Full wwPDB X-ray Structure Validation Report (i)

Mar 15, 2016 – 07:13 PM EDT

PDB ID	:	4YUU
Title	:	Crystal structure of oxygen-evolving photosystem II from a red alga
Authors	:	Ago, H.; Shen, J.-R.
Deposited on	:	2015-03-19
Resolution	:	2.77 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:

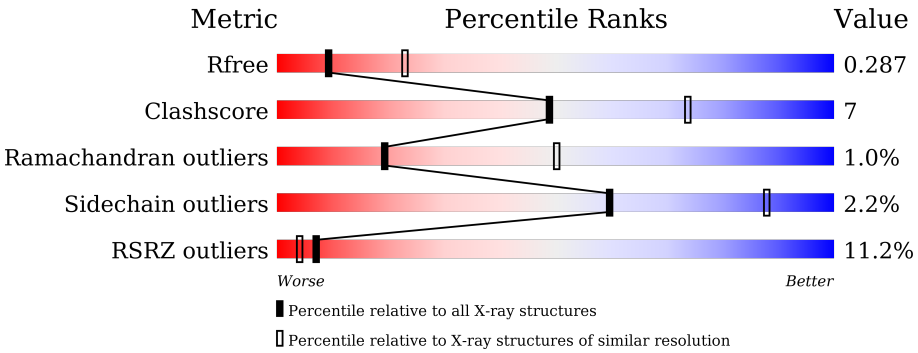
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 2.77 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	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (2.80-2.76)

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	344	3% 79% 20% ·
1	A2	344	7% 79% 16% · ·
1	a1	344	3% 96% · ·
1	a2	344	5% 95% · ·
2	B1	509	6% 78% 15% · 5%
2	B2	509	10% 83% 14% · ·

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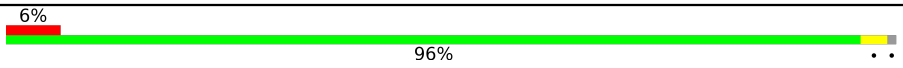
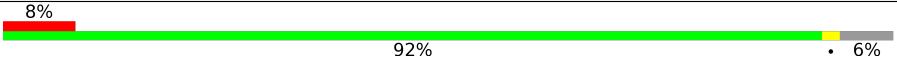
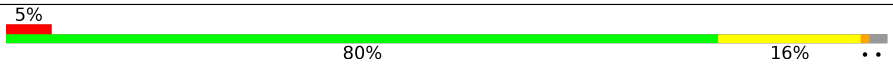
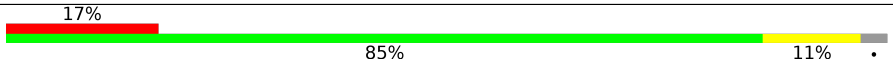
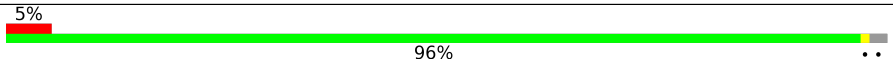
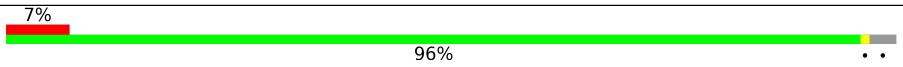
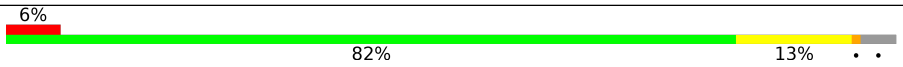
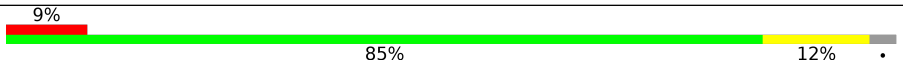
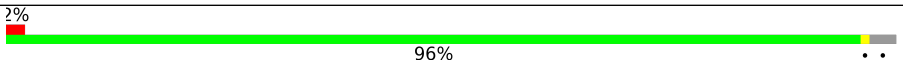
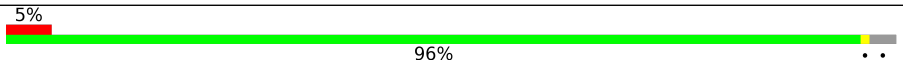
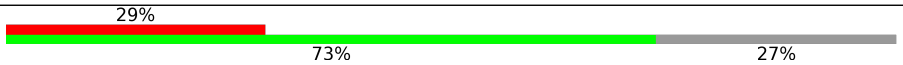
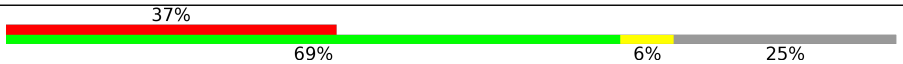
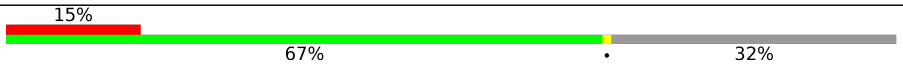
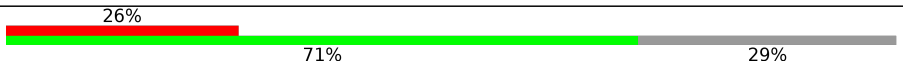
Mol	Chain	Length	Quality of chain
2	b1	509	
2	b2	509	
3	C1	460	
3	C2	460	
3	c1	460	
3	c2	460	
4	D1	351	
4	D2	351	
4	d1	351	
4	d2	351	
5	E1	84	
5	E2	84	
5	e1	84	
5	e2	84	
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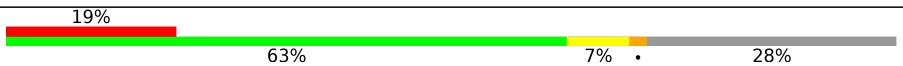
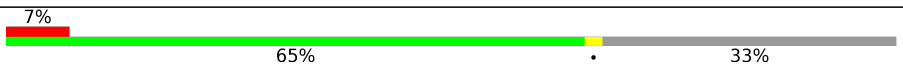
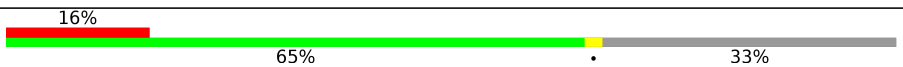
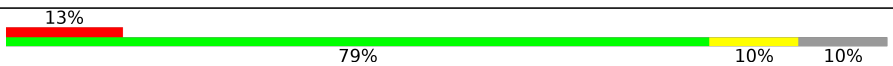
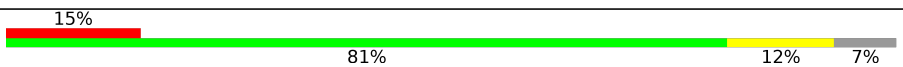
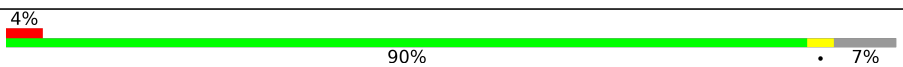
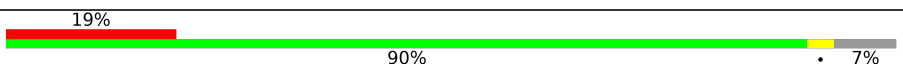
6	F2	43	
6	f1	43	
6	f2	43	
7	H1	67	
7	H2	67	
7	h1	67	
7	h2	67	
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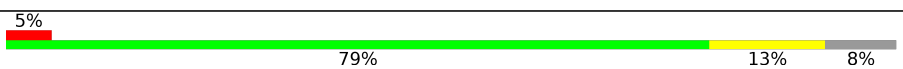
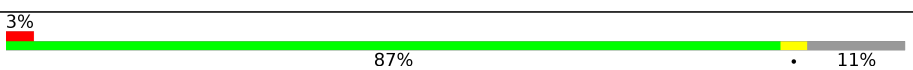
8	I2	38	
8	i1	38	

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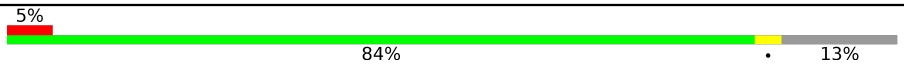
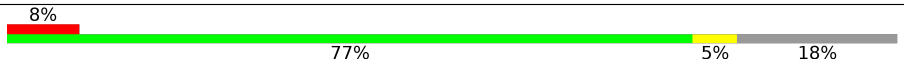
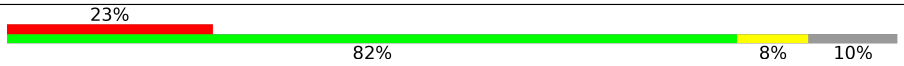
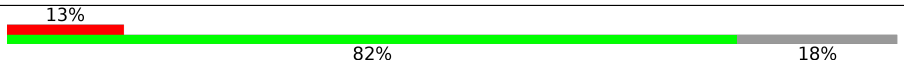
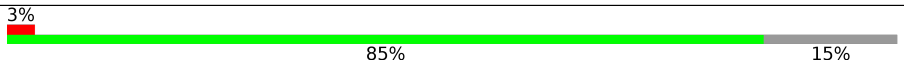
Mol	Chain	Length	Quality of chain
8	i2	38	
9	J1	39	
9	J2	39	
9	j1	39	
9	j2	39	
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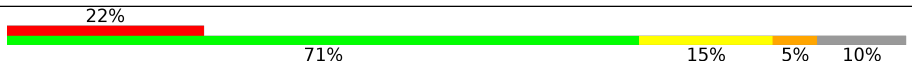
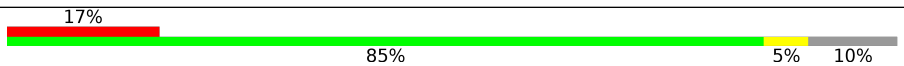
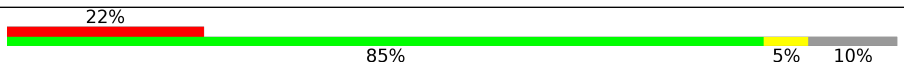
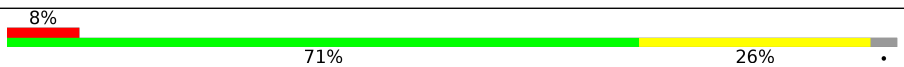
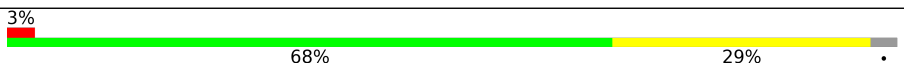
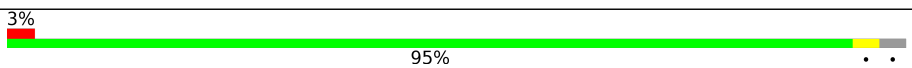
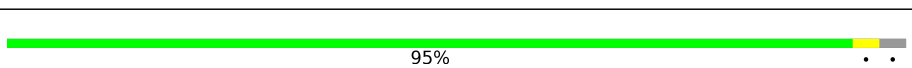
10	K2	41	
10	k1	41	
10	k2	41	
11	L1	38	
11	L2	38	
11	l1	38	
11	l2	38	
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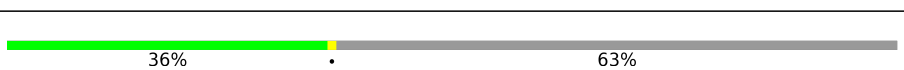
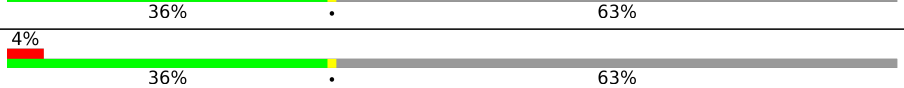
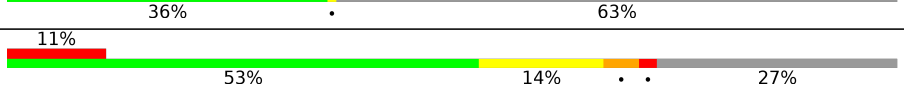
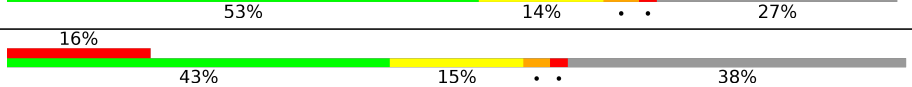
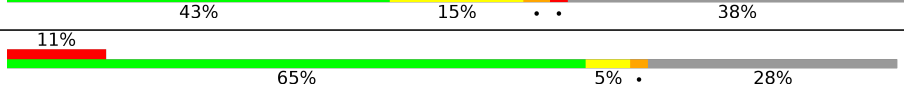
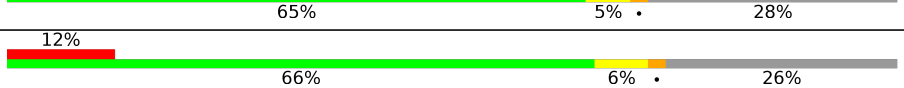
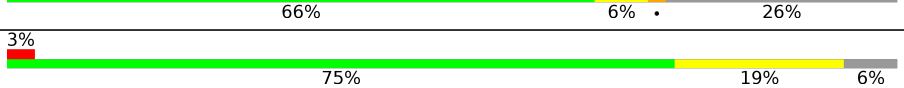
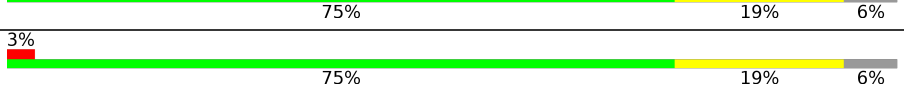
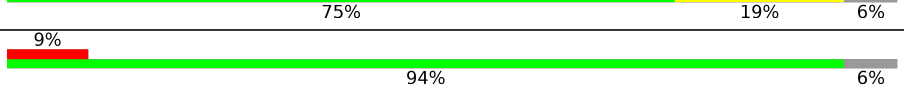
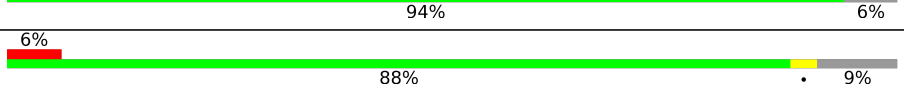
12	M2	108	
12	m1	108	
12	m2	108	
13	O1	329	
13	O2	329	
13	o1	329	
13	o2	329	
14	T1	32	
14	T2	32	
14	t1	32	
14	t2	32	

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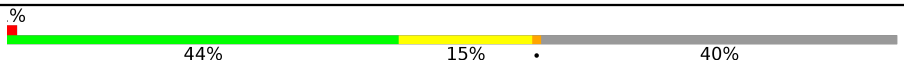
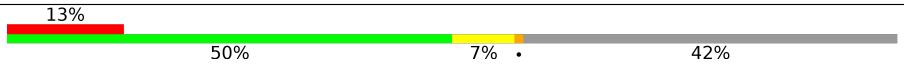
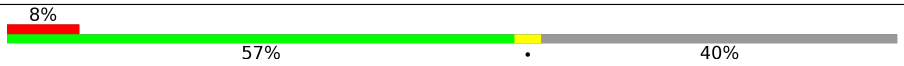
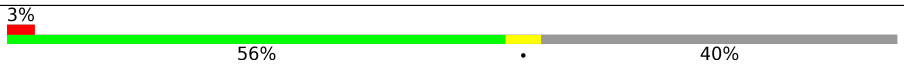
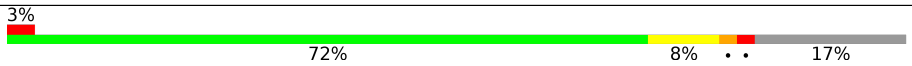
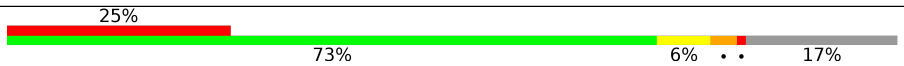
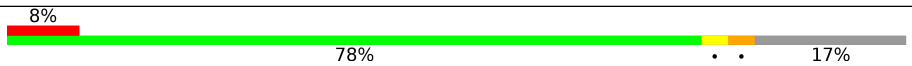
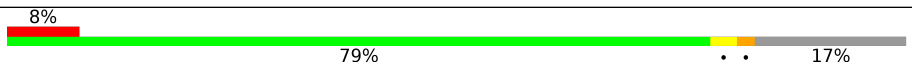
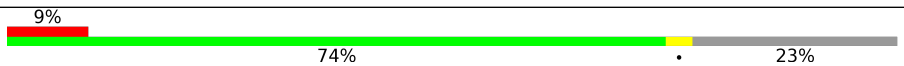
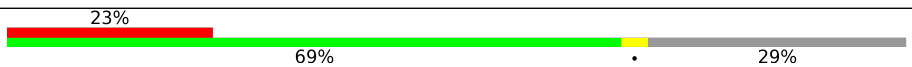
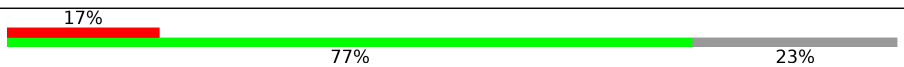
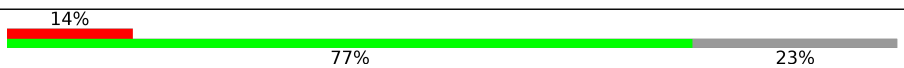
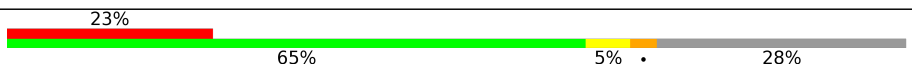
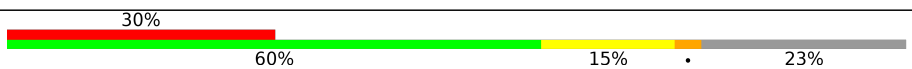
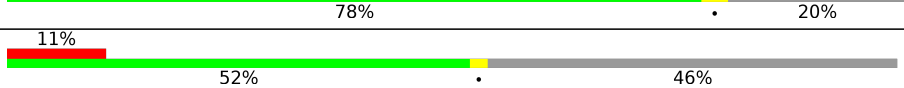
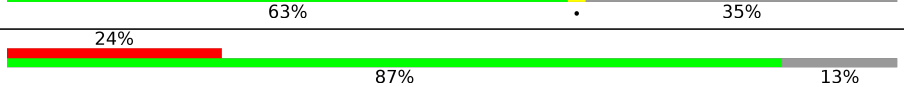
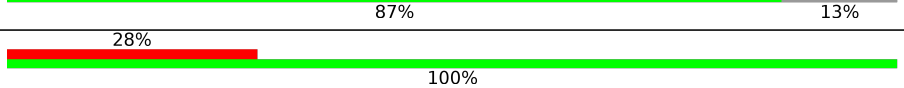
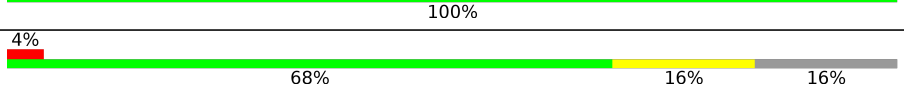
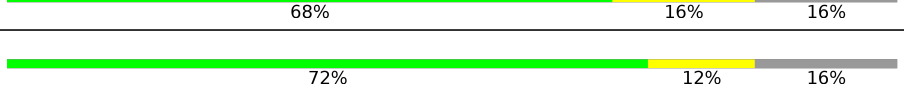
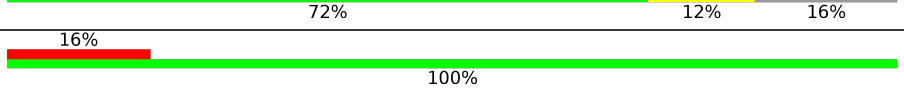
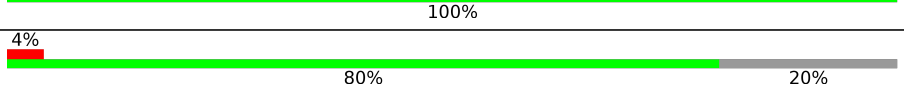
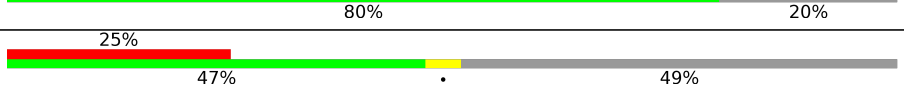
Mol	Chain	Length	Quality of chain
15	U1	155	
15	U2	155	
15	u1	155	
15	u2	155	
16	V1	155	
16	V2	155	
16	v1	155	
16	v2	155	
17	Y1	35	
17	Y2	35	
17	y1	35	
17	y2	35	
18	X1	40	
18	X2	40	
18	x1	40	
18	x2	40	
19	S1	46	
19	S2	46	
19	s1	46	
19	s2	46	
20	W1	25	
20	W2	25	
20	w1	25	
20	w2	25	
21	Q2	218	

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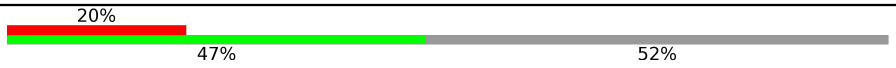
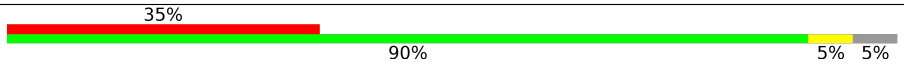
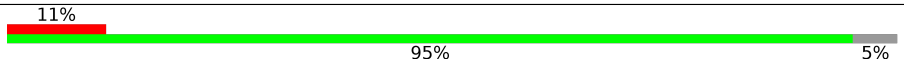
Mol	Chain	Length	Quality of chain
21	q1	218	
22	Z2	62	
22	z2	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	BCR	B1	602	-	-	-	X
23	BCR	H1	102	-	-	-	X
23	BCR	H2	103	-	-	-	X
23	BCR	J1	101	-	-	-	X
23	BCR	K1	101	-	-	-	X
23	BCR	K2	102	-	-	-	X
23	BCR	b1	602	-	-	-	X
23	BCR	b2	603	-	-	-	X
23	BCR	c1	502	-	-	-	X
23	BCR	c2	501	-	-	-	X
23	BCR	k1	101	-	-	-	X
23	BCR	z2	101	-	-	-	X
25	CLA	A1	403	X	-	-	-
25	CLA	A1	404	X	-	-	-
25	CLA	A1	405	X	-	-	-
25	CLA	A1	406	X	-	-	-
25	CLA	A2	402	X	-	-	-
25	CLA	A2	403	X	-	-	-
25	CLA	A2	404	X	-	-	-
25	CLA	B1	604	X	-	-	X
25	CLA	B1	605	X	-	-	-
25	CLA	B1	606	X	-	-	-
25	CLA	B1	607	X	-	-	-
25	CLA	B1	608	X	-	-	-
25	CLA	B1	609	X	-	-	-
25	CLA	B1	610	X	-	-	-
25	CLA	B1	611	X	-	-	-
25	CLA	B1	612	X	-	-	-
25	CLA	B1	613	X	-	-	-
25	CLA	B1	614	X	-	-	-
25	CLA	B1	615	X	-	-	-
25	CLA	B1	616	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B1	617	X	-	-	-
25	CLA	B1	618	X	-	-	-
25	CLA	B1	619	X	-	-	-
25	CLA	B2	604	X	-	-	-
25	CLA	B2	605	X	-	-	-
25	CLA	B2	606	X	-	-	X
25	CLA	B2	607	X	-	-	-
25	CLA	B2	608	X	-	-	-
25	CLA	B2	609	X	-	-	-
25	CLA	B2	610	X	-	-	-
25	CLA	B2	611	X	-	-	-
25	CLA	B2	612	X	-	-	-
25	CLA	B2	613	X	-	-	-
25	CLA	B2	614	X	-	-	-
25	CLA	B2	615	X	-	-	-
25	CLA	B2	616	X	-	-	-
25	CLA	B2	617	X	-	-	-
25	CLA	B2	618	X	-	-	-
25	CLA	B2	619	X	-	-	-
25	CLA	C1	502	X	-	-	X
25	CLA	C1	503	X	-	-	-
25	CLA	C1	504	X	-	-	-
25	CLA	C1	505	X	-	-	-
25	CLA	C1	506	X	-	-	-
25	CLA	C1	507	X	-	-	-
25	CLA	C1	508	X	-	-	-
25	CLA	C1	509	X	-	-	-
25	CLA	C1	510	X	-	-	-
25	CLA	C1	511	X	-	-	-
25	CLA	C1	512	X	-	-	-
25	CLA	C1	513	X	-	-	-
25	CLA	C1	514	X	-	-	-
25	CLA	C2	503	X	-	-	-
25	CLA	C2	504	X	-	-	-
25	CLA	C2	505	X	-	-	-
25	CLA	C2	506	X	-	-	X
25	CLA	C2	507	X	-	-	-
25	CLA	C2	508	X	-	-	-
25	CLA	C2	509	X	-	-	-
25	CLA	C2	510	X	-	-	-
25	CLA	C2	511	X	-	-	-
25	CLA	C2	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	C2	516	X	-	-	-
25	CLA	C2	518	X	-	-	-
25	CLA	D1	402	X	-	-	-
25	CLA	D1	403	X	-	-	-
25	CLA	D2	401	X	-	-	-
25	CLA	D2	404	X	-	-	-
25	CLA	D2	406	X	-	-	-
25	CLA	K2	101	X	-	-	-
25	CLA	a1	403	X	-	-	-
25	CLA	a1	404	X	-	-	-
25	CLA	a1	405	X	-	-	-
25	CLA	a2	404	X	-	-	-
25	CLA	a2	405	X	-	-	-
25	CLA	a2	413	X	-	-	-
25	CLA	b1	604	X	-	-	-
25	CLA	b1	605	X	-	-	-
25	CLA	b1	606	X	-	-	-
25	CLA	b1	607	X	-	-	-
25	CLA	b1	608	X	-	-	-
25	CLA	b1	609	X	-	-	-
25	CLA	b1	610	X	-	-	-
25	CLA	b1	611	X	-	-	-
25	CLA	b1	612	X	-	-	-
25	CLA	b1	613	X	-	-	-
25	CLA	b1	614	X	-	-	-
25	CLA	b1	615	X	-	-	-
25	CLA	b1	616	X	-	-	-
25	CLA	b1	617	X	-	-	-
25	CLA	b1	619	X	-	-	-
25	CLA	b1	620	X	-	-	-
25	CLA	b2	604	X	-	-	-
25	CLA	b2	606	X	-	-	-
25	CLA	b2	608	X	-	-	-
25	CLA	b2	609	X	-	-	-
25	CLA	b2	610	X	-	-	-
25	CLA	b2	611	X	-	-	-
25	CLA	b2	612	X	-	-	-
25	CLA	b2	613	X	-	-	-
25	CLA	b2	614	X	-	-	-
25	CLA	b2	615	X	-	-	-
25	CLA	b2	616	X	-	-	-
25	CLA	b2	617	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	b2	618	X	-	-	-
25	CLA	b2	619	X	-	-	-
25	CLA	b2	620	X	-	-	-
25	CLA	b2	624	X	-	-	-
25	CLA	c1	503	X	-	-	-
25	CLA	c1	504	X	-	-	-
25	CLA	c1	505	X	-	-	-
25	CLA	c1	506	X	-	-	-
25	CLA	c1	507	X	-	-	-
25	CLA	c1	508	X	-	-	-
25	CLA	c1	509	X	-	-	-
25	CLA	c1	510	X	-	-	-
25	CLA	c1	511	X	-	-	-
25	CLA	c1	512	X	-	-	-
25	CLA	c1	513	X	-	-	-
25	CLA	c1	515	X	-	-	-
25	CLA	c1	516	X	-	-	-
25	CLA	c2	502	X	-	-	-
25	CLA	c2	503	X	-	-	-
25	CLA	c2	504	X	-	-	-
25	CLA	c2	505	X	-	-	-
25	CLA	c2	506	X	-	-	-
25	CLA	c2	507	X	-	-	-
25	CLA	c2	508	X	-	-	-
25	CLA	c2	509	X	-	-	-
25	CLA	c2	510	X	-	-	-
25	CLA	c2	511	X	-	-	-
25	CLA	c2	512	X	-	-	-
25	CLA	c2	513	X	-	-	-
25	CLA	c2	515	X	-	-	-
25	CLA	d1	401	X	-	-	-
25	CLA	d1	404	X	-	-	-
25	CLA	d1	406	X	-	-	-
25	CLA	d2	402	X	-	-	-
25	CLA	d2	404	X	-	-	-
25	CLA	d2	405	X	-	-	-
28	UNL	A1	409	-	-	-	X
28	UNL	A2	408	-	-	-	X
28	UNL	B1	623	-	-	-	X
28	UNL	B1	624	-	-	-	X
28	UNL	B1	625	-	-	-	X
28	UNL	B2	622	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	UNL	B2	624	-	-	-	X
28	UNL	B2	625	-	-	-	X
28	UNL	C2	517	-	-	-	X
28	UNL	J2	101	-	-	-	X
28	UNL	a1	409	-	-	-	X
28	UNL	a2	401	-	-	-	X
28	UNL	a2	409	-	-	-	X
28	UNL	a2	411	-	-	-	X
28	UNL	b1	629	-	-	-	X
28	UNL	b1	630	-	-	-	X
28	UNL	b2	607	-	-	-	X
28	UNL	d1	410	-	-	-	X
28	UNL	d2	410	-	-	-	X
28	UNL	d2	411	-	-	-	X
28	UNL	j1	101	-	-	-	X
28	UNL	l1	103	-	-	-	X
28	UNL	m2	101	-	-	-	X
28	UNL	m2	102	-	-	-	X
28	UNL	t1	101	-	-	-	X
28	UNL	x1	101	-	-	-	X
29	LMG	B2	621	-	-	-	X
29	LMG	M1	101	-	-	-	X
29	LMG	b2	622	-	-	-	X
29	LMG	d1	411	-	-	-	X
29	LMG	j2	101	-	-	-	X
31	BCT	a1	413	-	-	-	X
32	GOL	B1	620	-	-	-	X
32	GOL	a2	415	-	-	-	X
32	GOL	c2	518	-	-	-	X
32	GOL	i1	101	-	-	-	X
33	LHG	B2	627	-	-	-	X
33	LHG	b2	625	-	-	-	X
35	LMT	a2	406	-	-	-	X
35	LMT	b2	621	-	-	-	X
35	LMT	c1	517	-	-	-	X
35	LMT	l1	101	-	-	-	X
35	LMT	m1	101	-	-	-	X
35	LMT	m2	103	-	-	-	X
35	LMT	m2	104	-	-	-	X
36	PL9	d2	409	-	-	-	X
37	SQD	B2	623	-	-	-	X
37	SQD	D1	409	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	SQD	b2	605	-	-	-	X
38	HEM	E1	101	-	-	-	X
38	HEM	e2	101	-	-	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 92765 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A1	344	Total	C	N	O	S	0	0	0
			2609	1708	425	462	14			
1	a1	334	Total	C	N	O	S	0	0	0
			2564	1676	421	454	13			
1	A2	332	Total	C	N	O	S	0	1	0
			2475	1607	411	444	13			
1	a2	334	Total	C	N	O	S	0	0	0
			2513	1638	410	452	13			

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B1	483	Total	C	N	O	S	0	0	0
			3703	2426	624	641	12			
2	b1	503	Total	C	N	O	S	0	1	0
			3881	2549	646	674	12			
2	B2	503	Total	C	N	O	S	0	0	0
			3770	2460	645	654	11			
2	b2	481	Total	C	N	O	S	0	0	0
			3681	2418	620	631	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C1	449	Total	C	N	O	S	0	0	0
			3392	2215	573	594	10			
3	c1	449	Total	C	N	O	S	0	2	0
			3439	2241	577	611	10			
3	C2	444	Total	C	N	O	S	0	0	0
			3145	2028	545	564	8			
3	c2	448	Total	C	N	O	S	0	0	0
			3386	2201	578	597	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D1	337	Total	C	N	O	S	0	0	0
			2615	1736	422	447	10			
4	d1	339	Total	C	N	O	S	0	0	0
			2678	1775	433	460	10			
4	D2	340	Total	C	N	O	S	0	0	0
			2585	1713	422	440	10			
4	d2	340	Total	C	N	O	S	0	0	0
			2643	1756	425	452	10			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E1	61	Total	C	N	O	0	0	0
			405	264	68	73			
5	e1	57	Total	C	N	O	0	0	0
			427	280	71	76			
5	E2	63	Total	C	N	O	0	0	0
			430	279	72	79			
5	e2	60	Total	C	N	O	0	0	0
			421	279	71	71			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F1	28	Total	C	N	O	S	0	0	0
			213	144	36	32	1			
6	f1	29	Total	C	N	O	S	0	0	0
			227	158	36	32	1			
6	F2	31	Total	C	N	O	S	0	0	0
			229	153	41	34	1			
6	f2	29	Total	C	N	O	S	0	0	0
			225	157	34	33	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H1	60	Total	C	N	O	S	0	0	0
			433	289	69	73	2			
7	h1	62	Total	C	N	O	S	0	0	0
			470	317	71	80	2			
7	H2	62	Total	C	N	O	S	0	0	0
			443	294	72	75	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	h2	62	Total	C	N	O	S	0	0	0
			450	302	69	77	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I1	34	Total	C	N	O	S	0	0	0
			274	184	42	45	3			
8	i1	34	Total	C	N	O	S	0	0	0
			280	188	44	45	3			
8	I2	35	Total	C	N	O	S	0	0	0
			265	177	41	45	2			
8	i2	33	Total	C	N	O	S	0	0	0
			261	174	40	44	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	J1	32	Total	C	N	O	0	0	0
			220	148	33	39			
9	j1	32	Total	C	N	O	0	0	0
			224	152	33	39			
9	J2	35	Total	C	N	O	0	0	0
			231	154	36	41			
9	j2	33	Total	C	N	O	0	0	0
			228	153	34	41			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K1	37	Total	C	N	O	S	0	0	0
			279	195	39	44	1			
10	k1	37	Total	C	N	O	S	0	0	0
			280	198	39	42	1			
10	K2	37	Total	C	N	O		0	0	0
			250	171	39	40				
10	k2	37	Total	C	N	O	S	0	0	0
			269	185	40	43	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L1	37	Total	C	N	O	0	0	0
			292	197	46	49			
11	l1	37	Total	C	N	O	0	0	0
			299	203	47	49			
11	L2	37	Total	C	N	O	0	0	0
			299	202	46	51			
11	l2	37	Total	C	N	O	0	0	0
			299	202	46	51			

- Molecule 12 is a protein called PHOTOSYSTEM II REACTION CENTER PROTEIN M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M1	40	Total	C	N	O	S	0	0	0
			285	189	44	50	2			
12	m1	40	Total	C	N	O	S	0	0	0
			285	189	44	50	2			
12	M2	40	Total	C	N	O	S	0	0	0
			284	188	46	48	2			
12	m2	40	Total	C	N	O	S	0	0	0
			287	189	46	50	2			

- Molecule 13 is a protein called PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE, PSBO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O1	240	Total	C	N	O	S	0	0	0
			1674	1074	276	316	8			
13	o1	238	Total	C	N	O	S	0	0	0
			1692	1070	282	332	8			
13	O2	205	Total	C	N	O	S	0	0	0
			1376	870	237	262	7			
13	o2	245	Total	C	N	O	S	0	0	0
			1768	1123	296	341	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T1	30	Total	C	N	O	S	0	0	0
			241	168	36	36	1			
14	t1	30	Total	C	N	O	S	0	0	0
			246	173	36	36	1			
14	T2	30	Total	C	N	O	S	0	0	0
			240	170	33	36	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	t2	29	Total	C	N	O	S	0	0	0
			235	167	32	35	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U1	93	Total	C	N	O	S	0	0	0
			691	445	116	129	1			
15	u1	93	Total	C	N	O	S	0	0	0
			703	449	119	134	1			
15	U2	90	Total	C	N	O	S	0	0	0
			577	355	103	118	1			
15	u2	93	Total	C	N	O	S	0	0	0
			708	455	120	132	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U1	-51	MET	-	initiating methionine	UNP Q9ZQS5
u1	-51	MET	-	initiating methionine	UNP Q9ZQS5
U2	-51	MET	-	initiating methionine	UNP Q9ZQS5
u2	-51	MET	-	initiating methionine	UNP Q9ZQS5

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V1	129	Total	C	N	O	S	0	0	0
			917	579	159	175	4			
16	v1	129	Total	C	N	O	S	0	0	0
			921	577	163	177	4			
16	V2	129	Total	C	N	O	S	0	0	0
			845	521	152	168	4			
16	v2	129	Total	C	N	O	S	0	0	0
			963	608	168	183	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	Y1	27	Total	C	N	O	0	0	0
			170	111	29	30			
17	y1	27	Total	C	N	O	0	0	0
			195	133	30	32			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
17	Y2	25	Total C N O 159 104 27 28	0	0	0
17	y2	27	Total C N O 188 126 30 32	0	0	0

- Molecule 18 is a protein called PHOTOSYSTEM II REACTION CENTER PROTEIN X.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
18	X1	29	Total C N O 197 135 30 32	0	0	0
18	x1	36	Total C N O S 255 174 38 42 1	0	0	0
18	X2	31	Total C N O S 215 149 33 32 1	0	0	0
18	x2	32	Total C N O 218 147 35 36	0	0	0

