1.59	0.43
3:AK:8:TYR:HA	3:AK:9:THR:HA	1.51	0.43
1:B3:12:ASP:C	1:B3:14:ARG:H	2.21	0.43
3:BE:44:TRP:HA	3:BE:45:ARG:HA	1.67	0.43
5:AL:200:PRO:HG2	5:AL:204:LYS:HB3	2.00	0.43
6:BM:290:VAL:HG12	6:BM:291:VAL:N	2.33	0.43
1:B1:43:TRP:C	1:B1:43:TRP:CD1	2.91	0.43
5:BL:105:VAL:O	5:BL:105:VAL:HG12	2.19	0.43
3:AU:12:THR:HA	3:AU:13:ASP:HA	1.55	0.43
4:AH:114:TRP:HB3	4:AH:232:LYS:HG3	2.00	0.43
5:BL:205:GLU:HG3	5:BL:207:ARG:HH21	1.84	0.43
5:BL:172:ALA:HB1	5:BL:246:LEU:HB3	2.01	0.43
5:AL:96:ALA:HB1	8:AL:303:BPH:H4C2	2.01	0.43
5:AL:208:THR:CB	5:AL:209:PRO:CD	2.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BP:36:LEU:HD11	7:BP:101:BCL:CBB	2.47	0.43
1:A2:15:ARG:CA	1:A2:19:ALA:HB3	2.37	0.43
7:BF:101:BCL:HAC1	7:BF:101:BCL:HHD	1.86	0.43
3:BY:6:LEU:HA	3:BY:7:GLY:HA2	1.68	0.43
3:BE:11:LEU:O	3:BE:12:THR:CB	2.62	0.43
5:AL:249:ILE:HG22	5:AL:250:ILE:CD1	2.48	0.43
3:B6:41:VAL:HG12	7:B6:101:BCL:CBC	2.43	0.43
1:B5:12:ASP:HB2	1:B5:13:PRO:CD	2.44	0.43
5:BL:15:THR:HG21	5:BL:33:PHE:HB2	1.98	0.43
3:AK:10:GLY:HA3	3:AK:11:LEU:HA	1.77	0.43
1:AZ:12:ASP:CB	1:AZ:13:PRO:HD3	2.45	0.43
1:BV:30:MET:HG3	1:BV:31:ILE:N	2.33	0.43
1:AV:46:ILE:O	1:AV:46:ILE:HG22	2.19	0.43
1:BN:8:TRP:O	1:BN:9:MET:HB2	2.17	0.43
7:B9:101:BCL:HMB3	7:BO:101:BCL:C1B	2.48	0.43
5:AL:176:ALA:HB2	5:AL:243:PHE:C	2.39	0.43
8:AM:403:BPH:H4C1	8:AM:403:BPH:H6C1	1.37	0.43
6:AM:177:TYR:HE1	12:AM:406:SPO:C23	2.32	0.43
1:BZ:12:ASP:HB2	1:BZ:13:PRO:HD3	2.00	0.43
7:AI:101:BCL:HMB2	7:AK:101:BCL:HMA3	1.99	0.43
4:BH:177:ARG:O	4:BH:193:MET:HB2	2.19	0.43
1:A2:43:TRP:HD1	1:A2:44:LEU:H	1.66	0.43
1:AJ:31:ILE:CG2	7:AJ:101:BCL:HMD3	2.41	0.43
3:BE:11:LEU:H	3:BE:11:LEU:CD1	2.28	0.43
3:A6:8:TYR:HA	3:A6:11:LEU:HD23	2.00	0.43
1:B7:26:LEU:HG	5:BL:40:PHE:CD1	2.48	0.43
3:A4:13:ASP:N	3:A4:13:ASP:OD1	2.51	0.43
3:BK:8:TYR:HA	3:BK:9:THR:HA	1.74	0.43
4:BH:246:PRO:HA	4:BH:247:LYS:HA	1.57	0.43
3:BG:8:TYR:CE1	3:BG:11:LEU:HD13	2.53	0.43
1:B2:24:LEU:HD12	1:B2:24:LEU:C	2.39	0.43
7:BI:101:BCL:HMA1	7:BK:101:BCL:CMA	2.45	0.43
3:BI:12:THR:HA	3:BI:13:ASP:HA	1.48	0.43
3:AG:45:ARG:HH21	3:AG:48:PHE:HA	1.84	0.43
1:AT:15:ARG:O	1:AT:20:GLN:N	2.51	0.43
4:AH:189:ARG:NH1	4:AH:218:THR:HG22	2.34	0.43
3:BS:20:HIS:HA	3:BS:24:MET:CB	2.49	0.43
7:BL:302:BCL:HAC1	7:BL:302:BCL:HHD	1.94	0.43
5:AL:178:SER:O	9:AL:304:U10:C19	2.67	0.43
7:AM:401:BCL:HHC	7:AM:402:BCL:H42	2.01	0.43
1:AD:31:ILE:HD13	7:AD:102:BCL:HMD3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B7:28:ALA:HB2	7:B8:101:BCL:HED2	2.01	0.43
6:BM:287:SER:HA	6:BM:294:TRP:HZ2	1.84	0.43
2:AB:17:THR:O	2:AB:18:ASN:C	2.56	0.43
4:AH:132:LYS:HB3	4:AH:136:ALA:HB3	2.01	0.43
3:AG:12:THR:HA	3:AG:13:ASP:HA	1.54	0.43
1:BF:16:VAL:HG22	1:BF:16:VAL:O	2.19	0.43
3:B9:35:ILE:HA	3:B9:38:HIS:ND1	2.34	0.43
6:AM:206:ILE:HA	7:AM:402:BCL:HMA3	2.01	0.43
7:AT:101:BCL:HMD2	7:AT:102:BCL:ND	2.33	0.43
4:BH:153:VAL:HG12	4:BH:154:ARG:N	2.34	0.43
3:BW:10:GLY:HA2	3:BW:11:LEU:HA	1.86	0.43
3:AY:44:TRP:HA	3:AY:45:ARG:HA	1.72	0.43
1:A7:38:THR:O	1:A7:39:PRO:C	2.56	0.43
5:AL:205:GLU:HG3	5:AL:207:ARG:NH2	2.33	0.43
5:AL:192:ALA:HB2	6:AM:270:ILE:HD12	1.99	0.43
3:BU:9:THR:HA	3:BU:10:GLY:HA3	1.63	0.43
3:BU:6:LEU:HA	3:BU:7:GLY:HA2	1.69	0.43
4:AH:17:ILE:HG13	4:AH:17:ILE:O	2.19	0.43
8:BL:304:BPH:H161	8:BL:304:BPH:H141	1.59	0.43
5:BL:41:PHE:CB	5:BL:96:ALA:HB2	2.49	0.43
6:AM:216:PHE:CD1	6:AM:219:HIS:HB3	2.54	0.43
6:BM:74:PHE:CG	6:BM:92:PHE:HB2	2.54	0.43
1:BF:43:TRP:NE1	7:BF:101:BCL:HHC	2.33	0.43
6:BM:9:GLN:N	6:BM:10:VAL:HG22	2.34	0.43
5:AL:9:TYR:OH	6:AM:247:ARG:NH1	2.52	0.43
1:BV:24:LEU:HG	1:BV:24:LEU:H	1.58	0.43
6:AM:293:ASN:HB3	6:AM:296:VAL:HG23	2.00	0.43
1:BP:46:ILE:O	1:BP:48:ALA:N	2.52	0.43
4:BH:40:TYR:HA	4:BH:41:PRO:C	2.39	0.43
5:AL:158:SER:C	5:AL:160:THR:N	2.72	0.43
4:AH:34:GLU:HG2	6:AM:267:ARG:HD2	2.01	0.43
3:B6:27:LEU:HA	3:B6:30:PHE:HB3	1.99	0.43
5:AL:137:VAL:O	5:AL:137:VAL:HG12	2.19	0.43
3:A8:12:THR:HA	3:A8:13:ASP:HA	1.73	0.43
5:BL:247:CYS:SG	5:BL:247:CYS:CA	2.97	0.42
3:AS:12:THR:H	3:AS:14:GLU:N	2.16	0.42
5:AL:233:GLY:HA2	6:AM:216:PHE:CD2	2.54	0.42
1:AT:43:TRP:CD1	7:AS:101:BCL:HBB1	2.54	0.42
3:BQ:35:ILE:HA	3:BQ:38:HIS:ND1	2.34	0.42
7:BZ:101:BCL:HHD	7:BZ:101:BCL:HBC3	2.01	0.42
1:B1:30:MET:SD	1:B1:31:ILE:N	2.92	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AW:9:THR:HA	3:AW:10:GLY:HA3	1.74	0.42
5:AL:214:THR:OG1	6:AM:20:MET:N	2.52	0.42
3:A8:44:TRP:C	3:A8:46:PRO:HD3	2.38	0.42
6:BM:286:LEU:HD22	6:BM:290:VAL:HG21	2.01	0.42
3:AW:35:ILE:HA	3:AW:38:HIS:ND1	2.34	0.42
1:B7:34:ILE:HD11	5:BL:47:ILE:HD13	2.01	0.42
4:BH:21:TRP:HA	4:BH:21:TRP:HE3	1.84	0.42
3:B6:38:HIS:HB3	3:B6:42:TYR:CE2	2.54	0.42
5:AL:265:TRP:CG	5:AL:265:TRP:O	2.72	0.42
5:BL:250:ILE:CD1	9:BL:306:U10:H371	2.49	0.42
1:A7:35:LEU:HD12	1:A7:43:TRP:HZ2	1.85	0.42
7:A7:101:BCL:HHD	7:A7:101:BCL:HAC1	1.88	0.42
1:A3:42:ASN:O	1:A3:43:TRP:CG	2.72	0.42
3:AI:41:VAL:CG1	7:AI:101:BCL:H2C	2.36	0.42
7:BD:101:BCL:HMA1	7:B8:101:BCL:HMA3	2.00	0.42
1:B5:31:ILE:HG23	1:B5:35:LEU:HD23	2.00	0.42
4:AH:40:TYR:HA	4:AH:41:PRO:C	2.39	0.42
3:AQ:6:LEU:HA	3:AQ:7:GLY:HA2	1.49	0.42
5:AL:66:VAL:O	5:AL:86:TRP:CD1	2.71	0.42
1:B7:41:TYR:HB3	1:B7:42:ASN:H	1.47	0.42
6:AM:66:TRP:CD1	6:AM:118:ALA:HB1	2.54	0.42
1:AT:38:THR:C	1:AT:40:SER:H	2.23	0.42
4:AH:164:VAL:HG11	4:AH:179:LEU:HD22	2.01	0.42
4:AH:55:PRO:C	4:AH:57:PRO:HD3	2.39	0.42
8:BM:402:BPH:HBB3	8:BM:402:BPH:CHC	2.49	0.42
5:AL:186:ALA:O	5:AL:229:ILE:HD11	2.18	0.42
5:AL:232:LEU:O	5:AL:236:LEU:CD1	2.64	0.42
6:AM:216:PHE:HD1	6:AM:216:PHE:HA	1.71	0.42
3:AG:42:TYR:HE1	7:AG:101:BCL:HHC	1.83	0.42
7:AP:101:BCL:CMA	7:AO:101:BCL:CMA	2.74	0.42
7:BD:102:BCL:HBA1	7:BD:102:BCL:H3A	1.80	0.42
6:BM:70:ILE:HG23	6:BM:177:TYR:HB3	2.02	0.42
1:BX:42:ASN:O	1:BX:43:TRP:CD2	2.72	0.42
3:BQ:27:LEU:O	3:BQ:31:SER:CB	2.66	0.42
4:BH:224:GLU:HG2	4:BH:226:THR:HG23	2.01	0.42
3:AY:9:THR:HG23	3:AY:11:LEU:HD12	2.01	0.42
5:BL:197:ALA:HA	5:BL:207:ARG:HB2	2.00	0.42
6:BM:287:SER:HA	6:BM:294:TRP:CZ2	2.54	0.42
3:BS:35:ILE:O	3:BS:35:ILE:HG22	2.18	0.42
4:AH:243:TYR:O	4:AH:246:PRO:HD3	2.18	0.42
3:A4:2:ASP:N	3:A4:2:ASP:OD2	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BL:254:ILE:HG13	5:BL:255:TRP:N	2.32	0.42
5:BL:107:ILE:HG22	5:BL:107:ILE:O	2.19	0.42
1:A2:18:VAL:CG1	1:A2:19:ALA:N	2.82	0.42
6:BM:6:ILE:HG22	6:BM:7:PHE:H	1.84	0.42
1:A3:12:ASP:HA	1:A3:16:VAL:HB	2.01	0.42
6:BM:70:ILE:HG21	6:BM:177:TYR:HB3	2.00	0.42
4:AH:75:VAL:HG11	6:AM:239:ALA:HA	2.00	0.42
7:BU:101:BCL:H3A	7:BU:101:BCL:HBA1	1.57	0.42
7:BV:101:BCL:HMD3	3:BW:41:VAL:HG21	2.00	0.42
3:AI:10:GLY:HA2	3:AI:11:LEU:HA	1.90	0.42
5:AL:205:GLU:HG2	5:AL:205:GLU:H	1.70	0.42
5:BL:135:ARG:H	5:BL:136:PRO:CD	2.33	0.42
1:BN:43:TRP:C	1:BN:43:TRP:CD1	2.93	0.42
4:BH:229:GLU:O	4:BH:233:ILE:HD12	2.19	0.42
3:AI:6:LEU:HD22	3:AI:7:GLY:CA	2.49	0.42
6:AM:14:GLY:HA2	6:AM:15:PRO:HD3	1.84	0.42
2:AB:17:THR:HG22	2:AB:18:ASN:N	2.34	0.42
2:AB:4:LYS:O	2:AB:5:THR:HB	2.19	0.42
5:AL:247:CYS:SG	5:AL:247:CYS:O	2.78	0.42
5:BL:170:ASN:HB3	5:BL:173:HIS:HB3	2.02	0.42
5:BL:243:PHE:CE1	9:BL:306:U10:H321	2.55	0.42
7:BL:301:BCL:CMD	7:BL:302:BCL:CAB	2.87	0.42
5:BL:61:PRO:HA	5:BL:64:ILE:HD12	2.01	0.42
5:AL:175:ILE:HD13	5:AL:175:ILE:HA	1.85	0.42
3:AO:11:LEU:HD12	3:AO:14:GLU:HG3	2.00	0.42
3:BE:11:LEU:HD22	3:BE:12:THR:HG22	2.00	0.42
4:AH:113:SER:HB2	6:AM:247:ARG:HH12	1.84	0.42
4:AH:131:ILE:CG2	4:AH:168:TRP:HE3	2.29	0.42
1:B3:43:TRP:O	1:B3:43:TRP:CD1	2.72	0.42
3:AQ:9:THR:HA	3:AQ:10:GLY:HA3	1.51	0.42
3:BG:6:LEU:HD22	3:BG:6:LEU:HA	1.92	0.42
3:A8:6:LEU:HD22	3:A8:7:GLY:N	2.33	0.42
1:BT:38:THR:HB	1:BT:39:PRO:HD2	2.01	0.42
3:B8:3:LYS:HB3	3:B8:4:SER:H	1.71	0.42
3:BY:47:TRP:O	3:BY:47:TRP:CG	2.71	0.42
5:BL:250:ILE:HD13	9:BL:306:U10:H371	2.02	0.42
7:BL:301:BCL:HBD	7:BL:301:BCL:HAA1	2.01	0.42
1:AD:36:LEU:HD21	1:AD:44:LEU:HD21	2.01	0.42
1:BJ:28:ALA:O	1:BJ:31:ILE:HG22	2.19	0.42
5:AL:154:LEU:HD22	6:AM:197:PHE:CE1	2.54	0.42
5:AL:60:ASN:O	5:AL:62:GLN:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AD:15:ARG:O	1:AD:19:ALA:HB3	2.20	0.42
3:A4:34:ALA:HB1	3:A4:38:HIS:HE1	1.85	0.42
1:A1:18:VAL:O	1:A1:18:VAL:HG22	2.19	0.42
5:BL:176:ALA:HB2	5:BL:243:PHE:HB3	2.02	0.42
5:BL:175:ILE:HG21	9:BL:306:U10:H23	2.02	0.42
3:A9:6:LEU:HD13	3:A9:7:GLY:CA	2.49	0.42
1:A1:35:LEU:CD1	1:A1:43:TRP:HZ3	2.31	0.42
4:BH:198:VAL:HG13	4:BH:203:VAL:HA	2.01	0.42
3:A4:10:GLY:HA2	3:A4:11:LEU:HA	1.76	0.42
2:BB:9:ASP:HB3	4:BH:249:LYS:HD3	2.02	0.42
5:AL:151:TRP:CE3	5:AL:154:LEU:HD12	2.54	0.42
1:AF:8:TRP:O	1:AF:10:ILE:N	2.52	0.42
1:AP:42:ASN:C	1:AP:44:LEU:N	2.73	0.42
5:BL:224:ILE:O	5:BL:224:ILE:HG12	2.19	0.42
1:BZ:45:GLU:HG3	1:BZ:45:GLU:O	2.20	0.42
3:AU:8:TYR:HD1	3:AU:11:LEU:HD22	1.84	0.42
1:AP:8:TRP:O	1:AP:10:ILE:N	2.47	0.42
4:AH:114:TRP:CD1	4:AH:232:LYS:HE2	2.54	0.42
1:BX:8:TRP:O	1:BX:9:MET:HB2	2.19	0.42
4:BH:148:PRO:HB2	4:BH:151:LEU:HD21	2.01	0.42
1:BV:35:LEU:H	1:BV:35:LEU:HG	1.69	0.42
5:BL:220:VAL:CG2	9:BL:306:U10:H1M2	2.49	0.42
6:BM:152:SER:CB	6:BM:152:SER:HG	2.14	0.42
5:AL:180:PHE:CD2	5:AL:240:ALA:HB1	2.55	0.42
5:AL:233:GLY:CA	6:AM:216:PHE:CZ	3.02	0.42
1:A7:35:LEU:HB2	1:A7:43:TRP:CH2	2.54	0.42
7:AV:101:BCL:CBD	7:AV:101:BCL:HAA2	2.50	0.42
7:B2:101:BCL:HAA2	7:B2:101:BCL:CBD	2.50	0.42
3:BI:8:TYR:HA	3:BI:10:GLY:CA	2.50	0.42
3:B9:6:LEU:HA	3:B9:7:GLY:HA2	1.73	0.42
3:B4:6:LEU:HA	3:B4:7:GLY:HA2	1.62	0.42
1:A3:12:ASP:HB2	3:A4:9:THR:HG23	2.02	0.42
5:AL:103:ARG:NH2	6:AM:255:THR:HG23	2.35	0.42
2:BB:12:ASN:O	2:BB:13:THR:CG2	2.59	0.42
4:BH:248:ARG:HG3	4:BH:249:LYS:HG2	2.01	0.42
3:B6:37:ALA:O	3:B6:41:VAL:HG23	2.20	0.42
3:AS:6:LEU:HD13	3:AS:7:GLY:N	2.29	0.42
5:BL:194:VAL:O	5:BL:194:VAL:HG12	2.20	0.42
1:A5:41:TYR:O	1:A5:42:ASN:HB2	2.19	0.42
9:BL:306:U10:O4	9:BL:306:U10:H3M3	2.20	0.42
6:BM:202:HIS:C	6:BM:202:HIS:ND1	2.73	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AZ:38:THR:O	1:AZ:40:SER:N	2.53	0.42
7:BZ:102:BCL:HBA1	7:BZ:102:BCL:H3A	1.59	0.42
1:BZ:26:LEU:HD21	6:BM:68:PHE:CE2	2.55	0.42
6:BM:116:LEU:O	6:BM:120:PHE:HB2	2.20	0.42
1:AT:12:ASP:N	1:AT:13:PRO:HD3	2.28	0.42
3:BG:33:VAL:O	3:BG:33:VAL:HG12	2.20	0.42
3:AG:8:TYR:HA	3:AG:9:THR:HA	1.73	0.42
4:AH:99:ALA:HA	4:AH:100:PRO:HD3	1.89	0.42
4:AH:142:VAL:HG13	4:AH:147:ASN:CB	2.49	0.42
6:BM:150:PHE:CB	8:BM:402:BPH:HMD3	2.47	0.42
5:AL:186:ALA:HB1	5:AL:229:ILE:CD1	2.50	0.42
8:AM:403:BPH:CHC	8:AM:403:BPH:HBB3	2.49	0.42
6:AM:10:VAL:CG1	6:AM:41:TRP:HZ3	2.30	0.42
7:A6:102:BCL:H3A	7:A6:102:BCL:HBA1	1.81	0.42
7:BP:101:BCL:HAC1	7:BP:101:BCL:HHD	1.87	0.42
3:BI:11:LEU:CD1	3:BI:11:LEU:C	2.88	0.42
1:BF:35:LEU:CD2	7:BF:102:BCL:HHD	2.50	0.42
7:BV:101:BCL:CBD	7:BV:101:BCL:HAA2	2.49	0.42
1:BJ:12:ASP:H	1:BJ:13:PRO:CD	2.33	0.42
6:BM:223:ILE:CG2	6:BM:223:ILE:O	2.67	0.42
4:BH:27:LEU:HD21	6:BM:271:TRP:CE3	2.55	0.42
3:BE:15:GLN:NE2	3:BE:19:LEU:HD13	2.34	0.42
6:AM:138:GLN:HG2	6:AM:138:GLN:O	2.20	0.42
3:AG:9:THR:HA	3:AG:10:GLY:HA3	1.64	0.42
3:AY:8:TYR:CD2	3:AY:8:TYR:N	2.88	0.42
1:BJ:29:VAL:O	1:BJ:33:LEU:HG	2.20	0.42
6:AM:69:THR:HB	6:AM:118:ALA:HB2	2.02	0.42
1:BV:31:ILE:HA	1:BV:34:ILE:HD12	2.01	0.42
3:AG:6:LEU:HA	3:AG:7:GLY:HA2	1.50	0.42
3:B8:12:THR:HA	3:B8:13:ASP:HA	1.55	0.42
5:BL:230:HIS:HB3	6:BM:220:GLY:HA2	2.01	0.42
4:BH:120:LEU:HD22	4:BH:120:LEU:HA	1.90	0.42
5:BL:168:HIS:CG	6:BM:183:LEU:HD22	2.55	0.41
7:BL:303:BCL:H101	8:BL:304:BPH:H18	2.01	0.41
8:BL:304:BPH:CED	6:BM:214:LEU:HD21	2.50	0.41
5:AL:224:ILE:HG13	6:AM:44:ASN:H	1.85	0.41
6:AM:273:ALA:O	8:AM:403:BPH:HBC1	2.20	0.41
7:AV:101:BCL:HBD	7:AV:101:BCL:HAA2	2.02	0.41
3:A6:44:TRP:HA	3:A6:45:ARG:HA	1.66	0.41
3:AK:5:ASP:O	3:AK:8:TYR:HB2	2.20	0.41
1:B2:15:ARG:HA	1:B2:19:ALA:HB3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AV:42:ASN:O	1:AV:43:TRP:CG	2.72	0.41
1:BN:41:TYR:O	1:BN:42:ASN:HB2	2.19	0.41
3:AE:9:THR:HG21	4:AH:92:VAL:CG1	2.50	0.41
1:A2:25:PHE:C	1:A2:27:LEU:N	2.73	0.41
1:B7:42:ASN:HB3	1:B7:45:GLU:CB	2.49	0.41
1:BT:43:TRP:CD1	1:BT:43:TRP:C	2.94	0.41
3:BG:8:TYR:HA	3:BG:9:THR:HA	1.73	0.41
3:BU:39:LEU:HA	3:BU:42:TYR:HD2	1.85	0.41
3:B4:15:GLN:C	3:B4:17:GLN:H	2.23	0.41
3:A4:32:ALA:HA	3:A4:35:ILE:HD12	2.02	0.41
5:BL:173:HIS:HE1	7:BL:302:BCL:HMC3	1.79	0.41
5:BL:37:ALA:O	5:BL:41:PHE:CD2	2.73	0.41
5:BL:184:ALA:CA	8:BM:402:BPH:CMC	2.97	0.41
5:AL:232:LEU:HD21	9:AL:304:U10:C11	2.51	0.41
5:AL:222:TYR:CD2	9:AL:304:U10:H1M3	2.49	0.41
6:AM:175:VAL:HA	6:AM:176:PRO:HD2	1.88	0.41
7:AF:101:BCL:HAA2	7:AF:101:BCL:CBD	2.50	0.41
1:AJ:12:ASP:O	1:AJ:16:VAL:HG12	2.20	0.41
1:AZ:31:ILE:CG2	7:AS:101:BCL:HMD3	2.50	0.41
3:BI:11:LEU:HD13	3:BI:11:LEU:C	2.40	0.41
1:BZ:11:PHE:HB3	1:BZ:14:ARG:HB3	2.01	0.41
5:BL:278:GLY:O	5:BL:279:ILE:HB	2.19	0.41
6:BM:6:ILE:HG22	6:BM:7:PHE:N	2.34	0.41
7:BD:101:BCL:HMC3	7:B8:101:BCL:HBB1	2.02	0.41
2:BB:14:ASN:H	2:BB:15:PRO:HD2	1.85	0.41
3:BE:6:LEU:HA	3:BE:7:GLY:HA2	1.51	0.41
5:AL:123:PHE:CD1	5:AL:238:LEU:HD13	2.55	0.41