- Molecule 19 is a protein called PEPTIDE CHAIN UNASSIGNED.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
19	S1	25	Total C N O 164 113 26 25	0	0	0
19	s1	40	Total C N O 263 182 41 40	0	0	0
19	S2	30	Total C N O 191 130 31 30	0	0	0
19	s2	46	Total C N O 281 188 47 46	0	0	0

- Molecule 20 is a protein called PEPTIDE CHAIN UNASSIGNED.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
20	W1	21	Total C N O 134 91 21 22	0	0	0
20	w1	25	Total C N O 152 101 25 26	0	0	0
20	W2	21	Total C N O 129 86 21 22	0	0	0
20	w2	20	Total C N O 127 86 20 21	0	0	0

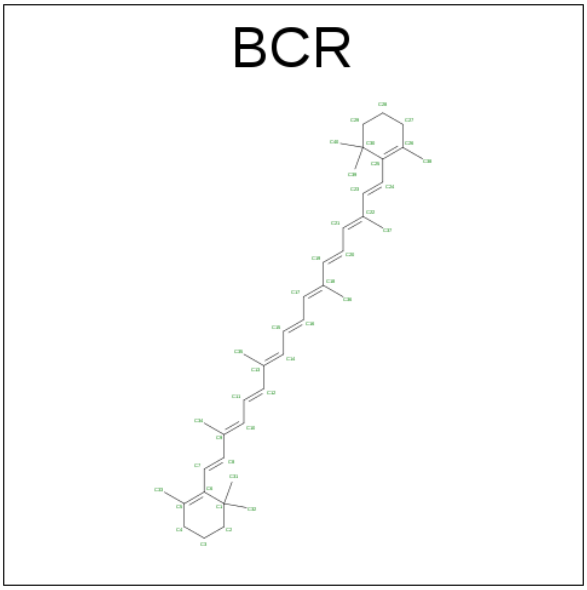
- Molecule 21 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	q1	105	Total	C	N	O	S	0	0	0
			645	399	115	127	4			
21	Q2	111	Total	C	N	O	S	0	0	0
			676	417	123	133	3			

- Molecule 22 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Z2	59	Total	C	N	O	S	0	0	0
			351	224	61	65	1			
22	z2	59	Total	C	N	O	S	0	0	0
			381	250	63	67	1			

- Molecule 23 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A1	1	Total	C	0	0
			40	40		
23	B1	1	Total	C	0	0
			40	40		
23	B1	1	Total	C	0	0
			40	40		
23	B1	1	Total	C	0	0
			40	40		
23	C1	1	Total	C	0	0
			40	40		
23	C1	1	Total	C	0	0
			40	40		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	D1	1	Total C 40 40	0	0
23	H1	1	Total C 22 22	0	0
23	J1	1	Total C 40 40	0	0
23	K1	1	Total C 31 31	0	0
23	a1	1	Total C 40 40	0	0
23	b1	1	Total C 40 40	0	0
23	b1	1	Total C 40 40	0	0
23	b1	1	Total C 40 40	0	0
23	c1	1	Total C 40 40	0	0
23	c1	1	Total C 40 40	0	0
23	d1	1	Total C 40 40	0	0
23	h1	1	Total C 40 40	0	0
23	k1	1	Total C 40 40	0	0
23	A2	1	Total C 40 40	0	0
23	B2	1	Total C 40 40	0	0
23	B2	1	Total C 40 40	0	0
23	B2	1	Total C 40 40	0	0
23	C2	1	Total C 40 40	0	0
23	F2	1	Total C 40 40	0	0
23	H2	1	Total C 24 24	0	0
23	K2	1	Total C 40 40	0	0

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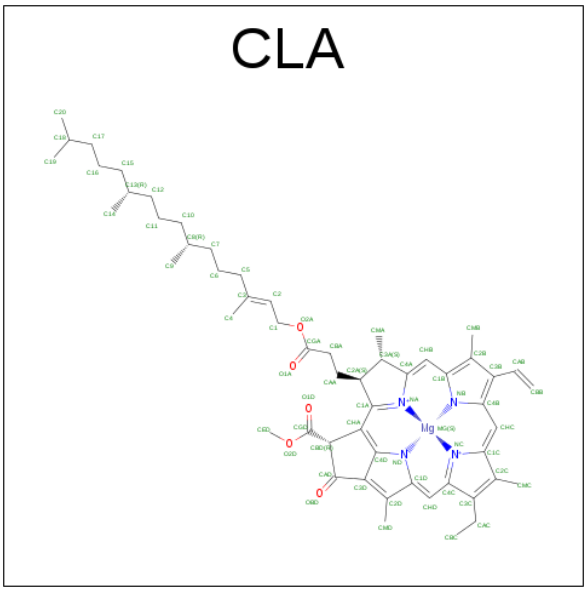
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	K2	1	Total C 29 29	0	0
23	a2	1	Total C 40 40	0	0
23	b2	1	Total C 40 40	0	0
23	b2	1	Total C 40 40	0	0
23	b2	1	Total C 40 40	0	0
23	c2	1	Total C 40 40	0	0
23	d2	1	Total C 40 40	0	0
23	h2	1	Total C 40 40	0	0
23	j2	1	Total C 40 40	0	0
23	k2	1	Total C 40 40	0	0
23	z2	1	Total C 40 40	0	0

- Molecule 24 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	a1	1	Total Cl 1 1	0	0
24	A2	1	Total Cl 1 1	0	0
24	A1	1	Total Cl 1 1	0	0
24	a2	1	Total Cl 1 1	0	0

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	A1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
25	A1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
25	A1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	B1	1	Total C Mg N O 65 55 1 4 5	0	0
25	B1	1	Total C Mg N O 65 55 1 4 5	0	0
25	B1	1	Total C Mg N O 65 55 1 4 5	0	0
25	B1	1	Total C Mg N O 65 55 1 4 5	0	0
25	B1	1	Total C Mg N O 58 48 1 4 5	0	0
25	B1	1	Total C Mg N O 65 55 1 4 5	0	0
25	C1	1	Total C Mg N O 65 55 1 4 5	0	0
25	C1	1	Total C Mg N O 60 50 1 4 5	0	0
25	C1	1	Total C Mg N O 65 55 1 4 5	0	0
25	C1	1	Total C Mg N O 65 55 1 4 5	0	0
25	C1	1	Total C Mg N O 65 55 1 4 5	0	0
25	C1	1	Total C Mg N O 65 55 1 4 5	0	0
25	C1	1	Total C Mg N O 65 55 1 4 5	0	0
25	C1	1	Total C Mg N O 65 55 1 4 5	0	0
25	C1	1	Total C Mg N O 65 55 1 4 5	0	0
25	C1	1	Total C Mg N O 65 55 1 4 5	0	0
25	C1	1	Total C Mg N O 65 55 1 4 5	0	0
25	C1	1	Total C Mg N O 61 51 1 4 5	0	0
25	C1	1	Total C Mg N O 45 35 1 4 5	0	0
25	D1	1	Total C Mg N O 65 55 1 4 5	0	0
25	D1	1	Total C Mg N O 51 41 1 4 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	a1	1	Total C Mg N O 65 55 1 4 5	0	0
25	a1	1	Total C Mg N O 60 50 1 4 5	0	0
25	a1	1	Total C Mg N O 50 40 1 4 5	0	0
25	b1	1	Total C Mg N O 65 55 1 4 5	0	0
25	b1	1	Total C Mg N O 65 55 1 4 5	0	0
25	b1	1	Total C Mg N O 65 55 1 4 5	0	0
25	b1	1	Total C Mg N O 65 55 1 4 5	0	0
25	b1	1	Total C Mg N O 65 55 1 4 5	0	0
25	b1	1	Total C Mg N O 65 55 1 4 5	0	0
25	b1	1	Total C Mg N O 65 55 1 4 5	0	0
25	b1	1	Total C Mg N O 65 55 1 4 5	0	0
25	b1	1	Total C Mg N O 65 55 1 4 5	0	0
25	b1	1	Total C Mg N O 65 55 1 4 5	0	0
25	b1	1	Total C Mg N O 65 55 1 4 5	0	0
25	b1	1	Total C Mg N O 59 49 1 4 5	0	0
25	b1	1	Total C Mg N O 65 55 1 4 5	0	0
25	b1	1	Total C Mg N O 65 55 1 4 5	0	0
25	b1	1	Total C Mg N O 65 55 1 4 5	0	0
25	b1	1	Total C Mg N O 65 55 1 4 5	0	0
25	c1	1	Total C Mg N O 65 55 1 4 5	0	0
25	c1	1	Total C Mg N O 65 55 1 4 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
25	c1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	c1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
25	c1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	A2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	A2	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
25	A2	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
25	B2	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
25	B2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	B2	1	Total C Mg N O 65 55 1 4 5	0	0
25	B2	1	Total C Mg N O 65 55 1 4 5	0	0
25	B2	1	Total C Mg N O 65 55 1 4 5	0	0
25	B2	1	Total C Mg N O 65 55 1 4 5	0	0
25	B2	1	Total C Mg N O 65 55 1 4 5	0	0
25	B2	1	Total C Mg N O 65 55 1 4 5	0	0
25	B2	1	Total C Mg N O 65 55 1 4 5	0	0
25	B2	1	Total C Mg N O 65 55 1 4 5	0	0
25	B2	1	Total C Mg N O 54 44 1 4 5	0	0
25	B2	1	Total C Mg N O 65 55 1 4 5	0	0
25	B2	1	Total C Mg N O 60 50 1 4 5	0	0
25	B2	1	Total C Mg N O 65 55 1 4 5	0	0
25	C2	1	Total C Mg N O 65 55 1 4 5	0	0
25	C2	1	Total C Mg N O 46 36 1 4 5	0	0
25	C2	1	Total C Mg N O 65 55 1 4 5	0	0
25	C2	1	Total C Mg N O 65 55 1 4 5	0	0
25	C2	1	Total C Mg N O 45 35 1 4 5	0	0
25	C2	1	Total C Mg N O 50 40 1 4 5	0	0
25	C2	1	Total C Mg N O 65 55 1 4 5	0	0
25	C2	1	Total C Mg N O 45 35 1 4 5	0	0
25	C2	1	Total C Mg N O 50 40 1 4 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C2	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
25	C2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
25	C2	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
25	D2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	D2	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
25	D2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	K2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
25	a2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
25	b2	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
25	b2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b2	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
25	b2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	b2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		

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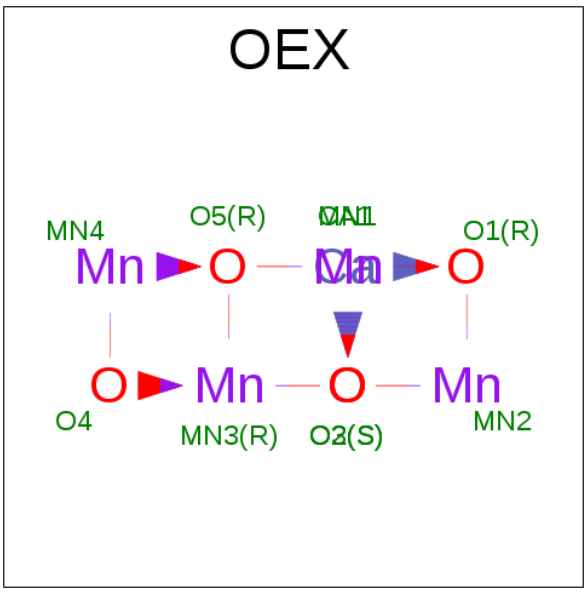
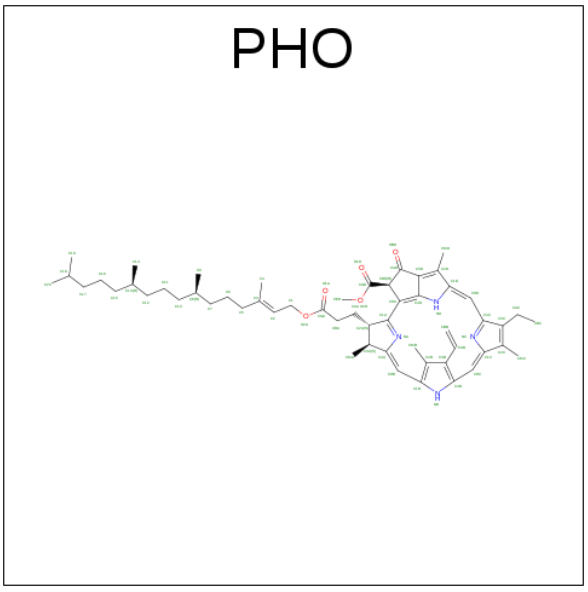
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	b2	1	Total C Mg N O 65 55 1 4 5	0	0
25	b2	1	Total C Mg N O 65 55 1 4 5	0	0
25	b2	1	Total C Mg N O 59 49 1 4 5	0	0
25	b2	1	Total C Mg N O 65 55 1 4 5	0	0
25	b2	1	Total C Mg N O 65 55 1 4 5	0	0
25	c2	1	Total C Mg N O 65 55 1 4 5	0	0
25	c2	1	Total C Mg N O 65 55 1 4 5	0	0
25	c2	1	Total C Mg N O 65 55 1 4 5	0	0
25	c2	1	Total C Mg N O 65 55 1 4 5	0	0
25	c2	1	Total C Mg N O 61 51 1 4 5	0	0
25	c2	1	Total C Mg N O 54 44 1 4 5	0	0
25	c2	1	Total C Mg N O 65 55 1 4 5	0	0
25	c2	1	Total C Mg N O 65 55 1 4 5	0	0
25	c2	1	Total C Mg N O 54 44 1 4 5	0	0
25	c2	1	Total C Mg N O 65 55 1 4 5	0	0
25	c2	1	Total C Mg N O 65 55 1 4 5	0	0
25	c2	1	Total C Mg N O 54 44 1 4 5	0	0
25	c2	1	Total C Mg N O 46 36 1 4 5	0	0
25	d2	1	Total C Mg N O 65 55 1 4 5	0	0
25	d2	1	Total C Mg N O 50 40 1 4 5	0	0
25	d2	1	Total C Mg N O 65 55 1 4 5	0	0

- Molecule 26 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A1	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
26	a1	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
26	A2	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
26	a2	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 27 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A1	1	Total C N O 64 55 4 5	0	0
27	D1	1	Total C N O 63 54 4 5	0	0
27	a1	1	Total C N O 64 55 4 5	0	0
27	d1	1	Total C N O 64 55 4 5	0	0
27	A2	1	Total C N O 64 55 4 5	0	0
27	D2	1	Total C N O 64 55 4 5	0	0
27	a2	1	Total C N O 64 55 4 5	0	0
27	d2	1	Total C N O 64 55 4 5	0	0

- Molecule 28 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	I2	2	Total C 31 31	0	0
28	d1	1	Total C 12 12	0	0
28	F2	1	Total C 16 16	0	0
28	m2	2	Total C 36 36	0	0
28	W2	1	Total C 9 9	0	0
28	c2	1	Total C 15 15	0	0
28	J2	1	Total C 10 10	0	0
28	A2	2	Total C 28 28	0	0
28	j1	1	Total C 17 17	0	0
28	i2	1	Total C 14 14	0	0
28	d2	2	Total C 25 25	0	0
28	B2	4	Total C 58 58	0	0

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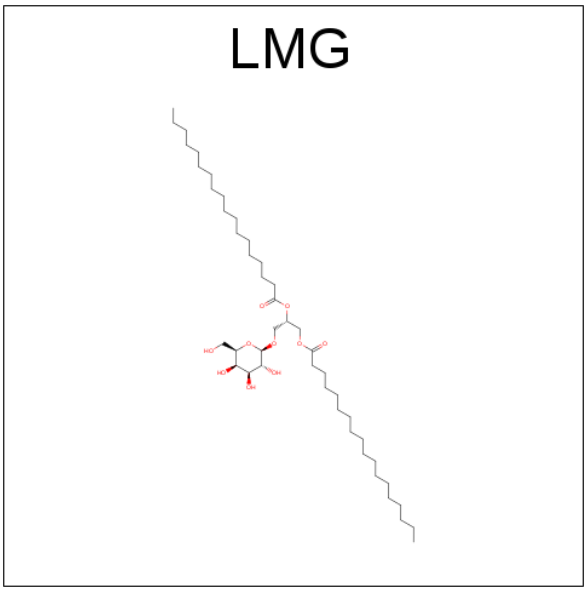
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	b1	7	Total C 92 92	0	0
28	t1	2	Total C 27 27	0	0
28	m1	1	Total C 6 6	0	0
28	a2	4	Total C 55 55	0	0
28	K2	1	Total C 5 5	0	0
28	A1	1	Total C 14 14	0	0
28	l1	1	Total C 12 12	0	0
28	b2	1	Total C 12 12	0	0
28	x1	1	Total C 15 15	0	0
28	X2	1	Total C 7 7	0	0
28	k2	4	Total C 30 30	0	0
28	a1	1	Total C 11 11	0	0
28	D1	1	Total C 6 6	0	0
28	H2	1	Total C 5 5	0	0
28	M2	1	Total C 11 11	0	0
28	C2	2	Total C 24 24	0	0
28	B1	3	Total C 41 41	0	0

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A1	1	Total 43	C 33	O 10	0	0
29	A1	1	Total 41	C 31	O 10	0	0
29	B1	1	Total 31	C 21	O 10	0	0
29	B1	1	Total 48	C 38	O 10	0	0
29	C1	1	Total 48	C 38	O 10	0	0
29	D1	1	Total 35	C 25	O 10	0	0
29	M1	1	Total 31	C 27	O 4	0	0
29	a1	1	Total 51	C 41	O 10	0	0
29	b1	1	Total 38	C 28	O 10	0	0
29	b1	1	Total 39	C 29	O 10	0	0
29	b1	1	Total 40	C 30	O 10	0	0
29	c1	1	Total 55	C 45	O 10	0	0
29	d1	1	Total 33	C 23	O 10	0	0
29	d1	1	Total 35	C 30	O 5	0	0

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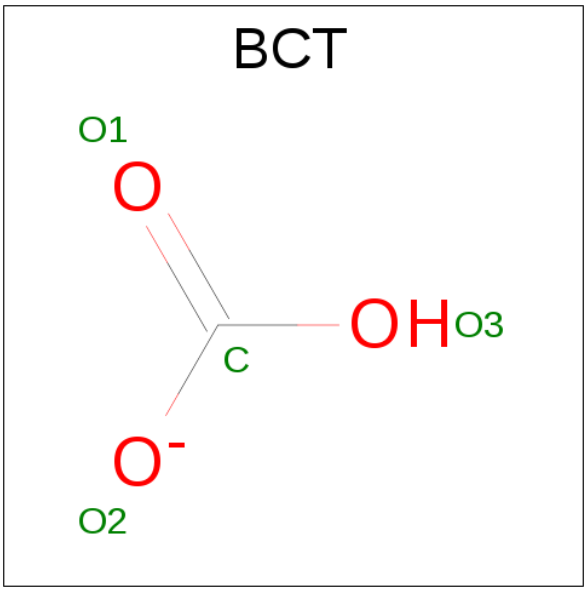
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A2	1	Total C O 29 19 10	0	0
29	B2	1	Total C O 40 30 10	0	0
29	B2	1	Total C O 37 27 10	0	0
29	C2	1	Total C O 24 14 10	0	0
29	F2	1	Total C O 35 25 10	0	0
29	I2	1	Total C O 34 24 10	0	0
29	a2	1	Total C O 44 34 10	0	0
29	b2	1	Total C O 39 29 10	0	0
29	c2	1	Total C O 26 16 10	0	0
29	d2	1	Total C O 27 17 10	0	0
29	j2	1	Total C O 50 40 10	0	0

- Molecule 30 is FE (III) ION (three-letter code: FE) (formula: Fe).

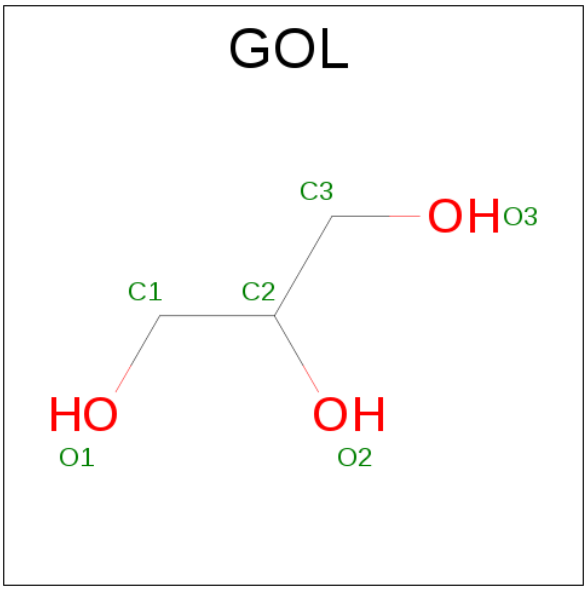
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	a1	1	Total Fe 1 1	0	0
30	A2	1	Total Fe 1 1	0	0
30	A1	1	Total Fe 1 1	0	0
30	a2	1	Total Fe 1 1	0	0

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



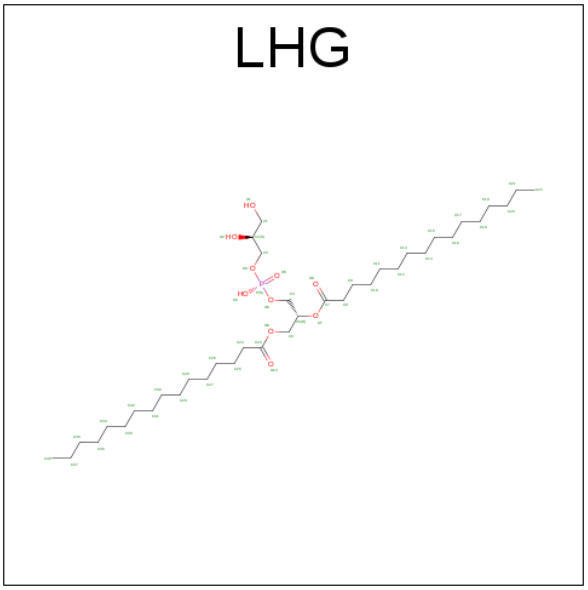
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A1	1	Total C O 4 1 3	0	0
31	a1	1	Total C O 4 1 3	0	0
31	A2	1	Total C O 4 1 3	0	0
31	a2	1	Total C O 4 1 3	0	0

- Molecule 32 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B1	1	Total	C	O	0	0
			6	3	3		
32	C1	1	Total	C	O	0	0
			6	3	3		
32	a1	1	Total	C	O	0	0
			6	3	3		
32	b1	1	Total	C	O	0	0
			6	3	3		
32	c1	1	Total	C	O	0	0
			6	3	3		
32	i1	1	Total	C	O	0	0
			6	3	3		
32	C2	1	Total	C	O	0	0
			6	3	3		
32	a2	1	Total	C	O	0	0
			6	3	3		
32	c2	1	Total	C	O	0	0
			6	3	3		

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B1	1	Total	C	O	P	0	0
			49	38	10	1		
33	D1	1	Total	C	O	P	0	0
			49	38	10	1		

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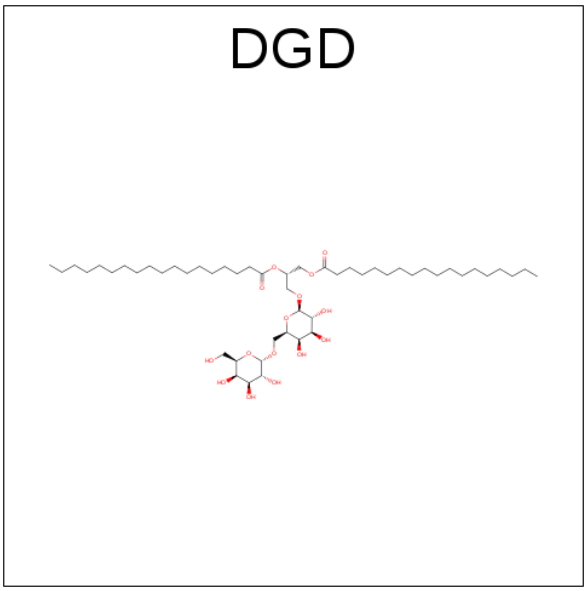
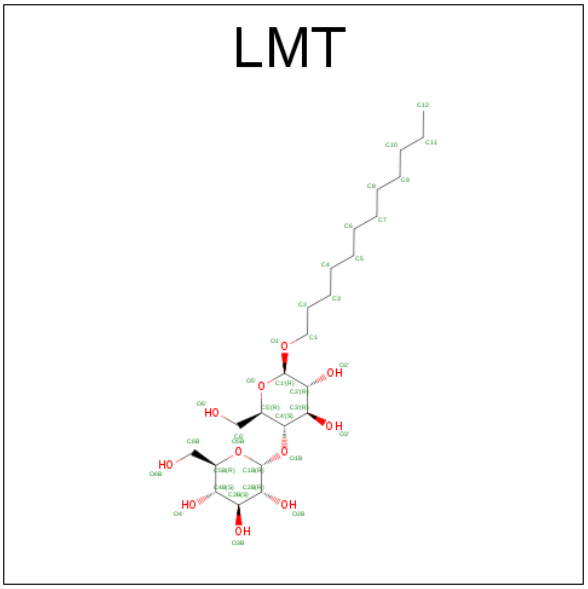
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	D1	1	Total	C	O	P	0	0
			49	38	10	1		
33	L1	1	Total	C	O	P	0	0
			41	30	10	1		
33	a1	1	Total	C	O	P	0	0
			43	32	10	1		
33	b1	1	Total	C	O	P	0	0
			49	38	10	1		
33	d1	1	Total	C	O	P	0	0
			32	21	10	1		
33	d1	1	Total	C	O	P	0	0
			49	38	10	1		
33	l1	1	Total	C	O	P	0	0
			49	38	10	1		
33	A2	1	Total	C	O	P	0	0
			33	22	10	1		
33	B2	1	Total	C	O	P	0	0
			42	31	10	1		
33	D2	1	Total	C	O	P	0	0
			49	38	10	1		
33	D2	1	Total	C	O	P	0	0
			49	38	10	1		
33	L2	1	Total	C	O	P	0	0
			49	38	10	1		
33	a2	1	Total	C	O	P	0	0
			30	19	10	1		
33	b2	1	Total	C	O	P	0	0
			43	32	10	1		
33	d2	1	Total	C	O	P	0	0
			49	38	10	1		
33	d2	1	Total	C	O	P	0	0
			49	38	10	1		
33	l2	1	Total	C	O	P	0	0
			44	33	10	1		

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	C1	1	Total C O 52 37 15	0	0
34	C1	1	Total C O 62 47 15	0	0
34	C1	1	Total C O 64 49 15	0	0
34	H1	1	Total C O 62 47 15	0	0
34	c1	1	Total C O 51 36 15	0	0
34	c1	1	Total C O 62 47 15	0	0
34	c1	1	Total C O 62 47 15	0	0
34	h1	1	Total C O 62 47 15	0	0
34	C2	1	Total C O 33 18 15	0	0
34	H2	1	Total C O 62 47 15	0	0
34	c2	1	Total C O 62 47 15	0	0
34	c2	1	Total C O 52 37 15	0	0
34	c2	1	Total C O 62 47 15	0	0
34	h2	1	Total C O 62 47 15	0	0

- Molecule 35 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C1	1	Total C O 35 24 11	0	0
35	L1	1	Total C 12 12	0	0
35	M1	1	Total C 11 11	0	0
35	M1	1	Total C O 24 18 6	0	0
35	T1	1	Total C 12 12	0	0
35	c1	1	Total C O 33 22 11	0	0
35	l1	1	Total C O 24 18 6	0	0
35	m1	1	Total C O 35 24 11	0	0
35	a2	1	Total C O 35 24 11	0	0
35	b2	1	Total C O 35 24 11	0	0
35	b2	1	Total C O 35 24 11	0	0
35	i2	1	Total C 7 7	0	0

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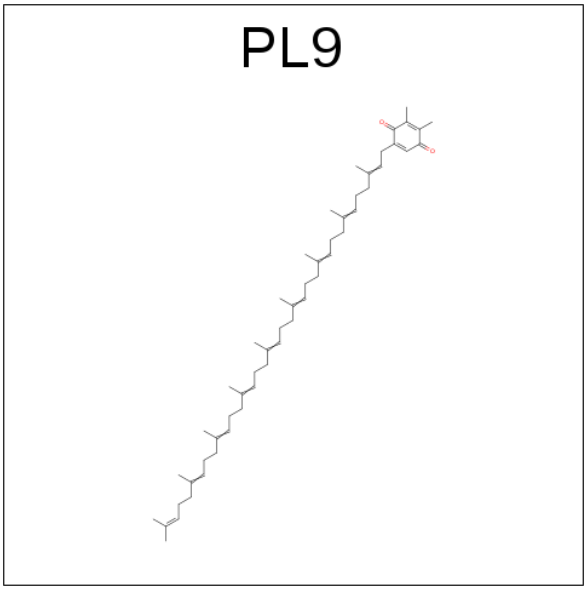
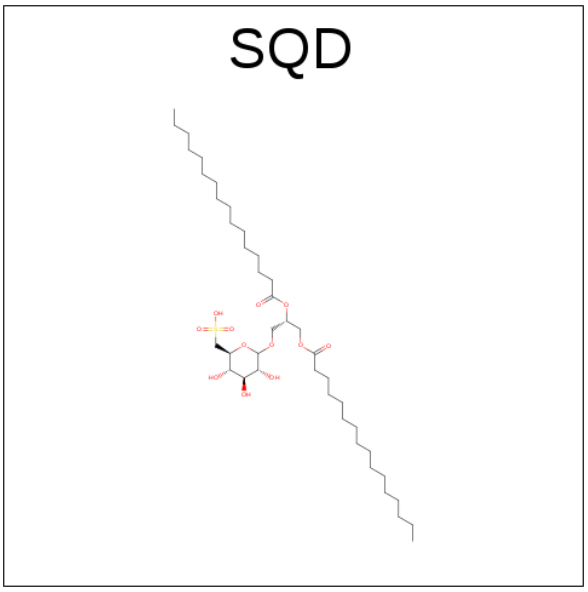
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	m2	1	Total C O 30 19 11	0	0
35	m2	1	Total C O 29 18 11	0	0

- Molecule 36 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



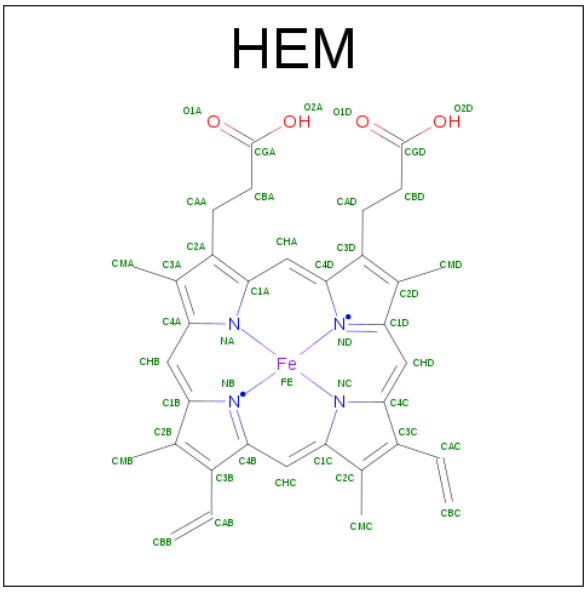
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	D1	1	Total C O 55 53 2	0	0
36	d1	1	Total C O 55 53 2	0	0
36	D2	1	Total C O 55 53 2	0	0
36	d2	1	Total C O 55 53 2	0	0

- Molecule 37 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	D1	1	Total	C	O	S	0	0
			35	22	12	1		
37	B2	1	Total	C	O	S	0	0
			45	32	12	1		
37	D2	1	Total	C	O	S	0	0
			25	12	12	1		
37	b2	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	E1	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	V1	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	f1	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	v1	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	E2	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	V2	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	e2	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	v2	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 39 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	O1	1	Total	Ca	0	0
			1	1		
39	o2	1	Total	Ca	0	0
			1	1		

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	A1	2	Total	O	0	0
			2	2		
40	B1	1	Total	O	0	0
			1	1		
40	a1	4	Total	O	0	0
			4	4		
40	c1	2	Total	O	0	0
			2	2		
40	A2	2	Total	O	0	0
			2	2		
40	a2	4	Total	O	0	0
			4	4		
40	b2	1	Total	O	0	0
			1	1		
40	c2	1	Total	O	0	0
			1	1		

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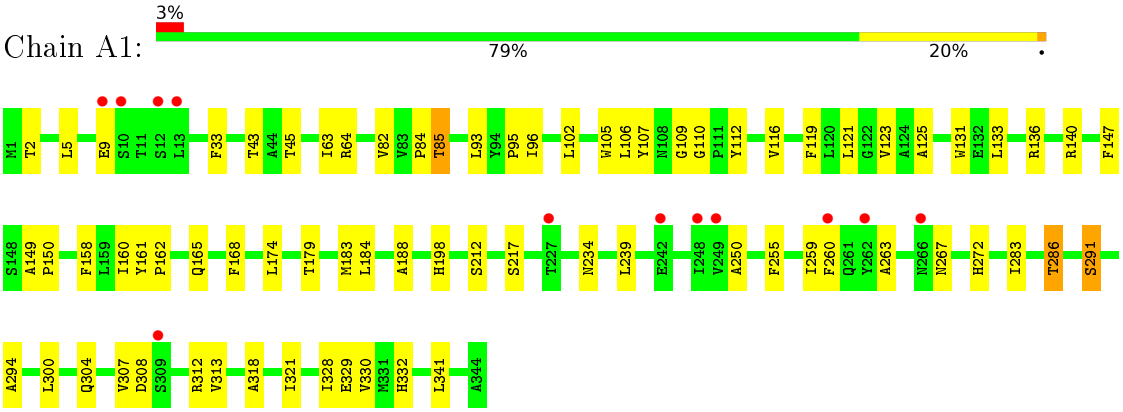
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	d2	1	Total O 1 1	0	0

3 Residue-property plots

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

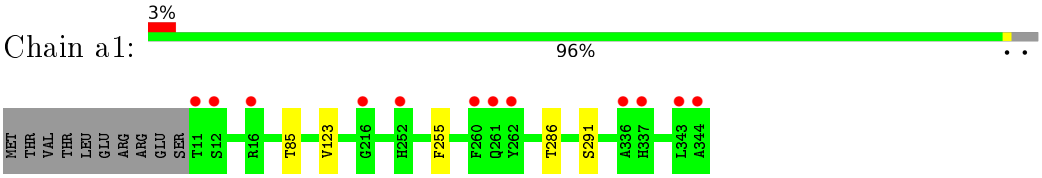
- Molecule 1: Photosystem II protein D1

Chain A1:



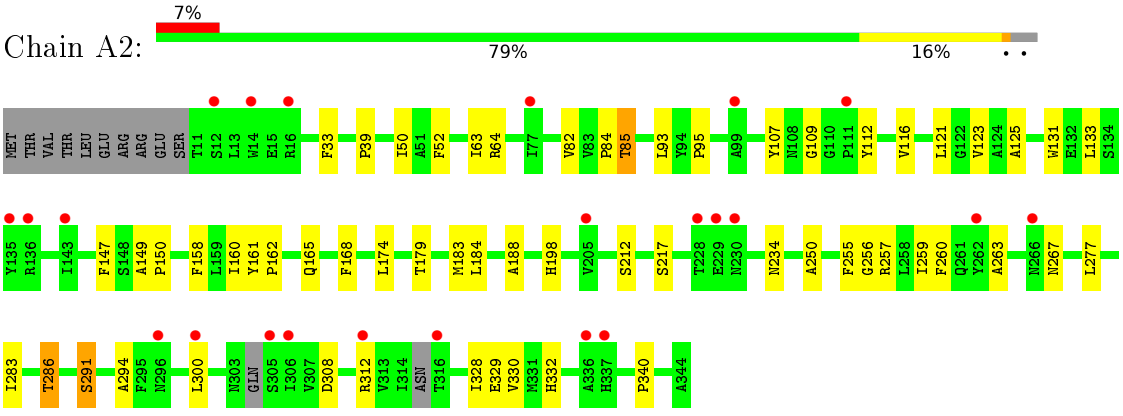
- Molecule 1: Photosystem II protein D1

Chain a1:



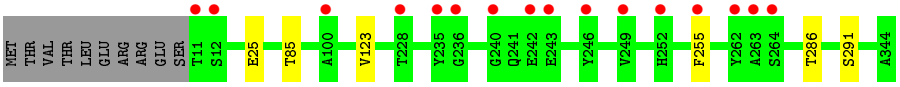
- Molecule 1: Photosystem II protein D1

Chain A2:



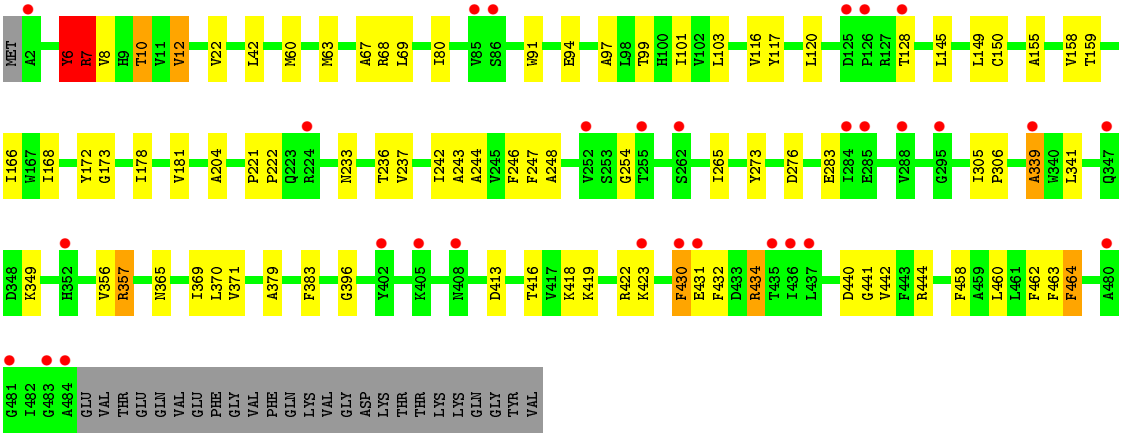
- Molecule 1: Photosystem II protein D1

Chain a2:



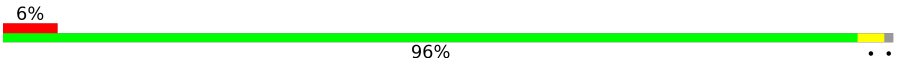
• Molecule 2: Photosystem II CP47 reaction center protein

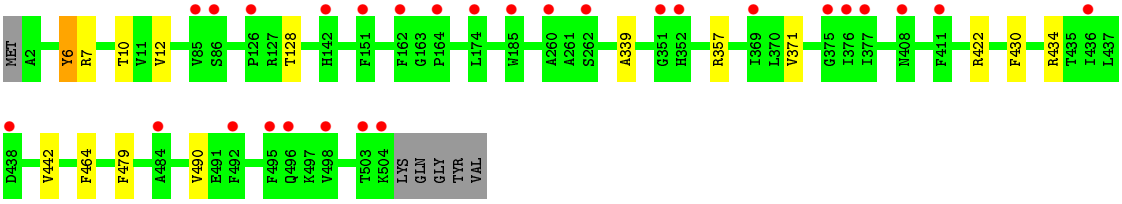
Chain B1:



• Molecule 2: Photosystem II CP47 reaction center protein

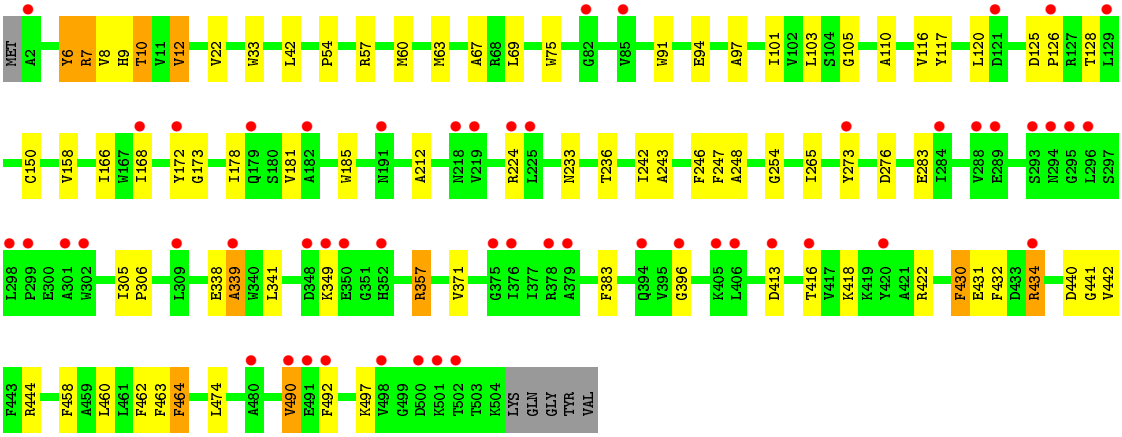
Chain b1:





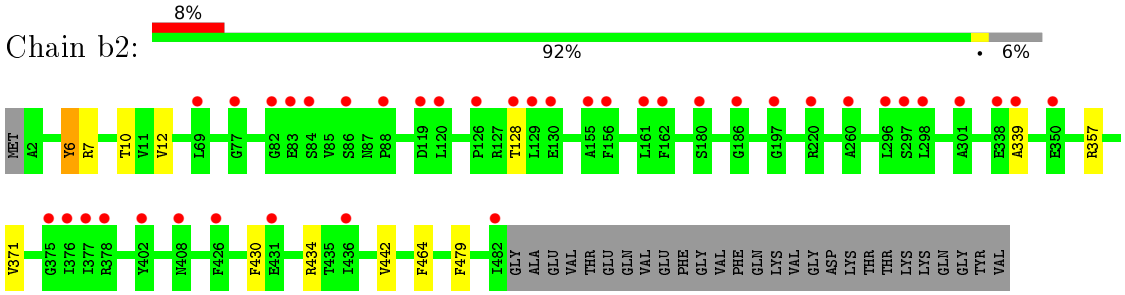
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B2:



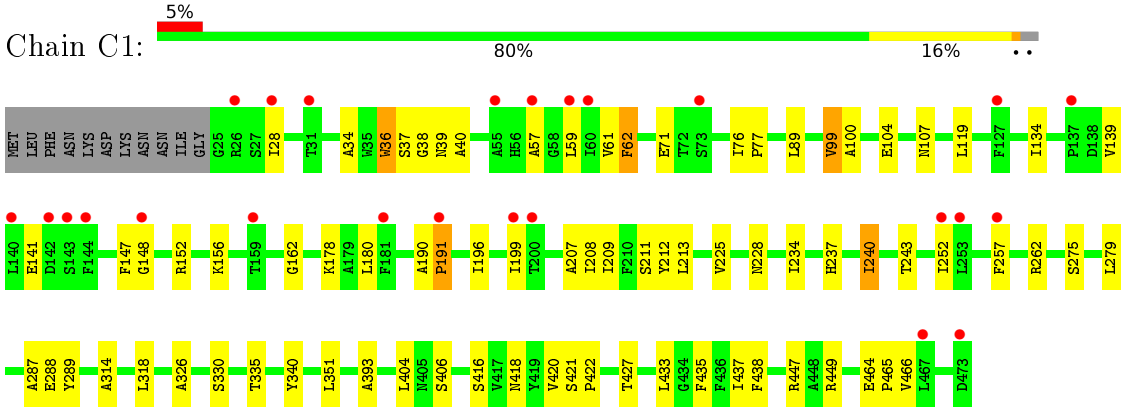
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b2:



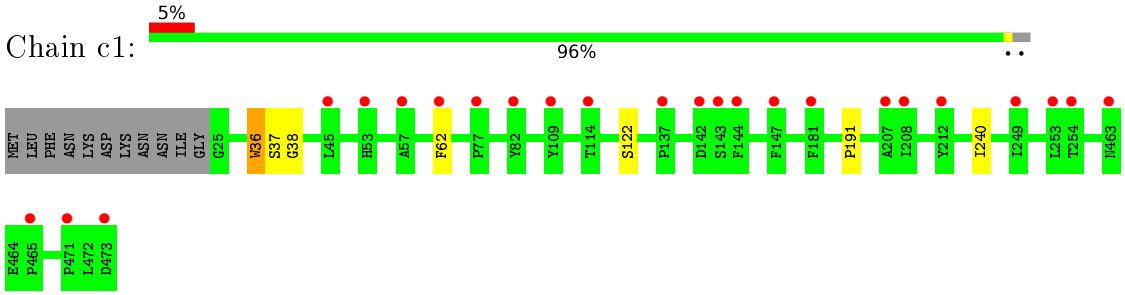
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C1:



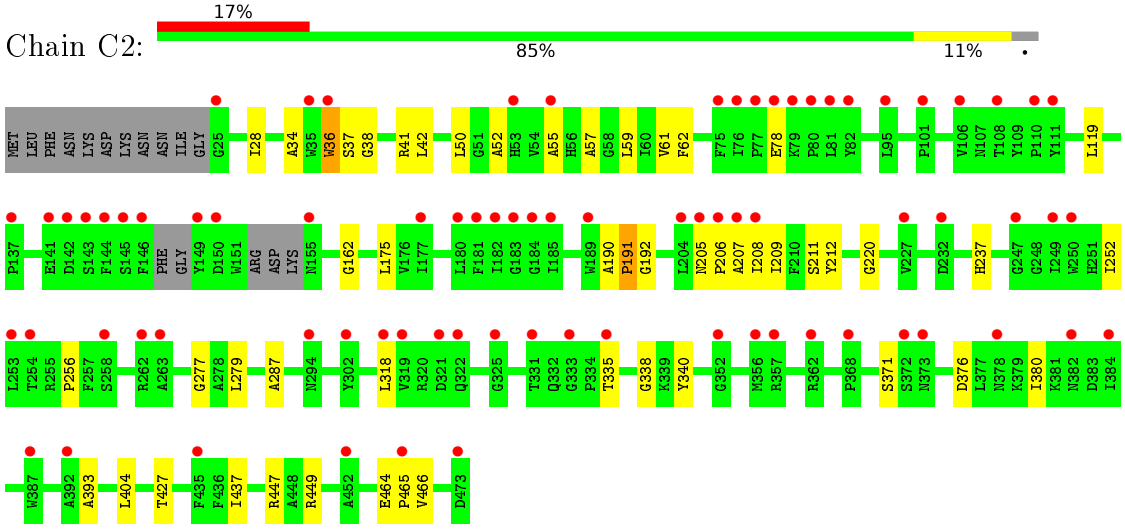
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c1:



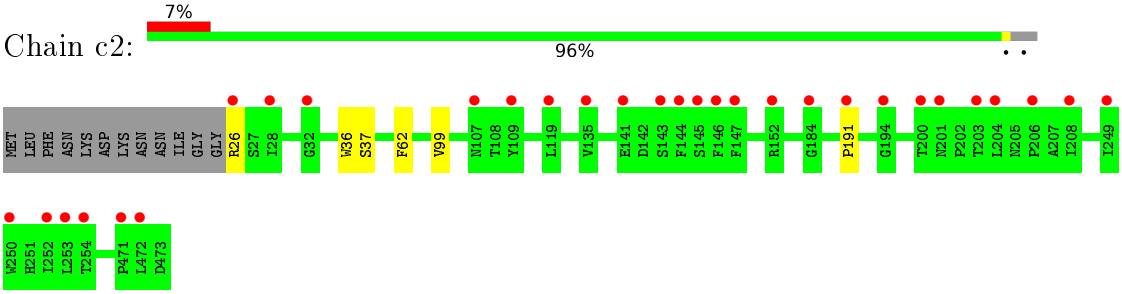
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C2:



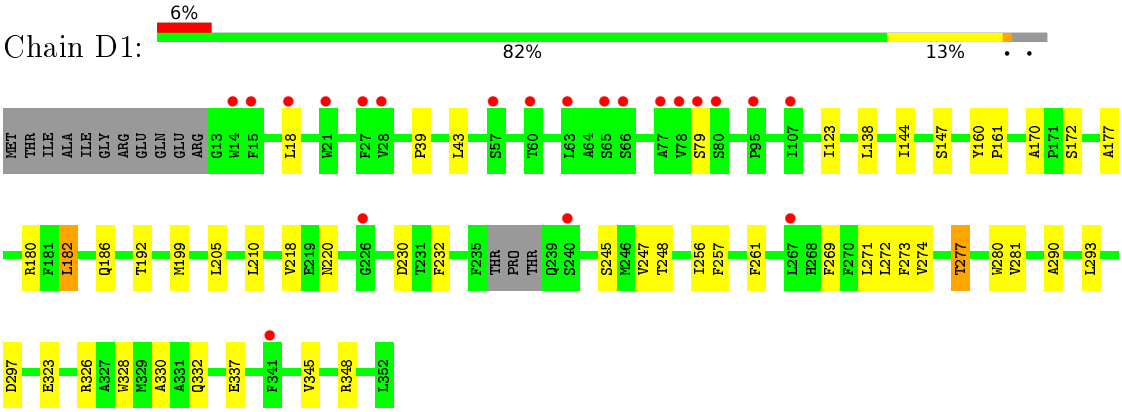
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c2:



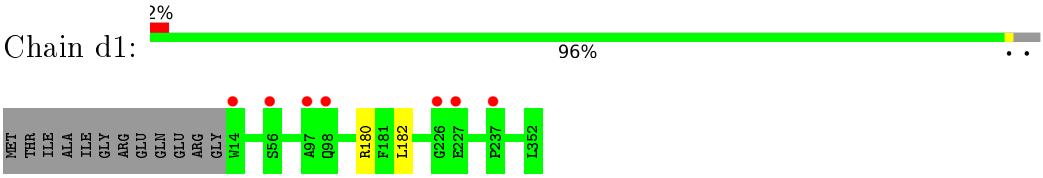
• Molecule 4: Photosystem II D2 protein

Chain D1:



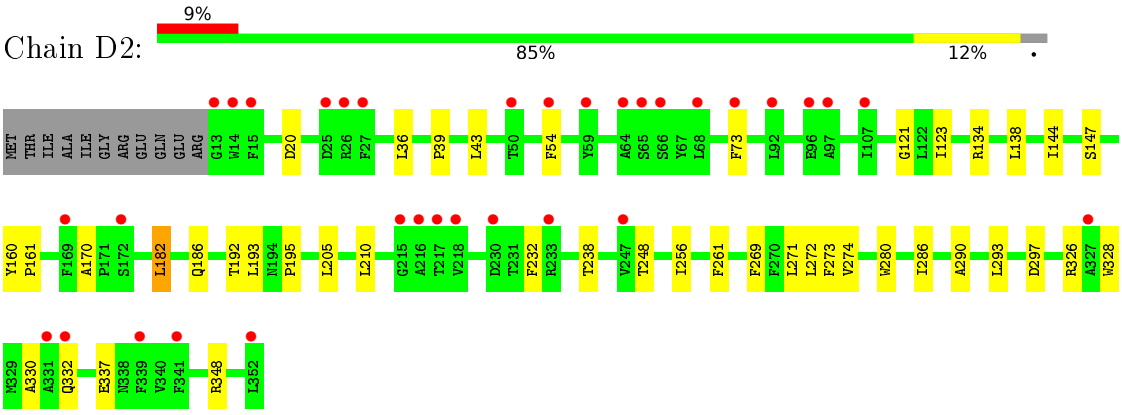
• Molecule 4: Photosystem II D2 protein

Chain d1:



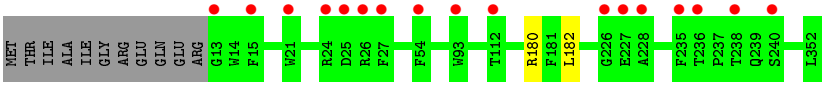
• Molecule 4: Photosystem II D2 protein

Chain D2:

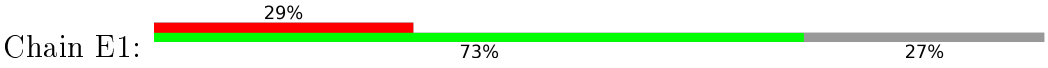


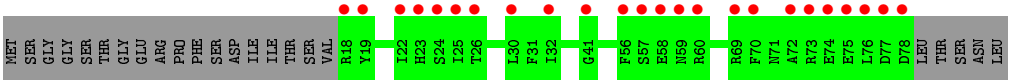
• Molecule 4: Photosystem II D2 protein

Chain d2:

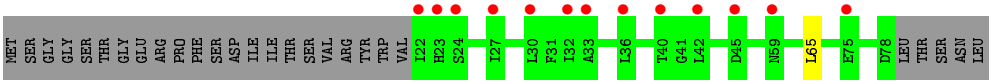


• Molecule 5: Cytochrome b559 subunit alpha

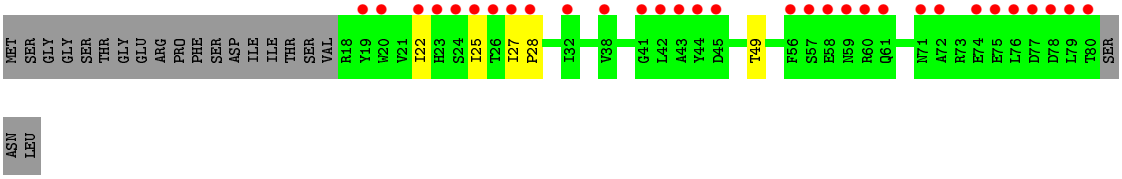




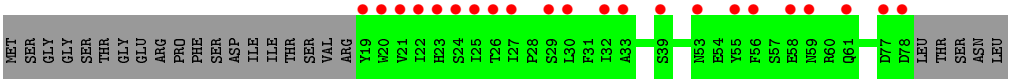
• Molecule 5: Cytochrome b559 subunit alpha



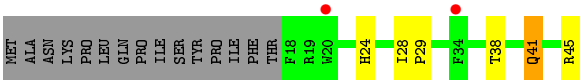
• Molecule 5: Cytochrome b559 subunit alpha



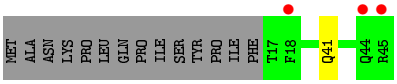
• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 6: Cytochrome b559 subunit beta

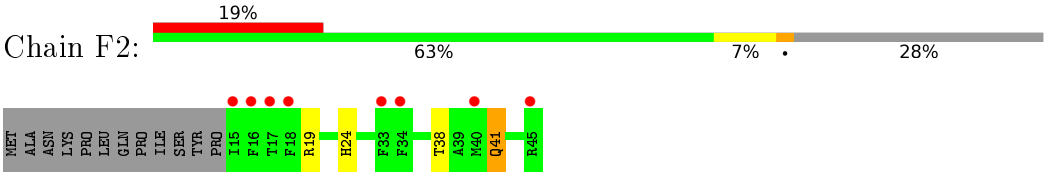


• Molecule 6: Cytochrome b559 subunit beta



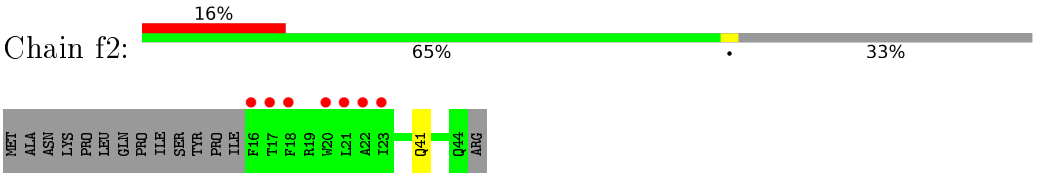
• Molecule 6: Cytochrome b559 subunit beta

Chain F2:



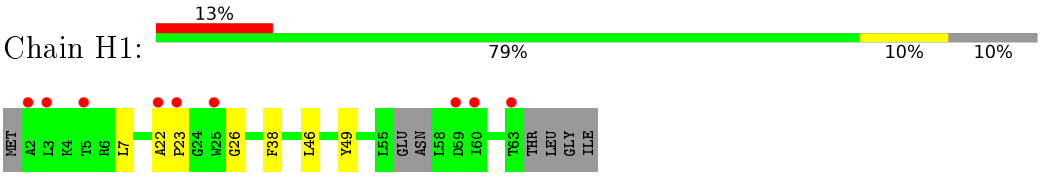
- Molecule 6: Cytochrome b559 subunit beta

Chain f2:



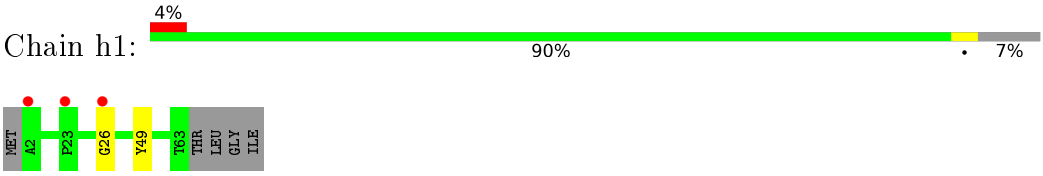
- Molecule 7: Photosystem II reaction center protein H

Chain H1:



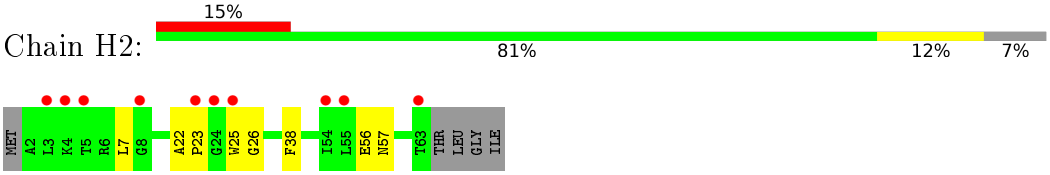
- Molecule 7: Photosystem II reaction center protein H

Chain h1:



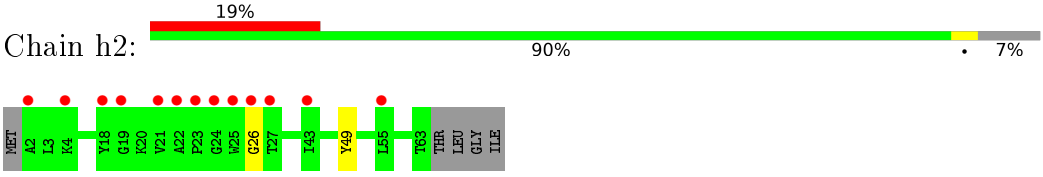
- Molecule 7: Photosystem II reaction center protein H

Chain H2:



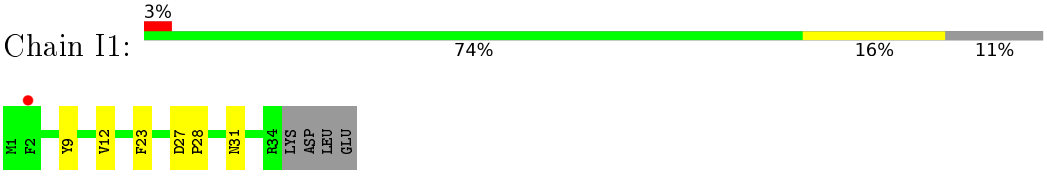
- Molecule 7: Photosystem II reaction center protein H

Chain h2:



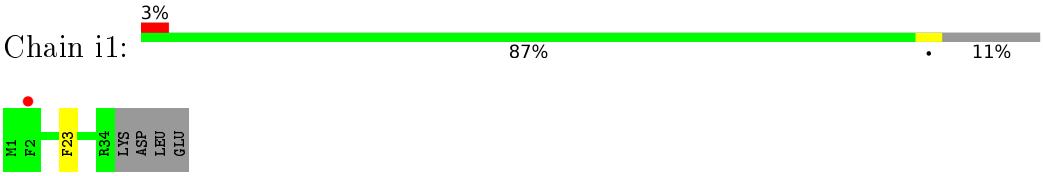
- Molecule 8: Photosystem II reaction center protein I

Chain I1:



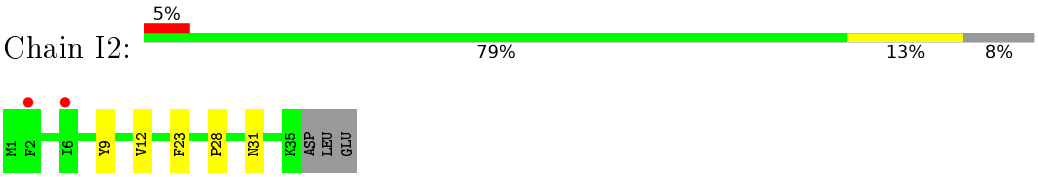
- Molecule 8: Photosystem II reaction center protein I

Chain i1:



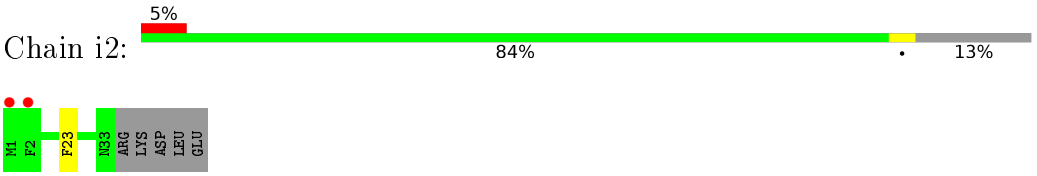
• Molecule 8: Photosystem II reaction center protein I

Chain I2:



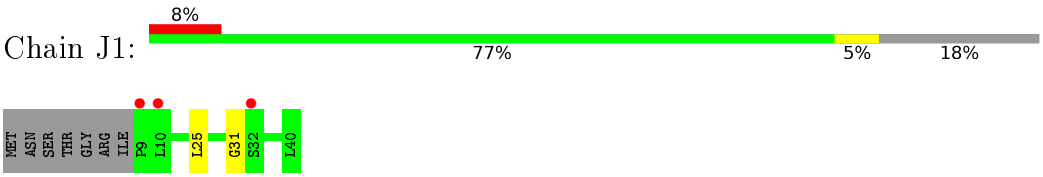
• Molecule 8: Photosystem II reaction center protein I

Chain i2:



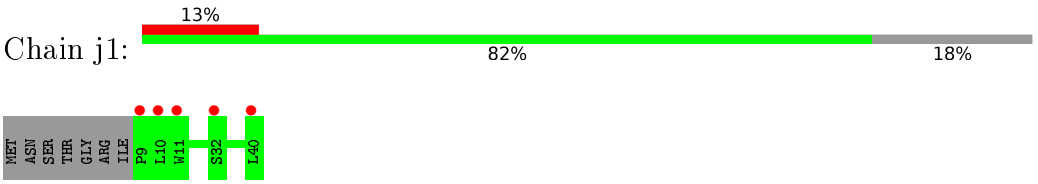
• Molecule 9: Photosystem II reaction center protein J

Chain J1:



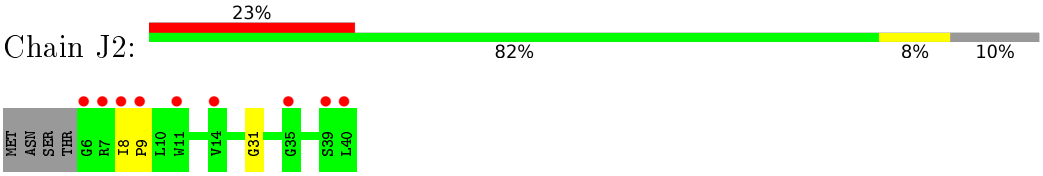
• Molecule 9: Photosystem II reaction center protein J

Chain j1:



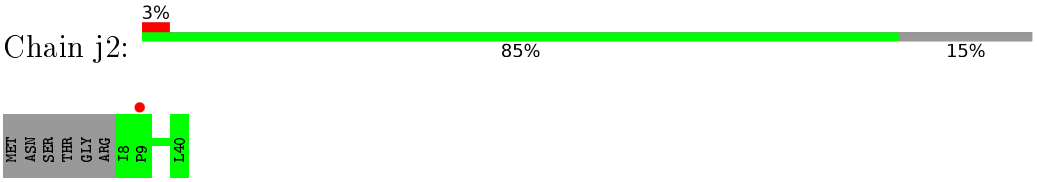
• Molecule 9: Photosystem II reaction center protein J

Chain J2:



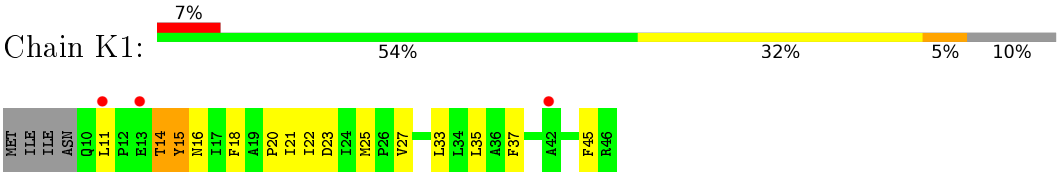
• Molecule 9: Photosystem II reaction center protein J

Chain j2:



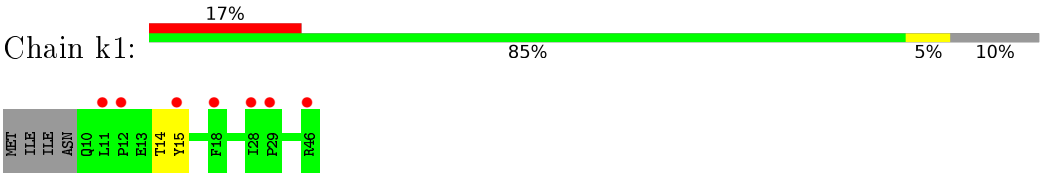
• Molecule 10: Photosystem II reaction center protein K

Chain K1:



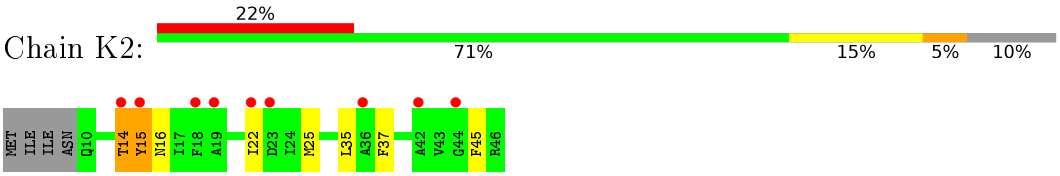
• Molecule 10: Photosystem II reaction center protein K

Chain k1:



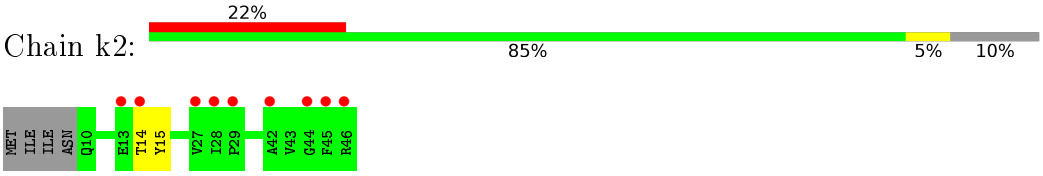
• Molecule 10: Photosystem II reaction center protein K

Chain K2:



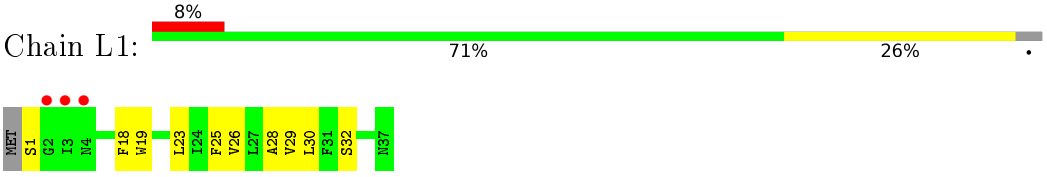
• Molecule 10: Photosystem II reaction center protein K

Chain k2:



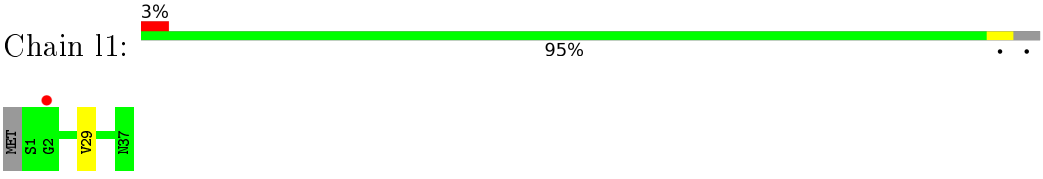
• Molecule 11: Photosystem II reaction center protein L

Chain L1:



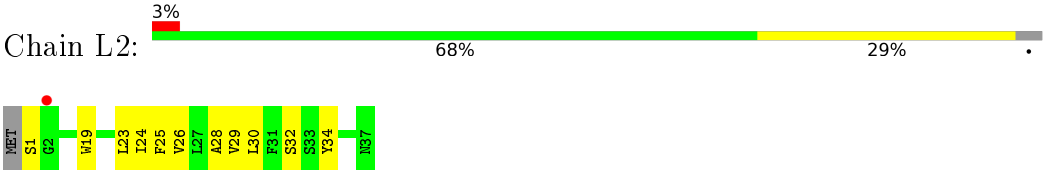
• Molecule 11: Photosystem II reaction center protein L

Chain l1:



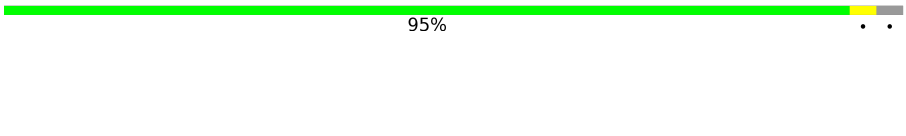
• Molecule 11: Photosystem II reaction center protein L

Chain L2:



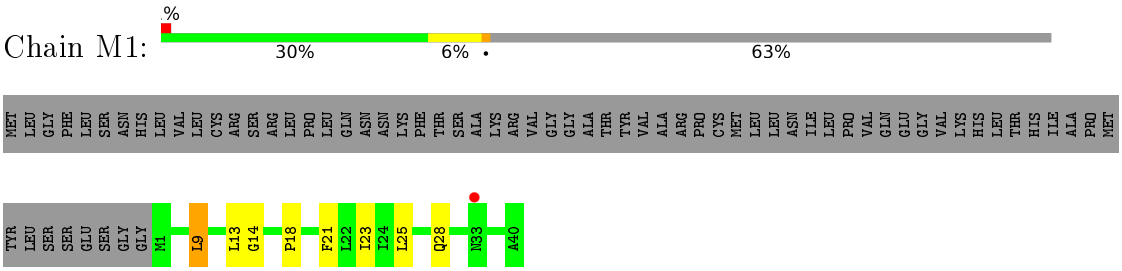
• Molecule 11: Photosystem II reaction center protein L

Chain l2:



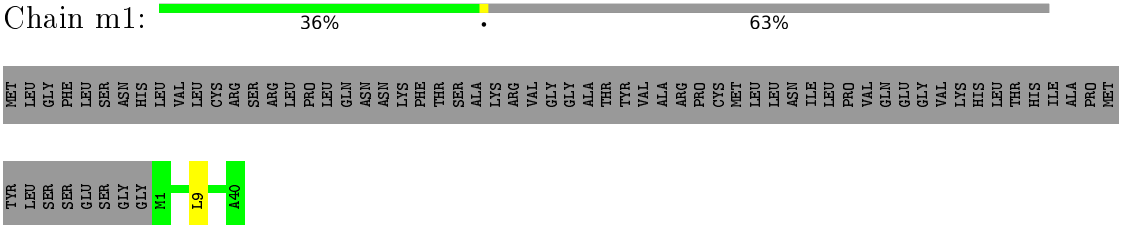
• Molecule 12: PHOTOSYSTEM II REACTION CENTER PROTEIN M

Chain M1:



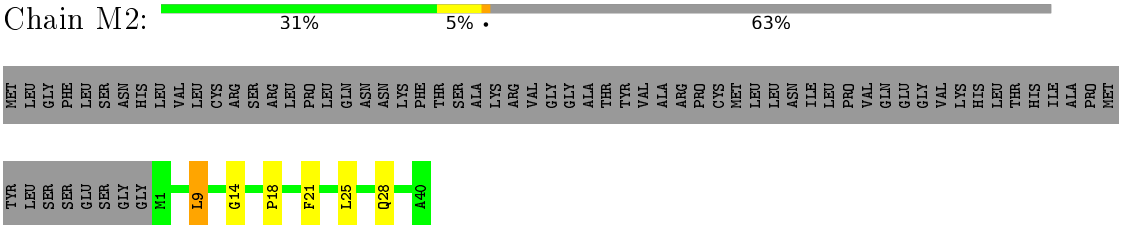
• Molecule 12: PHOTOSYSTEM II REACTION CENTER PROTEIN M

Chain m1:



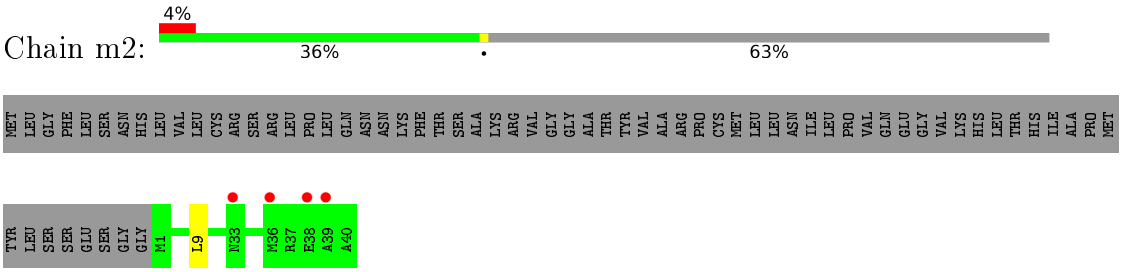
• Molecule 12: PHOTOSYSTEM II REACTION CENTER PROTEIN M

Chain M2:



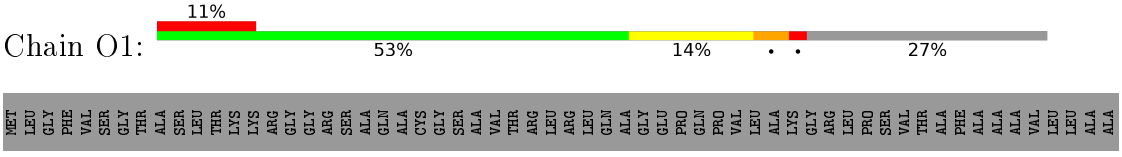
• Molecule 12: PHOTOSYSTEM II REACTION CENTER PROTEIN M