4:BH:60:LYS:CG	4:BH:61:PRO:HD2	2.51	0.41
3:AY:6:LEU:HA	3:AY:6:LEU:HD22	1.90	0.41
1:AD:12:ASP:HB2	1:AD:13:PRO:HD3	2.02	0.41
3:BE:38:HIS:HB3	3:BE:42:TYR:CD2	2.54	0.41
6:BM:294:TRP:HE3	6:BM:297:TRP:HB3	1.85	0.41
4:AH:234:CYS:HB3	6:AM:229:PHE:HA	2.01	0.41
8:BM:402:BPH:H4C1	8:BM:402:BPH:H6C1	1.37	0.41
5:AL:183:ASN:ND2	5:AL:236:LEU:HB2	2.35	0.41
6:AM:189:PHE:HB3	7:AM:402:BCL:HMD1	2.02	0.41
1:A2:18:VAL:HG13	1:A2:19:ALA:N	2.35	0.41
5:BL:278:GLY:H	6:BM:84:VAL:CG1	2.33	0.41
1:A2:33:LEU:HA	1:A2:36:LEU:HB2	2.03	0.41
1:AN:43:TRP:CD1	1:AN:43:TRP:C	2.93	0.41
5:BL:71:LEU:HA	5:BL:143:GLY:HA3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AH:86:ALA:H	4:AH:109:VAL:HG11	1.85	0.41
5:BL:113:ILE:HG22	6:BM:229:PHE:HE1	1.85	0.41
5:AL:154:LEU:HD13	6:AM:197:PHE:CD1	2.55	0.41
1:AP:42:ASN:HD22	1:AP:46:ILE:HD13	1.86	0.41
1:B2:46:ILE:HG23	1:B2:49:ALA:HB3	2.01	0.41
3:AQ:28:TRP:CD1	3:AQ:28:TRP:O	2.74	0.41
1:BX:12:ASP:N	1:BX:13:PRO:CD	2.83	0.41
4:AH:246:PRO:HA	4:AH:247:LYS:HA	1.59	0.41
1:AN:38:THR:HA	1:AN:39:PRO:HD3	1.89	0.41
7:BL:303:BCL:HMB1	7:BL:303:BCL:HBB2	2.03	0.41
7:BK:102:BCL:HMB1	7:BK:102:BCL:HBB3	2.01	0.41
7:B3:101:BCL:CGD	7:B3:101:BCL:HAA2	2.49	0.41
3:BO:8:TYR:HB3	3:BO:9:THR:OG1	2.21	0.41
5:AL:219:LEU:HD11	6:AM:133:THR:CG2	2.37	0.41
6:BM:9:GLN:N	6:BM:10:VAL:CA	2.78	0.41
3:AE:12:THR:HA	3:AE:13:ASP:HA	1.69	0.41
3:A4:7:GLY:O	3:A4:8:TYR:HB2	2.19	0.41
3:AW:11:LEU:HB2	3:AW:14:GLU:HB2	2.01	0.41
3:BU:44:TRP:HA	3:BU:45:ARG:HA	1.76	0.41
6:BM:227:SER:C	6:BM:229:PHE:H	2.24	0.41
3:BE:14:GLU:O	3:BE:18:GLU:HB2	2.20	0.41
6:BM:164:ARG:HB3	6:BM:165:PRO:CD	2.47	0.41
1:AX:43:TRP:C	1:AX:43:TRP:CD1	2.93	0.41
5:BL:200:PRO:HB2	5:BL:201:GLU:H	1.56	0.41
1:BJ:8:TRP:N	5:BL:202:LYS:O	2.52	0.41
6:AM:136:ARG:NH2	6:AM:139:ALA:HB2	2.36	0.41
3:AY:8:TYR:HA	3:AY:9:THR:HA	1.70	0.41
1:AD:12:ASP:O	1:AD:15:ARG:N	2.53	0.41
7:BL:303:BCL:C2B	8:BL:304:BPH:C19	2.95	0.41
7:BM:401:BCL:CGD	7:BM:401:BCL:HAA2	2.50	0.41
5:AL:31:VAL:CG2	9:AM:405:U10:H401	2.51	0.41
8:AL:303:BPH:H6C2	8:AL:303:BPH:H9C2	1.58	0.41
6:AM:11:GLN:O	6:AM:12:VAL:HG23	2.21	0.41
3:BQ:6:LEU:HA	3:BQ:7:GLY:HA2	1.68	0.41
1:AJ:31:ILE:HD12	7:AJ:101:BCL:HMD3	2.02	0.41
3:AE:11:LEU:CD2	3:AE:12:THR:H	2.23	0.41
6:BM:65:MET:HA	6:BM:68:PHE:HB2	2.02	0.41
2:AB:12:ASN:C	2:AB:13:THR:HG22	2.41	0.41
1:A5:16:VAL:O	1:A5:16:VAL:HG13	2.21	0.41
6:BM:159:VAL:HG11	6:BM:284:ILE:O	2.20	0.41
1:BN:27:LEU:HG	1:BP:25:PHE:CD1	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A6:101:BCL:HAA2	7:A6:101:BCL:HBD	2.03	0.41
5:BL:264:GLN:HB3	5:BL:264:GLN:HE21	1.71	0.41
5:BL:146:PHE:CD2	5:BL:147:PRO:O	2.74	0.41
5:BL:219:LEU:HA	6:BM:132:ARG:HH12	1.84	0.41
9:AM:405:U10:H201	9:AM:405:U10:H221	1.80	0.41
5:AL:172:ALA:HA	5:AL:175:ILE:HB	2.02	0.41
5:AL:177:ILE:HG21	7:AM:401:BCL:CAD	2.50	0.41
7:AM:401:BCL:HBB3	7:AM:401:BCL:CHC	2.51	0.41
1:AJ:10:ILE:HG12	1:AJ:15:ARG:HD3	2.03	0.41
3:A9:6:LEU:CG	3:A9:7:GLY:HA2	2.50	0.41
1:BJ:31:ILE:HG23	7:BK:102:BCL:HMD3	2.03	0.41
1:B7:9:MET:SD	4:BH:92:VAL:HB	2.60	0.41
5:BL:69:PRO:HG2	5:BL:142:TRP:HB2	2.03	0.41
5:BL:86:TRP:HE3	5:BL:87:GLN:HG3	1.85	0.41
1:A5:41:TYR:CE2	3:A6:46:PRO:HA	2.55	0.41
1:AZ:46:ILE:O	1:AZ:47:SER:C	2.58	0.41
3:BS:35:ILE:HA	3:BS:38:HIS:ND1	2.35	0.41
1:A1:29:VAL:HA	1:A1:32:HIS:ND1	2.35	0.41
1:BN:48:ALA:HB1	3:B9:48:PHE:HB2	2.03	0.41
1:BN:28:ALA:HB1	1:BN:32:HIS:CE1	2.55	0.41
5:BL:89:ILE:HG13	5:BL:89:ILE:H	1.72	0.41
7:BP:102:BCL:HAA1	3:BQ:38:HIS:HE1	1.84	0.41
5:BL:28:PRO:O	6:BM:254:TRP:HA	2.20	0.41
7:BY:102:BCL:HBA1	7:BY:102:BCL:H3A	1.78	0.41
4:BH:153:VAL:HG13	4:BH:203:VAL:HB	2.02	0.41
1:A3:32:HIS:HA	1:A3:35:LEU:CD1	2.50	0.41
3:A9:44:TRP:HA	3:A9:45:ARG:HA	1.66	0.41
5:BL:201:GLU:O	5:BL:202:LYS:HB2	2.20	0.41
3:AW:47:TRP:O	3:AW:47:TRP:CG	2.74	0.41
1:BT:12:ASP:N	1:BT:13:PRO:HD2	2.36	0.41
3:BI:6:LEU:HD22	3:BI:7:GLY:HA3	2.03	0.41
4:AH:90:THR:OG1	4:AH:97:PRO:O	2.39	0.41
1:B2:16:VAL:O	1:B2:16:VAL:HG22	2.21	0.41
6:AM:206:ILE:N	7:AM:402:BCL:HMA3	2.35	0.41
7:AD:102:BCL:HMB3	7:AF:101:BCL:C3A	2.50	0.41
1:B1:12:ASP:C	1:B1:14:ARG:N	2.74	0.41
1:BD:38:THR:HA	1:BD:39:PRO:HD3	1.80	0.41
5:AL:79:PRO:HB2	5:AL:80:LEU:H	1.59	0.41
5:AL:245:ALA:O	5:AL:249:ILE:HB	2.21	0.41
2:AB:55:LEU:N	2:AB:56:PRO:CD	2.84	0.41
3:AI:27:LEU:C	3:AI:29:LEU:H	2.24	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BL:131:LEU:HD23	5:BL:248:MET:HE2	2.02	0.41
3:AI:33:VAL:HG12	3:AI:33:VAL:O	2.19	0.41
3:BQ:14:GLU:HA	3:BQ:17:GLN:HB3	2.02	0.41
5:BL:120:ALA:HB1	5:BL:238:LEU:HD21	2.02	0.41
6:AM:59:SER:HB3	6:AM:129:TRP:CE3	2.53	0.41
5:AL:127:ALA:O	7:AL:301:BCL:H12	2.20	0.41
1:BZ:12:ASP:N	1:BZ:13:PRO:HD2	2.36	0.41
3:AE:44:TRP:HA	3:AE:45:ARG:CG	2.43	0.41
4:AH:154:ARG:HH21	4:AH:204:HIS:CG	2.39	0.41
7:BF:101:BCL:OBD	3:BG:38:HIS:CE1	2.74	0.41
3:AE:13:ASP:HB2	3:AE:16:ALA:HB3	2.02	0.41
3:A4:9:THR:HA	3:A4:10:GLY:HA3	1.69	0.41
5:AL:30:TYR:CD2	5:AL:103:ARG:NH1	2.83	0.41
3:B8:9:THR:HA	3:B8:10:GLY:HA2	1.80	0.41
4:BH:45:GLU:C	5:BL:7:ARG:HD2	2.41	0.41
3:A6:10:GLY:HA3	3:A6:11:LEU:HA	1.71	0.41
1:B5:31:ILE:HD13	1:B5:31:ILE:O	2.21	0.41
3:A6:43:ILE:C	3:A6:46:PRO:HD2	2.40	0.41
4:AH:144:ALA:CB	6:AM:2:GLU:HB2	2.50	0.41
1:A5:12:ASP:N	1:A5:13:PRO:CD	2.84	0.41
1:AP:15:ARG:HG2	1:AP:19:ALA:HB3	2.02	0.41
1:A2:10:ILE:CG1	1:A2:11:PHE:H	2.33	0.41
1:BJ:42:ASN:O	1:BJ:43:TRP:CG	2.74	0.41
1:BJ:15:ARG:NH1	1:B2:18:VAL:HB	2.36	0.41
1:BX:26:LEU:O	1:BX:30:MET:CG	2.68	0.41
5:BL:260:VAL:O	5:BL:260:VAL:CG2	2.67	0.41
6:BM:155:TRP:HA	6:BM:158:MET:HB2	2.03	0.41
1:AX:15:ARG:HA	1:AX:19:ALA:HB3	2.03	0.41
3:B9:15:GLN:HG3	3:B9:15:GLN:O	2.20	0.41
1:B2:28:ALA:HB1	1:B2:32:HIS:CE1	2.56	0.41
5:BL:176:ALA:HB2	5:BL:243:PHE:O	2.21	0.41
5:BL:250:ILE:O	5:BL:259:TRP:HZ2	2.04	0.41
7:BT:101:BCL:HMC2	7:BZ:102:BCL:HMB1	1.95	0.41
3:BO:11:LEU:HB3	3:BO:14:GLU:HB2	2.02	0.41
3:AI:44:TRP:HA	3:AI:45:ARG:HA	1.75	0.41
3:B6:12:THR:HA	3:B6:13:ASP:HA	1.50	0.41
3:BE:6:LEU:HA	3:BE:6:LEU:HD22	1.95	0.41
1:BX:41:TYR:O	1:BX:42:ASN:HB2	2.21	0.41
3:AE:38:HIS:HB3	3:AE:42:TYR:HD2	1.86	0.41
4:BH:12:LEU:HB2	4:BH:15:LEU:HD22	2.03	0.41
1:AT:46:ILE:O	1:AT:46:ILE:CG2	2.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AH:188:THR:C	4:AH:189:ARG:HG2	2.41	0.41
4:AH:248:ARG:HG3	4:AH:249:LYS:N	2.35	0.41
3:A4:34:ALA:HB1	3:A4:38:HIS:CE1	2.55	0.41
2:AB:43:LEU:HG	2:AB:44:LEU:HD12	2.04	0.41
5:BL:19:GLY:C	5:BL:21:LEU:H	2.24	0.41
3:A6:12:THR:HA	3:A6:13:ASP:HA	1.52	0.41
6:BM:216:PHE:HD1	6:BM:219:HIS:HB3	1.85	0.40
7:AD:101:BCL:HMA3	7:A8:101:BCL:HMB3	2.03	0.40
1:A1:42:ASN:O	1:A1:43:TRP:CD2	2.73	0.40
6:BM:9:GLN:H	6:BM:10:VAL:HG22	1.86	0.40
3:A4:6:LEU:HD13	3:A4:7:GLY:CA	2.51	0.40
1:A5:37:SER:O	1:A5:38:THR:OG1	2.38	0.40
3:BE:11:LEU:HD22	3:BE:12:THR:N	2.35	0.40
4:AH:37:ARG:NH2	4:AH:75:VAL:O	2.53	0.40
3:B6:43:ILE:O	3:B6:45:ARG:HA	2.22	0.40
3:BI:44:TRP:HA	3:BI:45:ARG:HA	1.82	0.40
4:BH:113:SER:HB2	6:BM:247:ARG:NH1	2.37	0.40
4:BH:35:ASN:O	6:BM:260:ALA:HA	2.21	0.40
3:AO:43:ILE:C	3:AO:46:PRO:HD2	2.42	0.40
1:B1:36:LEU:HG	1:B1:43:TRP:CZ3	2.56	0.40
6:AM:88:ASP:O	6:AM:90:PHE:N	2.53	0.40
4:BH:28:ILE:O	4:BH:28:ILE:CG2	2.69	0.40
6:AM:51:TYR:HB3	6:AM:132:ARG:NH2	2.37	0.40
1:AJ:38:THR:HA	1:AJ:39:PRO:HD3	1.94	0.40
1:B5:22:VAL:HA	1:B5:25:PHE:HB3	2.03	0.40
1:AX:26:LEU:HA	1:AX:29:VAL:HG12	2.03	0.40
3:BW:25:SER:C	3:BW:27:LEU:H	2.24	0.40
3:AY:25:SER:HA	3:AY:28:TRP:HB3	2.02	0.40
5:BL:128:TYR:HB2	7:BL:302:BCL:H61	2.03	0.40
3:BO:33:VAL:HG12	7:BO:101:BCL:HED3	2.03	0.40
7:AM:402:BCL:CAA	7:AM:402:BCL:CBD	2.99	0.40
7:BK:102:BCL:HBA1	7:BK:102:BCL:H3A	1.79	0.40
3:AO:35:ILE:HA	3:AO:38:HIS:HB2	2.03	0.40
6:BM:62:SER:CB	6:BM:121:PHE:O	2.51	0.40
6:BM:62:SER:O	6:BM:121:PHE:HB3	2.21	0.40
5:BL:208:THR:CB	5:BL:209:PRO:CD	2.93	0.40
5:BL:278:GLY:O	5:BL:280:ASN:N	2.52	0.40
6:AM:98:ALA:HB1	6:AM:99:PRO:CD	2.42	0.40
4:AH:28:ILE:O	4:AH:32:GLN:HB2	2.20	0.40
4:BH:117:ARG:O	4:BH:228:LEU:HB2	2.21	0.40
1:AP:42:ASN:O	1:AP:43:TRP:CG	2.74	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BP:38:THR:HA	1:BP:39:PRO:HD3	1.80	0.40
1:B5:42:ASN:O	1:B5:43:TRP:CG	2.75	0.40
3:BU:11:LEU:N	3:BU:14:GLU:HB2	2.36	0.40
1:A7:41:TYR:HB3	1:A7:42:ASN:H	1.47	0.40
1:BZ:42:ASN:C	1:BZ:44:LEU:H	2.23	0.40
1:BT:41:TYR:O	1:BT:42:ASN:HB2	2.21	0.40
1:BF:38:THR:HA	1:BF:39:PRO:HD3	1.88	0.40
1:AF:29:VAL:HG13	1:AF:30:MET:N	2.36	0.40
1:B3:26:LEU:C	1:B3:28:ALA:H	2.23	0.40
3:BE:29:LEU:HD23	3:BE:33:VAL:HG21	2.02	0.40
3:BK:15:GLN:HA	3:BK:15:GLN:HE21	1.86	0.40
5:BL:38:THR:HG22	8:BL:304:BPH:H4C2	2.03	0.40
6:AM:158:MET:CE	6:AM:158:MET:CG	2.97	0.40
1:AT:44:LEU:HD12	7:AS:101:BCL:HMC3	2.04	0.40
4:BH:198:VAL:HB	6:BM:7:PHE:HB3	2.03	0.40
3:B8:8:TYR:HA	3:B8:9:THR:HA	1.51	0.40
3:AQ:44:TRP:HA	3:AQ:45:ARG:HA	1.64	0.40
4:AH:111:PRO:HB2	4:AH:239:GLY:HA2	2.03	0.40
3:A8:6:LEU:HA	3:A8:7:GLY:HA2	1.57	0.40
1:AJ:29:VAL:CG1	1:AJ:30:MET:N	2.84	0.40
4:BH:48:THR:HG23	4:BH:49:PRO:HD2	2.01	0.40
3:AW:36:VAL:O	3:AW:39:LEU:HB2	2.21	0.40
7:BL:302:BCL:C17	8:BL:304:BPH:HMA3	2.50	0.40
3:AE:6:LEU:HD22	4:AH:48:THR:HG23	2.01	0.40
5:AL:113:ILE:CG2	6:AM:247:ARG:HB3	2.50	0.40
1:AN:8:TRP:HB3	3:AO:6:LEU:HD22	2.03	0.40
3:A4:44:TRP:CE3	3:A4:45:ARG:HG2	2.56	0.40
3:AU:6:LEU:HA	3:AU:7:GLY:HA2	1.72	0.40
1:B1:41:TYR:O	1:B1:42:ASN:HB2	2.22	0.40
4:BH:70:ARG:HH21	4:BH:120:LEU:HD12	1.86	0.40
3:B6:21:SER:O	3:B6:25:SER:HB3	2.22	0.40
5:BL:112:GLY:O	6:BM:228:ARG:HD2	2.22	0.40
5:AL:246:LEU:HD12	9:AL:304:U10:H362	2.04	0.40
5:AL:168:HIS:NE2	7:AL:301:BCL:HMC2	2.36	0.40
12:AM:406:SPO:H131	12:AM:406:SPO:H15	1.79	0.40
6:AM:44:ASN:N	6:AM:44:ASN:HD22	2.20	0.40
1:AP:35:LEU:HD21	7:AP:102:BCL:HHD	2.04	0.40
7:BI:101:BCL:H3A	7:BI:101:BCL:HBA1	1.49	0.40
1:A5:27:LEU:HD11	1:A7:29:VAL:HG21	2.04	0.40
4:AH:198:VAL:CG2	6:AM:8:SER:HB2	2.52	0.40
4:BH:52:ASN:HD22	4:BH:52:ASN:HA	1.64	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AM:274:VAL:O	6:AM:274:VAL:HG22	2.21	0.40
3:AI:8:TYR:HA	3:AI:9:THR:HA	1.77	0.40
3:BU:11:LEU:O	3:BU:11:LEU:HD13	2.21	0.40
3:BS:28:TRP:O	3:BS:32:ALA:HB3	2.21	0.40
3:AE:15:GLN:HA	3:AE:19:LEU:HD13	2.03	0.40
1:AN:14:ARG:C	1:AN:16:VAL:H	2.25	0.40
3:BI:27:LEU:HD13	3:BI:27:LEU:HA	1.94	0.40
1:AD:18:VAL:HG22	1:AD:18:VAL:O	2.21	0.40
1:B3:35:LEU:HG	1:B3:35:LEU:H	1.79	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	A1	40/58 (69%)	29 (72%)	8 (20%)	3 (8%)	1 21
1	A2	40/58 (69%)	27 (68%)	7 (18%)	6 (15%)	0 5
1	A3	40/58 (69%)	24 (60%)	13 (32%)	3 (8%)	1 21
1	A5	40/58 (69%)	23 (58%)	12 (30%)	5 (12%)	0 8
1	A7	40/58 (69%)	23 (58%)	11 (28%)	6 (15%)	0 5
1	AD	40/58 (69%)	22 (55%)	13 (32%)	5 (12%)	0 8
1	AF	40/58 (69%)	26 (65%)	12 (30%)	2 (5%)	3 31
1	AJ	40/58 (69%)	29 (72%)	7 (18%)	4 (10%)	1 14
1	AN	40/58 (69%)	29 (72%)	6 (15%)	5 (12%)	0 8
1	AP	40/58 (69%)	28 (70%)	10 (25%)	2 (5%)	3 31
1	AT	40/58 (69%)	26 (65%)	9 (22%)	5 (12%)	0 8
1	AV	40/58 (69%)	28 (70%)	11 (28%)	1 (2%)	7 46
1	AX	40/58 (69%)	25 (62%)	11 (28%)	4 (10%)	1 14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	AZ	40/58 (69%)	25 (62%)	11 (28%)	4 (10%)	1 14
1	B1	40/58 (69%)	28 (70%)	8 (20%)	4 (10%)	1 14
1	B2	40/58 (69%)	30 (75%)	7 (18%)	3 (8%)	1 21
1	B3	40/58 (69%)	27 (68%)	12 (30%)	1 (2%)	7 46
1	B5	40/58 (69%)	24 (60%)	12 (30%)	4 (10%)	1 14
1	B7	40/58 (69%)	23 (58%)	12 (30%)	5 (12%)	0 8
1	BD	40/58 (69%)	26 (65%)	11 (28%)	3 (8%)	1 21
1	BF	40/58 (69%)	25 (62%)	11 (28%)	4 (10%)	1 14
1	BJ	40/58 (69%)	27 (68%)	10 (25%)	3 (8%)	1 21
1	BN	40/58 (69%)	31 (78%)	8 (20%)	1 (2%)	7 46
1	BP	40/58 (69%)	26 (65%)	11 (28%)	3 (8%)	1 21
1	BT	40/58 (69%)	25 (62%)	13 (32%)	2 (5%)	3 31
1	BV	40/58 (69%)	29 (72%)	9 (22%)	2 (5%)	3 31
1	BX	40/58 (69%)	28 (70%)	11 (28%)	1 (2%)	7 46
1	BZ	40/58 (69%)	25 (62%)	11 (28%)	4 (10%)	1 14
2	AB	55/82 (67%)	24 (44%)	24 (44%)	7 (13%)	0 8
2	BB	55/82 (67%)	28 (51%)	22 (40%)	5 (9%)	1 17
3	A4	46/49 (94%)	30 (65%)	13 (28%)	3 (6%)	1 25
3	A6	46/49 (94%)	36 (78%)	9 (20%)	1 (2%)	8 49
3	A8	46/49 (94%)	30 (65%)	14 (30%)	2 (4%)	3 34
3	A9	46/49 (94%)	35 (76%)	8 (17%)	3 (6%)	1 25
3	AE	46/49 (94%)	34 (74%)	10 (22%)	2 (4%)	3 34
3	AG	46/49 (94%)	29 (63%)	16 (35%)	1 (2%)	8 49
3	AI	46/49 (94%)	34 (74%)	11 (24%)	1 (2%)	8 49
3	AK	46/49 (94%)	33 (72%)	10 (22%)	3 (6%)	1 25
3	AO	46/49 (94%)	33 (72%)	12 (26%)	1 (2%)	8 49
3	AQ	46/49 (94%)	40 (87%)	5 (11%)	1 (2%)	8 49
3	AS	46/49 (94%)	32 (70%)	12 (26%)	2 (4%)	3 34
3	AU	46/49 (94%)	31 (67%)	10 (22%)	5 (11%)	0 11
3	AW	46/49 (94%)	33 (72%)	11 (24%)	2 (4%)	3 34
3	AY	46/49 (94%)	31 (67%)	13 (28%)	2 (4%)	3 34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	B4	46/49 (94%)	27 (59%)	14 (30%)	5 (11%)	0 11
3	B6	46/49 (94%)	33 (72%)	12 (26%)	1 (2%)	8 49
3	B8	46/49 (94%)	30 (65%)	14 (30%)	2 (4%)	3 34
3	B9	46/49 (94%)	35 (76%)	8 (17%)	3 (6%)	1 25
3	BE	46/49 (94%)	33 (72%)	12 (26%)	1 (2%)	8 49
3	BG	46/49 (94%)	31 (67%)	15 (33%)	0	100 100
3	BI	46/49 (94%)	35 (76%)	11 (24%)	0	100 100
3	BK	46/49 (94%)	29 (63%)	15 (33%)	2 (4%)	3 34