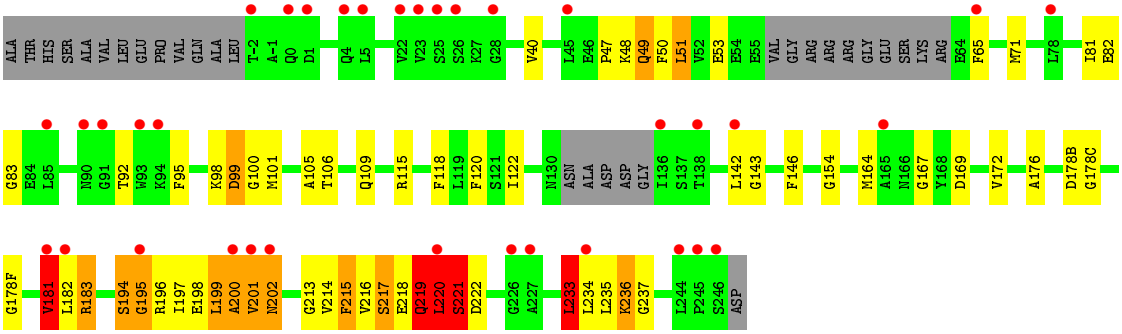
Chain m2:



• Molecule 13: PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE, PSBO

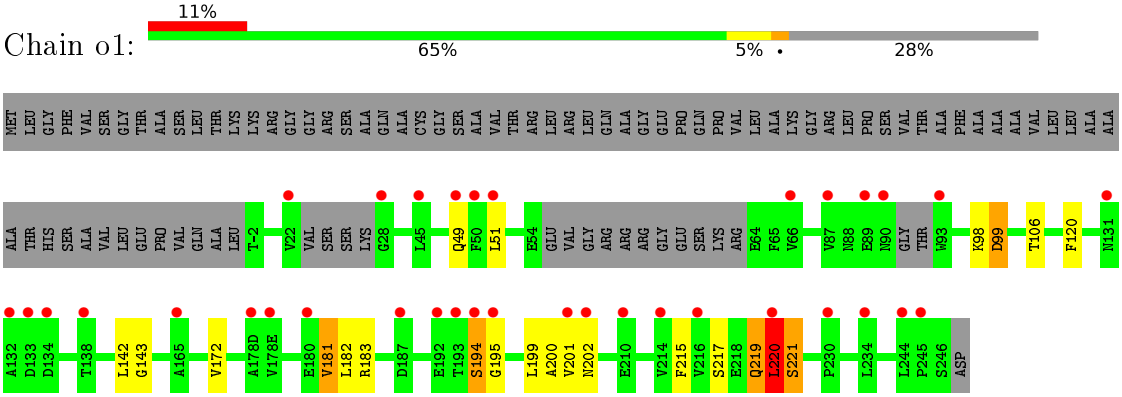
Chain O1:





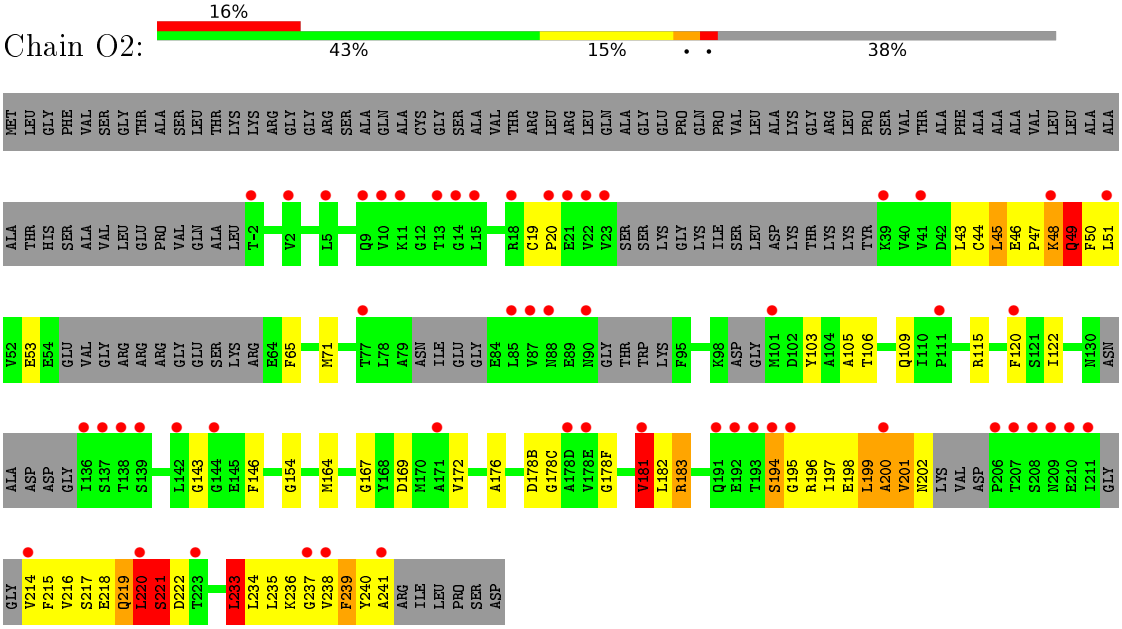
• Molecule 13: PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE, PSBO

Chain o1:



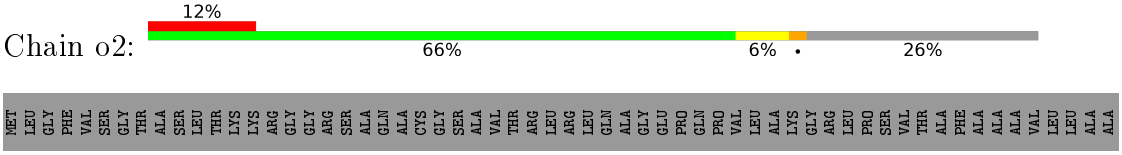
• Molecule 13: PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE, PSBO

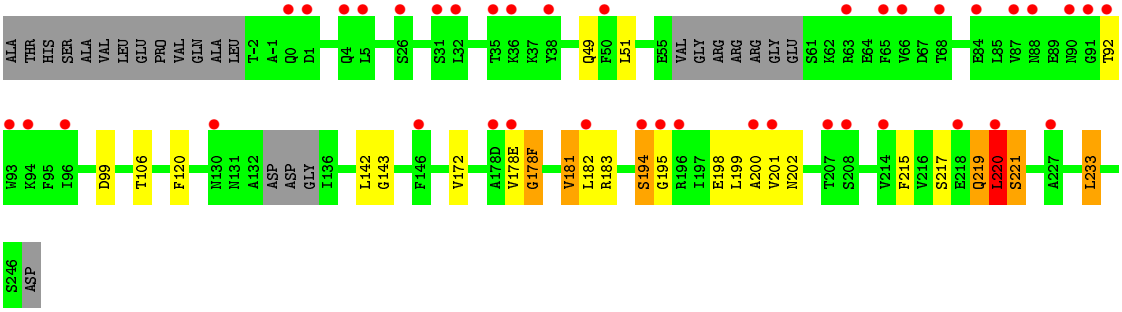
Chain O2:



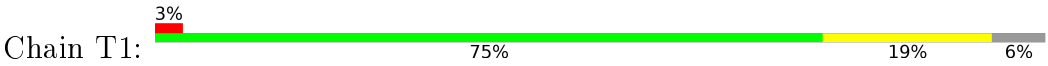
• Molecule 13: PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE, PSBO

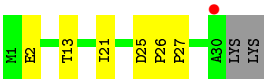
Chain o2:



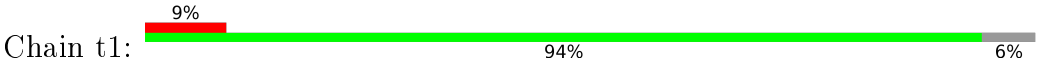


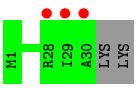
• Molecule 14: Photosystem II reaction center protein T



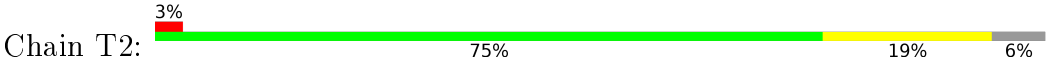


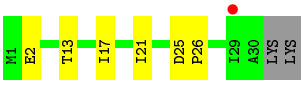
• Molecule 14: Photosystem II reaction center protein T



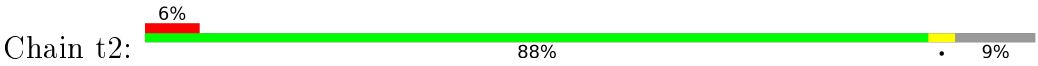


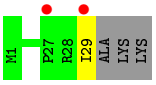
• Molecule 14: Photosystem II reaction center protein T



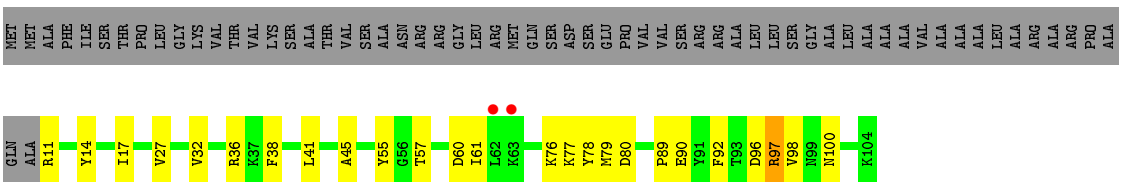


• Molecule 14: Photosystem II reaction center protein T



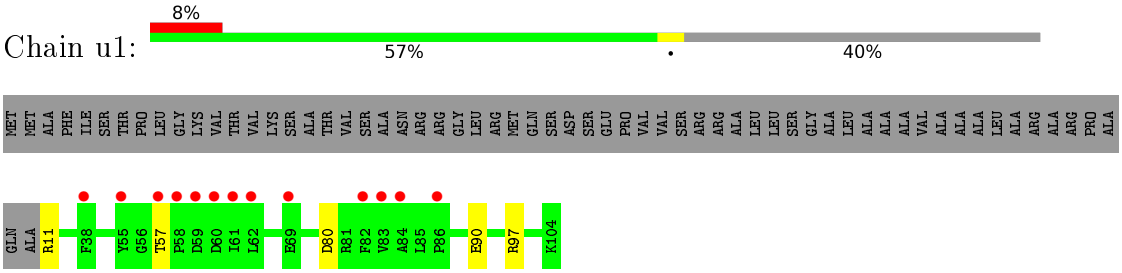


• Molecule 15: Photosystem II 12 kDa extrinsic protein, chloroplastic



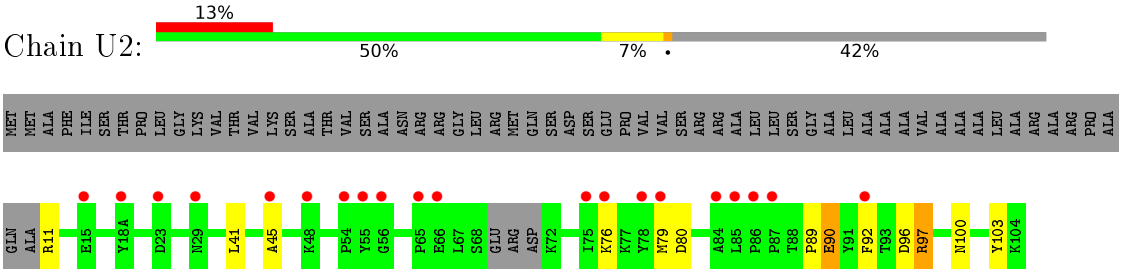
• Molecule 15: Photosystem II 12 kDa extrinsic protein, chloroplastic

Chain u1:



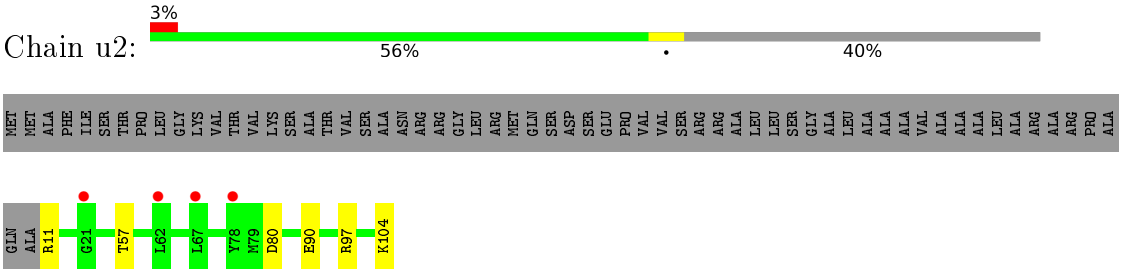
• Molecule 15: Photosystem II 12 kDa extrinsic protein, chloroplastic

Chain U2:



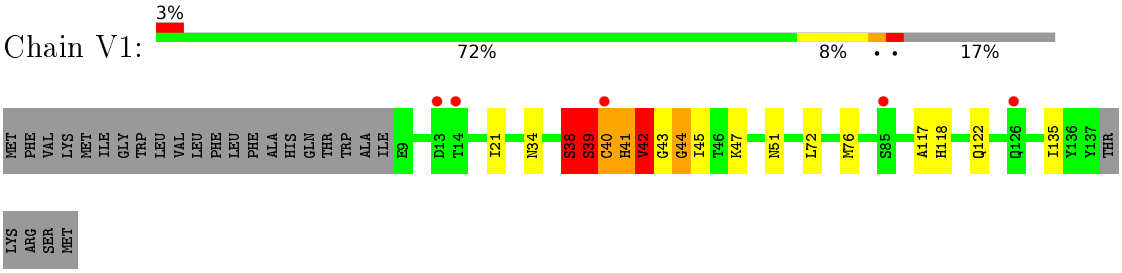
• Molecule 15: Photosystem II 12 kDa extrinsic protein, chloroplastic

Chain u2:



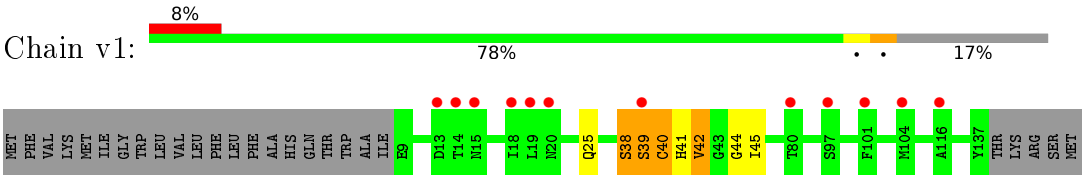
• Molecule 16: Cytochrome c-550

Chain V1:



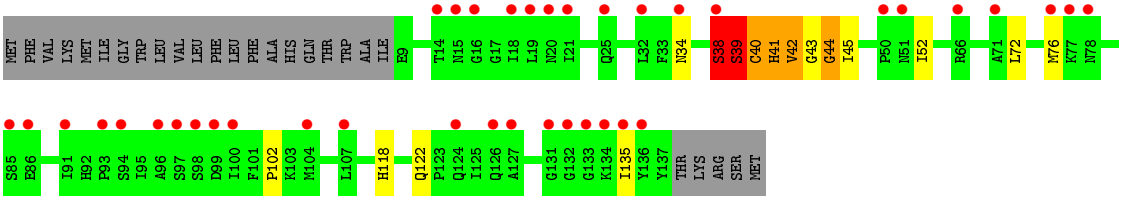
• Molecule 16: Cytochrome c-550

Chain v1:



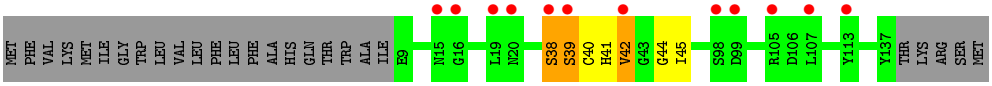
• Molecule 16: Cytochrome c-550

Chain V2:



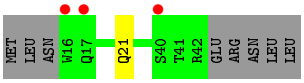
• Molecule 16: Cytochrome c-550

Chain v2:



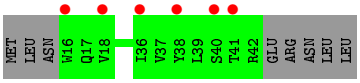
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y1:



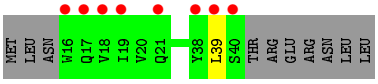
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y1:



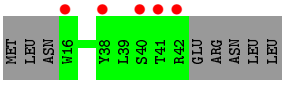
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y2:



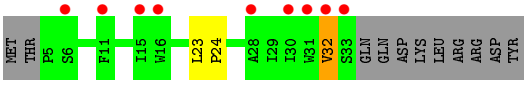
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y2:



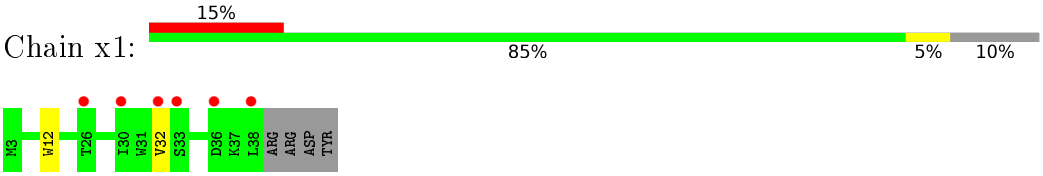
• Molecule 18: PHOTOSYSTEM II REACTION CENTER PROTEIN X

Chain X1:



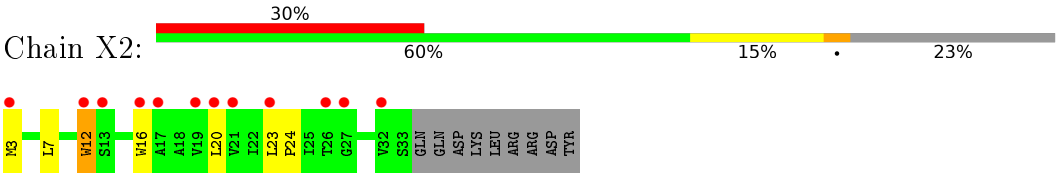
• Molecule 18: PHOTOSYSTEM II REACTION CENTER PROTEIN X

Chain x1:



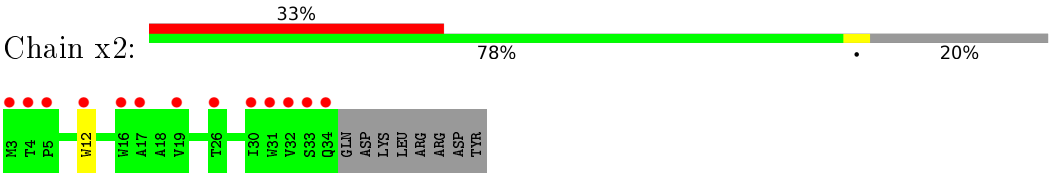
• Molecule 18: PHOTOSYSTEM II REACTION CENTER PROTEIN X

Chain X2:



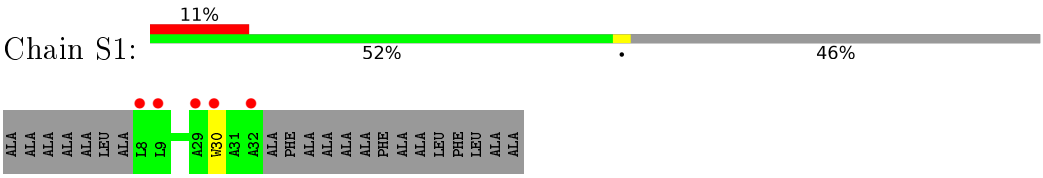
• Molecule 18: PHOTOSYSTEM II REACTION CENTER PROTEIN X

Chain x2:



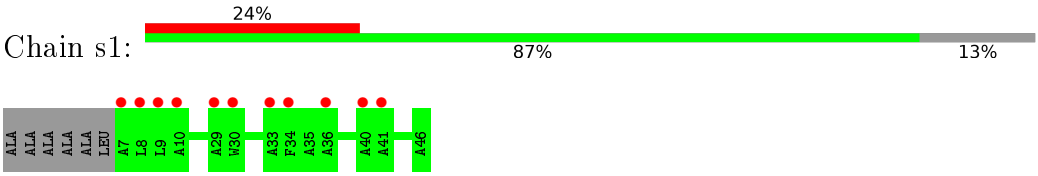
• Molecule 19: PEPTIDE CHAIN UNASSIGNED

Chain S1:



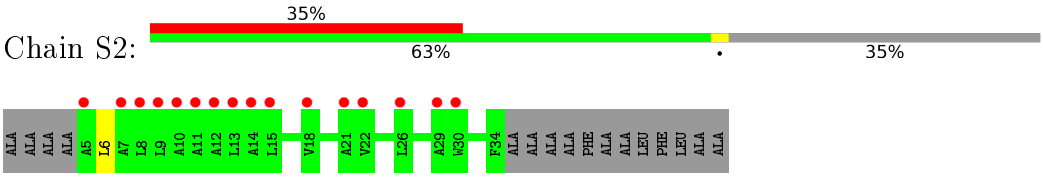
• Molecule 19: PEPTIDE CHAIN UNASSIGNED

Chain s1:



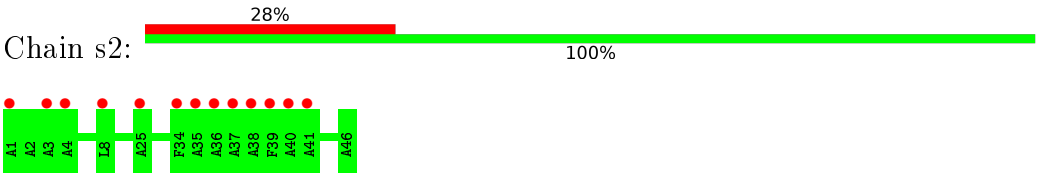
• Molecule 19: PEPTIDE CHAIN UNASSIGNED

Chain S2:



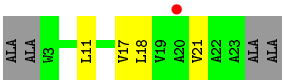
• Molecule 19: PEPTIDE CHAIN UNASSIGNED

Chain s2:



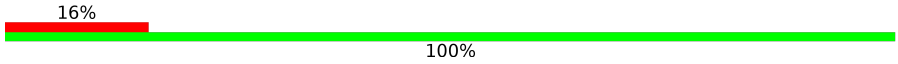
• Molecule 20: PEPTIDE CHAIN UNASSIGNED

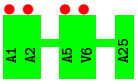
Chain W1:



• Molecule 20: PEPTIDE CHAIN UNASSIGNED

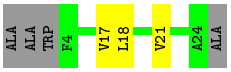
Chain w1:





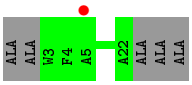
• Molecule 20: PEPTIDE CHAIN UNASSIGNED

Chain W2:



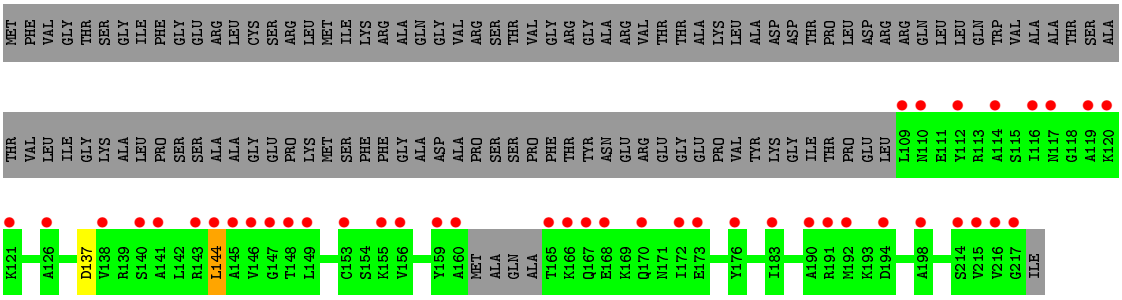
• Molecule 20: PEPTIDE CHAIN UNASSIGNED

Chain w2:



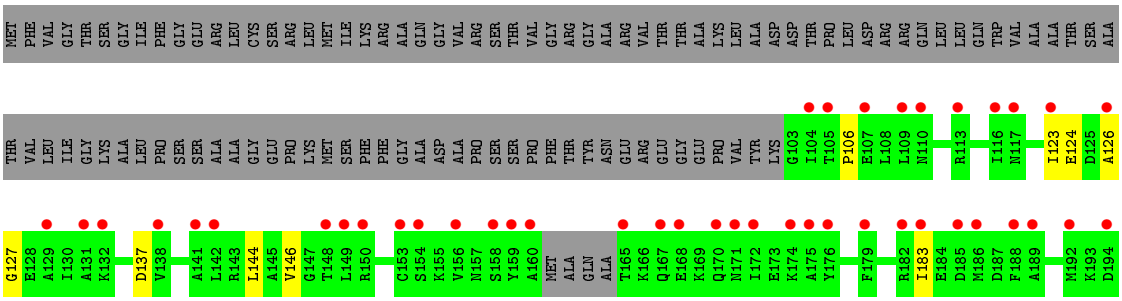
• Molecule 21: Extrinsic protein in photosystem II

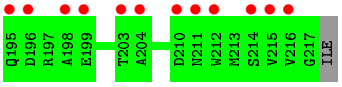
Chain q1:



• Molecule 21: Extrinsic protein in photosystem II

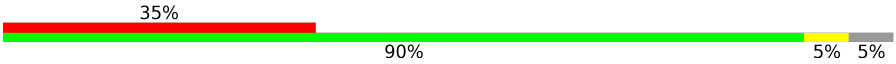
Chain Q2:

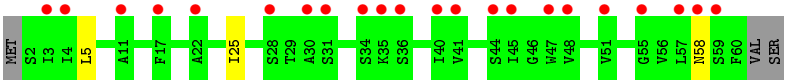




• Molecule 22: Photosystem II reaction center protein Z

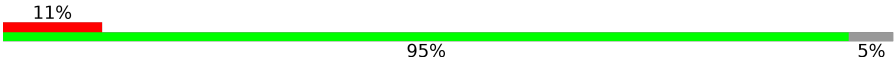
Chain Z2:

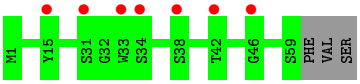




• Molecule 22: Photosystem II reaction center protein Z

Chain z2:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.44Å 240.31Å 300.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.77 29.78 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.7 (10.00-2.77) 99.5 (29.78-2.77)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.76Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.249 , 0.278 0.259 , 0.287	Depositor DCC
R_{free} test set	19164 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	68.0	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 55.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 382148 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	92765	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

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

[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: LHG, GOL, OEX, PHO, DGD, CL, CA, LMT, CLA, PL9, FE, BCT, HEM, LMG, UNL, BCR, SQD

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	0.28	0/2685	0.43	0/3673
1	A2	0.29	0/2548	0.43	0/3481
1	a1	0.28	0/2642	0.42	0/3612
1	a2	0.28	0/2586	0.43	0/3538
2	B1	0.33	0/3830	0.48	3/5227 (0.1%)
2	B2	0.33	0/3897	0.48	2/5323 (0.0%)
2	b1	0.36	1/4015 (0.0%)	0.49	2/5473 (0.0%)
2	b2	0.33	0/3808	0.48	2/5197 (0.0%)
3	C1	0.28	0/3501	0.43	0/4782
3	C2	0.27	0/3242	0.42	0/4441
3	c1	0.30	0/3555	0.43	0/4850
3	c2	0.27	0/3495	0.42	0/4773
4	D1	0.35	0/2704	0.46	0/3688
4	D2	0.34	0/2675	0.46	0/3655
4	d1	0.35	0/2772	0.46	0/3783
4	d2	0.35	0/2736	0.46	0/3734
5	E1	0.24	0/418	0.38	0/577
5	E2	0.25	0/443	0.39	0/614
5	e1	0.24	0/440	0.39	0/603
5	e2	0.24	0/434	0.37	0/598
6	F1	0.45	0/220	0.51	0/299
6	F2	0.43	0/236	0.51	0/320
6	f1	0.44	0/235	0.50	0/319
6	f2	0.45	0/234	0.49	0/318
7	H1	0.23	0/443	0.40	0/606
7	H2	0.23	0/453	0.38	0/619
7	h1	0.23	0/481	0.41	0/657
7	h2	0.23	0/461	0.38	0/631
8	I1	0.26	0/283	0.35	0/381
8	I2	0.26	0/273	0.35	0/371
8	i1	0.26	0/289	0.36	0/389

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	i2	0.27	0/270	0.34	0/364
9	J1	0.23	0/225	0.35	0/307
9	J2	0.22	0/236	0.35	0/324
9	j1	0.23	0/229	0.34	0/313
9	j2	0.22	0/233	0.36	0/319
10	K1	0.38	0/289	0.53	0/399
10	K2	0.38	0/258	0.52	0/359
10	k1	0.37	0/290	0.53	0/401
10	k2	0.38	0/278	0.52	0/385
11	L1	0.49	0/301	0.58	0/410
11	L2	0.47	0/308	0.57	0/419
11	l1	0.49	0/308	0.58	0/418
11	l2	0.48	0/308	0.58	0/418
12	M1	0.39	0/288	0.59	0/391
12	M2	0.38	0/287	0.58	0/390
12	m1	0.38	0/288	0.59	0/391
12	m2	0.38	0/290	0.59	0/394
13	O1	0.66	2/1700 (0.1%)	0.91	15/2315 (0.6%)
13	O2	0.63	1/1387 (0.1%)	0.85	7/1881 (0.4%)
13	o1	0.63	2/1716 (0.1%)	0.90	13/2330 (0.6%)
13	o2	0.65	2/1794 (0.1%)	0.91	14/2434 (0.6%)
14	T1	0.26	0/248	0.39	0/337
14	T2	0.25	0/247	0.38	0/337
14	t1	0.25	0/253	0.39	0/344
14	t2	0.26	0/242	0.39	0/330
15	U1	0.46	0/709	0.68	2/970 (0.2%)
15	U2	0.45	0/588	1.15	3/809 (0.4%)
15	u1	0.46	0/721	0.67	2/981 (0.2%)
15	u2	0.44	0/726	0.66	2/988 (0.2%)
16	V1	0.48	0/937	0.67	4/1281 (0.3%)
16	V2	0.46	1/858 (0.1%)	0.62	1/1177 (0.1%)
16	v1	0.47	0/941	0.67	4/1284 (0.3%)
16	v2	0.46	0/983	0.66	4/1337 (0.3%)
17	Y1	0.43	0/171	0.52	0/236
17	Y2	0.44	0/159	0.53	0/219
17	y1	0.41	0/198	0.50	0/274
17	y2	0.42	0/191	0.50	0/264
18	X1	0.26	0/202	0.43	0/278
18	X2	0.25	0/222	0.43	0/307
18	x1	0.29	0/262	0.44	0/363
18	x2	0.34	0/225	0.46	0/312
19	S1	0.25	0/167	0.36	0/231
19	S2	0.25	0/194	0.36	0/268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
19	s1	0.26	0/269	0.33	0/371
19	s2	0.24	0/285	0.34	0/395
20	W1	0.20	0/134	0.37	0/186
20	W2	0.20	0/129	0.38	0/179
20	w1	0.20	0/152	0.36	0/211
20	w2	0.21	0/127	0.37	0/176
21	Q2	0.41	0/682	0.47	0/937
21	q1	0.40	0/650	0.50	1/893 (0.1%)
22	Z2	0.20	0/353	0.37	0/487
22	z2	0.22	0/387	0.38	0/532
All	All	0.37	9/79929 (0.0%)	0.53	81/109188 (0.1%)

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
13	O1	0	2
13	O2	0	4
13	o1	0	3
13	o2	0	3
16	V1	0	3
16	V2	0	3
16	v1	0	3
16	v2	0	3
All	All	0	24

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	O1	221	SER	N-CA	6.20	1.58	1.46
13	o2	221	SER	N-CA	6.10	1.58	1.46
13	o1	221	SER	N-CA	6.00	1.58	1.46
13	O1	220	LEU	N-CA	5.81	1.57	1.46
13	o2	220	LEU	N-CA	5.81	1.57	1.46
13	o1	220	LEU	N-CA	5.73	1.57	1.46
13	O2	221	SER	N-CA	5.50	1.57	1.46
16	V2	42	VAL	CA-C	-5.45	1.38	1.52
2	b1	422	ARG	C-O	5.30	1.33	1.23

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	U2	11	ARG	NE-CZ-NH1	-19.49	110.56	120.30
15	U2	11	ARG	NE-CZ-NH2	17.62	129.11	120.30
13	o1	99	ASP	CB-CG-OD1	-10.04	109.26	118.30
15	U2	11	ARG	CD-NE-CZ	9.31	136.64	123.60
13	o1	195	GLY	CA-C-O	-8.28	105.69	120.60
13	o2	195	GLY	CA-C-O	-8.27	105.71	120.60
13	O1	195	GLY	CA-C-O	-8.20	105.83	120.60
16	v2	42	VAL	CA-C-N	-8.15	99.90	116.20
16	v1	42	VAL	CA-C-N	-8.14	99.93	116.20
16	V1	42	VAL	CA-C-N	-8.09	100.01	116.20
13	O1	215	PHE	C-N-CA	-7.67	102.53	121.70
13	o1	215	PHE	C-N-CA	-7.65	102.58	121.70
13	o2	215	PHE	C-N-CA	-7.64	102.61	121.70
13	O2	239	PHE	C-N-CA	-7.60	102.70	121.70
13	O1	194	SER	C-N-CA	-7.50	106.54	122.30
13	o1	194	SER	C-N-CA	-7.44	106.68	122.30
13	o2	194	SER	C-N-CA	-7.42	106.72	122.30
16	V2	42	VAL	CA-C-N	-7.04	102.13	116.20
13	o2	233	LEU	CB-CG-CD1	-6.98	99.13	111.00
15	U1	11	ARG	NE-CZ-NH2	-6.85	116.88	120.30
13	O1	220	LEU	CA-CB-CG	6.79	130.91	115.30
13	o1	99	ASP	CB-CG-OD2	6.77	124.39	118.30
15	u2	11	ARG	NE-CZ-NH2	-6.77	116.92	120.30
13	o2	220	LEU	CA-CB-CG	6.66	130.61	115.30
13	o1	220	LEU	CA-CB-CG	6.59	130.47	115.30
13	O1	219	GLN	N-CA-C	6.57	128.74	111.00
13	o2	219	GLN	N-CA-C	6.57	128.73	111.00
15	u1	11	ARG	NE-CZ-NH2	-6.54	117.03	120.30
13	o1	143	GLY	C-N-CA	-6.45	108.76	122.30
13	o2	143	GLY	C-N-CA	-6.42	108.81	122.30
13	O1	143	GLY	C-N-CA	-6.40	108.85	122.30
13	o1	219	GLN	N-CA-C	6.38	128.22	111.00
13	O1	220	LEU	C-N-CA	6.35	137.59	121.70
13	O2	220	LEU	C-N-CA	6.35	137.57	121.70
13	o2	220	LEU	C-N-CA	6.34	137.55	121.70
16	v2	42	VAL	N-CA-CB	6.33	125.44	111.50
16	V1	42	VAL	N-CA-CB	6.33	125.43	111.50
13	O2	194	SER	C-N-CA	-6.32	109.03	122.30
13	O2	233	LEU	CB-CG-CD1	-6.32	100.26	111.00
16	v1	42	VAL	N-CA-CB	6.29	125.35	111.50
13	o1	220	LEU	C-N-CA	6.16	137.10	121.70
13	O1	233	LEU	CB-CG-CD1	-6.08	100.66	111.00
2	B1	430	PHE	C-N-CA	-5.90	106.95	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	o2	217	SER	C-N-CA	-5.87	107.03	121.70
13	o2	221	SER	N-CA-C	5.86	126.82	111.00
13	O1	221	SER	N-CA-C	5.84	126.78	111.00
13	O1	217	SER	C-N-CA	-5.84	107.10	121.70
13	o2	219	GLN	C-N-CA	-5.78	107.25	121.70
13	O1	219	GLN	C-N-CA	-5.77	107.27	121.70
2	b1	430	PHE	C-N-CA	-5.73	107.38	121.70
13	o1	219	GLN	C-N-CA	-5.68	107.50	121.70
13	O1	220	LEU	CB-CG-CD2	5.67	120.64	111.00
15	u2	11	ARG	NE-CZ-NH1	5.62	123.11	120.30
15	u1	11	ARG	NE-CZ-NH1	5.57	123.08	120.30
13	o2	92	THR	C-N-CA	-5.54	107.84	121.70
13	O1	92	THR	C-N-CA	-5.54	107.85	121.70
13	o1	221	SER	N-CA-C	5.54	125.96	111.00
13	o2	220	LEU	CB-CG-CD2	5.48	120.31	111.00
15	U1	11	ARG	NE-CZ-NH1	5.46	123.03	120.30
16	v2	42	VAL	CA-C-O	5.45	131.55	120.10
13	o1	220	LEU	CB-CG-CD2	5.45	120.26	111.00
16	v1	42	VAL	CA-C-O	5.45	131.54	120.10
13	o1	217	SER	C-N-CA	-5.44	108.09	121.70
2	b2	430	PHE	C-N-CA	-5.42	108.14	121.70
13	O2	221	SER	N-CA-C	5.41	125.59	111.00
16	V1	42	VAL	CA-C-O	5.39	131.43	120.10
2	B2	430	PHE	C-N-CA	-5.39	108.23	121.70
21	q1	144	LEU	CA-CB-CG	5.34	127.59	115.30
13	O2	143	GLY	C-N-CA	-5.33	111.11	122.30
13	O2	220	LEU	O-C-N	5.31	131.20	122.70
13	o2	178(F)	GLY	N-CA-C	5.26	126.24	113.10
2	b2	339	ALA	N-CA-C	5.21	125.06	111.00
2	b1	339	ALA	N-CA-C	5.19	125.01	111.00
2	B1	339	ALA	N-CA-C	5.16	124.92	111.00
2	B2	339	ALA	N-CA-C	5.13	124.86	111.00
13	O1	221	SER	CB-CA-C	-5.09	100.43	110.10
16	V1	42	VAL	N-CA-C	-5.09	97.27	111.00
13	O1	236	LYS	C-N-CA	-5.08	111.63	122.30
16	v2	42	VAL	N-CA-C	-5.07	97.31	111.00
16	v1	42	VAL	N-CA-C	-5.03	97.43	111.00
2	B1	7	ARG	NE-CZ-NH1	-5.02	117.79	120.30

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	O1	194	SER	Peptide
13	O1	220	LEU	Peptide
13	O2	194	SER	Peptide
13	O2	220	LEU	Mainchain
13	O2	45	LEU	Mainchain
13	O2	49	GLN	Peptide
16	V1	38	SER	Peptide
16	V1	41	HIS	Peptide
16	V1	44	GLY	Peptide
16	V2	38	SER	Peptide
16	V2	41	HIS	Peptide
16	V2	44	GLY	Peptide
13	o1	194	SER	Peptide
13	o1	220	LEU	Peptide
13	o1	98	LYS	Peptide
13	o2	178(E)	VAL	Peptide
13	o2	194	SER	Peptide
13	o2	220	LEU	Peptide
16	v1	38	SER	Peptide
16	v1	41	HIS	Peptide
16	v1	44	GLY	Peptide
16	v2	38	SER	Peptide
16	v2	41	HIS	Peptide
16	v2	44	GLY	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	2609	0	2500	64	0
1	A2	2475	0	2296	51	0
1	a1	2564	0	2462	0	0
1	a2	2513	0	2376	0	0
2	B1	3703	0	3485	70	0
2	B2	3770	0	3462	67	0
2	b1	3881	0	3672	0	0
2	b2	3681	0	3452	0	0
3	C1	3392	0	3206	76	0
3	C2	3145	0	2751	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c1	3439	0	3293	0	0
3	c2	3386	0	3189	0	0
4	D1	2615	0	2465	49	0
4	D2	2585	0	2371	44	0
4	d1	2678	0	2544	0	0
4	d2	2643	0	2489	0	0
5	E1	405	0	304	0	0
5	E2	430	0	345	3	0
5	e1	427	0	374	0	0
5	e2	421	0	354	0	0
6	F1	213	0	198	5	0
6	F2	229	0	204	5	0
6	f1	227	0	221	0	0
6	f2	225	0	205	0	0
7	H1	433	0	407	5	0
7	H2	443	0	414	5	0
7	h1	470	0	474	0	0
7	h2	450	0	432	0	0
8	I1	274	0	262	6	0
8	I2	265	0	236	4	0
8	i1	280	0	276	0	0
8	i2	261	0	238	0	0
9	J1	220	0	209	2	0
9	J2	231	0	208	2	0
9	j1	224	0	223	0	0
9	j2	228	0	220	0	0
10	K1	279	0	268	17	0
10	K2	250	0	218	6	0
10	k1	280	0	280	0	0
10	k2	269	0	252	0	0
11	L1	292	0	284	9	0
11	L2	299	0	297	15	0
11	l1	299	0	304	0	0
11	l2	299	0	294	0	0
12	M1	285	0	295	8	0
12	M2	284	0	296	7	0
12	m1	285	0	295	0	0
12	m2	287	0	298	0	0
13	O1	1674	0	1534	64	0
13	O2	1376	0	1198	74	0
13	o1	1692	0	1547	0	0
13	o2	1768	0	1663	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	T1	241	0	248	5	0
14	T2	240	0	253	5	0
14	t1	246	0	264	0	0
14	t2	235	0	248	0	0
15	U1	691	0	628	15	0
15	U2	577	0	435	9	0
15	u1	703	0	645	0	0
15	u2	708	0	671	0	0
16	V1	917	0	847	21	0
16	V2	845	0	719	16	0
16	v1	921	0	842	0	0
16	v2	963	0	937	0	0
17	Y1	170	0	141	1	0
17	Y2	159	0	148	1	0
17	y1	195	0	194	0	0
17	y2	188	0	174	0	0
18	X1	197	0	192	2	0
18	X2	215	0	197	4	0
18	x1	255	0	245	0	0
18	x2	218	0	191	0	0
19	S1	164	0	161	1	0
19	S2	191	0	184	1	0
19	s1	263	0	260	0	0
19	s2	281	0	276	0	0
20	W1	134	0	149	4	0
20	W2	129	0	136	4	0
20	w1	152	0	165	0	0
20	w2	127	0	137	0	0
21	Q2	676	0	484	4	0
21	q1	645	0	462	0	0
22	Z2	351	0	280	2	0
22	z2	381	0	335	0	0
23	A1	40	0	56	9	0
23	A2	40	0	56	6	0
23	B1	120	0	168	21	0
23	B2	120	0	168	20	0
23	C1	80	0	112	12	0
23	C2	40	0	56	4	0
23	D1	40	0	56	3	0
23	F2	40	0	56	4	0
23	H1	22	0	29	5	0
23	H2	24	0	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	J1	40	0	56	6	0
23	K1	31	0	40	5	0
23	K2	69	0	97	8	0
23	a1	40	0	56	0	0
23	a2	40	0	56	0	0
23	b1	120	0	168	0	0
23	b2	120	0	168	0	0
23	c1	80	0	112	0	0
23	c2	40	0	56	0	0
23	d1	40	0	56	0	0
23	d2	40	0	56	0	0
23	h1	40	0	56	0	0
23	h2	40	0	56	0	0
23	j2	40	0	56	0	0
23	k1	40	0	56	0	0
23	k2	40	0	56	0	0
23	z2	40	0	56	0	0
24	A1	1	0	0	0	0
24	A2	1	0	0	0	0
24	a1	1	0	0	0	0
24	a2	1	0	0	0	0
25	A1	236	0	234	27	0
25	A2	177	0	174	20	0
25	B1	1002	0	1072	76	0
25	B2	1000	0	1072	69	0
25	C1	816	0	873	69	0
25	C2	636	0	572	29	0
25	D1	116	0	113	2	0
25	D2	191	0	205	12	0
25	K2	55	0	49	5	0
25	a1	175	0	170	0	0
25	a2	180	0	183	0	0
25	b1	1034	0	1138	0	0
25	b2	997	0	1060	0	0
25	c1	815	0	867	0	0
25	c2	789	0	814	0	0
25	d1	195	0	216	0	0
25	d2	180	0	183	0	0
26	A1	10	0	0	0	0
26	A2	10	0	0	0	0
26	a1	10	0	0	0	0
26	a2	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	A1	64	0	74	2	0
27	A2	64	0	74	4	0
27	D1	63	0	70	1	0
27	D2	64	0	74	3	0
27	a1	64	0	74	0	0
27	a2	64	0	74	0	0
27	d1	64	0	74	0	0
27	d2	64	0	74	0	0
28	A1	14	0	0	0	0
28	A2	28	0	0	0	0
28	B1	41	0	0	0	0
28	B2	58	0	0	0	0
28	C2	24	0	0	1	0
28	D1	6	0	0	0	0
28	F2	16	0	0	0	0
28	H2	5	0	0	0	0
28	I2	31	0	0	0	0
28	J2	10	0	0	0	0
28	K2	5	0	0	0	0
28	M2	11	0	0	0	0
28	W2	9	0	0	0	0
28	X2	7	0	0	0	0
28	a1	11	0	0	0	0
28	a2	55	0	0	0	0
28	b1	92	0	0	0	0
28	b2	12	0	0	0	0
28	c2	15	0	0	0	0
28	d1	12	0	0	0	0
28	d2	25	0	0	0	0
28	i2	14	0	0	0	0
28	j1	17	0	0	0	0
28	k2	30	0	0	0	0
28	l1	12	0	0	0	0
28	m1	6	0	0	0	0
28	m2	36	0	0	0	0
28	t1	27	0	0	0	0
28	x1	15	0	0	0	0
29	A1	84	0	108	6	0
29	A2	29	0	28	1	0
29	B1	79	0	98	3	0
29	B2	77	0	94	3	0
29	C1	48	0	66	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	C2	24	0	18	0	0
29	D1	35	0	40	1	0
29	F2	35	0	40	1	0
29	I2	34	0	38	2	0
29	M1	31	0	43	2	0
29	a1	51	0	72	0	0
29	a2	44	0	58	0	0
29	b1	117	0	144	0	0
29	b2	39	0	48	0	0
29	c1	55	0	86	0	0
29	c2	26	0	24	0	0
29	d1	68	0	85	0	0
29	d2	27	0	24	0	0
29	j2	50	0	73	0	0
30	A1	1	0	0	0	0
30	A2	1	0	0	0	0
30	a1	1	0	0	0	0
30	a2	1	0	0	0	0
31	A1	4	0	0	0	0
31	A2	4	0	0	0	0
31	a1	4	0	0	0	0
31	a2	4	0	0	0	0
32	B1	6	0	8	0	0
32	C1	6	0	8	0	0
32	C2	6	0	8	0	0
32	a1	6	0	8	0	0
32	a2	6	0	8	0	0
32	b1	6	0	8	0	0
32	c1	6	0	8	0	0
32	c2	6	0	8	0	0
32	i1	6	0	8	0	0
33	A2	33	0	36	3	0
33	B1	49	0	74	9	0
33	B2	42	0	57	2	0
33	D1	98	0	148	11	0
33	D2	98	0	148	19	0
33	L1	41	0	55	1	0
33	L2	49	0	74	10	0
33	a1	43	0	59	0	0
33	a2	30	0	32	0	0
33	b1	49	0	74	0	0
33	b2	43	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	d1	81	0	108	0	0
33	d2	98	0	148	0	0
33	l1	49	0	74	0	0
33	l2	44	0	61	0	0
34	C1	178	0	233	10	0
34	C2	33	0	26	0	0
34	H1	62	0	82	4	0
34	H2	62	0	82	3	0
34	c1	175	0	224	0	0
34	c2	176	0	226	0	0
34	h1	62	0	82	0	0
34	h2	62	0	82	0	0
35	C1	35	0	46	3	0
35	L1	12	0	23	1	0
35	M1	35	0	56	1	0
35	T1	12	0	23	0	0
35	a2	35	0	46	0	0
35	b2	70	0	92	0	0
35	c1	33	0	39	0	0
35	i2	7	0	10	0	0
35	l1	24	0	35	0	0
35	m1	35	0	46	0	0
35	m2	59	0	64	0	0
36	D1	55	0	80	10	0
36	D2	55	0	80	11	0
36	d1	55	0	80	0	0
36	d2	55	0	80	0	0
37	B2	45	0	57	1	0
37	D1	35	0	34	1	0
37	D2	25	0	15	0	0
37	b2	45	0	54	0	0
38	E1	43	0	30	3	0
38	E2	43	0	30	4	0
38	V1	43	0	30	5	0
38	V2	43	0	30	5	0
38	e2	43	0	30	0	0
38	f1	43	0	30	0	0
38	v1	43	0	30	0	0
38	v2	43	0	30	0	0
39	O1	1	0	0	0	0
39	o2	1	0	0	0	0
40	A1	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	A2	2	0	0	2	0
40	B1	1	0	0	0	0
40	a1	4	0	0	0	0
40	a2	4	0	0	0	0
40	b2	1	0	0	0	0
40	c1	2	0	0	0	0
40	c2	1	0	0	0	0
40	d2	1	0	0	0	0
All	All	92765	0	88715	982	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 7.