3	BO	46/49 (94%)	33 (72%)	10 (22%)	3 (6%)	1 25
3	BQ	46/49 (94%)	38 (83%)	8 (17%)	0	100 100
3	BS	46/49 (94%)	31 (67%)	12 (26%)	3 (6%)	1 25
3	BU	46/49 (94%)	29 (63%)	13 (28%)	4 (9%)	1 17
3	BW	46/49 (94%)	32 (70%)	12 (26%)	2 (4%)	3 34
3	BY	46/49 (94%)	33 (72%)	11 (24%)	2 (4%)	3 34
4	AH	248/260 (95%)	178 (72%)	59 (24%)	11 (4%)	3 33
4	BH	248/260 (95%)	198 (80%)	43 (17%)	7 (3%)	6 44
5	AL	279/282 (99%)	203 (73%)	61 (22%)	15 (5%)	2 29
5	BL	279/282 (99%)	208 (75%)	61 (22%)	10 (4%)	4 38
6	AM	303/308 (98%)	223 (74%)	63 (21%)	17 (6%)	2 28
6	BM	303/308 (98%)	232 (77%)	56 (18%)	15 (5%)	3 31
All	All	4178/4860 (86%)	2942 (70%)	997 (24%)	239 (6%)	2 28

All (239) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A5	38	THR
1	A7	39	PRO
1	A7	41	TYR
1	AD	10	ILE
1	A1	12	ASP
1	A2	22	VAL
1	A2	43	TRP
1	AZ	39	PRO
2	AB	13	THR
3	AS	12	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A9	12	THR
3	AK	8	TYR
5	AL	79	PRO
5	AL	202	LYS
6	AM	15	PRO
6	AM	24	VAL
6	AM	292	ASP
1	B7	39	PRO
1	B7	41	TYR
1	BD	10	ILE
1	BF	12	ASP
1	BF	42	ASN
1	B2	43	TRP
1	BZ	38	THR
3	BS	13	ASP
4	BH	138	ALA
4	BH	249	LYS
5	BL	23	ASP
6	BM	15	PRO
1	AV	15	ARG
1	A7	10	ILE
1	AD	18	VAL
1	A1	18	VAL
1	AJ	43	TRP
1	AN	47	SER
1	AZ	38	THR
1	AZ	42	ASN
2	AB	26	GLN
3	A9	8	TYR
3	AO	41	VAL
3	A6	8	TYR
3	AU	8	TYR
3	AU	47	TRP
3	AE	12	THR
3	AK	46	PRO
5	AL	240	ALA
6	AM	6	ILE
6	AM	8	SER
1	B5	42	ASN
1	BV	15	ARG
1	B7	10	ILE
1	BD	18	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B2	47	SER
1	BN	12	ASP
1	BP	47	SER
1	BZ	40	SER
2	BB	26	GLN
3	BS	12	THR
3	BS	45	ARG
3	B9	8	TYR
3	B6	8	TYR
3	BU	8	TYR
3	BE	12	THR
3	BK	8	TYR
5	BL	200	PRO
6	BM	57	VAL
6	BM	154	ILE
6	BM	255	THR
1	A5	9	MET
1	A5	37	SER
1	AT	43	TRP
1	AT	44	LEU
1	AT	47	SER
1	AX	15	ARG
1	A7	12	ASP
1	A7	38	THR
1	AD	12	ASP
1	AD	41	TYR
1	AD	44	LEU
1	AF	12	ASP
1	A1	41	TYR
1	AJ	9	MET
1	A2	10	ILE
1	A2	26	LEU
1	A2	47	SER
1	AN	12	ASP
1	AN	41	TYR
1	AP	42	ASN
2	AB	18	ASN
2	AB	53	ARG
3	AS	45	ARG
3	A9	26	GLY
3	AW	6	LEU
4	AH	52	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	AH	249	LYS
5	AL	112	GLY
5	AL	155	ASP
5	AL	200	PRO
6	AM	101	TYR
6	AM	141	GLY
6	AM	195	ASN
1	BT	43	TRP
1	BX	16	VAL
1	BD	12	ASP
1	BP	42	ASN
1	BZ	39	PRO
3	B9	12	THR
3	BO	46	PRO
3	BY	8	TYR
3	B4	8	TYR
3	B4	46	PRO
3	BK	46	PRO
4	BH	44	ASN
4	BH	111	PRO
5	BL	76	GLY
5	BL	79	PRO
5	BL	112	GLY
6	BM	89	LEU
1	AT	13	PRO
1	AX	9	MET
1	AX	42	ASN
1	A3	12	ASP
1	AF	41	TYR
1	AJ	12	ASP
1	AJ	41	TYR
1	A2	12	ASP
1	AN	48	ALA
1	AP	43	TRP
3	AU	4	SER
3	AU	45	ARG
3	AY	8	TYR
3	A4	8	TYR
3	A4	11	LEU
3	A4	12	THR
4	AH	171	ILE
5	AL	23	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AL	234	LEU
6	AM	89	LEU
6	AM	255	THR
6	AM	274	VAL
1	B5	38	THR
1	BV	42	ASN
1	B3	12	ASP
1	B7	38	THR
1	B1	12	ASP
1	B1	41	TYR
1	B2	12	ASP
1	BZ	42	ASN
2	BB	22	TRP
3	B9	31	SER
3	BW	18	GLU
4	BH	125	GLY
4	BH	171	ILE
5	BL	100	TRP
6	BM	56	GLY
1	A5	42	ASN
1	A5	44	LEU
1	AT	41	TYR
1	AX	39	PRO
1	A3	40	SER
1	A3	47	SER
1	A7	42	ASN
1	AN	43	TRP
1	AZ	40	SER
2	AB	12	ASN
3	AQ	8	TYR
3	AW	2	ASP
3	AY	12	THR
3	A8	8	TYR
3	AI	4	SER
4	AH	46	ASP
5	AL	61	PRO
5	AL	117	ILE
5	AL	119	PHE
5	AL	135	ARG
5	AL	142	TRP
5	AL	159	ASN
1	B5	37	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B7	42	ASN
1	B1	18	VAL
1	BJ	12	ASP
1	BJ	41	TYR
1	BP	12	ASP
2	BB	6	ILE
2	BB	52	GLY
3	BU	6	LEU
3	BU	12	THR
3	BW	6	LEU
3	BY	12	THR
3	B4	12	THR
3	B4	17	GLN
3	B8	8	TYR
5	BL	202	LYS
6	BM	8	SER
6	BM	29	ARG
6	BM	195	ASN
2	AB	50	VAL
3	A8	20	HIS
3	AE	29	LEU
3	AG	43	ILE
3	AK	43	ILE
4	AH	15	LEU
4	AH	19	SER
4	AH	49	PRO
4	AH	125	GLY
4	AH	235	GLY
6	AM	110	LYS
6	AM	302	GLY
1	BF	40	SER
3	BO	6	LEU
3	B8	7	GLY
5	BL	78	ALA
5	BL	83	GLY
6	BM	288	GLY
2	AB	36	GLY
3	AU	26	GLY
4	AH	150	GLY
6	AM	108	PRO
6	AM	154	ILE
1	B1	13	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	BH	192	PRO
6	BM	230	GLY
6	BM	238	ILE
6	BM	290	VAL
1	BT	13	PRO
1	BF	18	VAL
3	B4	43	ILE
5	AL	279	ILE
6	AM	230	GLY
1	B5	18	VAL
1	BJ	34	ILE
3	BU	26	GLY
5	BL	118	PRO
6	BM	10	VAL
4	AH	186	GLY
6	AM	290	VAL
2	BB	14	ASN
3	BO	41	VAL
6	BM	24	VAL

5.3.2 Protein sidechains (i)

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	A1	37/51 (72%)	31 (84%)	6 (16%)	3 20
1	A2	37/51 (72%)	31 (84%)	6 (16%)	3 20
1	A3	37/51 (72%)	29 (78%)	8 (22%)	1 9
1	A5	37/51 (72%)	33 (89%)	4 (11%)	8 35
1	A7	37/51 (72%)	27 (73%)	10 (27%)	0 5
1	AD	37/51 (72%)	32 (86%)	5 (14%)	5 27
1	AF	37/51 (72%)	32 (86%)	5 (14%)	5 27
1	AJ	37/51 (72%)	28 (76%)	9 (24%)	1 6
1	AN	37/51 (72%)	33 (89%)	4 (11%)	8 35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	AP	37/51 (72%)	30 (81%)	7 (19%)	2 13
1	AT	37/51 (72%)	33 (89%)	4 (11%)	8 35
1	AV	37/51 (72%)	29 (78%)	8 (22%)	1 9
1	AX	37/51 (72%)	26 (70%)	11 (30%)	0 3
1	AZ	37/51 (72%)	27 (73%)	10 (27%)	0 5
1	B1	37/51 (72%)	29 (78%)	8 (22%)	1 9
1	B2	37/51 (72%)	33 (89%)	4 (11%)	8 35
1	B3	37/51 (72%)	27 (73%)	10 (27%)	0 5
1	B5	37/51 (72%)	31 (84%)	6 (16%)	3 20
1	B7	37/51 (72%)	28 (76%)	9 (24%)	1 6
1	BD	37/51 (72%)	26 (70%)	11 (30%)	0 3
1	BF	37/51 (72%)	33 (89%)	4 (11%)	8 35
1	BJ	37/51 (72%)	29 (78%)	8 (22%)	1 9
1	BN	37/51 (72%)	31 (84%)	6 (16%)	3 20
1	BP	37/51 (72%)	27 (73%)	10 (27%)	0 5
1	BT	37/51 (72%)	30 (81%)	7 (19%)	2 13
1	BV	37/51 (72%)	30 (81%)	7 (19%)	2 13
1	BX	37/51 (72%)	29 (78%)	8 (22%)	1 9
1	BZ	37/51 (72%)	28 (76%)	9 (24%)	1 6
2	AB	46/66 (70%)	34 (74%)	12 (26%)	0 5
2	BB	46/66 (70%)	35 (76%)	11 (24%)	1 7
3	A4	39/40 (98%)	29 (74%)	10 (26%)	0 6
3	A6	39/40 (98%)	34 (87%)	5 (13%)	5 29
3	A8	39/40 (98%)	33 (85%)	6 (15%)	3 22
3	A9	39/40 (98%)	33 (85%)	6 (15%)	3 22
3	AE	39/40 (98%)	32 (82%)	7 (18%)	2 15
3	AG	39/40 (98%)	31 (80%)	8 (20%)	1 10
3	AI	39/40 (98%)	34 (87%)	5 (13%)	5 29
3	AK	39/40 (98%)	35 (90%)	4 (10%)	9 37
3	AO	39/40 (98%)	31 (80%)	8 (20%)	1 10
3	AQ	39/40 (98%)	36 (92%)	3 (8%)	16 52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	AS	39/40 (98%)	34 (87%)	5 (13%)	5 29
3	AU	39/40 (98%)	34 (87%)	5 (13%)	5 29
3	AW	39/40 (98%)	35 (90%)	4 (10%)	9 37
3	AY	39/40 (98%)	26 (67%)	13 (33%)	0 2
3	B4	39/40 (98%)	35 (90%)	4 (10%)	9 37
3	B6	39/40 (98%)	32 (82%)	7 (18%)	2 15
3	B8	39/40 (98%)	35 (90%)	4 (10%)	9 37
3	B9	39/40 (98%)	36 (92%)	3 (8%)	16 52
3	BE	39/40 (98%)	32 (82%)	7 (18%)	2 15
3	BG	39/40 (98%)	32 (82%)	7 (18%)	2 15
3	BI	39/40 (98%)	37 (95%)	2 (5%)	29 66
3	BK	39/40 (98%)	33 (85%)	6 (15%)	3 22
3	BO	39/40 (98%)	33 (85%)	6 (15%)	3 22
3	BQ	39/40 (98%)	36 (92%)	3 (8%)	16 52
3	BS	39/40 (98%)	31 (80%)	8 (20%)	1 10
3	BU	39/40 (98%)	36 (92%)	3 (8%)	16 52
3	BW	39/40 (98%)	36 (92%)	3 (8%)	16 52
3	BY	39/40 (98%)	32 (82%)	7 (18%)	2 15
4	AH	201/208 (97%)	166 (83%)	35 (17%)	2 17
4	BH	201/208 (97%)	176 (88%)	25 (12%)	6 30
5	AL	220/221 (100%)	183 (83%)	37 (17%)	2 19
5	BL	220/221 (100%)	183 (83%)	37 (17%)	2 19
6	AM	238/241 (99%)	203 (85%)	35 (15%)	4 24
6	BM	238/241 (99%)	199 (84%)	39 (16%)	3 19
All	All	3538/4020 (88%)	2944 (83%)	594 (17%)	2 19

All (594) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A5	15	ARG
1	A5	31	ILE
1	A5	35	LEU
1	A5	44	LEU
1	AT	27	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AT	31	ILE
1	AT	44	LEU
1	AT	45	GLU
1	AV	15	ARG
1	AV	24	LEU
1	AV	27	LEU
1	AV	31	ILE
1	AV	35	LEU
1	AV	38	THR
1	AV	43	TRP
1	AV	44	LEU
1	AX	8	TRP
1	AX	9	MET
1	AX	12	ASP
1	AX	14	ARG
1	AX	15	ARG
1	AX	16	VAL
1	AX	26	LEU
1	AX	27	LEU
1	AX	31	ILE
1	AX	35	LEU
1	AX	44	LEU
1	A3	15	ARG
1	A3	16	VAL
1	A3	24	LEU
1	A3	27	LEU
1	A3	31	ILE
1	A3	35	LEU
1	A3	43	TRP
1	A3	44	LEU
1	A7	9	MET
1	A7	14	ARG
1	A7	26	LEU
1	A7	27	LEU
1	A7	29	VAL
1	A7	31	ILE
1	A7	35	LEU
1	A7	41	TYR
1	A7	43	TRP
1	A7	45	GLU
1	AD	27	LEU
1	AD	31	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AD	40	SER
1	AD	43	TRP
1	AD	44	LEU
1	AF	14	ARG
1	AF	26	LEU
1	AF	27	LEU
1	AF	38	THR
1	AF	44	LEU
1	A1	15	ARG
1	A1	26	LEU
1	A1	27	LEU
1	A1	31	ILE
1	A1	43	TRP
1	A1	44	LEU
1	AJ	20	GLN
1	AJ	24	LEU
1	AJ	26	LEU
1	AJ	30	MET
1	AJ	31	ILE
1	AJ	35	LEU
1	AJ	41	TYR
1	AJ	44	LEU
1	AJ	45	GLU
1	A2	20	GLN
1	A2	24	LEU
1	A2	26	LEU
1	A2	27	LEU
1	A2	31	ILE
1	A2	35	LEU
1	AN	18	VAL
1	AN	31	ILE
1	AN	35	LEU
1	AN	43	TRP
1	AP	14	ARG
1	AP	23	PHE
1	AP	27	LEU
1	AP	31	ILE
1	AP	35	LEU
1	AP	43	TRP
1	AP	44	LEU
1	AZ	9	MET
1	AZ	15	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AZ	24	LEU
1	AZ	25	PHE
1	AZ	26	LEU
1	AZ	27	LEU
1	AZ	31	ILE
1	AZ	38	THR
1	AZ	43	TRP
1	AZ	44	LEU
2	AB	9	ASP
2	AB	10	HIS
2	AB	19	LEU
2	AB	20	ARG
2	AB	26	GLN
2	AB	27	MET
2	AB	29	LYS
2	AB	41	THR
2	AB	42	LEU
2	AB	43	LEU
2	AB	44	LEU
2	AB	49	ARG
3	AS	6	LEU
3	AS	11	LEU
3	AS	14	GLU
3	AS	24	MET
3	AS	45	ARG
3	A9	6	LEU
3	A9	11	LEU
3	A9	14	GLU
3	A9	22	VAL
3	A9	24	MET
3	A9	47	TRP
3	AO	5	ASP
3	AO	6	LEU
3	AO	22	VAL
3	AO	23	TYR
3	AO	24	MET
3	AO	27	LEU
3	AO	38	HIS
3	AO	41	VAL
3	AQ	6	LEU
3	AQ	11	LEU
3	AQ	39	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A6	2	ASP
3	A6	5	ASP
3	A6	6	LEU
3	A6	11	LEU
3	A6	44	TRP
3	AU	6	LEU
3	AU	11	LEU
3	AU	15	GLN
3	AU	17	GLN
3	AU	28	TRP
3	AW	9	THR
3	AW	11	LEU
3	AW	24	MET
3	AW	45	ARG
3	AY	2	ASP
3	AY	5	ASP
3	AY	6	LEU
3	AY	8	TYR
3	AY	9	THR
3	AY	15	GLN
3	AY	17	GLN
3	AY	33	VAL
3	AY	41	VAL
3	AY	42	TYR
3	AY	45	ARG
3	AY	47	TRP
3	AY	48	PHE
3	A4	2	ASP
3	A4	4	SER
3	A4	6	LEU
3	A4	11	LEU
3	A4	13	ASP
3	A4	14	GLU
3	A4	17	GLN
3	A4	18	GLU
3	A4	24	MET
3	A4	45	ARG
3	A8	5	ASP
3	A8	6	LEU
3	A8	9	THR
3	A8	11	LEU
3	A8	42	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A8	45	ARG
3	AE	8	TYR
3	AE	11	LEU
3	AE	15	GLN
3	AE	17	GLN
3	AE	27	LEU
3	AE	42	TYR
3	AE	47	TRP
3	AG	5	ASP
3	AG	6	LEU
3	AG	11	LEU
3	AG	19	LEU
3	AG	22	VAL
3	AG	27	LEU
3	AG	41	VAL
3	AG	48	PHE
3	AI	8	TYR
3	AI	11	LEU
3	AI	13	ASP
3	AI	15	GLN
3	AI	23	TYR
3	AK	6	LEU
3	AK	11	LEU
3	AK	28	TRP
3	AK	42	TYR
4	AH	11	ASP
4	AH	12	LEU
4	AH	19	SER
4	AH	21	TRP
4	AH	24	LEU
4	AH	28	ILE
4	AH	30	TYR
4	AH	35	ASN
4	AH	46	ASP
4	AH	52	ASN
4	AH	65	ILE
4	AH	70	ARG
4	AH	74	THR
4	AH	75	VAL
4	AH	85	ILE
4	AH	109	VAL
4	AH	135	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	AH	156	CYS
4	AH	167	ILE
4	AH	170	ASP
4	AH	188	THR
4	AH	191	LEU
4	AH	199	GLN
4	AH	201	ASN
4	AH	206	ASN
4	AH	218	THR
4	AH	219	ILE
4	AH	220	LYS
4	AH	225	VAL
4	AH	228	LEU
4	AH	233	ILE
4	AH	247	LYS
4	AH	248	ARG
4	AH	249	LYS
4	AH	258	GLU
5	AL	2	LEU
5	AL	7	ARG
5	AL	8	LYS
5	AL	11	VAL
5	AL	23	ASP
5	AL	25	TRP
5	AL	54	VAL
5	AL	55	LEU
5	AL	63	LEU
5	AL	67	TYR
5	AL	73	TYR
5	AL	113	ILE
5	AL	139	MET
5	AL	150	ILE
5	AL	160	THR
5	AL	163	THR
5	AL	167	PHE
5	AL	174	MET
5	AL	179	PHE
5	AL	180	PHE
5	AL	182	THR
5	AL	183	ASN
5	AL	185	LEU
5	AL	207	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AL	214	THR
5	AL	216	PHE
5	AL	226	THR
5	AL	232	LEU
5	AL	237	SER
5	AL	244	SER
5	AL	247	CYS
5	AL	250	ILE
5	AL	253	THR
5	AL	254	ILE
5	AL	265	TRP
5	AL	271	TRP
5	AL	280	ASN
6	AM	3	TYR
6	AM	11	GLN
6	AM	24	VAL
6	AM	26	LEU
6	AM	47	LEU
6	AM	74	PHE
6	AM	75	TRP
6	AM	86	LEU
6	AM	90	PHE
6	AM	100	GLU
6	AM	101	TYR
6	AM	110	LYS
6	AM	124	VAL
6	AM	132	ARG
6	AM	136	ARG
6	AM	138	GLN
6	AM	144	LYS
6	AM	146	THR
6	AM	151	LEU
6	AM	156	LEU
6	AM	157	TRP
6	AM	158	MET
6	AM	163	ILE
6	AM	164	ARG
6	AM	171	TRP
6	AM	197	PHE
6	AM	202	HIS
6	AM	214	LEU
6	AM	215	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	AM	216	PHE
6	AM	218	MET
6	AM	250	LEU
6	AM	278	LEU
6	AM	279	THR
6	AM	285	LEU
1	B5	11	PHE
1	B5	14	ARG
1	B5	15	ARG
1	B5	26	LEU
1	B5	31	ILE
1	B5	44	LEU
1	BT	26	LEU
1	BT	27	LEU
1	BT	31	ILE
1	BT	35	LEU
1	BT	36	LEU
1	BT	44	LEU
1	BT	45	GLU
1	BV	15	ARG
1	BV	24	LEU
1	BV	27	LEU
1	BV	31	ILE
1	BV	35	LEU
1	BV	43	TRP
1	BV	44	LEU
1	BX	12	ASP
1	BX	14	ARG
1	BX	16	VAL
1	BX	26	LEU
1	BX	27	LEU
1	BX	31	ILE
1	BX	35	LEU
1	BX	44	LEU
1	B3	15	ARG
1	B3	16	VAL
1	B3	17	PHE
1	B3	24	LEU
1	B3	27	LEU
1	B3	31	ILE
1	B3	35	LEU
1	B3	38	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B3	43	TRP
1	B3	44	LEU
1	B7	9	MET
1	B7	15	ARG
1	B7	24	LEU
1	B7	26	LEU
1	B7	27	LEU
1	B7	29	VAL
1	B7	31	ILE
1	B7	35	LEU
1	B7	43	TRP
1	BD	9	MET
1	BD	16	VAL
1	BD	22	VAL
1	BD	23	PHE
1	BD	24	LEU
1	BD	26	LEU
1	BD	27	LEU
1	BD	29	VAL
1	BD	31	ILE
1	BD	43	TRP
1	BD	44	LEU
1	BF	14	ARG
1	BF	27	LEU
1	BF	35	LEU
1	BF	43	TRP
1	B1	14	ARG
1	B1	15	ARG
1	B1	23	PHE
1	B1	27	LEU
1	B1	31	ILE
1	B1	43	TRP
1	B1	44	LEU
1	B1	45	GLU
1	BJ	26	LEU
1	BJ	30	MET
1	BJ	31	ILE
1	BJ	34	ILE
1	BJ	36	LEU
1	BJ	41	TYR
1	BJ	43	TRP
1	BJ	44	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B2	20	GLN
1	B2	24	LEU
1	B2	27	LEU
1	B2	31	ILE
1	BN	10	ILE
1	BN	26	LEU
1	BN	27	LEU
1	BN	31	ILE
1	BN	35	LEU
1	BN	43	TRP
1	BP	14	ARG
1	BP	20	GLN
1	BP	23	PHE
1	BP	26	LEU
1	BP	27	LEU
1	BP	29	VAL
1	BP	31	ILE
1	BP	35	LEU
1	BP	43	TRP
1	BP	44	LEU
1	BZ	8	TRP
1	BZ	9	MET
1	BZ	15	ARG
1	BZ	22	VAL
1	BZ	26	LEU
1	BZ	31	ILE
1	BZ	38	THR
1	BZ	40	SER
1	BZ	43	TRP
2	BB	8	ASN
2	BB	9	ASP
2	BB	18	ASN
2	BB	19	LEU
2	BB	26	GLN
2	BB	27	MET
2	BB	29	LYS
2	BB	41	THR
2	BB	43	LEU
2	BB	44	LEU
2	BB	49	ARG
3	BS	2	ASP