All (982) 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)
13:O2:44:CYS:O	13:O2:240:TYR:N	1.70	1.25
13:O2:201:VAL:HG12	13:O2:202:ASN:H	1.31	0.92
13:O1:195:GLY:CA	13:O1:220:LEU:H	1.86	0.89
13:O2:195:GLY:CA	13:O2:220:LEU:H	2.40	0.87
13:O2:46:GLU:N	13:O2:238:VAL:O	2.06	0.87
13:O2:44:CYS:N	13:O2:240:TYR:O	2.09	0.86
13:O1:199:LEU:HA	13:O1:215:PHE:HA	1.60	0.86
4:D2:186:GLN:HB2	25:D2:401:CLA:HBC1	1.58	0.86
13:O2:199:LEU:HA	13:O2:215:PHE:HA	1.70	0.86
16:V2:34:ASN:HA	16:V2:38:SER:HB3	1.59	0.85
16:V1:34:ASN:HA	16:V1:38:SER:HB3	1.60	0.84
25:B1:611:CLA:H2	25:B1:612:CLA:HBB2	1.61	0.82
13:O1:195:GLY:HA3	13:O1:219:GLN:HB2	1.63	0.81
3:C1:36:TRP:O	3:C1:38:GLY:N	2.15	0.81
13:O1:51:LEU:HB2	13:O1:234:LEU:HB3	1.64	0.80
2:B1:365:ASN:HD21	4:D1:323:GLU:HG2	1.51	0.80
4:D1:186:GLN:HB2	25:D1:402:CLA:HBC1	1.62	0.79
13:O1:201:VAL:HG12	13:O1:202:ASN:H	1.47	0.79
13:O2:195:GLY:HA3	13:O2:219:GLN:HB2	1.75	0.79
3:C2:36:TRP:O	3:C2:38:GLY:N	2.17	0.79
4:D1:192:THR:HG23	25:D1:402:CLA:HBC2	1.66	0.78
2:B1:222:PRO:HD2	25:B1:611:CLA:HED3	1.66	0.78
25:A2:402:CLA:HBB1	4:D2:182:LEU:HD21	1.63	0.78
38:E2:101:HEM:HBB2	38:E2:101:HEM:HHC	1.66	0.78
33:D2:405:LHG:H311	14:T2:21:ILE:HD11	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:339:ALA:H	2:B1:431:GLU:HB2	1.49	0.77
13:O2:46:GLU:O	13:O2:238:VAL:N	2.19	0.76
15:U2:76:LYS:O	15:U2:79:MET:HB2	1.84	0.76
15:U1:76:LYS:O	15:U1:79:MET:HB2	1.87	0.76
25:B1:610:CLA:HBB1	25:B1:610:CLA:HHC	1.68	0.76
25:B2:606:CLA:HBB2	25:B2:608:CLA:H193	1.68	0.76
16:V2:34:ASN:HA	16:V2:38:SER:CB	2.16	0.75
4:D2:192:THR:HG23	25:D2:401:CLA:HBC2	1.68	0.75
13:O2:221:SER:HB2	13:O2:233:LEU:HD11	1.70	0.75
13:O2:195:GLY:HA2	13:O2:220:LEU:H	1.98	0.75
1:A1:121:LEU:HD13	25:A1:405:CLA:HMB3	1.68	0.75
38:E1:101:HEM:HHC	38:E1:101:HEM:HBB2	1.69	0.75
13:O1:195:GLY:HA2	13:O1:220:LEU:H	1.52	0.75
38:V2:201:HEM:HHD	38:V2:201:HEM:HBC2	1.69	0.75
16:V1:34:ASN:HA	16:V1:38:SER:CB	2.17	0.74
25:B2:614:CLA:H171	25:B2:615:CLA:HBB2	1.97	0.74
25:D2:406:CLA:HAA2	36:D2:408:PL9:H371	1.69	0.74
25:B1:619:CLA:HBB1	29:M1:101:LMG:H371	1.69	0.74
25:A2:404:CLA:HHC	25:A2:404:CLA:HBB1	1.70	0.74
25:B2:617:CLA:H121	20:W2:18:LEU:HD21	1.68	0.74
2:B1:12:VAL:HG12	25:B1:614:CLA:HMC2	1.70	0.73
38:V1:201:HEM:HHD	38:V1:201:HEM:HBC2	1.71	0.73
13:O2:197:ILE:HG13	13:O2:217:SER:HB2	1.71	0.73
25:A1:404:CLA:HBB1	25:A1:404:CLA:HHC	3.58	0.72
25:A2:403:CLA:HHC	25:A2:403:CLA:HBB1	1.70	0.72
2:B2:12:VAL:HG12	25:B2:614:CLA:HMC2	1.77	0.72
25:B1:617:CLA:H121	20:W1:18:LEU:HD21	1.72	0.72
25:C1:508:CLA:HBB2	25:C1:509:CLA:H51	29.44	0.71
25:C1:512:CLA:H151	23:K1:101:BCR:H21C	1.70	0.71
13:O1:221:SER:HB2	13:O1:233:LEU:HD11	1.72	0.71
1:A1:121:LEU:HD13	25:A1:404:CLA:HMB3	44.22	0.70
1:A2:93:LEU:HG	1:A2:95:PRO:HD3	1.74	0.70
2:B1:339:ALA:N	2:B1:431:GLU:HB2	2.06	0.70
13:O1:82:GLU:N	13:O1:99:ASP:O	2.43	0.70
23:A1:401:BCR:H16C	25:A1:405:CLA:HBC2	1.74	0.70
25:C1:514:CLA:HMC2	23:K1:101:BCR:H373	1.73	0.70
25:A1:404:CLA:HBC1	29:B1:626:LMG:H171	60.84	0.70
4:D2:123:ILE:HD11	34:H2:101:DGD:HAW2	1.73	0.69
13:O2:45:LEU:HA	13:O2:239:PHE:HA	1.73	0.69
23:F2:401:BCR:H21C	23:F2:401:BCR:H361	1.72	0.69
13:O1:146:PHE:HE2	13:O1:197:ILE:N	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O2:201:VAL:HG12	13:O2:202:ASN:N	2.07	0.69
1:A1:93:LEU:HG	1:A1:95:PRO:HD3	1.74	0.68
29:C1:520:LMG:H181	10:K1:27:VAL:HG11	1.75	0.68
13:O1:195:GLY:HA2	13:O1:220:LEU:N	2.10	0.68
23:B2:602:BCR:HC8	29:B2:621:LMG:H211	1.75	0.68
25:B1:606:CLA:HBB2	25:B1:608:CLA:H193	1.76	0.68
13:O1:195:GLY:CA	13:O1:220:LEU:N	2.57	0.68
15:U1:36:ARG:NH1	16:V1:51:ASN:O	2.36	0.68
1:A2:121:LEU:HD13	25:A2:403:CLA:HMB3	1.76	0.68
13:O2:146:PHE:HE2	13:O2:197:ILE:N	2.00	0.68
13:O2:195:GLY:CA	13:O2:219:GLN:HA	2.23	0.68
25:B1:608:CLA:H192	25:B1:611:CLA:HBB2	2.51	0.68
13:O1:195:GLY:HA3	13:O1:219:GLN:CA	2.24	0.68
13:O1:51:LEU:HB3	13:O1:65:PHE:HB3	1.74	0.68
1:A2:161:TYR:OH	40:A2:501:HOH:O	6.99	0.68
23:K2:102:BCR:H21C	23:K2:102:BCR:H361	1.76	0.68
33:L2:101:LHG:H311	12:M2:18:PRO:HB3	1.75	0.68
13:O1:48:LYS:O	13:O1:236:LYS:O	2.14	0.68
12:M1:14:GLY:O	12:M1:18:PRO:HD2	1.94	0.67
3:C1:39:ASN:HB2	25:C1:509:CLA:CGA	2.24	0.67
12:M2:14:GLY:O	12:M2:18:PRO:HD2	1.95	0.67
13:O2:195:GLY:HA2	13:O2:220:LEU:N	2.60	0.67
2:B1:6:TYR:O	2:B1:8:VAL:N	2.31	0.67
13:O1:195:GLY:CA	13:O1:219:GLN:HA	2.25	0.67
13:O2:195:GLY:CA	13:O2:220:LEU:N	3.10	0.66
13:O1:48:LYS:O	13:O1:49:GLN:HB2	1.94	0.66
13:O1:197:ILE:HG13	13:O1:217:SER:HB2	1.79	0.66
13:O2:48:LYS:O	13:O2:49:GLN:HB2	2.20	0.66
1:A2:160:ILE:HG21	1:A2:291:SER:HB3	1.78	0.66
3:C1:39:ASN:HB2	25:C1:510:CLA:CGA	15.14	0.66
13:O2:48:LYS:O	13:O2:236:LYS:O	2.39	0.66
13:O2:199:LEU:HD12	13:O2:199:LEU:H	1.60	0.66
2:B2:103:LEU:HD21	25:B2:608:CLA:HMC3	1.78	0.66
25:A1:406:CLA:HAA2	36:D1:408:PL9:H371	1.78	0.65
25:A2:402:CLA:CBB	4:D2:182:LEU:HD21	2.26	0.65
13:O1:199:LEU:H	13:O1:199:LEU:HD12	1.61	0.65
6:F2:41:GLN:HG3	9:J2:31:GLY:HA3	1.78	0.65
2:B1:341:LEU:HD11	13:O1:178(C):GLY:HA3	1.78	0.65
23:D1:401:BCR:H391	9:J1:25:LEU:HD11	1.78	0.65
25:C1:504:CLA:HAB	25:C1:512:CLA:H141	5.19	0.65
3:C2:279:LEU:HD22	25:C2:510:CLA:HED2	27.90	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A2:404:CLA:H2	27:D2:407:PHO:HMB3	1.80	0.64
4:D1:172:SER:HB2	4:D1:177:ALA:HB1	1.79	0.64
4:D1:199:MET:HB2	4:D1:281:VAL:HG11	1.78	0.64
33:D1:405:LHG:H311	14:T1:21:ILE:HD11	1.77	0.64
25:D2:406:CLA:HMA2	36:D2:408:PL9:H421	1.79	0.64
13:O2:195:GLY:HA2	13:O2:219:GLN:HA	1.77	0.64
13:O1:49:GLN:O	13:O1:235:LEU:HA	1.98	0.64
2:B1:422:ARG:NH1	13:O1:169:ASP:OD2	2.29	0.64
1:A1:160:ILE:HG21	1:A1:291:SER:HB3	1.79	0.64
13:O1:154:GLY:HA2	13:O1:164:MET:HB2	1.79	0.64
13:O1:47:PRO:O	13:O1:48:LYS:HG2	1.97	0.64
13:O2:195:GLY:HA3	13:O2:219:GLN:CB	2.40	0.64
25:C1:506:CLA:HBB1	25:C1:506:CLA:H93	1.80	0.64
13:O2:195:GLY:HA3	13:O2:219:GLN:CA	2.42	0.64
1:A2:165:GLN:NE2	40:A2:501:HOH:O	8.26	0.64
13:O1:195:GLY:HA3	13:O1:219:GLN:CB	2.27	0.63
13:O2:197:ILE:HA	13:O2:217:SER:HA	1.80	0.63
2:B2:6:TYR:O	2:B2:8:VAL:N	2.31	0.63
13:O1:146:PHE:CE2	13:O1:197:ILE:N	2.67	0.63
1:A1:106:LEU:HD11	23:A1:401:BCR:H402	2.43	0.63
23:A1:401:BCR:H16C	25:A1:404:CLA:HBC2	43.62	0.63
3:C1:148:GLY:O	3:C1:156:LYS:NZ	2.41	0.63
13:O1:200:ALA:O	13:O1:201:VAL:O	2.16	0.63
13:O2:49:GLN:O	13:O2:235:LEU:HA	2.38	0.63
1:A1:5:LEU:HD23	3:C1:262:ARG:HG2	1.81	0.63
2:B2:458:PHE:CE2	25:B2:607:CLA:HBB1	2.34	0.63
25:A1:403:CLA:CBB	4:D1:182:LEU:HD21	2.29	0.63
2:B2:458:PHE:HB3	25:B2:607:CLA:HBC2	1.79	0.63
4:D2:332:GLN:OE1	4:D2:332:GLN:N	2.32	0.63
3:C1:447:ARG:NE	33:D1:404:LHG:O2	2.31	0.63
13:O2:146:PHE:CE2	13:O2:197:ILE:N	2.73	0.63
2:B1:103:LEU:HD21	25:B1:608:CLA:HMC3	1.81	0.62
2:B1:434:ARG:NH2	13:O1:178(F):GLY:O	2.32	0.62
16:V1:41:HIS:O	16:V1:43:GLY:N	2.31	0.62
25:C1:508:CLA:HMC2	25:C1:509:CLA:H101	28.52	0.62
13:O2:200:ALA:O	13:O2:201:VAL:O	2.33	0.62
3:C2:256:PRO:HA	25:C2:507:CLA:HED3	15.55	0.62
4:D1:332:GLN:N	4:D1:332:GLN:OE1	2.32	0.62
13:O2:154:GLY:HA2	13:O2:164:MET:HB2	1.81	0.62
16:V2:41:HIS:C	16:V2:43:GLY:H	2.03	0.62
1:A1:102:LEU:HB2	29:B1:626:LMG:HC3	70.38	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:B1:621:LHG:H192	4:D1:277:THR:HG22	1.81	0.62
36:D1:408:PL9:H352	11:L1:26:VAL:HG12	1.80	0.62
36:D1:408:PL9:H353	11:L1:30:LEU:HD22	1.81	0.62
16:V2:41:HIS:O	16:V2:43:GLY:N	2.32	0.62
3:C2:207:ALA:O	3:C2:211:SER:HB2	2.01	0.62
3:C1:466:VAL:HG21	4:D1:248:THR:HA	1.82	0.61
25:C1:512:CLA:H2	25:C1:512:CLA:HED2	6.86	0.61
2:B1:116:VAL:HG21	23:B1:603:BCR:H292	1.82	0.61
2:B1:370:LEU:HB2	2:B1:379:ALA:HB3	1.82	0.61
13:O1:195:GLY:N	13:O1:220:LEU:H	1.98	0.60
25:B2:608:CLA:H192	25:B2:610:CLA:HBB2	24.12	0.60
25:C2:503:CLA:H172	25:C2:509:CLA:HMB3	1.84	0.60
1:A2:291:SER:O	1:A2:294:ALA:HB3	2.00	0.60
23:B1:601:BCR:H332	12:M1:9:LEU:HD23	2.05	0.60
38:V1:201:HEM:HBB2	38:V1:201:HEM:HMB1	1.84	0.60
16:V2:41:HIS:C	16:V2:43:GLY:N	2.55	0.60
3:C1:209:ILE:HG23	23:C1:501:BCR:H403	1.84	0.60
38:E2:101:HEM:O1A	6:F2:19:ARG:NH1	2.35	0.60
13:O2:195:GLY:N	13:O2:220:LEU:H	2.35	0.60
2:B2:158:VAL:HG22	2:B2:166:ILE:HD11	1.84	0.60
3:C2:36:TRP:C	3:C2:38:GLY:H	2.08	0.60
2:B1:168:ILE:HD11	2:B1:181:VAL:HG22	1.86	0.59
2:B2:434:ARG:NH2	13:O2:178(F):GLY:O	2.71	0.59
2:B2:341:LEU:HD11	13:O2:178(C):GLY:HA3	2.00	0.59
3:C1:207:ALA:O	3:C1:211:SER:HB2	2.01	0.59
3:C1:288:GLU:HG3	34:C1:516:DGD:HB31	1.83	0.59
2:B2:458:PHE:HB3	25:B2:616:CLA:HBC2	20.39	0.59
25:A2:404:CLA:CBB	4:D2:182:LEU:HD21	12.57	0.59
3:C1:38:GLY:HA3	25:C1:513:CLA:HMD3	1.95	0.59
3:C1:99:VAL:HG23	3:C1:196:ILE:HD11	1.83	0.59
3:C1:36:TRP:C	3:C1:38:GLY:H	2.06	0.59
2:B1:458:PHE:HB3	25:B1:607:CLA:HBC2	1.83	0.59
3:C1:107:ASN:ND2	35:C1:519:LMT:O4'	2.36	0.59
16:V1:41:HIS:C	16:V1:43:GLY:H	2.06	0.59
23:A1:401:BCR:H373	29:A1:412:LMG:H301	1.83	0.59
25:B1:614:CLA:H171	25:B1:615:CLA:HBB2	1.83	0.59
13:O1:201:VAL:HG12	13:O1:202:ASN:N	2.17	0.59
2:B1:158:VAL:HG22	2:B1:166:ILE:HD11	1.85	0.59
2:B1:7:ARG:O	2:B1:10:THR:OG1	2.22	0.59
16:V1:42:VAL:HG13	16:V1:42:VAL:O	2.03	0.59
1:A2:149:ALA:HB3	1:A2:150:PRO:HD3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:D2:408:PL9:H353	11:L2:30:LEU:HD22	1.85	0.58
21:Q2:124:GLU:O	21:Q2:127:GLY:N	2.36	0.58
4:D1:326:ARG:O	4:D1:330:ALA:HB2	2.03	0.58
13:O2:221:SER:CB	13:O2:233:LEU:HD11	2.33	0.58
1:A1:131:TRP:CH2	25:C1:507:CLA:HAA2	16.37	0.58
11:L1:25:PHE:HB3	14:T1:13:THR:HG22	1.87	0.58
1:A1:149:ALA:HB3	1:A1:150:PRO:HD3	1.86	0.58
33:D2:403:LHG:H201	33:D2:403:LHG:H292	1.84	0.58
1:A1:9:GLU:HG3	19:S1:30:TRP:CZ2	2.39	0.58
2:B2:349:LYS:HE3	2:B2:396:GLY:HA3	1.86	0.58
2:B2:422:ARG:NH1	13:O2:169:ASP:OD2	2.61	0.58
3:C1:275:SER:HB3	25:C1:510:CLA:HED2	1.85	0.58
2:B1:349:LYS:HE3	2:B1:396:GLY:HA3	1.86	0.58
13:O1:81:ILE:HA	13:O1:100:GLY:HA3	1.86	0.58
23:B1:602:BCR:H341	25:B1:615:CLA:HMD3	2.59	0.58
11:L2:25:PHE:HB3	14:T2:13:THR:HG22	1.85	0.58
38:V2:201:HEM:HHC	38:V2:201:HEM:HBB2	1.86	0.58
25:A2:402:CLA:HHC	25:A2:402:CLA:HBB1	1.84	0.58
1:A1:291:SER:O	1:A1:294:ALA:HB3	2.02	0.58
2:B2:7:ARG:O	2:B2:10:THR:OG1	2.22	0.58
4:D2:326:ARG:O	4:D2:330:ALA:HB2	2.04	0.58
36:D2:408:PL9:H352	11:L2:26:VAL:HG12	1.85	0.58
13:O1:197:ILE:HA	13:O1:217:SER:HA	1.85	0.57
2:B1:458:PHE:CE2	25:B1:607:CLA:HBB1	2.66	0.57
3:C1:318:LEU:HD12	3:C1:340:TYR:HB3	1.88	0.57
25:C1:513:CLA:H2	23:C1:521:BCR:H281	1.86	0.57
2:B2:168:ILE:HD11	2:B2:181:VAL:HG22	1.85	0.57
1:A1:107:TYR:HB2	13:O1:71:MET:HE3	1.91	0.57
18:X2:3:MET:HG3	18:X2:7:LEU:HD23	1.86	0.57
1:A2:50:ILE:HG22	23:A2:401:BCR:H271	1.85	0.57
13:O2:45:LEU:H	13:O2:45:LEU:HD12	1.69	0.57
33:A2:405:LHG:O2	3:C2:447:ARG:NE	2.37	0.57
27:A1:408:PHO:HAB	4:D1:205:LEU:HD13	1.85	0.57
23:B1:602:BCR:H331	23:B1:602:BCR:HC8	1.87	0.57
23:B2:601:BCR:H332	12:M2:9:LEU:HD23	1.87	0.57
25:B2:612:CLA:H18	25:B2:615:CLA:H8	19.54	0.57
1:A1:184:LEU:HD21	4:D1:186:GLN:HG2	1.86	0.57
3:C2:42:LEU:HD21	25:K2:101:CLA:H2A	1.85	0.57
29:A1:410:LMG:H121	25:C1:506:CLA:H203	1.88	0.56
3:C2:318:LEU:HD12	3:C2:340:TYR:HB3	1.87	0.56
25:B1:614:CLA:HBB1	25:B1:614:CLA:HMB1	1.90	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B2:608:CLA:H192	25:B2:611:CLA:HBB2	1.87	0.56
33:D2:405:LHG:HC91	11:L2:19:TRP:HZ2	1.70	0.56
13:O2:200:ALA:N	13:O2:214:VAL:O	2.72	0.56
16:V1:41:HIS:C	16:V1:43:GLY:N	2.56	0.56
25:C2:503:CLA:C2D	25:C2:505:CLA:H2	2.35	0.56
3:C2:256:PRO:HA	25:C2:508:CLA:HED3	1.88	0.56
1:A2:107:TYR:HB2	13:O2:71:MET:HE3	1.99	0.56
3:C1:406:SER:HA	3:C1:420:VAL:HG23	1.88	0.56
3:C1:257:PHE:HD2	25:C1:508:CLA:HED3	17.44	0.56
25:C1:504:CLA:HMB3	35:C1:519:LMT:H62	1.88	0.56
33:B2:627:LHG:H322	4:D2:36:LEU:HB2	1.87	0.56
13:O2:201:VAL:CG1	13:O2:202:ASN:H	2.12	0.56
33:B1:621:LHG:H201	33:B1:621:LHG:H292	1.88	0.56
27:A2:407:PHO:HMB3	25:D2:406:CLA:H71	1.87	0.56
25:B1:611:CLA:HMC2	23:H1:102:BCR:H343	1.87	0.56
3:C1:433:LEU:HD22	25:C1:504:CLA:HMC3	18.15	0.56
38:E2:101:HEM:HBC2	38:E2:101:HEM:HMC1	1.87	0.56
13:O2:43:LEU:HD12	13:O2:240:TYR:O	2.05	0.56
25:C1:502:CLA:H151	25:C1:508:CLA:HMB3	1.88	0.56
1:A2:184:LEU:HD21	4:D2:186:GLN:HG2	1.94	0.56
13:O1:200:ALA:N	13:O1:214:VAL:O	2.42	0.56
2:B2:339:ALA:O	2:B2:431:GLU:N	2.39	0.56
2:B2:339:ALA:O	2:B2:430:PHE:HA	2.06	0.56
10:K2:35:LEU:HA	23:K2:102:BCR:H19C	1.86	0.56
4:D2:160:TYR:HA	4:D2:290:ALA:HB2	1.89	0.56
10:K1:23:ASP:OD2	17:Y1:21:GLN:NE2	2.38	0.56
33:D1:404:LHG:H132	33:D1:404:LHG:H321	1.88	0.55
38:V2:201:HEM:HMB1	38:V2:201:HEM:HBB2	4.69	0.55
1:A2:131:TRP:CH2	25:C2:507:CLA:HAA2	2.41	0.55
1:A2:161:TYR:HA	1:A2:294:ALA:HB1	1.87	0.55
4:D1:123:ILE:HD11	34:H1:101:DGD:HAW2	2.07	0.55
23:K1:101:BCR:H361	23:K1:101:BCR:H21C	4.41	0.55
25:C2:505:CLA:H193	25:C2:505:CLA:HMD2	1.87	0.55
2:B2:150:CYS:HB2	25:B2:606:CLA:HMC3	1.89	0.55
33:B2:627:LHG:HC42	4:D2:134:ARG:HG2	1.88	0.55
25:C1:503:CLA:C2D	25:C1:505:CLA:H2	17.57	0.55
23:B1:601:BCR:H362	25:B1:616:CLA:H112	1.89	0.55
25:K2:101:CLA:HMB2	23:K2:104:BCR:H382	1.87	0.55
3:C1:36:TRP:C	3:C1:38:GLY:N	2.60	0.55
12:M2:25:LEU:O	12:M2:28:GLN:HG3	2.06	0.55
1:A1:341:LEU:HD11	16:V1:47:LYS:HD3	1.91	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:22:VAL:HG22	25:B1:616:CLA:HMB3	1.90	0.55
33:B1:621:LHG:H141	11:L1:23:LEU:HD21	1.87	0.55
18:X2:23:LEU:HB3	18:X2:24:PRO:HD3	1.88	0.55
2:B1:339:ALA:O	2:B1:431:GLU:N	2.40	0.55
13:O1:195:GLY:HA3	13:O1:219:GLN:HA	1.88	0.55
16:V1:21:ILE:HD13	16:V1:117:ALA:HB1	1.89	0.55
2:B2:116:VAL:HG21	23:B2:603:BCR:H292	1.88	0.55
25:C1:505:CLA:H43	34:C1:517:DGD:HB32	1.88	0.55
2:B1:339:ALA:O	2:B1:430:PHE:HA	2.07	0.55
13:O2:181:VAL:O	13:O2:183:ARG:N	2.40	0.55
7:H1:46:LEU:HD11	34:H1:101:DGD:HA31	2.52	0.54
3:C2:52:ALA:HA	25:K2:101:CLA:HMB3	1.88	0.54
25:B1:619:CLA:HBA2	29:M1:101:LMG:H291	1.88	0.54
1:A1:161:TYR:HA	1:A1:294:ALA:HB1	1.90	0.54
1:A1:234:ASN:ND2	33:B1:621:LHG:O1	2.38	0.54
4:D1:160:TYR:HA	4:D1:290:ALA:HB2	1.88	0.54
25:C1:510:CLA:H2	25:C1:512:CLA:H12	6.68	0.54
13:O1:181:VAL:O	13:O1:183:ARG:N	2.41	0.54
18:X1:23:LEU:HB3	18:X1:24:PRO:HD3	1.88	0.54
23:B1:603:BCR:H342	25:B1:609:CLA:H71	2.36	0.54
2:B2:383:PHE:CZ	13:O2:167:GLY:HA2	2.73	0.54
25:C1:511:CLA:HBB1	25:C1:511:CLA:HMB1	2.15	0.54
13:O2:49:GLN:HB2	13:O2:236:LYS:HB2	2.18	0.54
3:C2:36:TRP:C	3:C2:38:GLY:N	2.61	0.54
33:D2:403:LHG:H111	33:L2:101:LHG:HC91	2.19	0.54
33:D2:403:LHG:H141	11:L2:23:LEU:HD21	1.90	0.54
25:B2:615:CLA:H51	33:D2:403:LHG:H352	1.89	0.54
3:C1:418:ASN:HD21	34:C1:515:DGD:HD4	1.72	0.54
1:A1:160:ILE:HD11	34:C1:516:DGD:HBT2	1.89	0.54
3:C2:59:LEU:HD13	25:C2:511:CLA:HMD2	18.73	0.54
38:E1:101:HEM:HBC2	38:E1:101:HEM:HMC1	1.89	0.54
11:L2:23:LEU:HD23	33:L2:101:LHG:H291	4.16	0.54
3:C1:28:ILE:HG13	10:K1:45:PHE:HE2	1.75	0.54
3:C2:393:ALA:HB1	38:V2:201:HEM:HBC1	2.00	0.53
23:D1:401:BCR:H372	29:D1:406:LMG:H301	1.89	0.53
2:B2:60:MET:HB3	2:B2:63:MET:HB2	1.90	0.53
13:O2:53:GLU:HA	13:O2:65:PHE:HA	1.89	0.53
1:A1:43:THR:HG22	23:A1:401:BCR:H16C	1.94	0.53
1:A1:131:TRP:CH2	25:C1:506:CLA:HAA2	2.43	0.53
12:M1:25:LEU:O	12:M1:28:GLN:HG3	2.07	0.53
4:D1:274:VAL:HG13	36:D1:408:PL9:H252	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:84:PRO:HA	1:A1:112:TYR:CG	2.44	0.53
1:A2:84:PRO:HA	1:A2:112:TYR:CG	2.44	0.53
2:B1:60:MET:HB3	2:B1:63:MET:HB2	1.90	0.53
25:B1:607:CLA:HBB1	25:B1:619:CLA:HBB2	1.91	0.53
15:U2:96:ASP:HB3	15:U2:100:ASN:HA	1.91	0.53
1:A2:85:THR:HA	1:A2:109:GLY:HA3	1.91	0.53
1:A1:85:THR:HA	1:A1:109:GLY:HA3	1.91	0.53
15:U2:92:PHE:O	15:U2:97:ARG:NH1	2.41	0.53
1:A2:183:MET:HA	25:A2:402:CLA:HMD2	1.90	0.53
13:O2:195:GLY:HA3	13:O2:219:GLN:HA	1.91	0.53
13:O2:43:LEU:HA	13:O2:241:ALA:HA	1.91	0.53
25:B1:609:CLA:H121	20:W1:11:LEU:HD11	4.09	0.53
1:A1:162:PRO:HB3	1:A1:168:PHE:HA	1.91	0.53
25:B2:616:CLA:H42	37:B2:623:SQD:H141	1.90	0.53
23:C1:501:BCR:H382	25:C1:513:CLA:HMB2	31.17	0.53
11:L1:28:ALA:O	11:L1:32:SER:HB3	2.09	0.53
1:A2:131:TRP:CH2	25:C2:506:CLA:HAA2	40.31	0.53
25:C1:512:CLA:HMA1	25:C1:512:CLA:H171	1.90	0.52
1:A2:162:PRO:HB3	1:A2:168:PHE:HA	1.91	0.52
2:B2:105:GLY:HA3	23:B2:602:BCR:H282	4.06	0.52
13:O1:195:GLY:HA2	13:O1:219:GLN:HA	1.90	0.52
1:A2:277:LEU:HA	33:A2:405:LHG:H291	1.91	0.52
3:C1:119:LEU:HG	23:C1:501:BCR:H10C	39.87	0.52
11:L2:28:ALA:O	11:L2:32:SER:HB3	2.10	0.52
25:A2:403:CLA:H43	29:I2:101:LMG:H111	1.92	0.52
23:B2:603:BCR:H311	25:B2:609:CLA:H72	2.54	0.52
13:O1:195:GLY:CA	13:O1:219:GLN:CA	2.87	0.52
17:Y2:39:LEU:HD21	22:Z2:25:ILE:HA	1.92	0.52
25:B1:613:CLA:H112	25:B1:615:CLA:H52	1.91	0.52
23:J1:101:BCR:H271	10:K1:37:PHE:HB3	1.91	0.52
3:C1:228:ASN:HB3	34:C1:516:DGD:HE62	1.90	0.52
3:C1:464:GLU:OE2	4:D1:245:SER:OG	2.20	0.52
23:A2:401:BCR:H14C	25:A2:403:CLA:HBC2	1.90	0.52
2:B1:357:ARG:NH2	4:D1:337:GLU:O	2.51	0.52
25:B2:612:CLA:H122	25:B2:617:CLA:HAA1	1.92	0.52
3:C1:59:LEU:HD13	25:C1:511:CLA:HMD2	1.92	0.52
3:C1:59:LEU:HD13	25:C1:512:CLA:HMD2	15.34	0.52
25:D2:404:CLA:HBC3	18:X2:20:LEU:HD13	1.91	0.52
36:D2:408:PL9:H513	36:D2:408:PL9:H451	1.91	0.52
11:L2:23:LEU:HD13	33:L2:101:LHG:H151	1.92	0.52
15:U1:96:ASP:HB3	15:U1:100:ASN:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C1:502:CLA:H172	25:C1:508:CLA:HMB3	1.92	0.52
29:A1:412:LMG:H141	25:C1:507:CLA:H172	27.26	0.51
13:O2:195:GLY:CA	13:O2:219:GLN:CA	2.97	0.51
16:V2:41:HIS:HA	16:V2:44:GLY:H	1.75	0.51
25:B1:611:CLA:HED2	25:B1:611:CLA:HAA1	1.91	0.51
13:O1:51:LEU:O	13:O1:234:LEU:N	2.43	0.51
2:B2:441:GLY:C	13:O2:176:ALA:HB3	2.30	0.51
13:O2:221:SER:OG	13:O2:222:ASP:N	2.43	0.51
13:O2:51:LEU:O	13:O2:234:LEU:N	2.91	0.51
2:B1:356:VAL:HG22	2:B1:370:LEU:HG	1.92	0.51
2:B1:150:CYS:HB2	25:B1:606:CLA:HMC3	1.95	0.51
1:A2:63:ILE:HB	3:C2:335:THR:HG21	1.91	0.51
2:B1:413:ASP:OD2	2:B1:416:THR:OG1	2.26	0.51
2:B1:462:PHE:CZ	25:B1:615:CLA:HMB3	2.46	0.51
25:B2:618:CLA:HBB1	25:B2:618:CLA:HHC	1.93	0.51
1:A1:131:TRP:HZ2	3:C1:449:ARG:HG3	1.82	0.51
16:V1:34:ASN:HA	16:V1:38:SER:OG	2.11	0.51
2:B2:120:LEU:HD13	25:B2:619:CLA:HMD2	37.68	0.51
3:C1:416:SER:HB2	16:V1:42:VAL:HG23	1.93	0.51
25:A1:405:CLA:HBB1	25:A1:405:CLA:HHC	1.91	0.51
3:C1:34:ALA:O	3:C1:38:GLY:N	2.48	0.51
25:C2:503:CLA:H52	25:C2:505:CLA:H91	1.91	0.51
3:C1:433:LEU:HD22	25:C1:503:CLA:HMC3	1.93	0.51
1:A2:64:ARG:NH1	13:O2:105:ALA:O	2.54	0.51
33:B1:621:LHG:H262	4:D1:277:THR:HG23	1.92	0.51
13:O2:199:LEU:HA	13:O2:215:PHE:CA	2.50	0.51
25:B2:614:CLA:HMB1	25:B2:614:CLA:HBB1	1.92	0.50
25:C1:502:CLA:C2D	25:C1:504:CLA:H2	2.42	0.50
3:C1:279:LEU:HD22	25:C1:510:CLA:HED3	1.92	0.50
15:U1:38:PHE:HB3	15:U1:78:TYR:CD1	2.47	0.50
15:U1:92:PHE:O	15:U1:97:ARG:NH1	2.40	0.50
16:V2:34:ASN:HA	16:V2:38:SER:OG	2.11	0.50
3:C1:435:PHE:HD1	34:C1:516:DGD:HBH2	1.75	0.50
3:C2:192:GLY:HA2	21:Q2:146:VAL:O	2.11	0.50
4:D1:232:PHE:CE2	33:D1:404:LHG:HC42	2.46	0.50
4:D2:161:PRO:HB3	4:D2:170:ALA:HB2	1.94	0.50
1:A1:308:ASP:OD1	1:A1:312:ARG:N	2.41	0.50
25:B1:617:CLA:H171	7:H1:7:LEU:HD21	1.92	0.50
4:D1:161:PRO:HB3	4:D1:170:ALA:HB2	1.94	0.50
7:H1:7:LEU:HB2	20:W1:21:VAL:HG11	2.05	0.50
25:B2:618:CLA:H122	20:W2:18:LEU:HD21	6.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C2:175:LEU:HD23	3:C2:237:HIS:CD2	2.48	0.50
29:I2:101:LMG:HC71	19:S2:6:LEU:HB3	1.93	0.50
13:O1:199:LEU:HA	13:O1:215:PHE:CA	2.38	0.50
13:O1:53:GLU:HA	13:O1:65:PHE:HA	2.01	0.50
2:B1:6:TYR:CD1	2:B1:7:ARG:HG3	2.46	0.50
25:C1:504:CLA:HMC3	35:C1:519:LMT:H122	1.92	0.50
4:D2:261:PHE:CZ	33:D2:405:LHG:HC81	2.46	0.50
1:A1:2:THR:HA	3:C1:152:ARG:HH11	1.77	0.50
1:A2:308:ASP:OD1	1:A2:312:ARG:N	2.41	0.50
2:B1:120:LEU:HD13	25:B1:619:CLA:HMD2	37.65	0.50
7:H1:38:PHE:HB2	23:H1:102:BCR:H10C	1.93	0.50
23:B1:601:BCR:H361	25:B1:616:CLA:HBB1	1.94	0.50
3:C2:220:GLY:H	28:C2:517:UNL:C1	2.24	0.50
16:V2:39:SER:O	16:V2:40:CYS:C	2.49	0.50
25:B2:610:CLA:H202	25:B2:613:CLA:H101	34.32	0.50
1:A1:217:SER:HA	4:D1:272:LEU:HD12	1.96	0.50
4:D2:73:PHE:CD1	29:F2:402:LMG:H291	2.47	0.49
2:B1:91:TRP:HE1	29:B1:622:LMG:HC91	1.76	0.49
3:C2:277:GLY:C	25:C2:506:CLA:HBC3	24.03	0.49
11:L2:26:VAL:HG11	33:L2:101:LHG:H201	1.94	0.49
2:B2:6:TYR:CD1	2:B2:7:ARG:HG3	2.46	0.49
1:A1:2:THR:HA	3:C1:152:ARG:HD2	1.94	0.49
4:D2:286:ILE:HG13	25:D2:401:CLA:HED2	1.93	0.49
25:C1:509:CLA:H8	25:C1:511:CLA:H51	1.93	0.49
33:D2:403:LHG:H101	33:D2:403:LHG:H332	1.94	0.49
13:O1:221:SER:OG	13:O1:222:ASP:N	2.42	0.49
25:B1:615:CLA:HBB1	25:B1:615:CLA:HMB1	1.99	0.49
3:C1:180:LEU:HD21	3:C1:234:ILE:HG21	1.95	0.49
21:Q2:123:ILE:O	21:Q2:126:ALA:HB3	2.13	0.49
15:U2:41:LEU:HA	15:U2:45:ALA:HB3	1.95	0.49
2:B2:413:ASP:OD2	2:B2:416:THR:OG1	2.26	0.49
3:C1:178:LYS:HB2	25:C1:504:CLA:H203	20.16	0.49
13:O1:221:SER:CB	13:O1:233:LEU:HD11	2.39	0.49
2:B1:103:LEU:HB2	25:B1:609:CLA:H62	2.29	0.49
3:C1:147:PHE:CD2	25:C1:514:CLA:H3A	2.47	0.49
16:V1:41:HIS:HA	16:V1:44:GLY:H	1.78	0.49
23:A2:401:BCR:H16C	25:A2:403:CLA:HBC2	1.95	0.49
2:B1:244:ALA:HA	25:B1:606:CLA:H121	1.95	0.49
25:C1:504:CLA:H72	25:C1:504:CLA:H112	1.58	0.49
33:B1:621:LHG:HC12	4:D1:269:PHE:CD2	2.48	0.49
13:O2:146:PHE:HE2	13:O2:197:ILE:H	1.70	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:45:THR:HG23	25:A1:406:CLA:H201	1.95	0.48
1:A2:183:MET:HB3	25:A2:402:CLA:HBC2	1.94	0.48
2:B1:243:ALA:HA	2:B1:246:PHE:CE2	2.48	0.48
25:B1:612:CLA:H142	25:B1:614:CLA:H2	2.07	0.48
2:B1:441:GLY:C	13:O1:176:ALA:HB3	2.41	0.48
1:A1:121:LEU:HG	34:C1:516:DGD:HAT2	1.93	0.48
27:A2:407:PHO:HAB	4:D2:205:LEU:HD13	1.94	0.48
23:B2:603:BCR:H321	25:B2:609:CLA:H52	2.40	0.48
1:A1:63:ILE:HB	3:C1:335:THR:HG21	1.95	0.48
15:U1:41:LEU:HA	15:U1:45:ALA:HB3	1.95	0.48
1:A1:198:HIS:HA	1:A1:286:THR:HG23	1.96	0.48
25:C1:509:CLA:H2	25:C1:511:CLA:H12	1.95	0.48
3:C2:119:LEU:HG	23:K2:104:BCR:H10C	1.95	0.48
13:O1:201:VAL:C	13:O1:213:GLY:HA3	2.37	0.48
3:C1:393:ALA:HB1	38:V1:201:HEM:HBC1	1.98	0.48
23:B1:601:BCR:H12C	23:B1:602:BCR:HC7	1.95	0.48
25:C2:509:CLA:H2	25:C2:511:CLA:H12	24.54	0.48
4:D1:257:PHE:O	33:D1:405:LHG:H322	2.13	0.48
25:A1:405:CLA:H2	8:I1:12:VAL:HG11	1.95	0.48
25:C2:509:CLA:H111	25:C2:509:CLA:H91	1.65	0.48
2:B1:432:PHE:HD2	13:O1:178(B):ASP:HB3	1.78	0.48
2:B2:357:ARG:NH2	4:D2:337:GLU:O	2.52	0.48
3:C1:237:HIS:HA	3:C1:240:ILE:HG22	1.95	0.48
25:C1:512:CLA:H112	25:C1:512:CLA:H152	2.91	0.48
1:A2:267:ASN:ND2	4:D2:232:PHE:O	2.46	0.48
16:V1:39:SER:O	16:V1:40:CYS:C	2.51	0.48
1:A2:217:SER:HA	4:D2:272:LEU:HD12	1.96	0.48
3:C2:34:ALA:O	3:C2:38:GLY:N	2.47	0.48
1:A1:250:ALA:HB1	4:D1:138:LEU:HD21	1.96	0.48
10:K2:14:THR:O	10:K2:16:ASN:N	2.47	0.48
15:U1:27:VAL:HG11	15:U1:61:ILE:HD11	1.97	0.48
25:A2:402:CLA:H72	25:A2:402:CLA:H112	1.66	0.48
1:A2:82:VAL:HB	1:A2:174:LEU:HB2	1.96	0.48
2:B2:243:ALA:HA	2:B2:246:PHE:CE2	2.48	0.48
25:C1:509:CLA:H12	25:C1:513:CLA:HBC2	1.96	0.48
2:B1:460:LEU:O	2:B1:463:PHE:HB3	2.15	0.48
2:B2:69:LEU:HD21	25:B2:606:CLA:HMD1	2.07	0.48
4:D1:210:LEU:HD21	36:D1:408:PL9:H13	1.96	0.48
23:B1:603:BCR:H321	25:B1:609:CLA:H52	1.96	0.47
25:B2:608:CLA:HMA1	25:B2:609:CLA:H3A	1.96	0.47
13:O2:44:CYS:O	13:O2:240:TYR:CA	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:149:LEU:HD23	25:B1:606:CLA:HBC1	2.13	0.47
25:B2:606:CLA:H192	25:B2:610:CLA:H152	8.50	0.47
4:D2:210:LEU:HD21	36:D2:408:PL9:H13	1.96	0.47
1:A2:198:HIS:HA	1:A2:286:THR:HG23	1.96	0.47
23:B1:601:BCR:H362	25:B1:616:CLA:H71	2.14	0.47
1:A2:257:ARG:NH1	2:B2:490:VAL:O	2.34	0.47
4:D2:269:PHE:CG	33:D2:403:LHG:HC12	2.59	0.47
13:O1:215:PHE:CE1	13:O1:237:GLY:HA3	2.59	0.47
3:C2:192:GLY:HA2	21:Q2:146:VAL:C	2.35	0.47
2:B1:419:LYS:HG2	2:B1:423:LYS:HE2	1.96	0.47
1:A1:300:LEU:HD23	3:C1:404:LEU:HB3	1.95	0.47
33:D2:405:LHG:O1	33:L2:101:LHG:O4	2.23	0.47
13:O1:201:VAL:CG1	13:O1:202:ASN:H	2.24	0.47
13:O2:197:ILE:CG1	13:O2:198:GLU:H	2.27	0.47
2:B2:22:VAL:HG22	25:B2:616:CLA:HMB3	1.96	0.47
25:C1:505:CLA:C4D	34:C1:515:DGD:HB21	2.45	0.47
23:J1:101:BCR:H21C	23:J1:101:BCR:H361	1.96	0.47
1:A1:179:THR:O	1:A1:183:MET:HG3	2.16	0.47
2:B2:462:PHE:CZ	25:B2:615:CLA:HMB3	2.54	0.47
10:K1:14:THR:O	10:K1:16:ASN:N	2.48	0.47
10:K1:11:LEU:HD11	10:K1:22:ILE:HD12	1.97	0.47
13:O1:146:PHE:HE2	13:O1:197:ILE:H	1.52	0.47
13:O1:198:GLU:N	13:O1:216:VAL:O	2.46	0.47
1:A2:179:THR:O	1:A2:183:MET:HG3	2.16	0.47
34:H1:101:DGD:HBF1	34:H1:101:DGD:HBE2	1.74	0.47
25:B2:606:CLA:H152	7:H2:38:PHE:HE2	1.80	0.47
13:O2:19:CYS:SG	13:O2:45:LEU:O	2.72	0.47
13:O2:215:PHE:CE1	13:O2:237:GLY:HA3	3.10	0.47
33:D2:405:LHG:H292	14:T2:17:ILE:HG23	1.96	0.47
14:T2:2:GLU:CD	14:T2:2:GLU:H	2.18	0.47
25:B2:615:CLA:H143	25:B2:615:CLA:H111	3.25	0.47
13:O1:118:PHE:CD1	13:O1:233:LEU:HD22	2.50	0.47
14:T1:2:GLU:CD	14:T1:2:GLU:H	2.18	0.47
1:A1:183:MET:HA	25:A1:403:CLA:HMD2	1.96	0.47
2:B1:120:LEU:HD13	25:B1:618:CLA:HMD2	1.97	0.47
2:B2:460:LEU:O	2:B2:463:PHE:HB3	2.15	0.47
3:C1:287:ALA:HB1	3:C1:427:THR:HG23	1.99	0.47
1:A1:330:VAL:HG21	4:D1:328:TRP:CE2	2.51	0.47
13:O2:197:ILE:HG13	13:O2:217:SER:CB	2.43	0.47
15:U1:92:PHE:HA	15:U1:97:ARG:HD3	1.98	0.47
2:B2:254:GLY:HA2	34:H2:101:DGD:HBW1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C2:371:SER:HB3	3:C2:376:ASP:HB2	1.96	0.47
13:O1:196:ARG:N	13:O1:218:GLU:O	2.48	0.47
23:B1:602:BCR:H11C	23:B1:602:BCR:H341	1.79	0.47
25:B2:617:CLA:H101	25:B2:617:CLA:H13	1.66	0.47
3:C2:287:ALA:HB1	3:C2:427:THR:HG23	1.98	0.47
2:B2:497:LYS:NZ	4:D2:20:ASP:OD1	2.31	0.47
25:B1:606:CLA:H62	25:B1:606:CLA:H41	1.93	0.46
4:D2:43:LEU:HD22	23:F2:401:BCR:H323	1.97	0.46
23:J1:101:BCR:H24C	23:J1:101:BCR:H371	1.70	0.46
25:C1:511:CLA:H203	10:K1:33:LEU:HD22	1.97	0.46
13:O2:198:GLU:N	13:O2:216:VAL:O	2.73	0.46
1:A1:283:ILE:HG13	27:A1:408:PHO:HBC3	1.96	0.46
33:A2:405:LHG:HC42	4:D2:232:PHE:CE2	2.50	0.46
23:B1:603:BCR:H341	23:B1:603:BCR:H11C	1.81	0.46
25:C1:508:CLA:H41	25:C1:508:CLA:H62	1.64	0.46
23:C2:502:BCR:H372	25:C2:510:CLA:HMC2	1.97	0.46
25:C2:505:CLA:H51	25:C2:505:CLA:H8	1.62	0.46
6:F1:41:GLN:HG3	9:J1:31:GLY:HA3	1.98	0.46
2:B1:117:TYR:HA	11:L1:1:SER:HB2	2.12	0.46
13:O1:83:GLY:HA3	13:O1:95:PHE:CE1	2.49	0.46
3:C1:40:ALA:N	25:C1:509:CLA:HAA2	2.31	0.46
33:D1:405:LHG:O1	33:L1:101:LHG:O4	2.20	0.46
1:A1:82:VAL:HB	1:A1:174:LEU:HB2	1.97	0.46
1:A2:131:TRP:HZ2	3:C2:449:ARG:HG3	1.80	0.46
2:B1:369:ILE:HD11	4:D1:345:VAL:HG21	2.04	0.46
25:B1:604:CLA:HAB	23:H1:102:BCR:H15C	1.98	0.46
25:C1:503:CLA:H72	25:C1:504:CLA:NB	2.30	0.46
25:B1:610:CLA:HBB2	4:D1:123:ILE:HG12	1.98	0.46
11:L2:24:ILE:HD11	33:L2:101:LHG:H292	4.43	0.46
15:U2:92:PHE:HA	15:U2:97:ARG:HD3	1.98	0.46
25:B1:613:CLA:HMD1	33:B1:621:LHG:O7	2.16	0.46
4:D1:273:PHE:CZ	4:D1:277:THR:HG21	2.50	0.46
23:F2:401:BCR:H341	23:F2:401:BCR:H11C	1.81	0.46
25:B1:608:CLA:H41	25:B1:608:CLA:H62	1.82	0.46
25:B2:613:CLA:H142	25:B2:613:CLA:H111	1.69	0.46
6:F1:28:ILE:HB	6:F1:29:PRO:HD3	1.99	0.46
23:H1:102:BCR:H351	23:H1:102:BCR:H15C	1.73	0.46
15:U1:38:PHE:HB2	15:U1:41:LEU:HD12	1.98	0.46
2:B2:212:ALA:HB2	25:B2:610:CLA:HMC3	21.89	0.46
29:A1:410:LMG:H352	34:C1:516:DGD:HB41	1.98	0.46
25:D2:404:CLA:H91	25:D2:404:CLA:H112	1.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K1:22:ILE:HA	10:K1:25:MET:HG2	1.98	0.46
3:C1:279:LEU:HD22	25:C1:511:CLA:HED2	13.75	0.46
25:C1:504:CLA:H8	25:C1:504:CLA:H51	1.83	0.46
20:W1:17:VAL:O	20:W1:21:VAL:HG23	2.17	0.46
1:A2:183:MET:HA	25:A2:404:CLA:HMD2	12.56	0.45
2:B1:237:VAL:HG22	25:B1:612:CLA:HBC2	1.98	0.45
23:B2:601:BCR:H15C	23:B2:601:BCR:H351	1.75	0.45
25:C1:507:CLA:H101	25:C1:507:CLA:H61	4.40	0.45
3:C2:41:ARG:NH1	25:K2:101:CLA:OBD	2.47	0.45
20:W2:17:VAL:O	20:W2:21:VAL:HG23	2.17	0.45
23:B1:602:BCR:H351	23:B1:602:BCR:H15C	1.86	0.45
2:B2:242:ILE:HG12	25:B2:612:CLA:HBB1	12.17	0.45
2:B2:338:GLU:HB2	2:B2:431:GLU:CB	2.46	0.45
25:C2:504:CLA:HMB1	25:C2:506:CLA:HMC3	1.96	0.45
23:K1:101:BCR:H341	23:K1:101:BCR:H11C	1.85	0.45
23:K2:102:BCR:H24C	23:K2:102:BCR:H371	1.70	0.45
1:A1:329:GLU:O	1:A1:332:HIS:ND1	2.49	0.45
1:A2:256:GLY:HA3	2:B2:492:PHE:HZ	1.81	0.45
4:D2:348:ARG:HH12	16:V2:135:ILE:HD11	1.81	0.45
25:B1:606:CLA:H72	25:B1:606:CLA:H112	1.54	0.45
4:D2:121:GLY:HA3	27:D2:407:PHO:H41	1.97	0.45
23:J1:101:BCR:HC31	10:K1:21:ILE:HD11	1.98	0.45
1:A1:304:GLN:HG2	1:A1:313:VAL:HG11	2.02	0.45
23:B1:601:BCR:HC8	23:B1:602:BCR:HC42	1.98	0.45
25:B1:616:CLA:H62	25:B1:616:CLA:H41	1.89	0.45
12:M1:13:LEU:HD23	12:M1:13:LEU:HA	1.78	0.45
25:A1:404:CLA:H2	8:I1:12:VAL:HG11	45.96	0.45
23:B1:603:BCR:H351	23:B1:603:BCR:H15C	1.82	0.45
25:B2:604:CLA:HAB	23:H2:103:BCR:H15C	1.99	0.45
25:B2:613:CLA:HMB1	25:B2:613:CLA:HBB1	1.99	0.45
14:T1:25:ASP:HA	14:T1:26:PRO:HD3	1.85	0.45
1:A1:105:TRP:NE1	1:A1:110:GLY:HA3	2.33	0.45
25:B2:612:CLA:H161	25:B2:612:CLA:H121	3.11	0.45
3:C1:208:ILE:O	3:C1:211:SER:HB3	2.17	0.45
4:D1:144:ILE:O	4:D1:147:SER:N	2.48	0.45
13:O1:200:ALA:O	13:O1:214:VAL:N	2.51	0.45
25:B2:606:CLA:C2D	25:B2:608:CLA:H2	3.29	0.45
4:D1:18:LEU:HA	18:X1:32:VAL:HG21	2.45	0.45
11:L2:23:LEU:HD13	33:L2:101:LHG:H142	3.34	0.45
2:B1:273:TYR:HA	2:B1:276:ASP:HB2	2.00	0.45
2:B2:110:ALA:HB2	23:B2:603:BCR:H17C	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:440:ASP:OD2	2:B2:444:ARG:NH2	2.37	0.45
23:B2:603:BCR:H371	23:B2:603:BCR:H24C	1.85	0.45
25:C2:503:CLA:H41	25:C2:503:CLA:H61	1.77	0.45
13:O2:196:ARG:N	13:O2:218:GLU:O	2.79	0.45
25:B1:616:CLA:H202	25:B1:616:CLA:H162	1.79	0.45
3:C1:100:ALA:HB3	3:C1:104:GLU:HB3	1.99	0.45
4:D2:273:PHE:CD1	33:D2:403:LHG:H242	2.52	0.45
13:O1:109:GLN:NE2	13:O1:115:ARG:HE	2.16	0.45
13:O2:197:ILE:HG12	13:O2:198:GLU:H	1.82	0.45
16:V1:72:LEU:O	16:V1:76:MET:HG3	2.17	0.45
25:B1:612:CLA:H203	25:B1:612:CLA:H161	1.87	0.44
25:B2:613:CLA:H2	25:B2:613:CLA:H61	1.79	0.44
3:C1:243:THR:HG22	25:C1:507:CLA:HMC1	1.99	0.44
3:C1:435:PHE:CD1	34:C1:516:DGD:HBH2	2.51	0.44
4:D1:261:PHE:CZ	33:D1:405:LHG:HC81	2.52	0.44
33:D1:405:LHG:HC92	36:D1:408:PL9:H111	1.99	0.44
36:D1:408:PL9:H352	11:L1:26:VAL:CG1	2.46	0.44
16:V2:39:SER:HB2	16:V2:40:CYS:H	1.39	0.44
25:A1:403:CLA:H193	25:A1:403:CLA:H161	2.17	0.44
25:A1:405:CLA:H42	8:I1:9:TYR:CE2	2.52	0.44
1:A2:329:GLU:O	1:A2:332:HIS:ND1	2.49	0.44
25:A2:403:CLA:H11	8:I2:9:TYR:CE1	2.52	0.44
1:A2:283:ILE:HG13	27:A2:407:PHO:HBC3	1.98	0.44
23:B2:602:BCR:H361	23:B2:602:BCR:H20C	1.85	0.44
25:B2:615:CLA:H112	25:B2:615:CLA:H72	2.57	0.44
12:M2:18:PRO:O	12:M2:21:PHE:HB3	2.17	0.44
1:A1:64:ARG:NH1	13:O1:105:ALA:O	2.48	0.44
13:O2:200:ALA:O	13:O2:214:VAL:N	2.77	0.44
2:B1:440:ASP:OD2	2:B1:444:ARG:NH2	2.38	0.44
3:C2:208:ILE:O	3:C2:211:SER:HB3	2.17	0.44
3:C2:55:ALA:HB1	23:K2:104:BCR:H373	1.98	0.44
4:D1:199:MET:HG2	36:D1:408:PL9:H311	1.99	0.44
4:D2:193:LEU:O	11:L2:34:TYR:OH	2.23	0.44
25:A1:404:CLA:H42	8:I1:9:TYR:CE2	48.79	0.44
7:H2:7:LEU:HB2	20:W2:21:VAL:HG11	2.00	0.44
2:B1:80:ILE:H	2:B1:80:ILE:HG13	1.59	0.44
1:A1:239:LEU:HD22	14:T1:27:PRO:HB2	2.06	0.44
15:U1:14:TYR:O	15:U1:17:ILE:HG13	2.17	0.44
25:C2:506:CLA:H62	25:C2:506:CLA:H102	4.97	0.44
1:A1:307:VAL:HB	6:F1:45:ARG:HD2	1.99	0.44
1:A1:188:ALA:HB2	1:A1:328:ILE:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:259:ILE:HG22	1:A2:260:PHE:CD2	2.52	0.44
2:B2:273:TYR:HA	2:B2:276:ASP:HB2	2.00	0.44
2:B2:413:ASP:OD1	2:B2:413:ASP:N	2.51	0.44
2:B2:248:ALA:HB2	25:B2:606:CLA:H61	2.61	0.44
25:B2:610:CLA:H62	25:B2:610:CLA:H92	1.93	0.44
3:C1:39:ASN:HB2	25:C1:510:CLA:O1A	15.21	0.44
25:B2:616:CLA:HMD1	12:M2:25:LEU:HD21	2.00	0.44
13:O2:45:LEU:N	13:O2:45:LEU:HD12	2.31	0.44
1:A2:340:PRO:HD3	15:U2:103:TYR:CZ	2.62	0.44
1:A1:96:ILE:HG12	1:A1:105:TRP:CE2	2.53	0.44
2:B1:221:PRO:HA	25:B1:611:CLA:HED3	3.14	0.44
2:B2:185:TRP:HB3	25:B2:604:CLA:HMA3	2.25	0.44
25:B2:606:CLA:H41	25:B2:606:CLA:H62	1.71	0.44
3:C1:139:VAL:HG13	3:C1:141:GLU:OE2	2.18	0.44
25:C1:512:CLA:H161	25:C1:512:CLA:H121	1.62	0.44
3:C2:437:ILE:HA	25:C2:511:CLA:HMC3	1.99	0.44
13:O2:197:ILE:CG1	13:O2:217:SER:HB2	2.45	0.44
16:V2:52:ILE:HB	38:V2:201:HEM:HAD2	2.00	0.44
23:B2:601:BCR:H12C	23:B2:602:BCR:HC7	2.00	0.44
25:B2:608:CLA:H41	25:B2:608:CLA:H61	1.77	0.44
1:A1:131:TRP:CZ2	3:C1:449:ARG:HG3	2.59	0.44
23:K1:101:BCR:H321	23:K1:101:BCR:HC8	2.00	0.44
10:K1:20:PRO:O	10:K1:23:ASP:HB2	2.17	0.44
13:O1:48:LYS:O	13:O1:49:GLN:CB	2.65	0.44
1:A1:259:ILE:HG22	1:A1:260:PHE:CD2	2.52	0.44
2:B1:247:PHE:HE1	25:B1:605:CLA:H8	1.83	0.44
3:C1:257:PHE:CD2	25:C1:508:CLA:HED3	18.20	0.44
3:C1:62:PHE:HD2	23:C1:501:BCR:H362	33.93	0.44
1:A2:300:LEU:HD23	3:C2:404:LEU:HB3	2.09	0.44
25:C2:506:CLA:NC	25:C2:506:CLA:H42	7.06	0.44
23:K2:102:BCR:H11C	23:K2:102:BCR:H341	1.82	0.44
14:T2:25:ASP:HA	14:T2:26:PRO:HD3	1.85	0.44
16:V1:39:SER:HB2	16:V1:40:CYS:H	1.33	0.44
1:A1:165:GLN:NE2	40:A1:501:HOH:O	8.36	0.43
1:A2:188:ALA:HB2	1:A2:328:ILE:HB	1.99	0.43
25:B1:619:CLA:H111	25:B1:619:CLA:H93	1.85	0.43
2:B2:305:ILE:HA	2:B2:306:PRO:HD3	1.85	0.43
9:J2:8:ILE:HA	9:J2:9:PRO:HD3	2.01	0.43
13:O2:109:GLN:NE2	13:O2:115:ARG:HE	2.16	0.43
16:V2:39:SER:O	16:V2:41:HIS:N	2.51	0.43
25:B1:613:CLA:H2	25:B1:613:CLA:H61	2.23	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B1:617:CLA:H92	25:B1:617:CLA:H61	1.87	0.43
3:C1:134:ILE:HD13	25:C1:513:CLA:H43	1.99	0.43
23:H2:103:BCR:H15C	23:H2:103:BCR:H351	1.85	0.43
7:H2:22:ALA:HA	7:H2:23:PRO:HD3	1.91	0.43
3:C1:71:GLU:OE1	3:C1:89:LEU:HG	2.19	0.43
23:C2:502:BCR:H15C	23:C2:502:BCR:H351	1.73	0.43
4:D2:144:ILE:O	4:D2:147:SER:N	2.49	0.43
2:B2:464:PHE:HB2	4:D2:280:TRP:CH2	2.67	0.43
22:Z2:5:LEU:HD11	22:Z2:58:ASN:HA	2.00	0.43
23:A2:401:BCR:H16C	25:A2:403:CLA:CBC	2.47	0.43
23:B1:602:BCR:H20C	23:B1:602:BCR:H361	1.93	0.43
25:B1:610:CLA:H42	25:B1:611:CLA:H72	2.00	0.43
3:C2:162:GLY:HA3	3:C2:252:ILE:HG13	2.01	0.43
10:K2:14:THR:HB	10:K2:15:TYR:H	1.68	0.43
10:K2:37:PHE:HB3	23:K2:102:BCR:H271	2.00	0.43
16:V1:135:ILE:H	16:V1:135:ILE:HG12	1.70	0.43
16:V2:72:LEU:O	16:V2:76:MET:HG3	2.19	0.43
2:B1:7:ARG:O	2:B1:8:VAL:C	2.62	0.43
23:B2:603:BCR:H351	23:B2:603:BCR:H15C	1.76	0.43
25:B2:614:CLA:H102	25:B2:614:CLA:H13	1.82	0.43
25:A1:406:CLA:H52	36:D1:408:PL9:H171	2.00	0.43
23:A1:401:BCR:H11C	23:A1:401:BCR:H341	1.85	0.43
3:C2:338:GLY:HA2	13:O2:103:TYR:OH	2.19	0.43
4:D1:297:ASP:OD1	4:D1:297:ASP:N	2.53	0.43
7:H1:22:ALA:HA	7:H1:23:PRO:HD3	1.91	0.43
2:B2:224:ARG:HD3	7:H2:25:TRP:CE2	2.78	0.43
13:O2:198:GLU:O	13:O2:216:VAL:N	2.90	0.43
27:A2:407:PHO:HMB2	25:D2:406:CLA:HMB2	2.01	0.43
2:B1:67:ALA:O	2:B1:178:ILE:HD11	2.18	0.43
2:B1:248:ALA:HA	25:B1:606:CLA:H42	2.00	0.43
23:B2:603:BCR:H20C	23:B2:603:BCR:H361	1.87	0.43
23:B2:603:BCR:H12C	25:B2:619:CLA:H143	37.06	0.43
3:C1:162:GLY:HA3	3:C1:252:ILE:HG13	2.01	0.43
3:C1:243:THR:HG22	25:C1:508:CLA:HMC1	16.83	0.43
3:C2:50:LEU:HD11	25:C2:510:CLA:HBB1	2.01	0.43
3:C2:466:VAL:HG21	4:D2:248:THR:HA	2.04	0.43
4:D2:39:PRO:HB2	25:D2:404:CLA:HAB	2.00	0.43
25:C1:511:CLA:HED3	10:K1:33:LEU:HD13	2.01	0.43
12:M1:18:PRO:O	12:M1:21:PHE:HB3	2.19	0.43
1:A2:259:ILE:HD11	27:D2:407:PHO:HED2	2.01	0.43
23:A2:401:BCR:H341	23:A2:401:BCR:H11C	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:254:GLY:HA2	34:H1:101:DGD:HBW1	2.10	0.43
3:C1:180:LEU:HD22	3:C1:199:ILE:O	2.19	0.43
25:C2:506:CLA:HBC2	25:C2:506:CLA:HMC1	4.33	0.43
1:A1:267:ASN:ND2	4:D1:232:PHE:O	2.59	0.43
12:M2:18:PRO:HA	12:M2:21:PHE:HB3	2.01	0.43
25:A1:403:CLA:H72	25:A1:403:CLA:H112	1.96	0.43
25:B1:606:CLA:H161	25:B1:606:CLA:H141	1.78	0.43
25:B1:613:CLA:H143	25:B1:613:CLA:H111	1.86	0.43
23:B2:602:BCR:H11C	23:B2:602:BCR:H341	1.77	0.43
25:B2:610:CLA:H141	25:B2:610:CLA:H162	2.55	0.43
8:I2:28:PRO:O	8:I2:31:ASN:ND2	2.53	0.43
13:O1:198:GLU:O	13:O1:216:VAL:N	2.44	0.43
4:D1:348:ARG:HH12	16:V1:135:ILE:HD11	1.95	0.43
38:V1:201:HEM:HMB2	38:V1:201:HEM:HBB2	3.40	0.43
25:A1:404:CLA:C4A	25:A1:404:CLA:HBA2	2.49	0.43
2:B1:173:GLY:HA3	2:B1:265:ILE:HD11	2.01	0.43
25:B1:608:CLA:H192	25:B1:608:CLA:H162	1.83	0.43
23:B2:601:BCR:H11C	23:B2:601:BCR:H341	1.85	0.43
25:C2:505:CLA:H112	25:C2:505:CLA:H72	1.42	0.43
13:O2:197:ILE:HG12	13:O2:198:GLU:N	2.34	0.43
15:U2:89:PRO:HA	15:U2:92:PHE:HB3	2.01	0.43
1:A1:133:LEU:HD23	4:D1:256:ILE:HG12	2.04	0.42
2:B1:305:ILE:HA	2:B1:306:PRO:HD3	1.85	0.42
23:B2:601:BCR:H371	23:B2:601:BCR:H24C	1.83	0.42
25:B2:608:CLA:H192	25:B2:608:CLA:H162	1.79	0.42
2:B2:67:ALA:O	2:B2:178:ILE:HD11	2.19	0.42
23:C2:502:BCR:H24C	23:C2:502:BCR:H371	1.86	0.42
29:A2:412:LMG:HC5	2:B2:75:TRP:HB3	65.27	0.42
25:B2:611:CLA:H161	25:B2:611:CLA:H203	4.00	0.42
4:D1:79:SER:HA	4:D1:172:SER:HB3	2.00	0.42
33:D2:403:LHG:H383	33:D2:403:LHG:HC81	2.00	0.42
33:D2:405:LHG:H151	25:D2:406:CLA:H61	2.01	0.42
5:E2:22:ILE:O	5:E2:25:ILE:HG22	2.19	0.42
12:M1:18:PRO:HA	12:M1:21:PHE:HB3	2.01	0.42
15:U1:55:TYR:HB3	15:U1:60:ASP:HB2	2.01	0.42
18:X2:12:TRP:HD1	18:X2:16:TRP:HE1	1.70	0.42
1:A2:52:PHE:CD1	36:D2:408:PL9:H48	2.54	0.42
2:B1:464:PHE:CE2	33:B1:621:LHG:H252	2.54	0.42
25:C1:512:CLA:H111	25:C1:512:CLA:H91	4.45	0.42
3:C2:209:ILE:O	3:C2:212:TYR:HB2	2.20	0.42
1:A2:330:VAL:HG21	4:D2:328:TRP:CE2	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:E2:101:HEM:ND	6:F2:24:HIS:NE2	2.67	0.42
16:V1:76:MET:HG2	38:V1:201:HEM:HMB3	3.33	0.42
23:A1:401:BCR:H361	23:A1:401:BCR:H20C	1.87	0.42
23:C1:501:BCR:H361	23:C1:501:BCR:H20C	2.01	0.42
6:F2:38:THR:O	6:F2:41:GLN:HB2	2.20	0.42
15:U2:90:GLU:HG3	15:U2:90:GLU:H	1.48	0.42
2:B1:204:ALA:CB	25:B1:605:CLA:HAB	2.65	0.42
2:B1:247:PHE:CD2	25:B1:606:CLA:H122	2.54	0.42
23:B2:602:BCR:H351	23:B2:602:BCR:H15C	1.82	0.42
23:C1:501:BCR:H351	23:C1:501:BCR:H15C	1.76	0.42
1:A2:250:ALA:HB1	4:D2:138:LEU:HD21	2.05	0.42
33:D2:403:LHG:H362	33:D2:403:LHG:H332	2.27	0.42
4:D2:274:VAL:HG13	36:D2:408:PL9:H252	2.00	0.42
13:O1:234:LEU:C	13:O1:235:LEU:HD23	2.41	0.42
1:A1:260:PHE:CE1	1:A1:263:ALA:HB2	2.55	0.42
1:A2:147:PHE:O	1:A2:150:PRO:HD2	2.20	0.42
25:B2:613:CLA:H72	25:B2:613:CLA:H112	1.82	0.42
25:C1:510:CLA:HAB	25:C1:512:CLA:HMA1	19.84	0.42
4:D1:261:PHE:HB2	36:D1:408:PL9:H522	2.01	0.42
23:H2:103:BCR:H341	23:H2:103:BCR:H11C	1.94	0.42
3:C2:28:ILE:HG13	10:K2:45:PHE:HE2	1.85	0.42
25:A1:403:CLA:CAB	25:A1:404:CLA:HMD2	2.50	0.42
1:A2:234:ASN:HD21	33:D2:403:LHG:HC11	1.85	0.42
2:B2:339:ALA:H	2:B2:431:GLU:CB	2.33	0.42
25:B2:608:CLA:HBB1	25:B2:609:CLA:H51	3.44	0.42
25:C2:507:CLA:CMD	25:C2:509:CLA:HAB	2.49	0.42
1:A1:136:ARG:NH1	8:I1:27:ASP:OD1	2.51	0.42
13:O2:122:ILE:HD12	13:O2:122:ILE:HA	1.93	0.42
13:O2:50:PHE:CD1	13:O2:235:LEU:HD22	2.69	0.42
3:C2:78:GLU:HB3	16:V2:102:PRO:O	2.22	0.42
1:A2:39:PRO:HB2	25:A2:403:CLA:HBB1	2.01	0.42
25:A2:403:CLA:H62	8:I2:12:VAL:HG12	2.02	0.42
33:B1:621:LHG:H332	33:B1:621:LHG:H101	2.02	0.42
2:B2:91:TRP:HE1	29:B2:620:LMG:HC91	1.84	0.42
23:C1:501:BCR:H24C	23:C1:501:BCR:H371	1.93	0.42
1:A1:212:SER:OG	4:D1:271:LEU:HB2	2.23	0.42
10:K1:22:ILE:HA	10:K1:25:MET:CG	2.50	0.42
13:O1:50:PHE:CD1	13:O1:235:LEU:HD22	2.55	0.42
25:B1:612:CLA:H51	25:B1:612:CLA:H8	2.38	0.42
25:B2:606:CLA:H93	25:B2:606:CLA:H112	2.01	0.42
25:B2:609:CLA:H91	25:B2:609:CLA:H112	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C2:205:ASN:HA	3:C2:206:PRO:HD3	1.94	0.42
4:D1:273:PHE:O	4:D1:277:THR:OG1	2.30	0.42
4:D2:54:PHE:O	5:E2:49:THR:OG1	2.23	0.42
13:O2:47:PRO:HA	13:O2:237:GLY:HA3	2.01	0.42
15:U1:32:VAL:HG23	15:U1:97:ARG:O	2.20	0.42
15:U1:89:PRO:HA	15:U1:92:PHE:HB3	2.02	0.42
23:A1:401:BCR:H371	23:A1:401:BCR:H24C	1.93	0.42
1:A1:183:MET:HB3	25:A1:403:CLA:HBC2	2.09	0.42
2:B2:117:TYR:HA	11:L2:1:SER:HB2	2.03	0.42
25:B2:612:CLA:H2	25:B2:612:CLA:H61	4.49	0.42
25:B2:612:CLA:H51	25:B2:612:CLA:H8	1.83	0.42
3:C1:190:ALA:HA	3:C1:191:PRO:HD3	1.91	0.42
25:C1:509:CLA:H91	25:C1:509:CLA:H111	4.17	0.42
23:C2:502:BCR:H341	23:C2:502:BCR:H11C	1.84	0.42
25:B1:605:CLA:H141	25:B1:605:CLA:H161	1.79	0.41
25:B1:610:CLA:H111	25:B1:610:CLA:H91	1.73	0.41
2:B2:42:LEU:HD13	2:B2:94:GLU:HG3	2.02	0.41
1:A1:147:PHE:O	1:A1:150:PRO:HD2	2.20	0.41
2:B1:383:PHE:CZ	13:O1:167:GLY:HA2	2.55	0.41
25:B1:610:CLA:CBB	4:D1:123:ILE:HG12	2.50	0.41
2:B1:145:LEU:HD11	25:B1:617:CLA:HMB2	2.05	0.41
2:B2:173:GLY:HA3	2:B2:265:ILE:HD11	2.02	0.41
3:C1:464:GLU:HA	3:C1:465:PRO:HD3	1.88	0.41
23:C1:521:BCR:H351	23:C1:521:BCR:H15C	1.77	0.41
23:J1:101:BCR:H19C	10:K1:35:LEU:HA	2.02	0.41
10:K1:14:THR:HB	10:K1:15:TYR:H	1.68	0.41
1:A2:33:PHE:O	1:A2:125:ALA:HB1	2.21	0.41
1:A2:260:PHE:CE1	1:A2:263:ALA:HB2	2.55	0.41
2:B2:22:VAL:HG22	25:B2:617:CLA:HMB3	20.00	0.41
2:B2:33:TRP:HE1	25:B2:619:CLA:C3C	2.33	0.41
3:C1:279:LEU:HD13	25:C1:510:CLA:HED1	2.02	0.41
25:C1:512:CLA:H152	25:C1:512:CLA:HMA2	2.01	0.41
3:C2:38:GLY:HA3	25:K2:101:CLA:HMD3	2.01	0.41
16:V1:42:VAL:CG1	16:V1:42:VAL:O	2.69	0.41
2:B1:172:TYR:CE1	2:B1:283:GLU:HB2	2.56	0.41
23:B2:603:BCR:H341	23:B2:603:BCR:H11C	1.79	0.41
2:B2:103:LEU:HB2	25:B2:609:CLA:H62	3.20	0.41
25:C1:506:CLA:H112	25:C1:506:CLA:H143	2.53	0.41
3:C1:437:ILE:HA	25:C1:510:CLA:HMC3	14.40	0.41
3:C1:57:ALA:O	3:C1:61:VAL:HG23	2.22	0.41
3:C1:76:ILE:HA	3:C1:77:PRO:HD3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C2:464:GLU:HA	3:C2:465:PRO:HD3	1.88	0.41
23:D1:401:BCR:H341	23:D1:401:BCR:H11C	1.77	0.41
25:A1:404:CLA:H2	27:D1:407:PHO:HMB3	2.02	0.41
8:I1:28:PRO:O	8:I1:31:ASN:ND2	2.54	0.41
33:D2:403:LHG:O2	33:L2:101:LHG:O5	2.37	0.41
13:O1:40:VAL:HB	13:O1:95:PHE:CE1	2.65	0.41
1:A1:161:TYR:HA	1:A1:294:ALA:CB	2.52	0.41
1:A1:161:TYR:HB3	1:A1:162:PRO:HD3	2.02	0.41
25:A1:406:CLA:HBA2	25:A1:406:CLA:C4A	2.51	0.41
29:A1:412:LMG:H352	29:A1:412:LMG:H381	1.91	0.41
2:B1:243:ALA:HA	2:B1:246:PHE:CD2	2.56	0.41
2:B1:413:ASP:N	2:B1:413:ASP:OD1	2.51	0.41
23:B1:601:BCR:H371	23:B1:601:BCR:H24C	1.82	0.41
25:B1:604:CLA:CAB	23:H1:102:BCR:H15C	2.50	0.41
25:B1:609:CLA:H161	25:B1:609:CLA:H192	4.33	0.41
3:C1:209:ILE:O	3:C1:212:TYR:HB2	2.20	0.41
3:C1:326:ALA:HB2	15:U1:98:VAL:HG21	2.21	0.41
23:C1:521:BCR:H371	23:C1:521:BCR:H24C	1.78	0.41
25:C2:505:CLA:H111	25:C2:505:CLA:H93	3.65	0.41
25:C2:513:CLA:HBA1	25:C2:513:CLA:H3A	1.82	0.41
4:D2:297:ASP:OD1	4:D2:297:ASP:N	2.54	0.41
4:D2:39:PRO:O	4:D2:43:LEU:HG	2.21	0.41
6:F2:38:THR:O	6:F2:41:GLN:N	2.53	0.41
13:O2:48:LYS:O	13:O2:49:GLN:CB	2.80	0.41
25:A2:403:CLA:H11	8:I2:9:TYR:CZ	2.55	0.41
2:B1:233:ASN:O	2:B1:236:THR:HG22	2.21	0.41
2:B2:172:TYR:CE1	2:B2:283:GLU:HB2	2.56	0.41
25:C1:507:CLA:H61	25:C1:507:CLA:H92	1.75	0.41
25:C1:507:CLA:H91	25:C1:507:CLA:H111	3.20	0.41
25:C2:503:CLA:HBA2	25:C2:503:CLA:HBD	2.81	0.41
6:F1:38:THR:O	6:F1:41:GLN:HB2	2.21	0.41
7:H2:56:GLU:HG3	7:H2:57:ASN:H	1.86	0.41
13:O1:122:ILE:HD12	13:O1:122:ILE:HA	1.91	0.41
23:A1:401:BCR:H351	23:A1:401:BCR:H15C	1.80	0.41
2:B1:68:ARG:HB3	2:B1:69:LEU:HD12	2.03	0.41
2:B2:125:ASP:HA	2:B2:126:PRO:HD3	1.88	0.41
25:B2:611:CLA:H162	25:B2:611:CLA:H141	1.65	0.41
23:B2:602:BCR:HC41	29:B2:621:LMG:H181	2.02	0.41
25:C1:506:CLA:HBB1	25:C1:506:CLA:HMB1	2.88	0.41
25:D2:406:CLA:H13	36:D2:408:PL9:H452	2.03	0.41
33:D1:405:LHG:HC91	11:L1:19:TRP:HZ2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:432:PHE:HD2	13:O2:178(B):ASP:HB3	2.21	0.41
1:A1:140:ARG:HB2	4:D1:220:ASN:HA	2.03	0.41
1:A2:161:TYR:HB3	1:A2:162:PRO:HD3	2.02	0.41
23:A2:401:BCR:H15C	23:A2:401:BCR:H351	1.85	0.41
2:B1:97:ALA:O	2:B1:101:ILE:HG12	2.21	0.41
2:B1:155:ALA:O	2:B1:159:THR:OG1	2.37	0.41
23:B1:603:BCR:H24C	23:B1:603:BCR:H371	1.95	0.41
25:B1:606:CLA:H18	25:B1:611:CLA:H8	4.28	0.41
2:B2:233:ASN:O	2:B2:236:THR:HG22	2.21	0.41
2:B2:243:ALA:HA	2:B2:246:PHE:CD2	2.56	0.41
23:C1:501:BCR:H313	10:K1:18:PHE:CD2	51.08	0.41
25:C2:503:CLA:CHA	25:C2:503:CLA:HBA1	2.47	0.41
4:D2:273:PHE:HD1	33:D2:403:LHG:H242	1.86	0.41
11:L1:18:PHE:HE1	35:L1:102:LMT:H72	1.85	0.41
1:A1:33:PHE:O	1:A1:125:ALA:HB1	2.21	0.41
25:A1:406:CLA:H62	25:A1:406:CLA:H92	1.89	0.41
25:A1:405:CLA:H43	29:A1:410:LMG:H111	2.02	0.41
1:A2:133:LEU:HD23	4:D2:256:ILE:HG12	2.02	0.41
1:A2:212:SER:OG	4:D2:271:LEU:HB2	2.25	0.41
2:B1:42:LEU:HD13	2:B1:94:GLU:HG3	2.03	0.41
23:B1:601:BCR:H351	23:B1:601:BCR:H15C	1.81	0.41
25:B2:605:CLA:H91	25:B2:605:CLA:H111	1.85	0.41
3:C1:225:VAL:HG13	3:C1:289:TYR:HA	2.03	0.41
4:D1:293:LEU:HA	4:D1:293:LEU:HD12	1.95	0.41
23:J1:101:BCR:H15C	23:J1:101:BCR:H351	1.80	0.41
1:A2:116:VAL:HG13	1:A2:158:PHE:HB3	2.03	0.41
23:B1:601:BCR:H11C	23:B1:601:BCR:H341	1.83	0.41
23:B1:602:BCR:H24C	23:B1:602:BCR:H371	1.81	0.41
25:B1:607:CLA:HMD2	25:B1:614:CLA:H203	2.03	0.41
2:B1:99:THR:HB	25:B1:609:CLA:H61	2.01	0.41
25:B1:612:CLA:C14	25:B1:614:CLA:H2	2.59	0.41
2:B2:474:LEU:HD11	25:B2:610:CLA:HAA2	2.03	0.41
25:B2:611:CLA:NC	23:H2:103:BCR:H332	2.36	0.41
25:B2:614:CLA:H171	25:B2:614:CLA:H13	1.81	0.41
25:B2:616:CLA:H92	33:L2:101:LHG:H372	2.02	0.41
2:B2:97:ALA:O	2:B2:101:ILE:HG12	2.21	0.41
3:C1:213:LEU:HD11	23:C1:501:BCR:C20	2.51	0.41
3:C1:34:ALA:HB2	4:D1:230:ASP:OD2	2.38	0.41
4:D1:39:PRO:O	4:D1:43:LEU:HG	2.21	0.41
12:M1:23:ILE:HD13	35:M1:102:LMT:H101	2.03	0.41
15:U1:76:LYS:O	15:U1:77:LYS:C	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V2:118:HIS:O	16:V2:122:GLN:HG2	2.22	0.41
1:A1:119:PHE:HE1	25:A1:403:CLA:H121	1.86	0.41
1:A2:161:TYR:HA	1:A2:294:ALA:CB	2.50	0.41
2:B1:242:ILE:HG12	25:B1:613:CLA:HBB1	2.02	0.41
25:B1:610:CLA:H142	25:B1:610:CLA:H112	1.79	0.41
25:B2:610:CLA:H8	25:B2:611:CLA:H13	2.03	0.41
3:C1:314:ALA:HB3	3:C1:351:LEU:HD13	2.03	0.41
3:C2:190:ALA:HA	3:C2:191:PRO:HD3	1.91	0.41
33:D2:405:LHG:HC92	36:D2:408:PL9:H111	2.03	0.41
38:E1:101:HEM:ND	6:F1:24:HIS:NE2	2.69	0.41
23:F2:401:BCR:H351	23:F2:401:BCR:H15C	1.77	0.41
3:C1:62:PHE:HE1	10:K1:25:MET:HE3	1.86	0.41
12:M1:25:LEU:HD23	12:M1:25:LEU:HA	1.90	0.41
16:V1:41:HIS:C	16:V1:44:GLY:H	2.24	0.41
25:B1:613:CLA:H72	25:B1:613:CLA:H111	2.02	0.40
25:B1:617:CLA:H13	25:B1:617:CLA:H101	1.60	0.40
25:B1:617:CLA:C1B	25:B1:617:CLA:H191	2.52	0.40
25:B1:619:CLA:H202	25:B1:619:CLA:H162	4.71	0.40
3:C1:421:SER:HA	3:C1:422:PRO:HD3	1.99	0.40
25:C1:509:CLA:H122	25:C1:509:CLA:H162	1.36	0.40
3:C2:57:ALA:O	3:C2:61:VAL:HG23	2.21	0.40
33:D1:404:LHG:H191	33:D1:404:LHG:H162	1.85	0.40
36:D2:408:PL9:H352	11:L2:26:VAL:CG1	2.49	0.40
5:E2:27:ILE:HB	5:E2:28:PRO:HD3	2.03	0.40
16:V1:118:HIS:O	16:V1:122:GLN:HG2	2.21	0.40
1:A1:318:ALA:O	1:A1:321:ILE:HG22	2.22	0.40
2:B2:54:PRO:HD2	2:B2:57:ARG:HG3	2.03	0.40
3:C1:438:PHE:CZ	25:C1:506:CLA:HAB	2.56	0.40
2:B1:464:PHE:HB2	4:D1:280:TRP:CZ2	2.63	0.40
4:D2:195:PRO:HD3	11:L2:34:TYR:CZ	2.56	0.40
34:H2:101:DGD:HBE2	34:H2:101:DGD:HBF1	1.82	0.40
15:U2:76:LYS:O	15:U2:79:MET:N	2.49	0.40
1:A1:116:VAL:HG13	1:A1:158:PHE:HB3	2.04	0.40
3:C1:466:VAL:HG11	4:D1:247:VAL:HG12	2.02	0.40
25:C1:509:CLA:HMD2	33:D1:404:LHG:H351	2.04	0.40
37:D1:409:SQD:H301	10:K1:37:PHE:CZ	2.56	0.40
10:K2:22:ILE:HA	10:K2:25:MET:CG	2.54	0.40
13:O2:197:ILE:CG1	13:O2:198:GLU:N	2.85	0.40
13:O2:46:GLU:O	13:O2:47:PRO:O	2.38	0.40
16:V2:41:HIS:C	16:V2:44:GLY:H	2.25	0.40
25:A1:403:CLA:H161	25:A1:403:CLA:H192	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B1:616:CLA:CGA	25:B1:616:CLA:C1A	3.02	0.40
2:B2:247:PHE:CD2	25:B2:606:CLA:H101	3.03	0.40
25:C1:503:CLA:H43	25:C1:504:CLA:H61	2.03	0.40
3:C2:376:ASP:O	3:C2:380:ILE:HG12	2.22	0.40
25:C2:503:CLA:CED	25:C2:503:CLA:H2A	4.64	0.40
1:A1:272:HIS:CD2	4:D1:218:VAL:HG21	2.65	0.40
4:D2:293:LEU:HA	4:D2:293:LEU:HD12	1.96	0.40
3:C1:330:SER:OG	13:O1:100:GLY:O	2.31	0.40
13:O1:82:GLU:O	13:O1:98:LYS:C	2.70	0.40
2:B1:418:LYS:O	2:B1:422:ARG:HG3	2.22	0.40
2:B2:418:LYS:O	2:B2:422:ARG:HG3	2.22	0.40
25:B2:605:CLA:H101	25:B2:611:CLA:H193	2.02	0.40
2:B2:9:HIS:CG	25:B2:612:CLA:O1A	17.65	0.40
13:O2:19:CYS:HA	13:O2:20:PRO:HD3	1.92	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	342/344 (99%)	328 (96%)	14 (4%)	0	100	100
1	A2	327/344 (95%)	318 (97%)	9 (3%)	0	100	100
1	a1	332/344 (96%)	323 (97%)	9 (3%)	0	100	100
1	a2	332/344 (96%)	323 (97%)	9 (3%)	0	100	100
2	B1	481/509 (94%)	456 (95%)	23 (5%)	2 (0%)	39	73
2	B2	501/509 (98%)	474 (95%)	26 (5%)	1 (0%)	52	84
2	b1	502/509 (99%)	474 (94%)	26 (5%)	2 (0%)	39	73
2	b2	479/509 (94%)	454 (95%)	23 (5%)	2 (0%)	39	73
3	C1	447/460 (97%)	424 (95%)	20 (4%)	3 (1%)	26	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C2	438/460 (95%)	416 (95%)	19 (4%)	3 (1%)	26 60
3	c1	449/460 (98%)	426 (95%)	19 (4%)	4 (1%)	21 53
3	c2	446/460 (97%)	424 (95%)	19 (4%)	3 (1%)	26 60
4	D1	333/351 (95%)	318 (96%)	15 (4%)	0	100 100
4	D2	338/351 (96%)	322 (95%)	16 (5%)	0	100 100
4	d1	337/351 (96%)	321 (95%)	16 (5%)	0	100 100
4	d2	338/351 (96%)	323 (96%)	15 (4%)	0	100 100
5	E1	59/84 (70%)	57 (97%)	2 (3%)	0	100 100
5	E2	61/84 (73%)	59 (97%)	2 (3%)	0	100 100
5	e1	55/84 (66%)	54 (98%)	1 (2%)	0	100 100
5	e2	58/84 (69%)	57 (98%)	1 (2%)	0	100 100
6	F1	26/43 (60%)	26 (100%)	0	0	100 100
6	F2	29/43 (67%)	29 (100%)	0	0	100 100
6	f1	27/43 (63%)	27 (100%)	0	0	100 100
6	f2	27/43 (63%)	26 (96%)	1 (4%)	0	100 100
7	H1	56/67 (84%)	53 (95%)	2 (4%)	1 (2%)	11 31
7	H2	60/67 (90%)	54 (90%)	5 (8%)	1 (2%)	11 33
7	h1	60/67 (90%)	57 (95%)	2 (3%)	1 (2%)	11 33
7	h2	60/67 (90%)	56 (93%)	3 (5%)	1 (2%)	11 33
8	I1	32/38 (84%)	32 (100%)	0	0	100 100
8	I2	33/38 (87%)	32 (97%)	1 (3%)	0	100 100
8	i1	32/38 (84%)	32 (100%)	0	0	100 100
8	i2	31/38 (82%)	31 (100%)	0	0	100 100
9	J1	30/39 (77%)	30 (100%)	0	0	100 100
9	J2	33/39 (85%)	33 (100%)	0	0	100 100
9	j1	30/39 (77%)	30 (100%)	0	0	100 100
9	j2	31/39 (80%)	31 (100%)	0	0	100 100
10	K1	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	2 5
10	K2	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	2 5
10	k1	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	2 5
10	k2	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	2 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	L1	35/38 (92%)	33 (94%)	1 (3%)	1 (3%)	6 18
11	L2	35/38 (92%)	33 (94%)	1 (3%)	1 (3%)	6 18
11	l1	35/38 (92%)	33 (94%)	1 (3%)	1 (3%)	6 18
11	l2	35/38 (92%)	33 (94%)	1 (3%)	1 (3%)	6 18
12	M1	38/108 (35%)	30 (79%)	8 (21%)	0	100 100
12	M2	38/108 (35%)	30 (79%)	8 (21%)	0	100 100
12	m1	38/108 (35%)	30 (79%)	8 (21%)	0	100 100
12	m2	38/108 (35%)	30 (79%)	8 (21%)	0	100 100
13	O1	234/329 (71%)	210 (90%)	14 (6%)	10 (4%)	3 9
13	O2	187/329 (57%)	165 (88%)	14 (8%)	8 (4%)	3 9
13	o1	230/329 (70%)	204 (89%)	16 (7%)	10 (4%)	3 9
13	o2	239/329 (73%)	212 (89%)	15 (6%)	12 (5%)	3 7
14	T1	28/32 (88%)	28 (100%)	0	0	100 100
14	T2	28/32 (88%)	28 (100%)	0	0	100 100
14	t1	28/32 (88%)	28 (100%)	0	0	100 100
14	t2	27/32 (84%)	27 (100%)	0	0	100 100
15	U1	91/155 (59%)	85 (93%)	6 (7%)	0	100 100
15	U2	86/155 (56%)	81 (94%)	5 (6%)	0	100 100
15	u1	91/155 (59%)	87 (96%)	4 (4%)	0	100 100
15	u2	91/155 (59%)	85 (93%)	6 (7%)	0	100 100
16	V1	127/155 (82%)	115 (91%)	7 (6%)	5 (4%)	4 11
16	V2	127/155 (82%)	115 (91%)	7 (6%)	5 (4%)	4 11
16	v1	127/155 (82%)	115 (91%)	7 (6%)	5 (4%)	4 11
16	v2	127/155 (82%)	115 (91%)	7 (6%)	5 (4%)	4 11
17	Y1	25/35 (71%)	24 (96%)	1 (4%)	0	100 100
17	Y2	23/35 (66%)	22 (96%)	1 (4%)	0	100 100
17	y1	25/35 (71%)	24 (96%)	1 (4%)	0	100 100
17	y2	25/35 (71%)	24 (96%)	1 (4%)	0	100 100
18	X1	27/40 (68%)	27 (100%)	0	0	100 100
18	X2	29/40 (72%)	29 (100%)	0	0	100 100
18	x1	34/40 (85%)	33 (97%)	1 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	x2	30/40 (75%)	30 (100%)	0	0	100	100
19	S1	23/46 (50%)	23 (100%)	0	0	100	100
19	S2	28/46 (61%)	27 (96%)	1 (4%)	0	100	100
19	s1	38/46 (83%)	34 (90%)	4 (10%)	0	100	100
19	s2	44/46 (96%)	37 (84%)	7 (16%)	0	100	100
20	W1	19/25 (76%)	19 (100%)	0	0	100	100
20	W2	19/25 (76%)	19 (100%)	0	0	100	100
20	w1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
20	w2	18/25 (72%)	18 (100%)	0	0	100	100
21	Q2	107/218 (49%)	102 (95%)	3 (3%)	2 (2%)	10	30
21	q1	101/218 (46%)	97 (96%)	3 (3%)	1 (1%)	19	50
22	Z2	57/62 (92%)	55 (96%)	2 (4%)	0	100	100
22	z2	57/62 (92%)	55 (96%)	2 (4%)	0	100	100
All	All	10304/12316 (84%)	9726 (94%)	479 (5%)	99 (1%)	19	50