3	BS	5	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	BS	6	LEU
3	BS	8	TYR
3	BS	11	LEU
3	BS	13	ASP
3	BS	18	GLU
3	BS	45	ARG
3	B9	6	LEU
3	B9	24	MET
3	B9	47	TRP
3	BO	5	ASP
3	BO	6	LEU
3	BO	11	LEU
3	BO	15	GLN
3	BO	24	MET
3	BO	48	PHE
3	BQ	11	LEU
3	BQ	24	MET
3	BQ	39	LEU
3	B6	6	LEU
3	B6	11	LEU
3	B6	19	LEU
3	B6	27	LEU
3	B6	44	TRP
3	B6	45	ARG
3	B6	48	PHE
3	BU	6	LEU
3	BU	11	LEU
3	BU	45	ARG
3	BW	9	THR
3	BW	24	MET
3	BW	48	PHE
3	BY	2	ASP
3	BY	6	LEU
3	BY	15	GLN
3	BY	17	GLN
3	BY	41	VAL
3	BY	42	TYR
3	BY	47	TRP
3	B4	6	LEU
3	B4	18	GLU
3	B4	44	TRP
3	B4	45	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B8	11	LEU
3	B8	24	MET
3	B8	42	TYR
3	B8	48	PHE
3	BE	6	LEU
3	BE	8	TYR
3	BE	11	LEU
3	BE	15	GLN
3	BE	17	GLN
3	BE	42	TYR
3	BE	47	TRP
3	BG	5	ASP
3	BG	6	LEU
3	BG	11	LEU
3	BG	15	GLN
3	BG	24	MET
3	BG	41	VAL
3	BG	47	TRP
3	BI	11	LEU
3	BI	13	ASP
3	BK	6	LEU
3	BK	9	THR
3	BK	11	LEU
3	BK	15	GLN
3	BK	23	TYR
3	BK	38	HIS
4	BH	12	LEU
4	BH	24	LEU
4	BH	30	TYR
4	BH	34	GLU
4	BH	46	ASP
4	BH	52	ASN
4	BH	58	LEU
4	BH	74	THR
4	BH	109	VAL
4	BH	120	LEU
4	BH	135	LYS
4	BH	151	LEU
4	BH	156	CYS
4	BH	167	ILE
4	BH	170	ASP
4	BH	191	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	BH	201	ASN
4	BH	206	ASN
4	BH	220	LYS
4	BH	225	VAL
4	BH	247	LYS
4	BH	249	LYS
4	BH	250	SER
4	BH	255	MET
4	BH	258	GLU
5	BL	2	LEU
5	BL	8	LYS
5	BL	21	LEU
5	BL	23	ASP
5	BL	25	TRP
5	BL	38	THR
5	BL	44	LEU
5	BL	49	ILE
5	BL	54	VAL
5	BL	60	ASN
5	BL	63	LEU
5	BL	67	TYR
5	BL	73	TYR
5	BL	129	LEU
5	BL	137	VAL
5	BL	139	MET
5	BL	174	MET
5	BL	175	ILE
5	BL	180	PHE
5	BL	182	THR
5	BL	183	ASN
5	BL	189	LEU
5	BL	207	ARG
5	BL	210	ASP
5	BL	216	PHE
5	BL	218	ASP
5	BL	220	VAL
5	BL	231	ARG
5	BL	232	LEU
5	BL	241	VAL
5	BL	249	ILE
5	BL	254	ILE
5	BL	257	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	BL	258	GLN
5	BL	261	ASP
5	BL	265	TRP
5	BL	271	TRP
6	BM	9	GLN
6	BM	10	VAL
6	BM	11	GLN
6	BM	18	LEU
6	BM	22	GLU
6	BM	24	VAL
6	BM	29	ARG
6	BM	38	LEU
6	BM	60	LEU
6	BM	75	TRP
6	BM	86	LEU
6	BM	90	PHE
6	BM	101	TYR
6	BM	123	PHE
6	BM	124	VAL
6	BM	136	ARG
6	BM	138	GLN
6	BM	144	LYS
6	BM	146	THR
6	BM	152	SER
6	BM	156	LEU
6	BM	163	ILE
6	BM	171	TRP
6	BM	173	GLU
6	BM	177	TYR
6	BM	180	PHE
6	BM	186	THR
6	BM	197	PHE
6	BM	198	TYR
6	BM	202	HIS
6	BM	214	LEU
6	BM	215	LEU
6	BM	216	PHE
6	BM	218	MET
6	BM	224	LEU
6	BM	250	LEU
6	BM	279	THR
6	BM	285	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	BM	287	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A5	32	HIS
1	AT	42	ASN
1	A3	32	HIS
1	A7	32	HIS
1	AJ	32	HIS
3	AS	15	GLN
3	A9	38	HIS
3	AO	15	GLN
3	AO	38	HIS
3	AQ	15	GLN
3	AU	15	GLN
3	AW	15	GLN
3	AY	15	GLN
3	A8	15	GLN
3	AE	15	GLN
3	AG	15	GLN
3	AI	38	HIS
4	AH	35	ASN
4	AH	52	ASN
4	AH	98	HIS
4	AH	147	ASN
4	AH	206	ASN
5	AL	153	HIS
5	AL	166	ASN
5	AL	173	HIS
5	AL	183	ASN
5	AL	264	GLN
6	AM	4	GLN
6	AM	44	ASN
6	AM	237	GLN
1	B5	32	HIS
1	B3	32	HIS
1	B7	32	HIS
1	BZ	42	ASN
3	BE	15	GLN
3	BK	15	GLN
3	BK	38	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	BH	52	ASN
4	BH	53	GLN
4	BH	147	ASN
4	BH	201	ASN
4	BH	206	ASN
5	BL	87	GLN
5	BL	153	HIS
5	BL	159	ASN
5	BL	173	HIS
5	BL	183	ASN
5	BL	230	HIS
5	BL	264	GLN
6	BM	9	GLN
6	BM	25	ASN
6	BM	44	ASN
6	BM	77	GLN
6	BM	188	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 76 ligands modelled in this entry, 2 are monoatomic - leaving 74 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	$\#\|Z\|>2$
7	BCL	A1	101	-	30,54,74	1.70	5 (16%)	33,91,115	1.91	6 (18%)
7	BCL	A2	101	-	30,54,74	1.64	5 (16%)	33,91,115	1.87	6 (18%)
7	BCL	A3	101	-	30,54,74	1.70	5 (16%)	33,91,115	1.92	6 (18%)
7	BCL	A4	101	-	30,54,74	1.69	5 (16%)	33,91,115	1.88	6 (18%)
7	BCL	A6	101	-	30,54,74	1.63	5 (16%)	33,91,115	1.86	7 (21%)
7	BCL	A6	102	-	30,54,74	1.70	6 (20%)	33,91,115	1.86	6 (18%)
7	BCL	A7	101	-	30,54,74	1.62	5 (16%)	33,91,115	1.85	7 (21%)
7	BCL	A8	101	-	30,54,74	1.60	5 (16%)	33,91,115	1.84	6 (18%)
7	BCL	A9	101	-	30,54,74	1.68	5 (16%)	33,91,115	1.85	6 (18%)
7	BCL	AD	101	-	30,54,74	1.62	5 (16%)	33,91,115	1.88	6 (18%)
7	BCL	AD	102	-	30,54,74	1.66	5 (16%)	33,91,115	1.83	6 (18%)
7	BCL	AF	101	-	30,54,74	1.61	5 (16%)	33,91,115	1.86	6 (18%)
7	BCL	AG	101	-	30,54,74	1.68	5 (16%)	33,91,115	1.87	6 (18%)
7	BCL	AI	101	-	30,54,74	1.66	6 (20%)	33,91,115	1.82	6 (18%)
7	BCL	AJ	101	-	30,54,74	1.68	5 (16%)	33,91,115	1.86	6 (18%)
7	BCL	AK	101	-	30,54,74	1.64	5 (16%)	33,91,115	1.88	6 (18%)
7	BCL	AL	301	-	53,74,74	1.39	6 (11%)	57,115,115	1.61	8 (14%)
7	BCL	AL	302	-	53,74,74	1.54	8 (15%)	57,115,115	1.65	8 (14%)
8	BPH	AL	303	-	64,70,70	2.56	14 (21%)	73,101,101	1.70	12 (16%)
9	U10	AL	304	-	48,48,63	1.14	2 (4%)	58,61,79	1.73	13 (22%)
10	PO4	AL	305	-	4,4,4	0.47	0	6,6,6	0.27	0
7	BCL	AM	401	-	53,74,74	1.35	6 (11%)	57,115,115	1.63	9 (15%)
7	BCL	AM	402	-	53,74,74	1.52	7 (13%)	57,115,115	1.60	7 (12%)
8	BPH	AM	403	-	64,70,70	2.47	11 (17%)	73,101,101	1.69	13 (17%)
9	U10	AM	405	-	48,48,63	1.78	4 (8%)	58,61,79	1.77	14 (24%)
12	SPO	AM	406	-	40,41,41	1.33	2 (5%)	45,50,50	2.08	12 (26%)
7	BCL	AN	101	-	30,54,74	1.68	5 (16%)	33,91,115	1.92	6 (18%)
7	BCL	AO	101	-	30,54,74	1.65	5 (16%)	33,91,115	1.81	6 (18%)
7	BCL	AP	101	-	30,54,74	1.61	5 (16%)	33,91,115	1.86	6 (18%)
7	BCL	AP	102	-	30,54,74	1.68	6 (20%)	33,91,115	1.83	6 (18%)
7	BCL	AS	101	-	30,54,74	1.66	5 (16%)	33,91,115	1.87	6 (18%)
7	BCL	AT	101	-	30,54,74	1.63	5 (16%)	33,91,115	1.85	7 (21%)
7	BCL	AT	102	-	30,54,74	1.70	6 (20%)	33,91,115	1.85	6 (18%)
7	BCL	AV	101	-	30,54,74	1.63	5 (16%)	33,91,115	1.87	6 (18%)
7	BCL	AW	101	-	30,54,74	1.62	5 (16%)	33,91,115	1.85	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	BCL	AY	101	-	30,54,74	1.69	5 (16%)	33,91,115	1.93	6 (18%)
7	BCL	AY	102	-	30,54,74	1.69	5 (16%)	33,91,115	1.86	6 (18%)
7	BCL	AZ	101	-	30,54,74	1.67	5 (16%)	33,91,115	1.87	6 (18%)
7	BCL	B1	101	-	30,54,74	1.69	5 (16%)	33,91,115	1.92	6 (18%)
7	BCL	B2	101	-	30,54,74	1.62	5 (16%)	33,91,115	1.89	6 (18%)
7	BCL	B3	101	-	30,54,74	1.69	5 (16%)	33,91,115	1.91	6 (18%)
7	BCL	B4	101	-	30,54,74	1.69	5 (16%)	33,91,115	1.88	6 (18%)
7	BCL	B5	101	-	30,54,74	1.63	5 (16%)	33,91,115	1.84	7 (21%)
7	BCL	B6	101	-	30,54,74	1.68	6 (20%)	33,91,115	1.85	6 (18%)
7	BCL	B7	101	-	30,54,74	1.63	5 (16%)	33,91,115	1.84	6 (18%)
7	BCL	B8	101	-	30,54,74	1.61	5 (16%)	33,91,115	1.82	6 (18%)
7	BCL	B9	101	-	30,54,74	1.68	5 (16%)	33,91,115	1.87	6 (18%)
7	BCL	BD	101	-	30,54,74	1.65	5 (16%)	33,91,115	1.89	6 (18%)
7	BCL	BD	102	-	30,54,74	1.67	5 (16%)	33,91,115	1.84	6 (18%)
7	BCL	BF	101	-	30,54,74	1.61	5 (16%)	33,91,115	1.87	6 (18%)
7	BCL	BF	102	-	30,54,74	1.68	5 (16%)	33,91,115	1.86	6 (18%)
7	BCL	BI	101	-	30,54,74	1.67	5 (16%)	33,91,115	1.83	6 (18%)
7	BCL	BK	101	-	30,54,74	1.61	5 (16%)	33,91,115	1.89	5 (15%)
7	BCL	BK	102	-	30,54,74	1.69	5 (16%)	33,91,115	1.87	6 (18%)
7	BCL	BL	301	-	53,74,74	1.45	6 (11%)	57,115,115	1.63	10 (17%)
7	BCL	BL	302	-	53,74,74	1.45	6 (11%)	57,115,115	1.61	7 (12%)
7	BCL	BL	303	-	53,74,74	1.49	8 (15%)	57,115,115	1.61	9 (15%)
8	BPH	BL	304	-	64,70,70	2.56	14 (21%)	73,101,101	1.70	12 (16%)
9	U10	BL	306	-	48,48,63	1.20	3 (6%)	58,61,79	1.73	13 (22%)
10	PO4	BL	307	-	4,4,4	0.46	0	6,6,6	0.27	0
7	BCL	BM	401	-	53,74,74	2.03	10 (18%)	57,115,115	1.66	11 (19%)
8	BPH	BM	402	-	64,70,70	2.47	11 (17%)	73,101,101	1.68	12 (16%)
7	BCL	BO	101	-	30,54,74	1.68	5 (16%)	33,91,115	1.91	6 (18%)
7	BCL	BO	102	-	30,54,74	1.66	5 (16%)	33,91,115	1.82	7 (21%)
7	BCL	BP	101	-	30,54,74	1.60	5 (16%)	33,91,115	1.87	6 (18%)
7	BCL	BP	102	-	30,54,74	1.68	6 (20%)	33,91,115	1.81	6 (18%)
7	BCL	BT	101	-	30,54,74	1.61	5 (16%)	33,91,115	1.84	7 (21%)
7	BCL	BU	101	-	30,54,74	1.69	6 (20%)	33,91,115	1.86	6 (18%)
7	BCL	BV	101	-	30,54,74	1.62	5 (16%)	33,91,115	1.87	6 (18%)
7	BCL	BV	102	-	30,54,74	1.60	5 (16%)	33,91,115	1.85	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	BCL	BY	101	-	30,54,74	1.71	5 (16%)	33,91,115	1.93	6 (18%)
7	BCL	BY	102	-	30,54,74	1.68	5 (16%)	33,91,115	1.83	6 (18%)
7	BCL	BZ	101	-	30,54,74	1.67	5 (16%)	33,91,115	1.89	6 (18%)
7	BCL	BZ	102	-	30,54,74	1.68	5 (16%)	33,91,115	1.86	6 (18%)

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
7	BCL	A1	101	-	-	0/11/113/137	0/0/9/9
7	BCL	A2	101	-	-	0/11/113/137	0/0/9/9
7	BCL	A3	101	-	-	0/11/113/137	0/0/9/9
7	BCL	A4	101	-	-	0/11/113/137	0/0/9/9
7	BCL	A6	101	-	-	0/11/113/137	0/0/9/9
7	BCL	A6	102	-	-	0/11/113/137	0/0/9/9
7	BCL	A7	101	-	-	0/11/113/137	0/0/9/9
7	BCL	A8	101	-	-	0/11/113/137	0/0/9/9
7	BCL	A9	101	-	-	0/11/113/137	0/0/9/9
7	BCL	AD	101	-	-	0/11/113/137	0/0/9/9
7	BCL	AD	102	-	-	0/11/113/137	0/0/9/9
7	BCL	AF	101	-	-	0/11/113/137	0/0/9/9
7	BCL	AG	101	-	-	0/11/113/137	0/0/9/9
7	BCL	AI	101	-	-	0/11/113/137	0/0/9/9
7	BCL	AJ	101	-	-	0/11/113/137	0/0/9/9
7	BCL	AK	101	-	-	0/11/113/137	0/0/9/9
7	BCL	AL	301	-	-	0/37/137/137	0/0/9/9
7	BCL	AL	302	-	-	0/37/137/137	0/0/9/9
8	BPH	AL	303	-	-	0/54/105/105	0/1/6/6
9	U10	AL	304	-	-	0/45/69/87	0/1/1/1
10	PO4	AL	305	-	-	0/0/0/0	0/0/0/0
7	BCL	AM	401	-	-	0/37/137/137	0/0/9/9
7	BCL	AM	402	-	-	0/37/137/137	0/0/9/9
8	BPH	AM	403	-	-	0/54/105/105	0/1/6/6
9	U10	AM	405	-	-	0/45/69/87	0/1/1/1
12	SPO	AM	406	-	-	0/47/47/47	0/0/0/0
7	BCL	AN	101	-	-	0/11/113/137	0/0/9/9
7	BCL	AO	101	-	-	0/11/113/137	0/0/9/9
7	BCL	AP	101	-	-	0/11/113/137	0/0/9/9
7	BCL	AP	102	-	-	0/11/113/137	0/0/9/9
7	BCL	AS	101	-	-	0/11/113/137	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	AT	101	-	-	0/11/113/137	0/0/9/9
7	BCL	AT	102	-	-	0/11/113/137	0/0/9/9
7	BCL	AV	101	-	-	0/11/113/137	0/0/9/9
7	BCL	AW	101	-	-	0/11/113/137	0/0/9/9
7	BCL	AY	101	-	-	0/11/113/137	0/0/9/9
7	BCL	AY	102	-	-	0/11/113/137	0/0/9/9
7	BCL	AZ	101	-	-	0/11/113/137	0/0/9/9
7	BCL	B1	101	-	-	0/11/113/137	0/0/9/9
7	BCL	B2	101	-	-	0/11/113/137	0/0/9/9
7	BCL	B3	101	-	-	0/11/113/137	0/0/9/9
7	BCL	B4	101	-	-	0/11/113/137	0/0/9/9
7	BCL	B5	101	-	-	0/11/113/137	0/0/9/9
7	BCL	B6	101	-	-	0/11/113/137	0/0/9/9
7	BCL	B7	101	-	-	0/11/113/137	0/0/9/9
7	BCL	B8	101	-	-	0/11/113/137	0/0/9/9
7	BCL	B9	101	-	-	0/11/113/137	0/0/9/9
7	BCL	BD	101	-	-	0/11/113/137	0/0/9/9
7	BCL	BD	102	-	-	0/11/113/137	0/0/9/9
7	BCL	BF	101	-	-	0/11/113/137	0/0/9/9
7	BCL	BF	102	-	-	0/11/113/137	0/0/9/9
7	BCL	BI	101	-	-	0/11/113/137	0/0/9/9
7	BCL	BK	101	-	-	0/11/113/137	0/0/9/9
7	BCL	BK	102	-	-	0/11/113/137	0/0/9/9
7	BCL	BL	301	-	-	0/37/137/137	0/0/9/9
7	BCL	BL	302	-	-	0/37/137/137	0/0/9/9
7	BCL	BL	303	-	-	0/37/137/137	0/0/9/9
8	BPH	BL	304	-	-	0/54/105/105	0/1/6/6
9	U10	BL	306	-	-	0/45/69/87	0/1/1/1
10	PO4	BL	307	-	-	0/0/0/0	0/0/0/0
7	BCL	BM	401	-	-	0/37/137/137	0/0/9/9
8	BPH	BM	402	-	-	0/54/105/105	0/1/6/6
7	BCL	BO	101	-	-	0/11/113/137	0/0/9/9
7	BCL	BO	102	-	-	0/11/113/137	0/0/9/9
7	BCL	BP	101	-	-	0/11/113/137	0/0/9/9
7	BCL	BP	102	-	-	1/11/113/137	0/0/9/9
7	BCL	BT	101	-	-	0/11/113/137	0/0/9/9
7	BCL	BU	101	-	-	0/11/113/137	0/0/9/9
7	BCL	BV	101	-	-	0/11/113/137	0/0/9/9
7	BCL	BV	102	-	-	0/11/113/137	0/0/9/9
7	BCL	BY	101	-	-	0/11/113/137	0/0/9/9
7	BCL	BY	102	-	-	0/11/113/137	0/0/9/9
7	BCL	BZ	101	-	-	0/11/113/137	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	BZ	102	-	-	0/11/113/137	0/0/9/9

All (405) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	BL	304	BPH	C3D-C4D	-13.04	1.24	1.41
8	AL	303	BPH	C3D-C4D	-12.98	1.24	1.41
8	BM	402	BPH	C3D-C4D	-12.94	1.24	1.41
8	AM	403	BPH	C3D-C4D	-12.91	1.24	1.41
8	BM	402	BPH	C1A-NA	-4.33	1.27	1.37
8	AM	403	BPH	C1A-NA	-4.32	1.27	1.37
8	BL	304	BPH	C14-C13	-4.18	1.38	1.52
8	AL	303	BPH	C14-C13	-4.18	1.38	1.52
8	AL	303	BPH	C1A-NA	-4.15	1.28	1.37
8	BL	304	BPH	C1A-NA	-4.12	1.28	1.37
8	BM	402	BPH	C4C-NC	-3.63	1.29	1.37
8	AM	403	BPH	C4C-NC	-3.63	1.29	1.37
8	BL	304	BPH	CHB-C4A	-3.45	1.34	1.40
8	AL	303	BPH	CHB-C4A	-3.44	1.34	1.40
8	BL	304	BPH	C9-C8	-3.27	1.41	1.52
8	AL	303	BPH	C9-C8	-3.25	1.41	1.52
8	BM	402	BPH	CHB-C4A	-3.11	1.34	1.40
8	AM	403	BPH	CHB-C4A	-3.10	1.34	1.40
8	BL	304	BPH	C4C-NC	-2.93	1.30	1.37
8	AL	303	BPH	C4C-NC	-2.93	1.30	1.37
7	B6	101	BCL	C3B-C2B	2.01	1.44	1.40
7	BL	303	BCL	C3B-C2B	2.01	1.44	1.40
7	AI	101	BCL	C3B-C2B	2.03	1.45	1.40
7	A6	102	BCL	C3B-C2B	2.03	1.45	1.40
7	BU	101	BCL	C3B-C2B	2.06	1.45	1.40
7	BM	401	BCL	C3B-C2B	2.06	1.45	1.40
7	AT	102	BCL	C3B-C2B	2.06	1.45	1.40
7	AL	302	BCL	C2-C3	2.06	1.37	1.33
8	AL	303	BPH	C1B-NB	2.07	1.42	1.38
8	BL	304	BPH	C1B-NB	2.08	1.43	1.38
7	AP	102	BCL	C3B-C2B	2.11	1.45	1.40
7	AM	402	BCL	O1A-CGA	2.11	1.29	1.22
7	BP	102	BCL	C3B-C2B	2.13	1.45	1.40
7	B8	101	BCL	C4B-CHC	2.18	1.45	1.39
7	B7	101	BCL	C4B-CHC	2.19	1.45	1.39
7	B5	101	BCL	C4B-CHC	2.19	1.45	1.39
7	AT	101	BCL	C4B-CHC	2.19	1.45	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A8	101	BCL	C4B-CHC	2.20	1.45	1.39
7	BV	102	BCL	C4B-CHC	2.20	1.45	1.39
7	BP	101	BCL	C4B-CHC	2.21	1.45	1.39
7	A6	101	BCL	C4B-CHC	2.21	1.45	1.39