All (99) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C1	36	TRP
3	C1	37	SER
10	K1	14	THR
13	O1	49	GLN
13	O1	99	ASP
13	O1	199	LEU
13	O1	201	VAL
13	O1	202	ASN
16	V1	39	SER
16	V1	40	CYS
3	c1	36	TRP
3	c1	37	SER
10	k1	14	THR
13	o1	49	GLN
13	o1	99	ASP
13	o1	199	LEU
13	o1	201	VAL
13	o1	202	ASN
16	v1	39	SER

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Mol	Chain	Res	Type
16	v1	40	CYS
3	C2	36	TRP
3	C2	37	SER
10	K2	14	THR
13	O2	49	GLN
13	O2	199	LEU
13	O2	200	ALA
13	O2	201	VAL
16	V2	39	SER
16	V2	40	CYS
16	V2	42	VAL
21	Q2	106	PRO
3	c2	36	TRP
3	c2	37	SER
10	k2	14	THR
13	o2	49	GLN
13	o2	99	ASP
13	o2	178(F)	GLY
13	o2	199	LEU
13	o2	201	VAL
13	o2	202	ASN
16	v2	39	SER
16	v2	40	CYS
2	B1	7	ARG
10	K1	15	TYR
13	O1	51	LEU
13	O1	181	VAL
13	O1	182	LEU
13	O1	200	ALA
16	V1	42	VAL
2	b1	7	ARG
10	k1	15	TYR
13	o1	51	LEU
13	o1	181	VAL
13	o1	182	LEU
13	o1	200	ALA
16	v1	42	VAL
2	B2	7	ARG
10	K2	15	TYR
13	O2	48	LYS
13	O2	181	VAL
13	O2	182	LEU

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Mol	Chain	Res	Type
2	b2	7	ARG
10	k2	15	TYR
13	o2	51	LEU
13	o2	181	VAL
13	o2	182	LEU
13	o2	200	ALA
16	v2	42	VAL
13	O1	120	PHE
16	V1	45	ILE
13	o1	120	PHE
16	v1	45	ILE
21	q1	144	LEU
13	O2	120	PHE
16	V2	45	ILE
21	Q2	144	LEU
13	o2	120	PHE
16	V1	38	SER
16	v1	38	SER
16	V2	38	SER
16	v2	38	SER
16	v2	45	ILE
2	B1	6	TYR
7	H1	26	GLY
7	h1	26	GLY
7	H2	26	GLY
2	b2	6	TYR
7	h2	26	GLY
3	C1	191	PRO
2	b1	6	TYR
3	c1	191	PRO
3	C2	191	PRO
3	c2	191	PRO
13	o2	198	GLU
11	l1	29	VAL
11	L2	29	VAL
11	l2	29	VAL
11	L1	29	VAL
3	c1	38	GLY

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	261/282 (93%)	256 (98%)	5 (2%)	65	90
1	A2	239/282 (85%)	234 (98%)	5 (2%)	61	88
1	a1	261/282 (93%)	256 (98%)	5 (2%)	65	90
1	a2	249/282 (88%)	243 (98%)	6 (2%)	57	86
2	B1	360/415 (87%)	351 (98%)	9 (2%)	55	85
2	B2	351/415 (85%)	341 (97%)	10 (3%)	51	83
2	b1	380/415 (92%)	369 (97%)	11 (3%)	50	82
2	b2	352/415 (85%)	342 (97%)	10 (3%)	51	83
3	C1	320/364 (88%)	317 (99%)	3 (1%)	84	96
3	C2	261/364 (72%)	260 (100%)	1 (0%)	93	98
3	c1	338/364 (93%)	334 (99%)	4 (1%)	78	94
3	c2	323/364 (89%)	320 (99%)	3 (1%)	84	96
4	D1	255/283 (90%)	252 (99%)	3 (1%)	78	94
4	D2	238/283 (84%)	236 (99%)	2 (1%)	86	96
4	d1	267/283 (94%)	265 (99%)	2 (1%)	88	97
4	d2	258/283 (91%)	256 (99%)	2 (1%)	86	96
5	E1	28/75 (37%)	28 (100%)	0	100	100
5	E2	34/75 (45%)	34 (100%)	0	100	100
5	e1	38/75 (51%)	37 (97%)	1 (3%)	54	85
5	e2	33/75 (44%)	33 (100%)	0	100	100
6	F1	18/36 (50%)	17 (94%)	1 (6%)	26	57
6	F2	17/36 (47%)	16 (94%)	1 (6%)	24	55
6	f1	20/36 (56%)	19 (95%)	1 (5%)	30	62
6	f2	19/36 (53%)	18 (95%)	1 (5%)	28	60
7	H1	39/58 (67%)	38 (97%)	1 (3%)	54	85
7	H2	38/58 (66%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	h1	47/58 (81%)	46 (98%)	1 (2%)	61 88
7	h2	42/58 (72%)	41 (98%)	1 (2%)	57 86
8	I1	30/36 (83%)	29 (97%)	1 (3%)	45 78
8	I2	26/36 (72%)	25 (96%)	1 (4%)	40 74
8	i1	32/36 (89%)	31 (97%)	1 (3%)	47 80
8	i2	28/36 (78%)	27 (96%)	1 (4%)	42 75
9	J1	20/32 (62%)	20 (100%)	0	100 100
9	J2	19/32 (59%)	19 (100%)	0	100 100
9	j1	22/32 (69%)	22 (100%)	0	100 100
9	j2	22/32 (69%)	22 (100%)	0	100 100
10	K1	26/36 (72%)	26 (100%)	0	100 100
10	K2	18/36 (50%)	18 (100%)	0	100 100
10	k1	27/36 (75%)	27 (100%)	0	100 100
10	k2	24/36 (67%)	24 (100%)	0	100 100
11	L1	31/35 (89%)	31 (100%)	0	100 100
11	L2	33/35 (94%)	33 (100%)	0	100 100
11	l1	33/35 (94%)	33 (100%)	0	100 100
11	l2	32/35 (91%)	32 (100%)	0	100 100
12	M1	26/88 (30%)	25 (96%)	1 (4%)	40 74
12	M2	26/88 (30%)	25 (96%)	1 (4%)	40 74
12	m1	26/88 (30%)	25 (96%)	1 (4%)	40 74
12	m2	27/88 (31%)	26 (96%)	1 (4%)	41 75
13	O1	148/266 (56%)	138 (93%)	10 (7%)	20 46
13	O2	110/266 (41%)	103 (94%)	7 (6%)	22 50
13	o1	156/266 (59%)	148 (95%)	8 (5%)	29 62
13	o2	168/266 (63%)	159 (95%)	9 (5%)	27 59
14	T1	24/28 (86%)	24 (100%)	0	100 100
14	T2	25/28 (89%)	25 (100%)	0	100 100
14	t1	26/28 (93%)	26 (100%)	0	100 100
14	t2	25/28 (89%)	24 (96%)	1 (4%)	38 72
15	U1	63/122 (52%)	59 (94%)	4 (6%)	22 51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	U2	40/122 (33%)	37 (92%)	3 (8%)	17 40
15	u1	66/122 (54%)	62 (94%)	4 (6%)	23 53
15	u2	69/122 (57%)	64 (93%)	5 (7%)	18 43
16	V1	88/132 (67%)	87 (99%)	1 (1%)	80 95
16	V2	70/132 (53%)	69 (99%)	1 (1%)	74 93
16	v1	88/132 (67%)	85 (97%)	3 (3%)	44 77
16	v2	100/132 (76%)	99 (99%)	1 (1%)	82 95
17	Y1	11/33 (33%)	11 (100%)	0	100 100
17	Y2	13/33 (39%)	13 (100%)	0	100 100
17	y1	18/33 (54%)	18 (100%)	0	100 100
17	y2	16/33 (48%)	16 (100%)	0	100 100
18	X1	17/34 (50%)	16 (94%)	1 (6%)	24 55
18	X2	16/34 (47%)	15 (94%)	1 (6%)	22 51
18	x1	23/34 (68%)	21 (91%)	2 (9%)	13 33
18	x2	17/34 (50%)	16 (94%)	1 (6%)	24 55
19	S1	10/20 (50%)	10 (100%)	0	100 100
19	S2	10/20 (50%)	10 (100%)	0	100 100
19	s1	15/20 (75%)	15 (100%)	0	100 100
19	s2	13/20 (65%)	13 (100%)	0	100 100
20	W1	12/13 (92%)	12 (100%)	0	100 100
20	W2	10/13 (77%)	10 (100%)	0	100 100
20	w1	11/13 (85%)	11 (100%)	0	100 100
20	w2	11/13 (85%)	11 (100%)	0	100 100
21	Q2	35/175 (20%)	33 (94%)	2 (6%)	25 56
21	q1	33/175 (19%)	32 (97%)	1 (3%)	48 81
22	Z2	22/54 (41%)	22 (100%)	0	100 100
22	z2	28/54 (52%)	28 (100%)	0	100 100
All	All	7221/10010 (72%)	7059 (98%)	162 (2%)	60 88