7	BF	101	BCL	C4B-CHC	2.22	1.46	1.39
7	AP	101	BCL	C4B-CHC	2.22	1.46	1.39
7	AF	101	BCL	C4B-CHC	2.23	1.46	1.39
7	A2	101	BCL	C4B-CHC	2.23	1.46	1.39
7	AW	101	BCL	C4B-CHC	2.23	1.46	1.39
7	BL	301	BCL	C4B-CHC	2.25	1.46	1.39
7	BT	101	BCL	C4B-CHC	2.25	1.46	1.39
7	AM	401	BCL	C4B-CHC	2.25	1.46	1.39
7	A7	101	BCL	C4B-CHC	2.27	1.46	1.39
7	AL	302	BCL	C1B-CHB	2.33	1.46	1.39
7	BL	303	BCL	C17-C18	2.35	1.69	1.51
7	BL	303	BCL	C1B-CHB	2.37	1.46	1.39
7	BV	101	BCL	C4B-CHC	2.40	1.46	1.39
7	B2	101	BCL	C4B-CHC	2.40	1.46	1.39
7	BO	102	BCL	C1B-CHB	2.50	1.46	1.39
7	AO	101	BCL	C1B-CHB	2.51	1.46	1.39
7	AL	301	BCL	C4B-CHC	2.53	1.46	1.39
7	BK	101	BCL	C4B-CHC	2.57	1.46	1.39
7	BD	102	BCL	C1B-CHB	2.60	1.47	1.39
7	B6	101	BCL	C1B-CHB	2.62	1.47	1.39
7	AM	402	BCL	C1B-CHB	2.62	1.47	1.39
7	AY	102	BCL	C1B-CHB	2.63	1.47	1.39
7	BI	101	BCL	C1B-CHB	2.63	1.47	1.39
7	BZ	102	BCL	C1B-CHB	2.63	1.47	1.39
7	AD	102	BCL	C1B-CHB	2.64	1.47	1.39
7	BY	102	BCL	C1B-CHB	2.64	1.47	1.39
7	BU	101	BCL	C1B-CHB	2.64	1.47	1.39
7	AJ	101	BCL	C1B-CHB	2.64	1.47	1.39
7	A6	102	BCL	C1B-CHB	2.64	1.47	1.39
7	AI	101	BCL	C1B-CHB	2.65	1.47	1.39
7	A9	101	BCL	C1B-CHB	2.66	1.47	1.39
7	AZ	101	BCL	C1B-CHB	2.67	1.47	1.39
7	BZ	101	BCL	C1B-CHB	2.68	1.47	1.39
7	AT	102	BCL	C1B-CHB	2.68	1.47	1.39
7	AG	101	BCL	C1B-CHB	2.70	1.47	1.39
7	BP	102	BCL	C1B-CHB	2.71	1.47	1.39
7	AP	102	BCL	C1B-CHB	2.71	1.47	1.39
7	BK	102	BCL	C1B-CHB	2.72	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	BF	102	BCL	C1B-CHB	2.72	1.47	1.39
7	B9	101	BCL	C1B-CHB	2.73	1.47	1.39
7	A4	101	BCL	C1B-CHB	2.76	1.47	1.39
7	BM	401	BCL	C1B-CHB	2.76	1.47	1.39
7	BL	302	BCL	CHD-C4C	2.76	1.49	1.41
7	BM	401	BCL	CBB-CAB	2.80	1.58	1.49
9	BL	306	U10	O3-C3M	2.81	1.52	1.45
7	B4	101	BCL	C1B-CHB	2.81	1.47	1.39
7	BL	301	BCL	CHD-C4C	2.84	1.49	1.41
7	B3	101	BCL	C1B-CHB	2.86	1.47	1.39
7	B1	101	BCL	C1B-CHB	2.88	1.47	1.39
7	AV	101	BCL	C4B-CHC	2.88	1.47	1.39
7	A1	101	BCL	C1B-CHB	2.89	1.47	1.39
7	AN	101	BCL	C1B-CHB	2.89	1.47	1.39
7	AS	101	BCL	C1B-CHB	2.90	1.47	1.39
7	A3	101	BCL	C1B-CHB	2.92	1.47	1.39
7	AK	101	BCL	C4B-CHC	2.92	1.47	1.39
7	AY	101	BCL	C1B-CHB	2.95	1.48	1.39
7	BY	101	BCL	C1B-CHB	2.96	1.48	1.39
7	BO	101	BCL	C1B-CHB	2.96	1.48	1.39
7	AL	301	BCL	CHD-C4C	2.97	1.50	1.41
7	BD	101	BCL	C1B-CHB	2.98	1.48	1.39
7	BP	101	BCL	CHD-C4C	2.98	1.50	1.41
7	AM	401	BCL	CHD-C4C	2.99	1.50	1.41
7	BK	101	BCL	CHD-C4C	2.99	1.50	1.41
7	B8	101	BCL	CHD-C4C	3.00	1.50	1.41
7	BV	102	BCL	CHD-C4C	3.01	1.50	1.41
7	BV	101	BCL	CHD-C4C	3.01	1.50	1.41
7	B2	101	BCL	CHD-C4C	3.02	1.50	1.41
7	BF	101	BCL	CHD-C4C	3.03	1.50	1.41
7	AP	101	BCL	CHD-C4C	3.03	1.50	1.41
7	AV	101	BCL	CHD-C4C	3.03	1.50	1.41
7	A7	101	BCL	CHD-C4C	3.04	1.50	1.41
7	A8	101	BCL	CHD-C4C	3.04	1.50	1.41
7	AF	101	BCL	CHD-C4C	3.04	1.50	1.41
7	AW	101	BCL	CHD-C4C	3.06	1.50	1.41
7	AD	101	BCL	CHD-C4C	3.06	1.50	1.41
7	B7	101	BCL	CHD-C4C	3.06	1.50	1.41
7	A2	101	BCL	CHD-C4C	3.07	1.50	1.41
7	AK	101	BCL	CHD-C4C	3.07	1.50	1.41
7	BL	302	BCL	C4B-CHC	3.08	1.48	1.39
7	BD	101	BCL	CHD-C4C	3.08	1.50	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	AD	101	BCL	C1B-CHB	3.08	1.48	1.39
7	AT	101	BCL	CHD-C4C	3.09	1.50	1.41
7	B5	101	BCL	CHD-C4C	3.10	1.50	1.41
9	AL	304	U10	C4-C3	3.10	1.49	1.35
7	BT	101	BCL	CHD-C4C	3.10	1.50	1.41
7	A6	101	BCL	CHD-C4C	3.10	1.50	1.41
7	AD	101	BCL	C4B-CHC	3.11	1.48	1.39
7	AS	101	BCL	CHD-C4C	3.12	1.50	1.41
9	AM	405	U10	C4-C3	3.13	1.49	1.35
7	AP	101	BCL	C1B-CHB	3.18	1.48	1.39
7	AL	302	BCL	C4B-CHC	3.21	1.48	1.39
7	AN	101	BCL	CHD-C4C	3.21	1.50	1.41
7	BP	101	BCL	C1B-CHB	3.21	1.48	1.39
7	AL	302	BCL	CHD-C4C	3.22	1.50	1.41
7	B9	101	BCL	CHD-C4C	3.23	1.50	1.41
7	AL	301	BCL	C1B-CHB	3.23	1.48	1.39
7	A8	101	BCL	C1B-CHB	3.24	1.48	1.39
7	BO	101	BCL	CHD-C4C	3.24	1.50	1.41
7	BZ	101	BCL	CHD-C4C	3.25	1.50	1.41
9	BL	306	U10	C4-C3	3.26	1.49	1.35
7	AK	101	BCL	C1B-CHB	3.26	1.48	1.39
7	BM	401	BCL	C4B-CHC	3.26	1.48	1.39
7	AZ	101	BCL	CHD-C4C	3.26	1.51	1.41
7	AY	101	BCL	CHD-C4C	3.27	1.51	1.41
7	B1	101	BCL	CHD-C4C	3.28	1.51	1.41
7	BO	102	BCL	CHD-C4C	3.28	1.51	1.41
7	B8	101	BCL	C1B-CHB	3.28	1.48	1.39
7	BF	101	BCL	C1B-CHB	3.28	1.48	1.39
7	A1	101	BCL	CHD-C4C	3.28	1.51	1.41
7	A3	101	BCL	CHD-C4C	3.29	1.51	1.41
7	AO	101	BCL	CHD-C4C	3.29	1.51	1.41
7	BL	302	BCL	C1B-CHB	3.29	1.48	1.39
7	BZ	102	BCL	CHD-C4C	3.29	1.51	1.41
7	BK	102	BCL	CHD-C4C	3.30	1.51	1.41
7	B3	101	BCL	CHD-C4C	3.30	1.51	1.41
7	AD	102	BCL	CHD-C4C	3.30	1.51	1.41
7	AJ	101	BCL	CHD-C4C	3.31	1.51	1.41
7	AF	101	BCL	C1B-CHB	3.31	1.49	1.39
7	B4	101	BCL	CHD-C4C	3.31	1.51	1.41
7	A9	101	BCL	CHD-C4C	3.31	1.51	1.41
7	AV	101	BCL	C1B-CHB	3.32	1.49	1.39
7	BD	101	BCL	C4B-CHC	3.32	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B2	101	BCL	C1B-CHB	3.33	1.49	1.39
7	AD	102	BCL	C4B-CHC	3.33	1.49	1.39
7	BY	101	BCL	CHD-C4C	3.33	1.51	1.41
7	AI	101	BCL	CHD-C4C	3.34	1.51	1.41
7	AO	101	BCL	C4B-CHC	3.34	1.49	1.39
7	BF	102	BCL	CHD-C4C	3.34	1.51	1.41
7	BK	101	BCL	C1B-CHB	3.34	1.49	1.39
7	A4	101	BCL	CHD-C4C	3.34	1.51	1.41
7	AM	402	BCL	C4B-CHC	3.36	1.49	1.39
7	BD	102	BCL	CHD-C4C	3.37	1.51	1.41
7	AM	401	BCL	C1B-CHB	3.37	1.49	1.39
7	BL	301	BCL	C1B-CHB	3.37	1.49	1.39
7	BL	303	BCL	C4B-CHC	3.37	1.49	1.39
7	AL	302	BCL	C4-C3	3.38	1.58	1.50
7	AG	101	BCL	CHD-C4C	3.39	1.51	1.41
7	BY	102	BCL	C4B-CHC	3.39	1.49	1.39
7	BD	102	BCL	C4B-CHC	3.40	1.49	1.39
7	BV	101	BCL	C1B-CHB	3.40	1.49	1.39
7	BV	102	BCL	C1B-CHB	3.40	1.49	1.39
7	AM	402	BCL	CHD-C4C	3.40	1.51	1.41
7	AP	102	BCL	CHD-C4C	3.41	1.51	1.41
7	BT	101	BCL	C1B-CHB	3.41	1.49	1.39
7	BP	102	BCL	C4B-CHC	3.41	1.49	1.39
7	B6	101	BCL	CHD-C4C	3.41	1.51	1.41
7	AI	101	BCL	C4B-CHC	3.41	1.49	1.39
7	BO	102	BCL	C4B-CHC	3.42	1.49	1.39
7	AP	102	BCL	C4B-CHC	3.42	1.49	1.39
7	A6	101	BCL	C1B-CHB	3.42	1.49	1.39
7	A2	101	BCL	C1B-CHB	3.42	1.49	1.39
7	BP	102	BCL	CHD-C4C	3.42	1.51	1.41
7	AY	102	BCL	CHD-C4C	3.42	1.51	1.41
7	BI	101	BCL	CHD-C4C	3.42	1.51	1.41
7	A7	101	BCL	C1B-CHB	3.42	1.49	1.39
7	BL	303	BCL	CHD-C4C	3.43	1.51	1.41
8	BM	402	BPH	CHC-C4B	3.43	1.48	1.40
8	AM	403	BPH	CHC-C4B	3.43	1.49	1.40
7	BU	101	BCL	CHD-C4C	3.44	1.51	1.41
7	AT	101	BCL	C1B-CHB	3.44	1.49	1.39
7	BY	102	BCL	CHD-C4C	3.44	1.51	1.41
7	BI	101	BCL	C4B-CHC	3.44	1.49	1.39
7	AW	101	BCL	C1B-CHB	3.45	1.49	1.39
7	B7	101	BCL	C1B-CHB	3.45	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	AT	102	BCL	CHD-C4C	3.45	1.51	1.41
7	B5	101	BCL	C1B-CHB	3.46	1.49	1.39
7	B6	101	BCL	C4B-CHC	3.47	1.49	1.39
7	AS	101	BCL	C4B-CHC	3.49	1.49	1.39
7	A6	102	BCL	CHD-C4C	3.49	1.51	1.41
7	BO	101	BCL	C4B-CHC	3.51	1.49	1.39
7	BF	102	BCL	C4B-CHC	3.52	1.49	1.39
7	AT	102	BCL	C4B-CHC	3.52	1.49	1.39
7	BZ	102	BCL	C4B-CHC	3.54	1.49	1.39
7	BU	101	BCL	C4B-CHC	3.54	1.49	1.39
7	AY	101	BCL	C4B-CHC	3.55	1.49	1.39
7	A6	102	BCL	C4B-CHC	3.55	1.49	1.39
7	A9	101	BCL	C4B-CHC	3.55	1.49	1.39
7	AZ	101	BCL	C4B-CHC	3.56	1.49	1.39
7	AG	101	BCL	C4B-CHC	3.56	1.49	1.39
7	AY	102	BCL	C4B-CHC	3.56	1.49	1.39
7	AN	101	BCL	C4B-CHC	3.57	1.49	1.39
7	B9	101	BCL	C4B-CHC	3.57	1.49	1.39
7	BZ	101	BCL	C4B-CHC	3.59	1.49	1.39
7	AJ	101	BCL	C4B-CHC	3.59	1.49	1.39
7	A3	101	BCL	C4B-CHC	3.60	1.49	1.39
7	A4	101	BCL	C4B-CHC	3.60	1.49	1.39
7	B4	101	BCL	C4B-CHC	3.61	1.49	1.39
7	BM	401	BCL	CHD-C4C	3.61	1.52	1.41
7	B1	101	BCL	C4B-CHC	3.63	1.49	1.39
7	BY	101	BCL	C4B-CHC	3.64	1.49	1.39
7	BK	102	BCL	C4B-CHC	3.65	1.49	1.39
7	B3	101	BCL	C4B-CHC	3.65	1.49	1.39
7	A1	101	BCL	C4B-CHC	3.68	1.50	1.39
8	BL	304	BPH	CHD-C4C	3.90	1.48	1.38
8	AL	303	BPH	CHD-C4C	3.93	1.48	1.38
7	AL	301	BCL	O2A-CGA	4.04	1.45	1.33
7	AM	401	BCL	O2A-CGA	4.05	1.45	1.33
7	BL	301	BCL	OBD-CAD	4.06	1.28	1.22
7	AD	101	BCL	OBD-CAD	4.07	1.28	1.22
8	AM	403	BPH	O2A-CGA	4.15	1.45	1.33
9	AM	405	U10	C38-C39	4.15	1.45	1.32
8	BM	402	BPH	O2A-CGA	4.15	1.45	1.33
12	AM	406	SPO	C24-C23	4.15	1.59	1.50
7	AM	401	BCL	OBD-CAD	4.16	1.28	1.22
7	BT	101	BCL	OBD-CAD	4.17	1.28	1.22
7	AI	101	BCL	OBD-CAD	4.18	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	BV	102	BCL	OBD-CAD	4.18	1.28	1.22
7	A7	101	BCL	OBD-CAD	4.22	1.28	1.22
7	B8	101	BCL	OBD-CAD	4.23	1.28	1.22
7	AT	101	BCL	OBD-CAD	4.25	1.28	1.22
7	A6	101	BCL	OBD-CAD	4.25	1.28	1.22
8	AL	303	BPH	O2A-CGA	4.25	1.46	1.33
7	AV	101	BCL	OBD-CAD	4.26	1.28	1.22
7	BK	101	BCL	OBD-CAD	4.26	1.28	1.22
7	AF	101	BCL	OBD-CAD	4.26	1.28	1.22
7	BP	101	BCL	OBD-CAD	4.27	1.28	1.22
7	B5	101	BCL	OBD-CAD	4.27	1.28	1.22
7	AK	101	BCL	OBD-CAD	4.27	1.28	1.22
7	BL	303	BCL	OBD-CAD	4.27	1.28	1.22
7	AZ	101	BCL	OBD-CAD	4.27	1.28	1.22
8	BL	304	BPH	O2A-CGA	4.27	1.46	1.33
7	AP	102	BCL	OBD-CAD	4.27	1.28	1.22
7	BF	101	BCL	OBD-CAD	4.27	1.28	1.22
7	AW	101	BCL	OBD-CAD	4.28	1.28	1.22
7	AL	302	BCL	OBD-CAD	4.28	1.28	1.22
7	AG	101	BCL	OBD-CAD	4.28	1.28	1.22
7	BI	101	BCL	OBD-CAD	4.28	1.28	1.22
7	BY	102	BCL	OBD-CAD	4.28	1.28	1.22
7	B7	101	BCL	OBD-CAD	4.28	1.28	1.22
7	BP	102	BCL	OBD-CAD	4.28	1.28	1.22
7	A9	101	BCL	OBD-CAD	4.28	1.28	1.22
7	A8	101	BCL	OBD-CAD	4.29	1.28	1.22
8	BM	402	BPH	CHD-C4C	4.29	1.49	1.38
8	AM	403	BPH	CHD-C4C	4.29	1.49	1.38
7	BU	101	BCL	OBD-CAD	4.30	1.28	1.22
7	AS	101	BCL	OBD-CAD	4.30	1.28	1.22
7	B2	101	BCL	OBD-CAD	4.30	1.28	1.22
7	BK	102	BCL	OBD-CAD	4.30	1.28	1.22
7	AP	101	BCL	OBD-CAD	4.30	1.28	1.22
7	B9	101	BCL	OBD-CAD	4.30	1.28	1.22
7	BD	102	BCL	OBD-CAD	4.30	1.28	1.22
7	B1	101	BCL	OBD-CAD	4.31	1.28	1.22
7	AY	101	BCL	OBD-CAD	4.31	1.28	1.22
7	BD	101	BCL	OBD-CAD	4.31	1.28	1.22
7	BZ	102	BCL	OBD-CAD	4.32	1.28	1.22
7	AY	102	BCL	OBD-CAD	4.32	1.29	1.22
7	A2	101	BCL	OBD-CAD	4.32	1.29	1.22
7	BO	102	BCL	OBD-CAD	4.32	1.29	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	BV	101	BCL	OBD-CAD	4.33	1.29	1.22
8	BL	304	BPH	CHC-C4B	4.33	1.51	1.40
7	BO	101	BCL	OBD-CAD	4.33	1.29	1.22
7	BF	102	BCL	OBD-CAD	4.33	1.29	1.22
7	B6	101	BCL	OBD-CAD	4.33	1.29	1.22
7	AJ	101	BCL	OBD-CAD	4.33	1.29	1.22
8	AL	303	BPH	OBD-CAD	4.34	1.29	1.22
7	B3	101	BCL	OBD-CAD	4.34	1.29	1.22
7	AD	102	BCL	OBD-CAD	4.34	1.29	1.22
7	A4	101	BCL	OBD-CAD	4.34	1.29	1.22
8	BL	304	BPH	OBD-CAD	4.34	1.29	1.22
7	A1	101	BCL	OBD-CAD	4.35	1.29	1.22
8	AL	303	BPH	CHC-C4B	4.35	1.51	1.40
8	AM	403	BPH	OBD-CAD	4.35	1.29	1.22
7	A6	102	BCL	OBD-CAD	4.35	1.29	1.22
7	AT	102	BCL	OBD-CAD	4.36	1.29	1.22
7	BZ	101	BCL	OBD-CAD	4.36	1.29	1.22
7	AO	101	BCL	OBD-CAD	4.36	1.29	1.22
8	BM	402	BPH	OBD-CAD	4.36	1.29	1.22
7	AN	101	BCL	OBD-CAD	4.36	1.29	1.22
7	BM	401	BCL	OBD-CAD	4.37	1.29	1.22
7	BY	101	BCL	OBD-CAD	4.37	1.29	1.22
7	B4	101	BCL	OBD-CAD	4.37	1.29	1.22
7	A3	101	BCL	OBD-CAD	4.38	1.29	1.22
7	AM	402	BCL	OBD-CAD	4.43	1.29	1.22
7	BL	302	BCL	OBD-CAD	4.51	1.29	1.22
7	AL	302	BCL	O2A-CGA	4.54	1.47	1.33
7	AL	301	BCL	OBD-CAD	4.54	1.29	1.22
7	BL	303	BCL	O2A-CGA	4.56	1.47	1.33
7	BL	302	BCL	O2A-CGA	4.63	1.47	1.33
8	AL	303	BPH	CHA-C1A	4.67	1.48	1.37
8	BL	304	BPH	CHA-C1A	4.70	1.48	1.37
7	BL	301	BCL	O2D-CGD	4.71	1.45	1.33
8	AM	403	BPH	CHA-C1A	4.74	1.48	1.37
8	BM	402	BPH	CHA-C1A	4.75	1.48	1.37
7	BM	401	BCL	O2A-CGA	4.79	1.47	1.33
7	AM	401	BCL	O2D-CGD	4.93	1.45	1.33
8	AL	303	BPH	O2D-CGD	4.95	1.45	1.33
8	BL	304	BPH	O2D-CGD	4.95	1.45	1.33
7	A4	101	BCL	O2D-CGD	4.95	1.45	1.33
7	BF	102	BCL	O2D-CGD	4.95	1.45	1.33
7	A8	101	BCL	O2D-CGD	4.96	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B3	101	BCL	O2D-CGD	4.96	1.45	1.33
7	B4	101	BCL	O2D-CGD	4.96	1.45	1.33
7	AJ	101	BCL	O2D-CGD	4.96	1.45	1.33
7	AW	101	BCL	O2D-CGD	4.97	1.45	1.33
7	AY	101	BCL	O2D-CGD	4.97	1.45	1.33
7	AG	101	BCL	O2D-CGD	4.97	1.45	1.33
7	BI	101	BCL	O2D-CGD	4.97	1.45	1.33
7	BP	101	BCL	O2D-CGD	4.97	1.45	1.33
7	B1	101	BCL	O2D-CGD	4.97	1.45	1.33
7	BV	102	BCL	O2D-CGD	4.97	1.45	1.33
7	B6	101	BCL	O2D-CGD	4.97	1.45	1.33
7	BM	401	BCL	O2D-CGD	4.97	1.45	1.33
7	A3	101	BCL	O2D-CGD	4.98	1.45	1.33
7	A1	101	BCL	O2D-CGD	4.98	1.45	1.33
7	AP	101	BCL	O2D-CGD	4.98	1.45	1.33
7	BY	101	BCL	O2D-CGD	4.98	1.45	1.33
7	BT	101	BCL	O2D-CGD	4.98	1.45	1.33
7	BP	102	BCL	O2D-CGD	4.98	1.45	1.33
7	AS	101	BCL	O2D-CGD	4.98	1.45	1.33
7	AO	101	BCL	O2D-CGD	4.98	1.45	1.33
7	AV	101	BCL	O2D-CGD	4.99	1.45	1.33
7	AK	101	BCL	O2D-CGD	4.99	1.45	1.33
7	AZ	101	BCL	O2D-CGD	4.99	1.45	1.33
7	B8	101	BCL	O2D-CGD	4.99	1.45	1.33
7	BK	101	BCL	O2D-CGD	4.99	1.45	1.33
7	AT	101	BCL	O2D-CGD	4.99	1.45	1.33
7	BZ	102	BCL	O2D-CGD	4.99	1.45	1.33
7	AY	102	BCL	O2D-CGD	4.99	1.45	1.33
7	BV	101	BCL	O2D-CGD	4.99	1.45	1.33
7	AF	101	BCL	O2D-CGD	4.99	1.45	1.33
7	BZ	101	BCL	O2D-CGD	4.99	1.45	1.33
7	AT	102	BCL	O2D-CGD	5.00	1.46	1.33
7	B2	101	BCL	O2D-CGD	5.00	1.46	1.33
7	AM	402	BCL	O2D-CGD	5.00	1.46	1.33
7	BD	101	BCL	O2D-CGD	5.00	1.46	1.33
7	B5	101	BCL	O2D-CGD	5.00	1.46	1.33
7	A9	101	BCL	O2D-CGD	5.00	1.46	1.33
7	BF	101	BCL	O2D-CGD	5.00	1.46	1.33
7	A6	102	BCL	O2D-CGD	5.00	1.46	1.33
7	BO	102	BCL	O2D-CGD	5.00	1.46	1.33
7	AN	101	BCL	O2D-CGD	5.00	1.46	1.33
7	BU	101	BCL	O2D-CGD	5.01	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B9	101	BCL	O2D-CGD	5.01	1.46	1.33
7	BD	102	BCL	O2D-CGD	5.01	1.46	1.33
7	BO	101	BCL	O2D-CGD	5.01	1.46	1.33
7	AP	102	BCL	O2D-CGD	5.01	1.46	1.33
7	A6	101	BCL	O2D-CGD	5.01	1.46	1.33
7	AD	101	BCL	O2D-CGD	5.01	1.46	1.33
7	BK	102	BCL	O2D-CGD	5.02	1.46	1.33
7	A2	101	BCL	O2D-CGD	5.02	1.46	1.33
7	B7	101	BCL	O2D-CGD	5.02	1.46	1.33
7	AD	102	BCL	O2D-CGD	5.02	1.46	1.33
7	AI	101	BCL	O2D-CGD	5.02	1.46	1.33
7	A7	101	BCL	O2D-CGD	5.02	1.46	1.33
7	BL	303	BCL	O2D-CGD	5.02	1.46	1.33
7	BL	302	BCL	O2D-CGD	5.03	1.46	1.33
7	BY	102	BCL	O2D-CGD	5.03	1.46	1.33
8	BM	402	BPH	O2D-CGD	5.03	1.46	1.33
8	AM	403	BPH	O2D-CGD	5.04	1.46	1.33
7	AL	301	BCL	O2D-CGD	5.06	1.46	1.33
7	AL	302	BCL	O2D-CGD	5.12	1.46	1.33
7	AM	402	BCL	O2A-CGA	5.45	1.49	1.33
12	AM	406	SPO	C22-C23	5.60	1.43	1.35
7	BL	301	BCL	O2A-CGA	5.70	1.50	1.33
8	AM	403	BPH	CHB-C1B	5.80	1.50	1.38
8	BM	402	BPH	CHB-C1B	5.82	1.50	1.38
9	BL	306	U10	C6-C1	5.92	1.49	1.35
8	BL	304	BPH	CHB-C1B	6.00	1.50	1.38
8	AL	303	BPH	CHB-C1B	6.02	1.50	1.38
9	AL	304	U10	C6-C1	6.04	1.49	1.35
9	AM	405	U10	C6-C1	6.12	1.49	1.35
7	BM	401	BCL	C2-C3	6.50	1.45	1.33
7	BM	401	BCL	C4-C3	6.79	1.67	1.50
9	AM	405	U10	C41-C39	8.37	1.75	1.50

All (513) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	AM	406	SPO	C21-C22-C23	-5.39	119.42	127.20
7	AY	101	BCL	C1D-CHD-C4C	-5.21	118.12	126.07
7	BY	101	BCL	C1D-CHD-C4C	-5.19	118.14	126.07
7	A3	101	BCL	C1D-CHD-C4C	-5.13	118.23	126.07
7	BO	101	BCL	C1D-CHD-C4C	-5.11	118.27	126.07
7	AN	101	BCL	C1D-CHD-C4C	-5.10	118.28	126.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B3	101	BCL	C1D-CHD-C4C	-5.09	118.31	126.07
7	A1	101	BCL	C1D-CHD-C4C	-5.03	118.39	126.07
7	B1	101	BCL	C1D-CHD-C4C	-4.99	118.45	126.07
7	BD	101	BCL	C1D-CHD-C4C	-4.91	118.57	126.07
7	AD	101	BCL	C1D-CHD-C4C	-4.90	118.58	126.07
7	AK	101	BCL	C1D-CHD-C4C	-4.90	118.58	126.07
7	BL	302	BCL	C1D-CHD-C4C	-4.89	118.61	126.07
7	AV	101	BCL	C1D-CHD-C4C	-4.87	118.63	126.07
7	AS	101	BCL	C1D-CHD-C4C	-4.87	118.63	126.07
7	BK	101	BCL	C1D-CHD-C4C	-4.67	118.94	126.07
7	B2	101	BCL	C1D-CHD-C4C	-4.67	118.94	126.07
7	B4	101	BCL	C1D-CHD-C4C	-4.66	118.96	126.07
7	BV	101	BCL	C1D-CHD-C4C	-4.53	119.16	126.07
7	BF	101	BCL	C1D-CHD-C4C	-4.46	119.26	126.07
7	BZ	101	BCL	C1D-CHD-C4C	-4.46	119.26	126.07
12	AM	406	SPO	C15-C14-C12	-4.43	120.80	127.20
7	B9	101	BCL	C1D-CHD-C4C	-4.37	119.40	126.07
7	BK	102	BCL	C1D-CHD-C4C	-4.35	119.42	126.07
7	A4	101	BCL	C1D-CHD-C4C	-4.35	119.43	126.07
7	AM	401	BCL	C1D-CHD-C4C	-4.35	119.44	126.07
7	BP	101	BCL	C1D-CHD-C4C	-4.33	119.46	126.07
7	AL	301	BCL	C1D-CHD-C4C	-4.31	119.49	126.07
7	AF	101	BCL	C1D-CHD-C4C	-4.31	119.49	126.07
7	A2	101	BCL	C1D-CHD-C4C	-4.27	119.54	126.07
12	AM	406	SPO	C10-C9-C7	-4.21	121.11	127.20
7	AP	101	BCL	C1D-CHD-C4C	-4.20	119.66	126.07
7	AG	101	BCL	C1D-CHD-C4C	-4.18	119.69	126.07
12	AM	406	SPO	C20-C19-C17	-4.16	121.19	127.20
7	A6	101	BCL	C1D-CHD-C4C	-4.15	119.73	126.07
7	AW	101	BCL	C1D-CHD-C4C	-4.14	119.75	126.07
7	A9	101	BCL	C1D-CHD-C4C	-4.13	119.77	126.07
7	BL	301	BCL	C1D-CHD-C4C	-4.09	119.83	126.07
7	A7	101	BCL	C1D-CHD-C4C	-4.08	119.84	126.07
7	AZ	101	BCL	C1D-CHD-C4C	-4.08	119.84	126.07
7	AJ	101	BCL	C1D-CHD-C4C	-4.07	119.85	126.07
7	BZ	102	BCL	C1D-CHD-C4C	-4.07	119.86	126.07
7	A8	101	BCL	C1D-CHD-C4C	-4.05	119.88	126.07
7	AT	101	BCL	C1D-CHD-C4C	-4.05	119.89	126.07
7	BT	101	BCL	C1D-CHD-C4C	-4.03	119.92	126.07
7	BF	102	BCL	C1D-CHD-C4C	-4.01	119.95	126.07
12	AM	406	SPO	C4-C5-C6	-3.97	119.03	124.67
7	BV	102	BCL	C1D-CHD-C4C	-3.96	120.02	126.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	AY	102	BCL	C1D-CHD-C4C	-3.93	120.07	126.07
7	BU	101	BCL	C1D-CHD-C4C	-3.93	120.07	126.07
7	B5	101	BCL	C1D-CHD-C4C	-3.92	120.08	126.07
7	A6	102	BCL	C1D-CHD-C4C	-3.91	120.09	126.07
7	B8	101	BCL	C1D-CHD-C4C	-3.85	120.19	126.07
7	B7	101	BCL	C1D-CHD-C4C	-3.85	120.20	126.07
7	B6	101	BCL	C1D-CHD-C4C	-3.83	120.22	126.07
7	AT	102	BCL	C1D-CHD-C4C	-3.74	120.36	126.07
7	AD	102	BCL	C1D-CHD-C4C	-3.71	120.40	126.07
7	AM	402	BCL	C1D-CHD-C4C	-3.66	120.48	126.07
9	AL	304	U10	C7-C8-C9	-3.60	120.60	126.70
7	BD	102	BCL	C1D-CHD-C4C	-3.59	120.59	126.07
9	BL	306	U10	C27-C28-C29	-3.55	120.05	127.76
7	BY	102	BCL	C1D-CHD-C4C	-3.52	120.69	126.07
7	AP	102	BCL	C1D-CHD-C4C	-3.51	120.72	126.07
7	BI	101	BCL	C1D-CHD-C4C	-3.48	120.76	126.07
9	AM	405	U10	C7-C8-C9	-3.47	120.82	126.70
7	BO	102	BCL	C1D-CHD-C4C	-3.46	120.79	126.07
9	AL	304	U10	C17-C18-C19	-3.45	120.26	127.76
7	AI	101	BCL	C1D-CHD-C4C	-3.43	120.83	126.07
9	BL	306	U10	C7-C8-C9	-3.37	120.99	126.70
7	AO	101	BCL	C1D-CHD-C4C	-3.36	120.95	126.07
9	AM	405	U10	C27-C28-C29	-3.34	120.50	127.76
9	AL	304	U10	C27-C28-C29	-3.33	120.52	127.76
9	AL	304	U10	C22-C23-C24	-3.33	120.52	127.76
7	BP	102	BCL	C1D-CHD-C4C	-3.30	121.03	126.07
9	AM	405	U10	C12-C13-C14	-3.25	120.70	127.76
9	BL	306	U10	C12-C13-C14	-3.21	120.78	127.76
7	BM	401	BCL	C1D-CHD-C4C	-3.21	121.17	126.07
9	AM	405	U10	C37-C38-C39	-3.18	115.48	127.73
9	AL	304	U10	C32-C33-C34	-3.18	120.84	127.76
9	AM	405	U10	C22-C23-C24	-3.17	120.86	127.76
9	AM	405	U10	C17-C18-C19	-3.16	120.90	127.76
9	AL	304	U10	C12-C13-C14	-3.14	120.93	127.76
9	BL	306	U10	C17-C18-C19	-3.12	120.97	127.76
7	AL	302	BCL	C1D-CHD-C4C	-3.12	121.30	126.07
12	AM	406	SPO	C31-C32-C33	-3.11	121.00	127.76
9	AM	405	U10	C32-C33-C34	-3.09	121.05	127.76
9	BL	306	U10	C32-C33-C34	-3.07	121.09	127.76
9	BL	306	U10	C22-C23-C24	-3.06	121.10	127.76
7	AM	402	BCL	O1D-CGD-CBD	-2.88	120.50	124.62
7	BK	101	BCL	O1D-CGD-CBD	-2.88	120.50	124.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	BL	301	BCL	O1D-CGD-CBD	-2.87	120.50	124.62
8	BM	402	BPH	O1D-CGD-CBD	-2.85	120.54	124.62
7	BD	101	BCL	O1D-CGD-CBD	-2.85	120.54	124.62
7	AL	302	BCL	O1D-CGD-CBD	-2.84	120.55	124.62
7	BL	303	BCL	C1D-CHD-C4C	-2.84	121.73	126.07
7	AD	101	BCL	O1D-CGD-CBD	-2.84	120.55	124.62
7	AV	101	BCL	O1D-CGD-CBD	-2.84	120.55	124.62
8	AM	403	BPH	O1D-CGD-CBD	-2.83	120.56	124.62
7	AY	101	BCL	O1D-CGD-CBD	-2.83	120.57	124.62
7	AP	101	BCL	O1D-CGD-CBD	-2.83	120.57	124.62
7	AK	101	BCL	O1D-CGD-CBD	-2.81	120.59	124.62
7	AM	401	BCL	O1D-CGD-CBD	-2.81	120.59	124.62
7	BP	101	BCL	O1D-CGD-CBD	-2.80	120.61	124.62
7	BM	401	BCL	O1D-CGD-CBD	-2.79	120.62	124.62
7	AN	101	BCL	O1D-CGD-CBD	-2.79	120.62	124.62
12	AM	406	SPO	C5-C6-C7	-2.79	121.49	125.75
7	A4	101	BCL	O1D-CGD-CBD	-2.79	120.62	124.62
7	BO	101	BCL	O1D-CGD-CBD	-2.78	120.63	124.62
8	BL	304	BPH	O1D-CGD-CBD	-2.78	120.64	124.62
7	B1	101	BCL	O1D-CGD-CBD	-2.78	120.64	124.62
7	BM	401	BCL	C5-C3-C2	-2.78	115.79	121.05
7	AZ	101	BCL	O1D-CGD-CBD	-2.78	120.64	124.62
7	BL	302	BCL	O1D-CGD-CBD	-2.77	120.65	124.62
8	AL	303	BPH	O1D-CGD-CBD	-2.77	120.65	124.62
7	A6	101	BCL	O1D-CGD-CBD	-2.77	120.65	124.62
7	A2	101	BCL	O1D-CGD-CBD	-2.77	120.66	124.62
9	AM	405	U10	C40-C39-C38	-2.76	113.72	122.61
7	B8	101	BCL	O1D-CGD-CBD	-2.76	120.66	124.62
7	A7	101	BCL	O1D-CGD-CBD	-2.76	120.66	124.62
7	B7	101	BCL	O1D-CGD-CBD	-2.76	120.66	124.62
7	BL	303	BCL	O1D-CGD-CBD	-2.76	120.67	124.62
7	B6	101	BCL	O1D-CGD-CBD	-2.76	120.67	124.62
7	AY	102	BCL	O1D-CGD-CBD	-2.75	120.67	124.62
7	B5	101	BCL	O1D-CGD-CBD	-2.75	120.67	124.62
7	BY	101	BCL	O1D-CGD-CBD	-2.75	120.68	124.62
7	BT	101	BCL	O1D-CGD-CBD	-2.75	120.68	124.62
7	BZ	101	BCL	O1D-CGD-CBD	-2.75	120.68	124.62
7	BV	102	BCL	O1D-CGD-CBD	-2.75	120.68	124.62
7	AJ	101	BCL	O1D-CGD-CBD	-2.75	120.68	124.62
7	B2	101	BCL	O1D-CGD-CBD	-2.75	120.68	124.62
7	BD	102	BCL	O1D-CGD-CBD	-2.75	120.68	124.62
7	BI	101	BCL	O1D-CGD-CBD	-2.75	120.69	124.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A3	101	BCL	O1D-CGD-CBD	-2.75	120.69	124.62
7	A8	101	BCL	O1D-CGD-CBD	-2.75	120.69	124.62
7	BF	102	BCL	O1D-CGD-CBD	-2.74	120.69	124.62
7	B4	101	BCL	O1D-CGD-CBD	-2.74	120.70	124.62
7	A1	101	BCL	O1D-CGD-CBD	-2.74	120.70	124.62
7	B3	101	BCL	O1D-CGD-CBD	-2.74	120.70	124.62
7	AI	101	BCL	O1D-CGD-CBD	-2.74	120.70	124.62
7	BP	102	BCL	O1D-CGD-CBD	-2.73	120.70	124.62
7	A6	102	BCL	O1D-CGD-CBD	-2.73	120.70	124.62
7	BV	101	BCL	O1D-CGD-CBD	-2.73	120.71	124.62
7	AD	102	BCL	O1D-CGD-CBD	-2.73	120.72	124.62
7	AP	102	BCL	O1D-CGD-CBD	-2.72	120.72	124.62
7	BU	101	BCL	O1D-CGD-CBD	-2.72	120.73	124.62
7	AT	102	BCL	O1D-CGD-CBD	-2.72	120.73	124.62
7	BK	102	BCL	O1D-CGD-CBD	-2.71	120.73	124.62
7	AG	101	BCL	O1D-CGD-CBD	-2.71	120.74	124.62
7	AF	101	BCL	O1D-CGD-CBD	-2.71	120.74	124.62
7	BY	102	BCL	O1D-CGD-CBD	-2.70	120.75	124.62
7	AW	101	BCL	O1D-CGD-CBD	-2.70	120.75	124.62
7	AT	101	BCL	O1D-CGD-CBD	-2.70	120.75	124.62
7	AO	101	BCL	O1D-CGD-CBD	-2.70	120.75	124.62
7	A9	101	BCL	O1D-CGD-CBD	-2.69	120.76	124.62
7	BF	101	BCL	O1D-CGD-CBD	-2.69	120.76	124.62
7	B9	101	BCL	O1D-CGD-CBD	-2.69	120.77	124.62
7	AL	301	BCL	O1D-CGD-CBD	-2.69	120.77	124.62
7	BZ	102	BCL	O1D-CGD-CBD	-2.69	120.77	124.62
7	BO	102	BCL	O1D-CGD-CBD	-2.68	120.78	124.62
7	AS	101	BCL	O1D-CGD-CBD	-2.68	120.78	124.62
8	AM	403	BPH	CMD-C2D-C3D	-2.38	120.44	125.09
8	BM	402	BPH	CMD-C2D-C3D	-2.37	120.45	125.09
7	AL	302	BCL	O2D-CGD-O1D	-2.32	119.00	123.79
8	BL	304	BPH	CMD-C2D-C3D	-2.30	120.58	125.09
8	AL	303	BPH	CMD-C2D-C3D	-2.30	120.60	125.09
7	AT	101	BCL	O2D-CGD-O1D	-2.29	119.07	123.79
7	BF	101	BCL	O2D-CGD-O1D	-2.28	119.08	123.79
7	AM	401	BCL	O2D-CGD-O1D	-2.28	119.08	123.79
7	AW	101	BCL	O2D-CGD-O1D	-2.28	119.09	123.79
7	AM	402	BCL	O2D-CGD-O1D	-2.27	119.10	123.79
7	B9	101	BCL	O2D-CGD-O1D	-2.27	119.10	123.79
7	BU	101	BCL	O2D-CGD-O1D	-2.27	119.10	123.79
7	AL	301	BCL	O2D-CGD-O1D	-2.27	119.10	123.79
7	BO	102	BCL	O2D-CGD-O1D	-2.27	119.10	123.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	BK	101	BCL	O2D-CGD-O1D	-2.27	119.11	123.79
7	BZ	102	BCL	O2D-CGD-O1D	-2.27	119.11	123.79
7	AG	101	BCL	O2D-CGD-O1D	-2.27	119.11	123.79
7	BP	101	BCL	O2D-CGD-O1D	-2.27	119.11	123.79
7	BL	301	BCL	O2D-CGD-O1D	-2.26	119.11	123.79
7	BY	102	BCL	O2D-CGD-O1D	-2.26	119.12	123.79
7	BV	102	BCL	O2D-CGD-O1D	-2.26	119.12	123.79
7	AF	101	BCL	O2D-CGD-O1D	-2.26	119.12	123.79
7	A3	101	BCL	O2D-CGD-O1D	-2.26	119.12	123.79
7	A8	101	BCL	O2D-CGD-O1D	-2.26	119.13	123.79
7	AD	101	BCL	O2D-CGD-O1D	-2.26	119.13	123.79
7	BZ	101	BCL	O2D-CGD-O1D	-2.26	119.13	123.79
7	AN	101	BCL	O2D-CGD-O1D	-2.26	119.13	123.79
7	BD	101	BCL	O2D-CGD-O1D	-2.26	119.13	123.79
7	BK	102	BCL	O2D-CGD-O1D	-2.25	119.14	123.79
7	B3	101	BCL	O2D-CGD-O1D	-2.25	119.14	123.79
7	A7	101	BCL	O2D-CGD-O1D	-2.25	119.14	123.79
7	B2	101	BCL	O2D-CGD-O1D	-2.25	119.14	123.79
7	A1	101	BCL	O2D-CGD-O1D	-2.25	119.14	123.79
7	BY	101	BCL	O2D-CGD-O1D	-2.25	119.15	123.79
7	AT	102	BCL	O2D-CGD-O1D	-2.25	119.15	123.79
7	AK	101	BCL	O2D-CGD-O1D	-2.25	119.15	123.79
7	A6	102	BCL	O2D-CGD-O1D	-2.25	119.15	123.79
7	BL	302	BCL	O2D-CGD-O1D	-2.25	119.15	123.79
7	BD	102	BCL	O2D-CGD-O1D	-2.25	119.15	123.79
7	BF	102	BCL	O2D-CGD-O1D	-2.25	119.15	123.79
7	BI	101	BCL	O2D-CGD-O1D	-2.24	119.16	123.79
7	AS	101	BCL	O2D-CGD-O1D	-2.24	119.16	123.79
7	AP	101	BCL	O2D-CGD-O1D	-2.24	119.16	123.79
7	A9	101	BCL	O2D-CGD-O1D	-2.24	119.16	123.79
7	AY	102	BCL	O2D-CGD-O1D	-2.24	119.16	123.79
7	BL	303	BCL	O2D-CGD-O1D	-2.24	119.16	123.79
7	BV	101	BCL	O2D-CGD-O1D	-2.24	119.16	123.79
7	AZ	101	BCL	O2D-CGD-O1D	-2.24	119.16	123.79
7	A6	101	BCL	O2D-CGD-O1D	-2.24	119.17	123.79
7	B5	101	BCL	O2D-CGD-O1D	-2.24	119.17	123.79
8	BM	402	BPH	O2D-CGD-O1D	-2.24	119.17	123.79
7	B1	101	BCL	O2D-CGD-O1D	-2.24	119.17	123.79
7	AJ	101	BCL	O2D-CGD-O1D	-2.24	119.17	123.79
7	AI	101	BCL	O2D-CGD-O1D	-2.24	119.17	123.79
8	AL	303	BPH	O2D-CGD-O1D	-2.24	119.17	123.79
7	A4	101	BCL	O2D-CGD-O1D	-2.24	119.17	123.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	AM	403	BPH	O2D-CGD-O1D	-2.24	119.17	123.79
7	BP	102	BCL	O2D-CGD-O1D	-2.24	119.17	123.79
7	BO	101	BCL	O2D-CGD-O1D	-2.24	119.17	123.79
7	A2	101	BCL	O2D-CGD-O1D	-2.23	119.18	123.79
7	B7	101	BCL	O2D-CGD-O1D	-2.23	119.18	123.79
7	B8	101	BCL	O2D-CGD-O1D	-2.23	119.18	123.79
7	B6	101	BCL	O2D-CGD-O1D	-2.23	119.19	123.79
7	AP	102	BCL	O2D-CGD-O1D	-2.23	119.19	123.79
7	AD	102	BCL	O2D-CGD-O1D	-2.23	119.19	123.79
7	AY	101	BCL	O2D-CGD-O1D	-2.23	119.19	123.79
7	AO	101	BCL	O2D-CGD-O1D	-2.23	119.19	123.79
8	BL	304	BPH	O2D-CGD-O1D	-2.22	119.20	123.79
7	BM	401	BCL	O2D-CGD-O1D	-2.22	119.20	123.79
7	B4	101	BCL	O2D-CGD-O1D	-2.22	119.20	123.79
7	AV	101	BCL	O2D-CGD-O1D	-2.22	119.21	123.79
7	BT	101	BCL	O2D-CGD-O1D	-2.21	119.22	123.79
8	AL	303	BPH	CBC-CAC-C3C	-2.16	108.28	113.57
8	BL	304	BPH	CBC-CAC-C3C	-2.16	108.30	113.57
12	AM	406	SPO	C18-C17-C19	-2.12	119.77	122.90
12	AM	406	SPO	C15-C16-C17	-2.12	120.08	126.32
7	BL	301	BCL	CMD-C2D-C3D	-2.10	120.97	125.09
8	AM	403	BPH	C3B-C2B-C1B	-2.09	102.41	105.77
8	BM	402	BPH	C3B-C2B-C1B	-2.07	102.45	105.77
7	BL	303	BCL	CMD-C2D-C3D	-2.07	121.04	125.09
7	BM	401	BCL	CMD-C2D-C3D	-2.05	121.07	125.09
7	AM	401	BCL	CMD-C2D-C3D	-2.04	121.10	125.09
7	BV	102	BCL	CMD-C2D-C3D	-2.02	121.13	125.09
7	BT	101	BCL	CMD-C2D-C3D	-2.02	121.14	125.09
7	AW	101	BCL	CMD-C2D-C3D	-2.02	121.14	125.09
7	A6	101	BCL	CMD-C2D-C3D	-2.02	121.14	125.09
7	AT	101	BCL	CMD-C2D-C3D	-2.01	121.15	125.09
7	AK	101	BCL	CMD-C2D-C3D	-2.01	121.15	125.09
7	BL	301	BCL	CAA-CBA-CGA	-2.01	107.44	113.32
8	AM	403	BPH	CAA-C2A-C1A	-2.00	107.59	112.86
7	B5	101	BCL	CMD-C2D-C3D	-2.00	121.17	125.09
7	BO	102	BCL	CMD-C2D-C3D	-2.00	121.17	125.09
7	A7	101	BCL	CMD-C2D-C3D	-2.00	121.17	125.09
7	AV	101	BCL	CMB-C2B-C3B	2.00	129.00	125.09
7	AD	101	BCL	CMB-C2B-C3B	2.01	129.01	125.09
7	B2	101	BCL	CMB-C2B-C3B	2.03	129.05	125.09
7	BL	301	BCL	CMB-C2B-C3B	2.03	129.06	125.09
7	B3	101	BCL	CMB-C2B-C3B	2.03	129.06	125.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	AL	303	BPH	CMB-C2B-C1B	2.03	128.37	125.06
8	BL	304	BPH	CMB-C2B-C1B	2.03	128.37	125.06
7	A1	101	BCL	CMB-C2B-C3B	2.04	129.08	125.09
7	AY	101	BCL	CMB-C2B-C3B	2.04	129.08	125.09
7	BV	101	BCL	CMB-C2B-C3B	2.04	129.08	125.09
7	AS	101	BCL	CMB-C2B-C3B	2.04	129.08	125.09
7	BY	101	BCL	CMB-C2B-C3B	2.05	129.09	125.09
7	BD	101	BCL	CMB-C2B-C3B	2.05	129.09	125.09
7	BO	101	BCL	CMB-C2B-C3B	2.05	129.10	125.09
7	BM	401	BCL	CMB-C2B-C3B	2.06	129.11	125.09
7	AN	101	BCL	CMB-C2B-C3B	2.07	129.13	125.09
7	AL	302	BCL	O2A-CGA-CBA	2.07	118.21	111.90
7	AL	301	BCL	CMB-C2B-C3B	2.07	129.14	125.09
7	AM	401	BCL	CMB-C2B-C3B	2.07	129.14	125.09
7	A3	101	BCL	CMB-C2B-C3B	2.08	129.16	125.09
7	AF	101	BCL	CMB-C2B-C3B	2.08	129.16	125.09
7	AW	101	BCL	CMB-C2B-C3B	2.08	129.16	125.09
7	AD	102	BCL	CMB-C2B-C3B	2.09	129.17	125.09
7	BF	101	BCL	CMB-C2B-C3B	2.09	129.17	125.09
7	B1	101	BCL	CMB-C2B-C3B	2.09	129.17	125.09
7	BT	101	BCL	CMB-C2B-C3B	2.09	129.18	125.09
7	A4	101	BCL	CMB-C2B-C3B	2.09	129.19	125.09
7	B4	101	BCL	CMB-C2B-C3B	2.10	129.19	125.09
7	AM	402	BCL	CMB-C2B-C3B	2.10	129.19	125.09
7	A2	101	BCL	CMB-C2B-C3B	2.11	129.21	125.09
7	BP	101	BCL	CMB-C2B-C3B	2.11	129.22	125.09
7	BZ	101	BCL	CMB-C2B-C3B	2.11	129.22	125.09
7	BV	102	BCL	CMB-C2B-C3B	2.11	129.22	125.09
7	B9	101	BCL	CMB-C2B-C3B	2.12	129.23	125.09
7	A6	101	BCL	CMB-C2B-C3B	2.12	129.23	125.09
7	A8	101	BCL	CMB-C2B-C3B	2.12	129.24	125.09
7	A7	101	BCL	CMB-C2B-C3B	2.12	129.24	125.09
7	BM	401	BCL	OBB-CAB-CBB	2.12	125.22	120.13
7	AG	101	BCL	CMB-C2B-C3B	2.13	129.25	125.09
7	BF	102	BCL	CMB-C2B-C3B	2.13	129.25	125.09
7	AP	101	BCL	CMB-C2B-C3B	2.13	129.25	125.09
9	BL	306	U10	C41-C39-C40	2.13	119.87	114.64
9	AL	304	U10	C41-C39-C40	2.13	119.87	114.64
7	BK	102	BCL	CMB-C2B-C3B	2.13	129.25	125.09
7	AZ	101	BCL	CMB-C2B-C3B	2.13	129.25	125.09
7	AT	101	BCL	CMB-C2B-C3B	2.14	129.26	125.09
7	AL	302	BCL	CMB-C2B-C3B	2.14	129.28	125.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	BI	101	BCL	CMB-C2B-C3B	2.14	129.28	125.09
7	A9	101	BCL	CMB-C2B-C3B	2.15	129.28	125.09
7	AI	101	BCL	CMB-C2B-C3B	2.15	129.29	125.09
7	AY	102	BCL	CMB-C2B-C3B	2.15	129.30	125.09
12	AM	406	SPO	C40-C38-C39	2.15	119.94	114.64
7	AO	101	BCL	CMB-C2B-C3B	2.16	129.31	125.09
7	B5	101	BCL	CMB-C2B-C3B	2.16	129.32	125.09
7	AT	102	BCL	CMB-C2B-C3B	2.16	129.32	125.09
7	BZ	102	BCL	CMB-C2B-C3B	2.17	129.32	125.09
7	BP	102	BCL	CMB-C2B-C3B	2.17	129.33	125.09
7	BO	102	BCL	CMB-C2B-C3B	2.17	129.34	125.09
7	A6	102	BCL	CMB-C2B-C3B	2.17	129.34	125.09
7	AJ	101	BCL	CMB-C2B-C3B	2.18	129.35	125.09
7	BD	102	BCL	CMB-C2B-C3B	2.18	129.35	125.09
7	B8	101	BCL	CMB-C2B-C3B	2.19	129.36	125.09
7	B6	101	BCL	CMB-C2B-C3B	2.19	129.37	125.09
7	B7	101	BCL	CMB-C2B-C3B	2.19	129.38	125.09
7	BY	102	BCL	CMB-C2B-C3B	2.19	129.38	125.09
7	BL	303	BCL	CMB-C2B-C3B	2.20	129.38	125.09
7	AP	102	BCL	CMB-C2B-C3B	2.20	129.40	125.09
7	BU	101	BCL	CMB-C2B-C3B	2.24	129.47	125.09
8	BM	402	BPH	CMB-C2B-C1B	2.25	128.72	125.06
8	BL	304	BPH	C4A-NA-C1A	2.26	110.23	108.21
8	AL	303	BPH	C4A-NA-C1A	2.28	110.24	108.21
8	AM	403	BPH	CMB-C2B-C1B	2.28	128.76	125.06
7	BL	301	BCL	O2A-CGA-CBA	2.33	118.99	111.90
8	BM	402	BPH	C4A-NA-C1A	2.56	110.50	108.21
8	AM	403	BPH	C4A-NA-C1A	2.61	110.55	108.21
8	BM	402	BPH	O2A-CGA-CBA	2.62	119.88	111.90
8	AM	403	BPH	O2A-CGA-CBA	2.62	119.89	111.90
8	BM	402	BPH	C2B-C1B-NB	2.67	113.73	109.73
7	BL	303	BCL	O2A-CGA-CBA	2.68	120.07	111.90
8	AM	403	BPH	C2B-C1B-NB	2.69	113.76	109.73
8	BL	304	BPH	O2A-CGA-CBA	2.70	120.12	111.90
8	AL	303	BPH	O2A-CGA-CBA	2.70	120.14	111.90
7	AM	401	BCL	O2A-CGA-CBA	2.72	120.19	111.90
9	AM	405	U10	C35-C34-C36	2.77	119.63	115.41
8	AL	303	BPH	C2B-C1B-NB	2.77	113.88	109.73
8	BL	304	BPH	C2B-C1B-NB	2.77	113.88	109.73
7	AL	301	BCL	O2A-CGA-CBA	2.77	120.34	111.90
7	BL	302	BCL	O2A-CGA-CBA	2.77	120.34	111.90
9	AL	304	U10	C20-C19-C21	2.78	119.65	115.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	AM	403	BPH	C4-C3-C5	2.79	119.67	115.41
8	BM	402	BPH	C4-C3-C5	2.79	119.67	115.41
12	AM	406	SPO	C29-C28-C30	2.81	119.70	115.41
7	BM	401	BCL	C4-C3-C5	2.85	119.76	115.41
9	AM	405	U10	C30-C29-C31	2.87	119.79	115.41
7	BM	401	BCL	O2A-CGA-CBA	2.89	120.70	111.90
7	AL	301	BCL	C4-C3-C5	2.92	119.86	115.41
7	BL	302	BCL	C4-C3-C5	2.92	119.87	115.41
9	AM	405	U10	C10-C9-C11	2.93	119.89	115.41
7	AM	402	BCL	C4-C3-C5	2.94	119.90	115.41
7	BK	101	BCL	C4A-NA-C1A	2.95	110.17	106.36
7	AL	301	BCL	C4A-NA-C1A	2.95	110.17	106.36
9	AM	405	U10	C25-C24-C26	2.96	119.93	115.41
7	AM	401	BCL	C4-C3-C5	2.96	119.93	115.41
12	AM	406	SPO	C34-C33-C35	2.97	119.94	115.41
8	AL	303	BPH	C4-C3-C5	2.97	119.94	115.41
9	AL	304	U10	C25-C24-C26	2.97	119.95	115.41
7	BV	101	BCL	C4A-NA-C1A	2.97	110.20	106.36
9	BL	306	U10	C15-C14-C16	2.97	119.95	115.41
8	BL	304	BPH	C4-C3-C5	2.98	119.95	115.41
9	AL	304	U10	C30-C29-C31	3.01	120.00	115.41
9	BL	306	U10	C10-C9-C11	3.01	120.00	115.41
7	BL	301	BCL	C4-C3-C5	3.01	120.00	115.41
9	AM	405	U10	C15-C14-C16	3.01	120.01	115.41
9	AL	304	U10	C10-C9-C11	3.02	120.01	115.41
7	AV	101	BCL	C4A-NA-C1A	3.02	110.26	106.36
9	AL	304	U10	C15-C14-C16	3.02	120.03	115.41
7	BL	303	BCL	C4-C3-C5	3.03	120.03	115.41
7	B2	101	BCL	C4A-NA-C1A	3.03	110.28	106.36
9	BL	306	U10	C20-C19-C21	3.04	120.05	115.41
9	AM	405	U10	C20-C19-C21	3.05	120.06	115.41
9	AL	304	U10	C35-C34-C36	3.05	120.06	115.41
9	BL	306	U10	C35-C34-C36	3.06	120.08	115.41
7	BF	101	BCL	C4A-NA-C1A	3.07	110.33	106.36
7	AK	101	BCL	C4A-NA-C1A	3.09	110.35	106.36
7	AM	401	BCL	C4A-NA-C1A	3.10	110.37	106.36
7	BP	101	BCL	C4A-NA-C1A	3.13	110.40	106.36
7	AD	101	BCL	C4A-NA-C1A	3.13	110.41	106.36
7	A8	101	BCL	C4A-NA-C1A	3.15	110.43	106.36
7	BL	302	BCL	C4A-NA-C1A	3.15	110.43	106.36
7	AP	101	BCL	C4A-NA-C1A	3.16	110.44	106.36
9	BL	306	U10	C25-C24-C26	3.16	120.24	115.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A7	101	BCL	C4A-NA-C1A	3.19	110.48	106.36
7	BD	101	BCL	C4A-NA-C1A	3.20	110.50	106.36
7	AF	101	BCL	C4A-NA-C1A	3.20	110.50	106.36
7	BT	101	BCL	C4A-NA-C1A	3.21	110.51	106.36
7	AW	101	BCL	C4A-NA-C1A	3.22	110.52	106.36
7	A2	101	BCL	C4A-NA-C1A	3.22	110.53	106.36
7	BL	301	BCL	C4A-NA-C1A	3.23	110.53	106.36
7	A6	101	BCL	C4A-NA-C1A	3.24	110.55	106.36
7	BV	102	BCL	C4A-NA-C1A	3.28	110.60	106.36
7	B8	101	BCL	C4A-NA-C1A	3.28	110.60	106.36
7	B5	101	BCL	C4A-NA-C1A	3.29	110.62	106.36
7	AT	101	BCL	C4A-NA-C1A	3.30	110.63	106.36
9	BL	306	U10	C30-C29-C31	3.35	120.52	115.41
7	B7	101	BCL	C4A-NA-C1A	3.35	110.69	106.36
7	BO	101	BCL	C4A-NA-C1A	3.35	110.69	106.36
7	AL	302	BCL	C4A-NA-C1A	3.36	110.70	106.36
7	AS	101	BCL	C4A-NA-C1A	3.37	110.72	106.36
7	BM	401	BCL	C4A-NA-C1A	3.44	110.81	106.36
7	AY	101	BCL	C4A-NA-C1A	3.44	110.81	106.36
7	BZ	101	BCL	C4A-NA-C1A	3.45	110.82	106.36
7	AN	101	BCL	C4A-NA-C1A	3.45	110.82	106.36
7	B3	101	BCL	C4A-NA-C1A	3.50	110.88	106.36
7	A3	101	BCL	C4A-NA-C1A	3.50	110.88	106.36
7	BL	303	BCL	C4A-NA-C1A	3.50	110.88	106.36
7	A1	101	BCL	C4A-NA-C1A	3.50	110.89	106.36
7	B4	101	BCL	C4A-NA-C1A	3.51	110.89	106.36
7	AZ	101	BCL	C4A-NA-C1A	3.51	110.90	106.36
7	B9	101	BCL	C4A-NA-C1A	3.52	110.91	106.36
7	BO	102	BCL	C4A-NA-C1A	3.52	110.91	106.36
7	A9	101	BCL	C4A-NA-C1A	3.53	110.92	106.36
7	AD	102	BCL	C4A-NA-C1A	3.53	110.92	106.36
7	A4	101	BCL	C4A-NA-C1A	3.53	110.92	106.36
7	B1	101	BCL	C4A-NA-C1A	3.55	110.94	106.36
7	AO	101	BCL	C4A-NA-C1A	3.56	110.96	106.36
7	BY	101	BCL	C4A-NA-C1A	3.56	110.96	106.36
7	BP	102	BCL	C4A-NA-C1A	3.57	110.97	106.36
7	BZ	102	BCL	C4A-NA-C1A	3.57	110.98	106.36
7	AI	101	BCL	C4A-NA-C1A	3.59	111.00	106.36
7	BD	102	BCL	C4A-NA-C1A	3.59	111.00	106.36
7	BK	102	BCL	C4A-NA-C1A	3.59	111.00	106.36
7	AY	102	BCL	C4A-NA-C1A	3.59	111.01	106.36
7	AL	302	BCL	C4-C3-C5	3.60	120.90	115.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	AJ	101	BCL	C4A-NA-C1A	3.60	111.02	106.36
7	B6	101	BCL	C4A-NA-C1A	3.60	111.02	106.36
7	A6	102	BCL	C4A-NA-C1A	3.61	111.03	106.36
7	BY	102	BCL	C4A-NA-C1A	3.62	111.04	106.36
7	BF	102	BCL	C4A-NA-C1A	3.62	111.05	106.36
7	BI	101	BCL	C4A-NA-C1A	3.64	111.06	106.36
7	AP	102	BCL	C4A-NA-C1A	3.65	111.07	106.36
7	BU	101	BCL	C4A-NA-C1A	3.66	111.09	106.36
7	AG	101	BCL	C4A-NA-C1A	3.67	111.10	106.36
7	AM	402	BCL	C4A-NA-C1A	3.67	111.11	106.36
7	AT	102	BCL	C4A-NA-C1A	3.69	111.13	106.36
8	AM	403	BPH	C4D-C3D-C2D	3.97	112.21	107.08
8	BM	402	BPH	C4D-C3D-C2D	4.00	112.25	107.08
8	AL	303	BPH	C4D-C3D-C2D	4.07	112.34	107.08
8	BL	304	BPH	C4D-C3D-C2D	4.09	112.36	107.08
8	BM	402	BPH	C3C-C4C-NC	5.23	113.17	107.93
8	AM	403	BPH	C3C-C4C-NC	5.25	113.19	107.93
8	BL	304	BPH	C3C-C4C-NC	6.00	113.94	107.93
8	AL	303	BPH	C3C-C4C-NC	6.01	113.95	107.93
7	AO	101	BCL	O2D-CGD-CBD	6.38	120.06	111.30
7	AS	101	BCL	O2D-CGD-CBD	6.39	120.06	111.30
7	A9	101	BCL	O2D-CGD-CBD	6.40	120.08	111.30
7	B4	101	BCL	O2D-CGD-CBD	6.41	120.10	111.30
7	AP	102	BCL	O2D-CGD-CBD	6.41	120.10	111.30
7	AD	102	BCL	O2D-CGD-CBD	6.41	120.10	111.30
7	BT	101	BCL	O2D-CGD-CBD	6.41	120.10	111.30
7	BO	102	BCL	O2D-CGD-CBD	6.42	120.11	111.30
7	BZ	102	BCL	O2D-CGD-CBD	6.43	120.12	111.30
7	BV	101	BCL	O2D-CGD-CBD	6.43	120.12	111.30
7	AT	102	BCL	O2D-CGD-CBD	6.43	120.12	111.30
7	BP	102	BCL	O2D-CGD-CBD	6.43	120.13	111.30
7	AL	301	BCL	O2D-CGD-CBD	6.44	120.13	111.30
7	AI	101	BCL	O2D-CGD-CBD	6.44	120.13	111.30
7	BY	102	BCL	O2D-CGD-CBD	6.44	120.13	111.30
7	BK	102	BCL	O2D-CGD-CBD	6.44	120.13	111.30
7	B9	101	BCL	O2D-CGD-CBD	6.44	120.14	111.30
7	B6	101	BCL	O2D-CGD-CBD	6.45	120.14	111.30
7	AF	101	BCL	O2D-CGD-CBD	6.45	120.14	111.30
7	A6	102	BCL	O2D-CGD-CBD	6.45	120.14	111.30
7	AJ	101	BCL	O2D-CGD-CBD	6.45	120.15	111.30
7	AW	101	BCL	O2D-CGD-CBD	6.45	120.16	111.30
7	AG	101	BCL	O2D-CGD-CBD	6.46	120.16	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B8	101	BCL	O2D-CGD-CBD	6.46	120.16	111.30
7	A1	101	BCL	O2D-CGD-CBD	6.46	120.16	111.30
7	B7	101	BCL	O2D-CGD-CBD	6.46	120.16	111.30
7	B5	101	BCL	O2D-CGD-CBD	6.46	120.16	111.30
7	BI	101	BCL	O2D-CGD-CBD	6.46	120.16	111.30
7	BF	102	BCL	O2D-CGD-CBD	6.46	120.16	111.30
7	BF	101	BCL	O2D-CGD-CBD	6.46	120.16	111.30
7	A2	101	BCL	O2D-CGD-CBD	6.46	120.16	111.30
7	B3	101	BCL	O2D-CGD-CBD	6.46	120.16	111.30
7	AY	102	BCL	O2D-CGD-CBD	6.46	120.17	111.30
8	BL	304	BPH	O2D-CGD-CBD	6.46	120.17	111.30
7	BD	102	BCL	O2D-CGD-CBD	6.46	120.17	111.30
7	BL	303	BCL	O2D-CGD-CBD	6.47	120.17	111.30
7	BU	101	BCL	O2D-CGD-CBD	6.47	120.17	111.30
7	BY	101	BCL	O2D-CGD-CBD	6.47	120.17	111.30
7	B2	101	BCL	O2D-CGD-CBD	6.47	120.18	111.30
7	AT	101	BCL	O2D-CGD-CBD	6.47	120.18	111.30
7	BM	401	BCL	O2D-CGD-CBD	6.47	120.18	111.30
7	A6	101	BCL	O2D-CGD-CBD	6.47	120.18	111.30
8	AL	303	BPH	O2D-CGD-CBD	6.47	120.18	111.30
7	A8	101	BCL	O2D-CGD-CBD	6.48	120.19	111.30
7	A3	101	BCL	O2D-CGD-CBD	6.48	120.19	111.30
7	B1	101	BCL	O2D-CGD-CBD	6.48	120.19	111.30
7	BZ	101	BCL	O2D-CGD-CBD	6.48	120.19	111.30
7	AZ	101	BCL	O2D-CGD-CBD	6.48	120.19	111.30
7	A7	101	BCL	O2D-CGD-CBD	6.48	120.20	111.30
7	BO	101	BCL	O2D-CGD-CBD	6.49	120.20	111.30
7	BV	102	BCL	O2D-CGD-CBD	6.49	120.20	111.30
7	BL	302	BCL	O2D-CGD-CBD	6.49	120.20	111.30
7	A4	101	BCL	O2D-CGD-CBD	6.49	120.21	111.30
7	AV	101	BCL	O2D-CGD-CBD	6.52	120.24	111.30
7	AY	101	BCL	O2D-CGD-CBD	6.52	120.24	111.30
7	AN	101	BCL	O2D-CGD-CBD	6.52	120.25	111.30
7	AK	101	BCL	O2D-CGD-CBD	6.53	120.26	111.30
8	AM	403	BPH	O2D-CGD-CBD	6.54	120.27	111.30
7	AP	101	BCL	O2D-CGD-CBD	6.54	120.28	111.30
7	BP	101	BCL	O2D-CGD-CBD	6.55	120.28	111.30
8	BM	402	BPH	O2D-CGD-CBD	6.56	120.30	111.30
7	AD	101	BCL	O2D-CGD-CBD	6.57	120.32	111.30
7	BD	101	BCL	O2D-CGD-CBD	6.58	120.33	111.30
7	AM	401	BCL	O2D-CGD-CBD	6.58	120.33	111.30
7	BL	301	BCL	O2D-CGD-CBD	6.62	120.38	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	BK	101	BCL	O2D-CGD-CBD	6.63	120.39	111.30
7	AM	402	BCL	O2D-CGD-CBD	6.64	120.41	111.30
7	AL	302	BCL	O2D-CGD-CBD	6.67	120.45	111.30

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	BP	102	BCL	CED-O2D-CGD-CBD

There are no ring outliers.

72 monomers are involved in 682 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A1	101	BCL	2	0
7	A2	101	BCL	3	0
7	A3	101	BCL	6	0
7	A4	101	BCL	6	0
7	A6	101	BCL	1	0
7	A6	102	BCL	13	0
7	A7	101	BCL	9	0
7	A8	101	BCL	9	0
7	A9	101	BCL	11	0
7	AD	101	BCL	9	0
7	AD	102	BCL	13	0
7	AF	101	BCL	12	0
7	AG	101	BCL	2	0
7	AI	101	BCL	11	0
7	AJ	101	BCL	8	0
7	AK	101	BCL	6	0
7	AL	301	BCL	34	0
7	AL	302	BCL	22	0
8	AL	303	BPH	27	0
9	AL	304	U10	21	0
7	AM	401	BCL	28	0
7	AM	402	BCL	23	0
8	AM	403	BPH	18	0
9	AM	405	U10	12	0
12	AM	406	SPO	9	0
7	AN	101	BCL	4	0
7	AO	101	BCL	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	AP	101	BCL	13	0
7	AP	102	BCL	8	0
7	AS	101	BCL	15	0
7	AT	101	BCL	7	0
7	AT	102	BCL	14	0
7	AV	101	BCL	6	0
7	AW	101	BCL	1	0
7	AY	101	BCL	3	0
7	AY	102	BCL	4	0
7	AZ	101	BCL	12	0
7	B1	101	BCL	2	0
7	B2	101	BCL	9	0
7	B3	101	BCL	7	0
7	B4	101	BCL	3	0
7	B5	101	BCL	1	0
7	B6	101	BCL	5	0
7	B7	101	BCL	3	0
7	B8	101	BCL	11	0
7	B9	101	BCL	7	0
7	BD	101	BCL	8	0
7	BD	102	BCL	6	0
7	BF	101	BCL	12	0
7	BF	102	BCL	1	0
7	BI	101	BCL	12	0
7	BK	101	BCL	9	0
7	BK	102	BCL	9	0
7	BL	301	BCL	16	0
7	BL	302	BCL	48	0
7	BL	303	BCL	28	0
8	BL	304	BPH	45	0
9	BL	306	U10	20	0
7	BM	401	BCL	27	0
8	BM	402	BPH	26	0
7	BO	101	BCL	6	0
7	BO	102	BCL	19	0
7	BP	101	BCL	16	0
7	BP	102	BCL	12	0
7	BT	101	BCL	7	0
7	BU	101	BCL	6	0
7	BV	101	BCL	8	0
7	BV	102	BCL	5	0
7	BY	101	BCL	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	BY	102	BCL	5	0
7	BZ	101	BCL	11	0
7	BZ	102	BCL	18	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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, 95^{th} 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	A1	42/58 (72%)	-0.83	0 100 100	135, 231, 388, 456	0
1	A2	42/58 (72%)	-0.65	0 100 100	182, 298, 500, 500	0
1	A3	42/58 (72%)	-0.57	0 100 100	162, 348, 498, 500	0
1	A5	42/58 (72%)	-0.82	0 100 100	87, 166, 318, 335	0
1	A7	42/58 (72%)	-0.27	1 (2%) 62 58	217, 396, 500, 500	0
1	AD	42/58 (72%)	-0.68	0 100 100	120, 190, 361, 392	0
1	AF	42/58 (72%)	-0.48	1 (2%) 62 58	235, 399, 499, 500	0
1	AJ	42/58 (72%)	-0.80	0 100 100	42, 331, 460, 498	0
1	AN	42/58 (72%)	-0.69	0 100 100	149, 330, 490, 500	0
1	AP	42/58 (72%)	-0.72	0 100 100	163, 285, 365, 402	0
1	AT	42/58 (72%)	-0.61	0 100 100	171, 353, 500, 500	0
1	AV	42/58 (72%)	-0.58	0 100 100	310, 453, 500, 500	0
1	AX	42/58 (72%)	-0.36	1 (2%) 62 58	270, 446, 500, 500	0
1	AZ	42/58 (72%)	-0.56	0 100 100	123, 321, 500, 500	0
1	B1	42/58 (72%)	-0.46	1 (2%) 62 58	230, 429, 500, 500	0
1	B2	42/58 (72%)	-0.39	0 100 100	177, 354, 500, 500	0
1	B3	42/58 (72%)	-0.47	0 100 100	307, 434, 500, 500	0
1	B5	42/58 (72%)	-0.64	0 100 100	146, 321, 429, 492	0
1	B7	42/58 (72%)	-0.61	0 100 100	162, 245, 500, 500	0
1	BD	42/58 (72%)	-0.61	1 (2%) 62 58	137, 211, 374, 482	0
1	BF	42/58 (72%)	-0.44	0 100 100	206, 417, 500, 500	0
1	BJ	42/58 (72%)	-0.61	0 100 100	204, 333, 500, 500	0
1	BN	42/58 (72%)	-0.78	0 100 100	113, 245, 500, 500	0
1	BP	42/58 (72%)	-0.12	1 (2%) 62 58	182, 415, 500, 500	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	BT	42/58 (72%)	-0.53	0 100 100	214, 397, 484, 500	0
1	BV	42/58 (72%)	-0.32	0 100 100	295, 443, 500, 500	0
1	BX	42/58 (72%)	0.23	3 (7%) 19 22	285, 448, 500, 500	0
1	BZ	42/58 (72%)	-0.46	0 100 100	243, 355, 499, 500	0
2	AB	57/82 (69%)	-0.90	0 100 100	145, 257, 378, 461	0
2	BB	57/82 (69%)	-0.33	0 100 100	306, 464, 500, 500	0
3	A4	48/49 (97%)	-0.74	0 100 100	220, 382, 500, 500	0
3	A6	48/49 (97%)	-1.10	0 100 100	89, 180, 383, 405	0
3	A8	48/49 (97%)	-0.68	0 100 100	258, 408, 497, 500	0
3	A9	48/49 (97%)	-0.84	0 100 100	250, 475, 500, 500	0
3	AE	48/49 (97%)	-0.73	0 100 100	237, 329, 457, 500	0
3	AG	48/49 (97%)	-0.19	0 100 100	149, 384, 500, 500	0
3	AI	48/49 (97%)	-0.66	0 100 100	233, 385, 491, 500	0
3	AK	48/49 (97%)	-0.82	0 100 100	235, 383, 499, 500	0
3	AO	48/49 (97%)	-0.77	0 100 100	117, 342, 494, 500	0
3	AQ	48/49 (97%)	-0.61	0 100 100	94, 446, 500, 500	0
3	AS	48/49 (97%)	-0.76	0 100 100	170, 319, 496, 500	0
3	AU	48/49 (97%)	-0.71	0 100 100	331, 417, 500, 500	0
3	AW	48/49 (97%)	-0.44	1 (2%) 67 62	232, 405, 500, 500	0
3	AY	48/49 (97%)	-0.62	0 100 100	262, 396, 500, 500	0
3	B4	48/49 (97%)	-0.57	0 100 100	202, 353, 489, 500	0
3	B6	48/49 (97%)	-0.94	0 100 100	116, 241, 375, 438	0
3	B8	48/49 (97%)	-0.27	1 (2%) 67 62	225, 472, 500, 500	0
3	B9	48/49 (97%)	-0.74	0 100 100	187, 374, 462, 494	0
3	BE	48/49 (97%)	-0.55	0 100 100	177, 387, 500, 500	0
3	BG	48/49 (97%)	-0.21	1 (2%) 67 62	274, 482, 500, 500	0
3	BI	48/49 (97%)	-0.52	0 100 100	242, 480, 500, 500	0
3	BK	48/49 (97%)	-0.34	0 100 100	356, 448, 500, 500	0
3	BO	48/49 (97%)	-0.65	0 100 100	206, 396, 500, 500	0
3	BQ	48/49 (97%)	-0.69	0 100 100	159, 401, 500, 500	0
3	BS	48/49 (97%)	-0.54	1 (2%) 67 62	235, 426, 500, 500	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
3	BU	48/49 (97%)	-0.41	0 100 100	225, 487, 500, 500	0
3	BW	48/49 (97%)	-0.63	0 100 100	210, 382, 500, 500	0
3	BY	48/49 (97%)	-0.57	1 (2%) 67 62	279, 460, 500, 500	0
4	AH	250/260 (96%)	-0.78	0 100 100	2, 101, 447, 500	0
4	BH	250/260 (96%)	-0.59	0 100 100	16, 193, 470, 500	0
5	AL	281/282 (99%)	-0.94	1 (0%) 93 90	2, 2, 194, 460	0
5	BL	281/282 (99%)	-0.92	0 100 100	2, 9, 249, 370	0
6	AM	304/308 (98%)	-0.82	0 100 100	2, 2, 215, 459	0
6	BM	304/308 (98%)	-0.75	0 100 100	2, 9, 269, 492	0
All	All	4304/4860 (88%)	-0.67	15 (0%) 94 92	2, 273, 500, 500	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BX	19	ALA	3.4
1	B1	12	ASP	3.4
1	A7	18	VAL	3.3
1	BX	21	GLY	3.3
3	BS	5	ASP	2.9
1	AF	49	ALA	2.8
1	BP	15	ARG	2.8
3	BG	4	SER	2.7
3	BY	1	ALA	2.3
1	BX	49	ALA	2.3
3	AW	1	ALA	2.3
1	AX	13	PRO	2.2
1	BD	18	VAL	2.1
3	B8	16	ALA	2.1
5	AL	274	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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, 95^{th} 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
7	BCL	B5	101	46/66	0.81	0.39	4.06	460,484,500,500	0
7	BCL	BO	101	46/66	0.81	0.37	3.92	500,500,500,500	0
7	BCL	BL	303	66/66	0.92	0.30	2.53	2,2,2,2	0
7	BCL	AO	101	46/66	0.92	0.31	2.50	247,260,266,272	0
7	BCL	A6	101	46/66	0.90	0.30	2.04	391,461,488,498	0
7	BCL	B9	101	46/66	0.84	0.38	1.82	500,500,500,500	0
7	BCL	B6	101	46/66	0.88	0.30	1.77	268,314,325,333	0
7	BCL	AY	101	46/66	0.94	0.25	1.63	438,471,494,500	0
7	BCL	BL	302	66/66	0.95	0.26	1.60	2,2,2,2	0
12	SPO	AM	406	42/42	0.94	0.27	1.59	2,2,2,2	0
8	BPH	BL	304	65/65	0.90	0.25	1.57	2,2,2,2	0
7	BCL	AK	101	46/66	0.88	0.27	1.57	422,500,500,500	0
7	BCL	B4	101	46/66	0.86	0.29	1.54	467,500,500,500	0
7	BCL	BK	101	46/66	0.88	0.28	1.53	471,500,500,500	0
7	BCL	AM	401	66/66	0.97	0.22	1.44	2,2,2,2	0
7	BCL	BL	301	66/66	0.94	0.25	1.39	2,2,2,2	0
8	BPH	AL	303	65/65	0.96	0.26	1.32	2,2,2,2	0
9	U10	AM	405	48/63	0.94	0.26	1.27	2,2,2,2	0
8	BPH	AM	403	65/65	0.95	0.26	1.27	2,2,2,2	0
7	BCL	AY	102	46/66	0.91	0.22	1.26	360,384,441,448	0
7	BCL	AM	402	66/66	0.97	0.23	1.24	2,2,2,2	0
7	BCL	AT	102	46/66	0.91	0.28	1.20	368,404,465,495	0
9	U10	AL	304	48/63	0.95	0.21	1.14	2,2,2,2	0
9	U10	BL	306	48/63	0.94	0.22	1.09	2,2,2,2	0
7	BCL	BZ	101	46/66	0.91	0.32	1.08	411,455,500,500	0
7	BCL	BM	401	66/66	0.95	0.23	1.03	2,2,2,2	0
7	BCL	A1	101	46/66	0.96	0.19	0.97	317,355,399,417	0
7	BCL	AL	301	66/66	0.97	0.23	0.96	2,2,2,2	0
7	BCL	BF	102	46/66	0.90	0.31	0.94	418,498,500,500	0
7	BCL	AL	302	66/66	0.95	0.25	0.92	2,2,2,2	0
7	BCL	A6	102	46/66	0.95	0.22	0.91	205,301,379,402	0
7	BCL	AV	101	46/66	0.87	0.27	0.90	313,363,409,416	0
7	BCL	BU	101	46/66	0.85	0.28	0.86	292,480,500,500	0
7	BCL	AN	101	46/66	0.92	0.23	0.79	263,334,370,376	0
7	BCL	BI	101	46/66	0.90	0.22	0.77	449,481,500,500	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	BCL	AD	102	46/66	0.96	0.18	0.73	145,169,200,210	0
7	BCL	AD	101	46/66	0.96	0.18	0.72	133,145,160,169	0
7	BCL	AG	101	46/66	0.94	0.20	0.71	329,398,418,422	0
7	BCL	AZ	101	46/66	0.93	0.26	0.67	500,500,500,500	0
7	BCL	AJ	101	46/66	0.94	0.25	0.66	241,343,392,401	0
7	BCL	B1	101	46/66	0.91	0.20	0.64	221,405,460,480	0
7	BCL	A4	101	46/66	0.92	0.19	0.60	289,335,362,369	0
7	BCL	BV	101	46/66	0.94	0.28	0.52	326,464,500,500	0
7	BCL	AP	101	46/66	0.92	0.26	0.47	196,268,280,290	0
7	BCL	AI	101	46/66	0.93	0.16	0.44	277,287,302,304	0
7	BCL	B3	101	46/66	0.92	0.18	0.43	442,492,500,500	0
7	BCL	BD	102	46/66	0.93	0.27	0.37	313,347,446,472	0
7	BCL	BZ	102	46/66	0.84	0.26	0.34	340,425,460,469	0
7	BCL	AP	102	46/66	0.90	0.23	0.33	212,236,270,272	0
7	BCL	A2	101	46/66	0.96	0.18	0.33	451,500,500,500	0
8	BPH	BM	402	65/65	0.94	0.20	0.27	2,2,2,2	0
7	BCL	B2	101	46/66	0.89	0.25	0.23	171,220,230,232	0
7	BCL	B7	101	46/66	0.93	0.26	0.21	159,184,195,199	0
7	BCL	A9	101	46/66	0.96	0.14	0.16	318,386,396,414	0
7	BCL	A8	101	46/66	0.96	0.19	0.15	301,369,400,413	0
7	BCL	AW	101	46/66	0.93	0.24	0.11	388,435,462,478	0
7	BCL	A7	101	46/66	0.92	0.18	0.10	180,198,207,213	0
7	BCL	BF	101	46/66	0.90	0.19	0.07	374,453,480,499	0
7	BCL	AT	101	46/66	0.93	0.18	0.02	241,267,280,281	0
7	BCL	AF	101	46/66	0.97	0.16	-0.05	204,214,229,239	0
7	BCL	BO	102	46/66	0.97	0.20	-0.05	152,179,187,204	0
7	BCL	BK	102	46/66	0.94	0.24	-0.06	321,390,455,471	0
10	PO4	BL	307	5/5	0.97	0.17	-0.07	2,2,2,2	0
7	BCL	BV	102	46/66	0.95	0.20	-0.15	332,395,420,424	0
7	BCL	AS	101	46/66	0.95	0.17	-0.17	275,321,356,360	0
10	PO4	AL	305	5/5	0.98	0.12	-0.19	2,2,2,2	0
7	BCL	BT	101	46/66	0.92	0.19	-0.23	274,316,329,331	0
7	BCL	BD	101	46/66	0.95	0.20	-0.24	233,299,305,307	0
7	BCL	B8	101	46/66	0.95	0.19	-0.39	233,268,304,309	0
7	BCL	BY	102	46/66	0.95	0.17	-0.53	192,221,234,245	0
7	BCL	BY	101	46/66	0.94	0.17	-0.56	283,306,315,316	0
7	BCL	BP	101	46/66	0.97	0.14	-0.60	142,147,153,161	0
7	BCL	A3	101	46/66	0.95	0.14	-0.65	245,269,314,322	0
7	BCL	BP	102	46/66	0.95	0.13	-0.67	172,203,216,217	0
11	FE2	AM	404	1/1	0.97	0.05	-1.59	2,2,2,2	0
11	FE2	BL	305	1/1	0.94	0.10	-2.09	2,2,2,2	0

6.5 Other polymers (i)

There are no such residues in this entry.