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	85	THR

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Mol	Chain	Res	Type
1	A1	123	VAL
1	A1	255	PHE
1	A1	286	THR
1	A1	291	SER
2	B1	6	TYR
2	B1	10	THR
2	B1	12	VAL
2	B1	128	THR
2	B1	357	ARG
2	B1	371	VAL
2	B1	434	ARG
2	B1	442	VAL
2	B1	464	PHE
3	C1	62	PHE
3	C1	99	VAL
3	C1	240	ILE
4	D1	180	ARG
4	D1	182	LEU
4	D1	277	THR
6	F1	41	GLN
7	H1	49	TYR
8	I1	23	PHE
12	M1	9	LEU
13	O1	101	MET
13	O1	106	THR
13	O1	142	LEU
13	O1	172	VAL
13	O1	181	VAL
13	O1	183	ARG
13	O1	219	GLN
13	O1	220	LEU
13	O1	221	SER
13	O1	233	LEU
15	U1	57	THR
15	U1	80	ASP
15	U1	90	GLU
15	U1	97	ARG
16	V1	39	SER
18	X1	32	VAL
1	a1	85	THR
1	a1	123	VAL
1	a1	255	PHE

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Mol	Chain	Res	Type
1	a1	286	THR
1	a1	291	SER
2	b1	6	TYR
2	b1	10	THR
2	b1	12	VAL
2	b1	128	THR
2	b1	357	ARG
2	b1	371	VAL
2	b1	434	ARG
2	b1	442	VAL
2	b1	464	PHE
2	b1	479	PHE
2	b1	490	VAL
3	c1	36	TRP
3	c1	62	PHE
3	c1	122	SER
3	c1	240	ILE
4	d1	180	ARG
4	d1	182	LEU
5	e1	65	LEU
6	f1	41	GLN
7	h1	49	TYR
8	i1	23	PHE
12	m1	9	LEU
13	o1	106	THR
13	o1	142	LEU
13	o1	172	VAL
13	o1	181	VAL
13	o1	183	ARG
13	o1	219	GLN
13	o1	220	LEU
13	o1	221	SER
15	u1	57	THR
15	u1	80	ASP
15	u1	90	GLU
15	u1	97	ARG
16	v1	25	GLN
16	v1	39	SER
16	v1	40	CYS
18	x1	12	TRP
18	x1	32	VAL
21	q1	137	ASP

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Mol	Chain	Res	Type
1	A2	85	THR
1	A2	123	VAL
1	A2	255	PHE
1	A2	286	THR
1	A2	291	SER
2	B2	6	TYR
2	B2	10	THR
2	B2	12	VAL
2	B2	128	THR
2	B2	357	ARG
2	B2	371	VAL
2	B2	434	ARG
2	B2	442	VAL
2	B2	464	PHE
2	B2	490	VAL
3	C2	62	PHE
4	D2	182	LEU
4	D2	238	THR
6	F2	41	GLN
8	I2	23	PHE
12	M2	9	LEU
13	O2	106	THR
13	O2	172	VAL
13	O2	181	VAL
13	O2	183	ARG
13	O2	219	GLN
13	O2	221	SER
13	O2	233	LEU
15	U2	80	ASP
15	U2	90	GLU
15	U2	97	ARG
16	V2	39	SER
18	X2	12	TRP
21	Q2	137	ASP
21	Q2	183	ILE
1	a2	25	GLU
1	a2	85	THR
1	a2	123	VAL
1	a2	255	PHE
1	a2	286	THR
1	a2	291	SER
2	b2	6	TYR

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Mol	Chain	Res	Type
2	b2	10	THR
2	b2	12	VAL
2	b2	128	THR
2	b2	357	ARG
2	b2	371	VAL
2	b2	434	ARG
2	b2	442	VAL
2	b2	464	PHE
2	b2	479	PHE
3	c2	26	ARG
3	c2	62	PHE
3	c2	99	VAL
4	d2	180	ARG
4	d2	182	LEU
6	f2	41	GLN
7	h2	49	TYR
8	i2	23	PHE
12	m2	9	LEU
13	o2	106	THR
13	o2	142	LEU
13	o2	172	VAL
13	o2	181	VAL
13	o2	183	ARG
13	o2	219	GLN
13	o2	220	LEU
13	o2	221	SER
13	o2	233	LEU
14	t2	29	ILE
15	u2	57	THR
15	u2	80	ASP
15	u2	90	GLU
15	u2	97	ARG
15	u2	104	LYS
16	v2	39	SER
18	x2	12	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	234	ASN
2	B1	216	HIS
2	B1	223	GLN

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Mol	Chain	Res	Type
2	B1	365	ASN
3	C1	56	HIS
3	C1	107	ASN
3	C1	418	ASN
13	O1	109	GLN
2	b1	216	HIS
2	b1	223	GLN
2	b1	365	ASN
2	b1	489	GLN
3	c1	56	HIS
3	c1	418	ASN
13	o1	109	GLN
21	q1	170	GLN
2	B2	216	HIS
3	C2	56	HIS
13	O2	109	GLN
16	V2	122	GLN
2	b2	216	HIS
2	b2	365	ASN
3	c2	56	HIS
13	o2	109	GLN
18	x2	34	GLN

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 353 ligands modelled in this entry, 52 are unknown and 10 are monoatomic - leaving 291 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	$\#\|Z\| > 2$
23	BCR	A1	401	-	41,41,41	0.67	0	56,56,56	1.74	11 (19%)
25	CLA	A1	403	-	57,73,73	1.17	6 (10%)	61,113,113	1.15	7 (11%)
25	CLA	A1	404	-	43,59,73	1.30	4 (9%)	43,96,113	1.30	6 (13%)
25	CLA	A1	405	-	47,63,73	1.26	6 (12%)	49,101,113	1.26	6 (12%)
25	CLA	A1	406	-	57,73,73	1.11	5 (8%)	61,113,113	1.19	7 (11%)
26	OEX	A1	407	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
27	PHO	A1	408	-	67,69,69	2.05	17 (25%)	86,99,99	1.97	23 (26%)
29	LMG	A1	410	-	43,43,55	1.00	2 (4%)	51,51,63	1.14	4 (7%)
29	LMG	A1	412	-	41,41,55	1.03	2 (4%)	49,49,63	1.03	3 (6%)
31	BCT	A1	413	30	0,3,3	0.00	-	0,3,3	0.00	-
23	BCR	A2	401	-	41,41,41	0.69	0	56,56,56	2.05	16 (28%)
25	CLA	A2	402	-	57,73,73	1.16	6 (10%)	61,113,113	1.18	7 (11%)
25	CLA	A2	403	-	53,69,73	1.16	5 (9%)	55,108,113	1.16	6 (10%)
25	CLA	A2	404	-	43,59,73	1.31	5 (11%)	43,96,113	1.27	6 (13%)
33	LHG	A2	405	-	32,32,48	1.10	2 (6%)	33,38,54	1.03	2 (6%)
26	OEX	A2	406	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
27	PHO	A2	407	-	67,69,69	2.06	16 (23%)	86,99,99	1.99	22 (25%)
29	LMG	A2	412	-	29,29,55	1.03	2 (6%)	37,37,63	1.11	2 (5%)
31	BCT	A2	413	30	0,3,3	0.00	-	0,3,3	0.00	-
23	BCR	B1	601	-	41,41,41	0.69	0	56,56,56	1.92	16 (28%)
23	BCR	B1	602	-	41,41,41	0.68	0	56,56,56	1.96	14 (25%)
23	BCR	B1	603	-	41,41,41	0.68	0	56,56,56	1.71	11 (19%)
25	CLA	B1	604	-	34,50,73	1.43	6 (17%)	37,85,113	1.29	6 (16%)
25	CLA	B1	605	-	57,73,73	1.14	4 (7%)	61,113,113	1.12	6 (9%)
25	CLA	B1	606	-	57,73,73	1.12	4 (7%)	61,113,113	1.13	7 (11%)
25	CLA	B1	607	-	52,68,73	1.21	5 (9%)	55,107,113	1.17	5 (9%)
25	CLA	B1	608	-	57,73,73	1.12	4 (7%)	61,113,113	1.12	7 (11%)
25	CLA	B1	609	-	57,73,73	1.14	5 (8%)	61,113,113	1.45	10 (16%)
25	CLA	B1	610	-	57,73,73	1.11	4 (7%)	61,113,113	1.13	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	B1	611	-	54,70,73	1.16	5 (9%)	57,109,113	1.22	6 (10%)
25	CLA	B1	612	-	57,73,73	1.13	4 (7%)	61,113,113	1.18	6 (9%)
25	CLA	B1	613	-	57,73,73	1.17	5 (8%)	61,113,113	1.22	6 (9%)
25	CLA	B1	614	-	57,73,73	1.13	4 (7%)	61,113,113	1.18	7 (11%)
25	CLA	B1	615	-	57,73,73	1.11	4 (7%)	61,113,113	1.16	6 (9%)
25	CLA	B1	616	-	57,73,73	1.14	6 (10%)	61,113,113	1.09	7 (11%)
25	CLA	B1	617	-	57,73,73	1.12	4 (7%)	61,113,113	1.19	7 (11%)
25	CLA	B1	618	-	50,66,73	1.19	5 (10%)	52,104,113	1.25	6 (11%)
25	CLA	B1	619	40	57,73,73	1.11	4 (7%)	61,113,113	1.19	7 (11%)
32	GOL	B1	620	-	5,5,5	0.33	0	5,5,5	0.26	0
33	LHG	B1	621	-	48,48,48	0.90	2 (4%)	49,54,54	1.02	3 (6%)
29	LMG	B1	622	-	31,31,55	1.16	2 (6%)	39,39,63	1.22	4 (10%)
29	LMG	B1	626	-	48,48,55	0.96	2 (4%)	56,56,63	1.20	4 (7%)
23	BCR	B2	601	-	41,41,41	0.69	0	56,56,56	1.94	16 (28%)
23	BCR	B2	602	-	41,41,41	0.68	0	56,56,56	2.00	14 (25%)
23	BCR	B2	603	-	41,41,41	0.68	0	56,56,56	1.83	11 (19%)
25	CLA	B2	604	-	32,49,73	1.46	4 (12%)	35,84,113	1.40	6 (17%)
25	CLA	B2	605	-	57,73,73	1.13	4 (7%)	61,113,113	1.19	6 (9%)
25	CLA	B2	606	-	57,73,73	1.13	4 (7%)	61,113,113	1.13	5 (8%)
25	CLA	B2	607	-	57,73,73	1.14	5 (8%)	61,113,113	1.22	8 (13%)
25	CLA	B2	608	-	57,73,73	1.14	4 (7%)	61,113,113	1.13	5 (8%)
25	CLA	B2	609	-	57,73,73	1.12	5 (8%)	61,113,113	1.22	8 (13%)
25	CLA	B2	610	-	57,73,73	1.10	4 (7%)	61,113,113	1.18	6 (9%)
25	CLA	B2	611	-	57,73,73	1.13	5 (8%)	61,113,113	1.18	7 (11%)
25	CLA	B2	612	-	57,73,73	1.12	4 (7%)	61,113,113	1.16	5 (8%)
25	CLA	B2	613	-	57,73,73	1.13	4 (7%)	61,113,113	1.30	7 (11%)
25	CLA	B2	614	-	57,73,73	1.12	4 (7%)	61,113,113	1.16	8 (13%)
25	CLA	B2	615	-	57,73,73	1.10	4 (7%)	61,113,113	1.16	6 (9%)
25	CLA	B2	616	-	46,62,73	1.26	5 (10%)	47,99,113	1.23	7 (14%)
25	CLA	B2	617	-	57,73,73	1.13	4 (7%)	61,113,113	1.18	7 (11%)
25	CLA	B2	618	-	52,68,73	1.18	5 (9%)	55,107,113	1.23	6 (10%)
25	CLA	B2	619	-	57,73,73	1.12	4 (7%)	61,113,113	1.16	5 (8%)
29	LMG	B2	620	-	40,40,55	1.04	2 (5%)	48,48,63	1.08	4 (8%)
29	LMG	B2	621	-	37,37,55	0.91	2 (5%)	45,45,63	1.16	3 (6%)
37	SQD	B2	623	-	44,45,54	1.85	4 (9%)	53,56,65	1.40	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	LHG	B2	627	-	41,41,48	1.00	2 (4%)	42,47,54	1.11	3 (7%)
23	BCR	C1	501	-	41,41,41	0.69	0	56,56,56	1.80	14 (25%)
25	CLA	C1	502	-	57,73,73	1.11	5 (8%)	61,113,113	1.18	6 (9%)
25	CLA	C1	503	-	52,68,73	1.18	4 (7%)	55,107,113	1.20	7 (12%)
25	CLA	C1	504	-	57,73,73	1.14	4 (7%)	61,113,113	1.09	6 (9%)
25	CLA	C1	505	-	57,73,73	1.10	4 (7%)	61,113,113	1.20	6 (9%)
25	CLA	C1	506	-	57,73,73	1.15	4 (7%)	61,113,113	1.17	8 (13%)
25	CLA	C1	507	-	57,73,73	1.13	5 (8%)	61,113,113	1.18	8 (13%)
25	CLA	C1	508	-	57,73,73	1.13	4 (7%)	61,113,113	1.15	6 (9%)
25	CLA	C1	509	-	57,73,73	1.14	4 (7%)	61,113,113	1.35	8 (13%)
25	CLA	C1	510	-	57,73,73	1.13	4 (7%)	61,113,113	1.11	6 (9%)
25	CLA	C1	511	-	57,73,73	1.12	4 (7%)	61,113,113	1.16	5 (8%)
25	CLA	C1	512	-	57,73,73	1.12	4 (7%)	61,113,113	1.16	7 (11%)
25	CLA	C1	513	3	53,69,73	1.18	4 (7%)	55,108,113	1.21	5 (9%)
25	CLA	C1	514	-	34,53,73	1.42	4 (11%)	37,89,113	1.35	7 (18%)
34	DGD	C1	515	-	53,53,67	0.93	2 (3%)	67,67,81	1.05	4 (5%)
34	DGD	C1	516	-	63,63,67	0.83	2 (3%)	77,77,81	1.00	3 (3%)
34	DGD	C1	517	-	65,65,67	0.83	2 (3%)	79,79,81	0.87	3 (3%)
32	GOL	C1	518	-	5,5,5	0.35	0	5,5,5	0.20	0
35	LMT	C1	519	-	36,36,36	0.35	0	47,47,47	0.70	1 (2%)
29	LMG	C1	520	-	48,48,55	0.95	2 (4%)	56,56,63	1.01	3 (5%)
23	BCR	C1	521	-	41,41,41	0.69	0	56,56,56	1.93	15 (26%)
23	BCR	C2	502	-	41,41,41	0.70	0	56,56,56	1.86	11 (19%)
25	CLA	C2	503	-	57,73,73	1.11	4 (7%)	61,113,113	1.20	6 (9%)
25	CLA	C2	504	-	38,54,73	1.38	5 (13%)	41,90,113	1.32	6 (14%)
25	CLA	C2	505	-	57,73,73	1.12	4 (7%)	61,113,113	1.15	7 (11%)
25	CLA	C2	506	-	57,73,73	1.12	5 (8%)	61,113,113	1.19	7 (11%)
25	CLA	C2	507	-	34,53,73	1.43	4 (11%)	37,89,113	1.36	7 (18%)
25	CLA	C2	508	-	42,58,73	1.30	4 (9%)	44,95,113	1.39	8 (18%)
25	CLA	C2	509	-	57,73,73	1.14	4 (7%)	61,113,113	1.14	6 (9%)
25	CLA	C2	510	-	34,53,73	1.41	4 (11%)	37,89,113	1.33	6 (16%)
25	CLA	C2	511	-	42,58,73	1.31	5 (11%)	44,95,113	1.42	7 (15%)
34	DGD	C2	512	-	34,34,67	1.27	2 (5%)	46,47,81	1.07	2 (4%)
25	CLA	C2	513	-	45,61,73	1.28	4 (8%)	46,98,113	1.25	6 (13%)
32	GOL	C2	514	-	5,5,5	0.35	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	LMG	C2	515	-	24,24,55	1.14	2 (8%)	32,32,63	0.97	2 (6%)
25	CLA	C2	516	-	38,54,73	1.36	4 (10%)	41,90,113	1.30	6 (14%)
25	CLA	C2	518	-	32,49,73	1.45	4 (12%)	35,84,113	1.51	8 (22%)
23	BCR	D1	401	-	41,41,41	0.71	0	56,56,56	1.97	13 (23%)
25	CLA	D1	402	-	57,73,73	1.13	4 (7%)	61,113,113	1.14	6 (9%)
25	CLA	D1	403	-	43,59,73	1.29	4 (9%)	43,96,113	1.34	6 (13%)
33	LHG	D1	404	-	48,48,48	0.91	2 (4%)	49,54,54	1.05	3 (6%)
33	LHG	D1	405	-	48,48,48	0.91	2 (4%)	49,54,54	1.02	3 (6%)
29	LMG	D1	406	-	35,35,55	1.08	2 (5%)	43,43,63	1.09	3 (6%)
27	PHO	D1	407	-	66,68,69	2.12	16 (24%)	84,97,99	1.99	22 (26%)
36	PL9	D1	408	-	54,55,55	0.61	2 (3%)	68,69,69	1.89	19 (27%)
37	SQD	D1	409	-	34,35,54	2.16	4 (11%)	43,46,65	1.51	8 (18%)
25	CLA	D2	401	-	57,73,73	1.13	4 (7%)	61,113,113	1.16	7 (11%)
37	SQD	D2	402	-	24,25,54	2.70	4 (16%)	31,35,65	1.88	7 (22%)
33	LHG	D2	403	-	48,48,48	0.89	2 (4%)	49,54,54	1.04	3 (6%)
25	CLA	D2	404	-	53,69,73	1.18	4 (7%)	55,108,113	1.23	7 (12%)
33	LHG	D2	405	-	48,48,48	0.90	2 (4%)	49,54,54	1.04	3 (6%)
25	CLA	D2	406	-	57,73,73	1.12	4 (7%)	61,113,113	1.14	6 (9%)
27	PHO	D2	407	-	67,69,69	2.09	17 (25%)	86,99,99	2.03	24 (27%)
36	PL9	D2	408	-	54,55,55	0.60	1 (1%)	68,69,69	1.85	19 (27%)
38	HEM	E1	101	5,6	24,50,50	2.34	7 (29%)	16,82,82	1.25	0
38	HEM	E2	101	5	24,50,50	2.33	7 (29%)	16,82,82	1.29	0
23	BCR	F2	401	-	41,41,41	0.71	0	56,56,56	2.18	18 (32%)
29	LMG	F2	402	-	35,35,55	1.10	2 (5%)	43,43,63	1.06	4 (9%)
34	DGD	H1	101	-	63,63,67	0.85	2 (3%)	77,77,81	0.94	3 (3%)
23	BCR	H1	102	-	22,22,41	0.70	0	29,29,56	1.74	6 (20%)
34	DGD	H2	101	-	63,63,67	0.86	2 (3%)	77,77,81	0.92	3 (3%)
23	BCR	H2	103	-	24,24,41	0.72	0	31,31,56	1.70	8 (25%)
29	LMG	I2	101	-	34,34,55	1.12	2 (5%)	42,42,63	1.15	3 (7%)
23	BCR	J1	101	-	41,41,41	0.74	0	56,56,56	2.09	15 (26%)
23	BCR	K1	101	-	30,31,41	0.68	0	38,40,56	2.17	11 (28%)
25	CLA	K2	101	-	47,63,73	1.26	4 (8%)	49,101,113	1.20	4 (8%)
23	BCR	K2	102	-	41,41,41	0.71	0	56,56,56	2.06	17 (30%)
23	BCR	K2	104	-	28,29,41	0.58	0	38,41,56	1.79	10 (26%)
33	LHG	L1	101	-	40,40,48	0.98	2 (5%)	41,46,54	1.11	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	LMT	L1	102	-	11,11,36	0.25	0	10,10,47	0.57	0
33	LHG	L2	101	-	48,48,48	0.91	2 (4%)	49,54,54	1.12	3 (6%)
29	LMG	M1	101	-	30,30,55	1.16	3 (10%)	32,32,63	1.33	3 (9%)
35	LMT	M1	102	-	10,10,36	0.25	0	9,9,47	0.57	0
35	LMT	M1	103	-	24,24,36	0.44	0	29,29,47	0.59	0
35	LMT	T1	101	-	11,11,36	0.25	0	10,10,47	0.58	0
38	HEM	V1	201	16	24,50,50	2.36	7 (29%)	16,82,82	1.30	1 (6%)
38	HEM	V2	201	16	24,50,50	2.40	7 (29%)	16,82,82	1.33	2 (12%)
23	BCR	a1	401	-	41,41,41	0.69	0	56,56,56	1.74	13 (23%)
25	CLA	a1	403	-	57,73,73	1.16	6 (10%)	61,113,113	1.15	4 (6%)
25	CLA	a1	404	-	52,68,73	1.19	5 (9%)	55,107,113	1.16	5 (9%)
25	CLA	a1	405	-	42,58,73	1.31	4 (9%)	44,95,113	1.39	7 (15%)
32	GOL	a1	406	-	5,5,5	0.33	0	5,5,5	0.24	0
33	LHG	a1	407	-	42,42,48	0.98	2 (4%)	43,48,54	1.10	3 (6%)
26	OEX	a1	408	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
27	PHO	a1	411	-	67,69,69	2.07	17 (25%)	86,99,99	1.92	23 (26%)
29	LMG	a1	412	-	51,51,55	0.93	2 (3%)	59,59,63	1.11	4 (6%)
31	BCT	a1	413	30	0,3,3	0.00	-	0,3,3	0.00	-
23	BCR	a2	402	-	41,41,41	0.67	0	56,56,56	1.63	12 (21%)
25	CLA	a2	404	-	57,73,73	1.16	5 (8%)	61,113,113	1.15	7 (11%)
25	CLA	a2	405	-	57,73,73	1.12	4 (7%)	61,113,113	1.17	6 (9%)
35	LMT	a2	406	-	36,36,36	0.44	0	47,47,47	0.67	1 (2%)
33	LHG	a2	407	-	29,29,48	1.22	2 (6%)	28,34,54	1.06	1 (3%)
26	OEX	a2	408	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
29	LMG	a2	412	-	44,44,55	0.98	2 (4%)	52,52,63	1.16	5 (9%)
25	CLA	a2	413	-	42,58,73	1.32	4 (9%)	44,95,113	1.31	7 (15%)
32	GOL	a2	415	-	5,5,5	0.36	0	5,5,5	0.32	0
27	PHO	a2	416	-	67,69,69	2.07	16 (23%)	86,99,99	1.94	22 (25%)
31	BCT	a2	417	30	0,3,3	0.00	-	0,3,3	0.00	-
23	BCR	b1	601	-	41,41,41	0.68	0	56,56,56	1.84	14 (25%)
23	BCR	b1	602	-	41,41,41	0.68	0	56,56,56	2.04	18 (32%)
23	BCR	b1	603	-	41,41,41	0.72	0	56,56,56	1.75	10 (17%)
25	CLA	b1	604	-	57,73,73	1.14	4 (7%)	61,113,113	1.10	7 (11%)
25	CLA	b1	605	-	57,73,73	1.13	5 (8%)	61,113,113	1.19	7 (11%)
25	CLA	b1	606	-	57,73,73	1.13	4 (7%)	61,113,113	1.17	8 (13%)
25	CLA	b1	607	-	57,73,73	1.16	5 (8%)	61,113,113	1.18	7 (11%)
25	CLA	b1	608	-	57,73,73	1.13	5 (8%)	61,113,113	1.16	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	b1	609	-	57,73,73	1.14	4 (7%)	61,113,113	1.16	7 (11%)
25	CLA	b1	610	-	57,73,73	1.12	4 (7%)	61,113,113	1.18	8 (13%)
25	CLA	b1	611	-	57,73,73	1.13	4 (7%)	61,113,113	1.17	8 (13%)
25	CLA	b1	612	-	57,73,73	1.14	4 (7%)	61,113,113	1.18	7 (11%)
25	CLA	b1	613	-	57,73,73	1.16	6 (10%)	61,113,113	1.26	7 (11%)
25	CLA	b1	614	-	57,73,73	1.12	5 (8%)	61,113,113	1.24	8 (13%)
25	CLA	b1	615	-	51,67,73	1.18	4 (7%)	53,105,113	1.24	7 (13%)
25	CLA	b1	616	-	57,73,73	1.14	6 (10%)	61,113,113	1.10	8 (13%)
25	CLA	b1	617	-	57,73,73	1.14	4 (7%)	61,113,113	1.13	5 (8%)
32	GOL	b1	618	-	5,5,5	0.33	0	5,5,5	0.37	0
25	CLA	b1	619	-	57,73,73	1.12	5 (8%)	61,113,113	1.16	7 (11%)
25	CLA	b1	620	-	57,73,73	1.12	4 (7%)	61,113,113	1.14	7 (11%)
29	LMG	b1	621	-	38,38,55	1.09	2 (5%)	46,46,63	1.09	2 (4%)
33	LHG	b1	622	-	48,48,48	0.89	2 (4%)	49,54,54	1.05	4 (8%)
29	LMG	b1	624	-	39,39,55	1.05	2 (5%)	47,47,63	1.42	4 (8%)
29	LMG	b1	631	-	40,40,55	1.06	2 (5%)	48,48,63	1.29	5 (10%)
23	BCR	b2	601	-	41,41,41	0.69	0	56,56,56	1.98	16 (28%)
23	BCR	b2	602	-	41,41,41	0.69	0	56,56,56	2.14	16 (28%)
23	BCR	b2	603	-	41,41,41	0.69	0	56,56,56	1.90	13 (23%)
25	CLA	b2	604	-	34,50,73	1.42	4 (11%)	37,85,113	1.31	6 (16%)
37	SQD	b2	605	-	44,45,54	1.82	4 (9%)	53,56,65	1.34	4 (7%)
25	CLA	b2	606	-	57,73,73	1.12	4 (7%)	61,113,113	1.16	8 (13%)
25	CLA	b2	608	-	57,73,73	1.14	4 (7%)	61,113,113	1.11	6 (9%)
25	CLA	b2	609	-	53,69,73	1.18	5 (9%)	55,108,113	1.21	7 (12%)
25	CLA	b2	610	-	57,73,73	1.13	4 (7%)	61,113,113	1.16	7 (11%)
25	CLA	b2	611	-	57,73,73	1.12	4 (7%)	61,113,113	1.17	6 (9%)
25	CLA	b2	612	-	57,73,73	1.16	6 (10%)	61,113,113	1.26	9 (14%)
25	CLA	b2	613	-	57,73,73	1.13	4 (7%)	61,113,113	1.13	6 (9%)
25	CLA	b2	614	-	57,73,73	1.13	4 (7%)	61,113,113	1.16	7 (11%)
25	CLA	b2	615	-	52,68,73	1.17	4 (7%)	55,107,113	1.20	7 (12%)
25	CLA	b2	616	-	52,68,73	1.20	4 (7%)	55,107,113	1.20	6 (10%)
25	CLA	b2	617	-	57,73,73	1.12	4 (7%)	61,113,113	1.12	5 (8%)
25	CLA	b2	618	-	57,73,73	1.14	4 (7%)	61,113,113	1.16	7 (11%)
25	CLA	b2	619	-	51,67,73	1.20	5 (9%)	53,105,113	1.17	5 (9%)
25	CLA	b2	620	40	57,73,73	1.12	4 (7%)	61,113,113	1.25	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	LMT	b2	621	-	36,36,36	0.40	0	47,47,47	0.71	0
29	LMG	b2	622	-	39,39,55	1.04	2 (5%)	47,47,63	1.03	3 (6%)
35	LMT	b2	623	-	36,36,36	0.37	0	47,47,47	0.88	1 (2%)
25	CLA	b2	624	-	57,73,73	1.11	4 (7%)	61,113,113	1.18	6 (9%)
33	LHG	b2	625	-	42,42,48	0.98	2 (4%)	43,48,54	1.10	3 (6%)
23	BCR	c1	501	-	41,41,41	0.70	0	56,56,56	2.10	12 (21%)
23	BCR	c1	502	-	41,41,41	0.74	0	56,56,56	2.06	14 (25%)
25	CLA	c1	503	-	57,73,73	1.11	4 (7%)	61,113,113	1.19	7 (11%)
25	CLA	c1	504	-	57,73,73	1.14	4 (7%)	61,113,113	1.17	6 (9%)
25	CLA	c1	505	-	57,73,73	1.12	4 (7%)	61,113,113	1.13	7 (11%)
25	CLA	c1	506	40	57,73,73	1.11	4 (7%)	61,113,113	1.19	5 (8%)
25	CLA	c1	507	-	57,73,73	1.16	4 (7%)	61,113,113	1.15	6 (9%)
25	CLA	c1	508	-	42,58,73	1.33	5 (11%)	44,95,113	1.40	8 (18%)
25	CLA	c1	509	40	57,73,73	1.15	4 (7%)	61,113,113	1.09	6 (9%)
25	CLA	c1	510	-	57,73,73	1.13	6 (10%)	61,113,113	1.25	8 (13%)
25	CLA	c1	511	-	57,73,73	1.12	4 (7%)	61,113,113	1.21	5 (8%)
25	CLA	c1	512	-	57,73,73	1.12	4 (7%)	61,113,113	1.18	5 (8%)
25	CLA	c1	513	3	52,68,73	1.19	4 (7%)	55,107,113	1.21	5 (9%)
34	DGD	c1	514	-	52,52,67	0.94	2 (3%)	66,66,81	1.07	5 (7%)
25	CLA	c1	515	-	47,63,73	1.24	4 (8%)	49,101,113	1.31	8 (16%)
25	CLA	c1	516	-	57,73,73	1.11	4 (7%)	61,113,113	1.16	5 (8%)
35	LMT	c1	517	-	34,34,36	0.43	0	45,45,47	0.67	1 (2%)
34	DGD	c1	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.00	4 (5%)
29	LMG	c1	519	-	55,55,55	0.88	2 (3%)	63,63,63	0.96	2 (3%)
34	DGD	c1	520	-	63,63,67	0.85	2 (3%)	77,77,81	0.89	3 (3%)
32	GOL	c1	521	-	5,5,5	0.34	0	5,5,5	0.27	0
23	BCR	c2	501	-	41,41,41	0.80	1 (2%)	56,56,56	3.44	20 (35%)
25	CLA	c2	502	-	57,73,73	1.12	5 (8%)	61,113,113	1.13	6 (9%)
25	CLA	c2	503	-	57,73,73	1.13	4 (7%)	61,113,113	1.18	9 (14%)
25	CLA	c2	504	-	57,73,73	1.14	4 (7%)	61,113,113	1.14	6 (9%)
25	CLA	c2	505	-	57,73,73	1.11	4 (7%)	61,113,113	1.18	5 (8%)
25	CLA	c2	506	-	53,69,73	1.17	4 (7%)	55,108,113	1.32	6 (10%)
25	CLA	c2	507	-	46,62,73	1.26	4 (8%)	47,99,113	1.29	6 (12%)
25	CLA	c2	508	40	57,73,73	1.14	4 (7%)	61,113,113	1.11	6 (9%)
25	CLA	c2	509	-	57,73,73	1.12	4 (7%)	61,113,113	1.30	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	c2	510	-	46,62,73	1.27	4 (8%)	47,99,113	1.22	6 (12%)
25	CLA	c2	511	-	57,73,73	1.13	4 (7%)	61,113,113	1.14	6 (9%)
25	CLA	c2	512	3	57,73,73	1.14	4 (7%)	61,113,113	1.12	5 (8%)
25	CLA	c2	513	-	46,62,73	1.25	4 (8%)	47,99,113	1.30	6 (12%)
34	DGD	c2	514	-	63,63,67	0.85	2 (3%)	77,77,81	0.98	4 (5%)
25	CLA	c2	515	-	38,54,73	1.34	4 (10%)	41,90,113	1.33	7 (17%)
34	DGD	c2	516	-	53,53,67	0.93	2 (3%)	67,67,81	1.06	4 (5%)
34	DGD	c2	517	-	63,63,67	0.86	2 (3%)	77,77,81	0.85	2 (2%)
32	GOL	c2	518	-	5,5,5	0.35	0	5,5,5	0.21	0
29	LMG	c2	519	-	25,26,55	1.46	2 (8%)	33,33,63	1.51	3 (9%)
25	CLA	d1	401	-	57,73,73	1.12	4 (7%)	61,113,113	1.18	6 (9%)
33	LHG	d1	402	-	31,31,48	1.13	2 (6%)	32,37,54	1.38	3 (9%)
27	PHO	d1	403	-	67,69,69	2.10	16 (23%)	86,99,99	1.95	20 (23%)
25	CLA	d1	404	40	57,73,73	1.11	5 (8%)	61,113,113	1.22	7 (11%)
23	BCR	d1	405	-	41,41,41	0.70	0	56,56,56	1.85	12 (21%)
25	CLA	d1	406	-	57,73,73	1.10	4 (7%)	61,113,113	1.20	6 (9%)
33	LHG	d1	407	-	48,48,48	0.89	2 (4%)	49,54,54	1.07	3 (6%)
29	LMG	d1	408	-	33,33,55	1.12	2 (6%)	41,41,63	1.12	3 (7%)
36	PL9	d1	409	-	54,55,55	0.61	2 (3%)	68,69,69	1.89	21 (30%)
29	LMG	d1	411	-	34,34,55	1.07	2 (5%)	36,36,63	1.15	3 (8%)
23	BCR	d2	401	-	41,41,41	0.70	0	56,56,56	2.15	14 (25%)
25	CLA	d2	402	-	57,73,73	1.10	4 (7%)	61,113,113	1.19	6 (9%)
33	LHG	d2	403	-	48,48,48	0.91	2 (4%)	49,54,54	1.03	3 (6%)
25	CLA	d2	404	-	42,58,73	1.30	4 (9%)	44,95,113	1.37	7 (15%)
25	CLA	d2	405	-	57,73,73	1.13	4 (7%)	61,113,113	1.12	7 (11%)
33	LHG	d2	406	-	48,48,48	0.89	2 (4%)	49,54,54	1.01	3 (6%)
29	LMG	d2	407	-	27,27,55	1.35	2 (7%)	35,35,63	1.29	3 (8%)
27	PHO	d2	408	-	67,69,69	2.08	16 (23%)	86,99,99	1.96	23 (26%)
36	PL9	d2	409	-	54,55,55	0.61	1 (1%)	68,69,69	1.84	19 (27%)
38	HEM	e2	101	5,6	24,50,50	2.35	7 (29%)	16,82,82	1.26	0
38	HEM	f1	101	6	24,50,50	2.35	7 (29%)	16,82,82	1.19	0
34	DGD	h1	101	-	63,63,67	0.85	2 (3%)	77,77,81	0.98	4 (5%)
23	BCR	h1	102	-	41,41,41	0.68	0	56,56,56	1.89	18 (32%)
23	BCR	h2	101	-	41,41,41	0.67	0	56,56,56	1.78	13 (23%)
34	DGD	h2	102	-	63,63,67	0.85	2 (3%)	77,77,81	0.92	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	GOL	i1	101	-	5,5,5	0.41	0	5,5,5	0.16	0
35	LMT	i2	102	-	6,6,36	0.28	0	5,5,47	0.43	0
29	LMG	j2	101	-	50,50,55	0.91	2 (4%)	58,58,63	1.05	3 (5%)
23	BCR	j2	102	-	41,41,41	0.73	0	56,56,56	2.08	17 (30%)
23	BCR	k1	101	-	41,41,41	0.70	0	56,56,56	2.01	14 (25%)
23	BCR	k2	501	-	41,41,41	0.67	0	56,56,56	2.04	14 (25%)
35	LMT	l1	101	-	24,24,36	0.46	0	29,29,47	0.93	2 (6%)
33	LHG	l1	102	-	48,48,48	0.90	2 (4%)	49,54,54	1.09	3 (6%)
33	LHG	l2	101	-	43,43,48	0.97	2 (4%)	44,49,54	1.09	4 (9%)
35	LMT	m1	101	-	36,36,36	0.42	0	47,47,47	0.68	0
35	LMT	m2	103	-	31,31,36	0.43	0	42,42,47	0.96	2 (4%)
35	LMT	m2	104	-	30,30,36	0.46	0	41,41,47	0.84	1 (2%)
38	HEM	v1	201	16	24,50,50	2.36	6 (25%)	16,82,82	1.37	1 (6%)
38	HEM	v2	201	16	24,50,50	2.36	6 (25%)	16,82,82	1.25	0
23	BCR	z2	101	-	41,41,41	0.69	0	56,56,56	1.74	9 (16%)

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
23	BCR	A1	401	-	-	0/29/63/63	0/2/2/2
25	CLA	A1	403	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	A1	404	-	3/3/17/25	0/21/119/135	0/0/9/9
25	CLA	A1	405	-	3/3/18/25	0/25/123/135	0/0/9/9
25	CLA	A1	406	-	3/3/20/25	0/37/135/135	0/0/9/9
26	OEX	A1	407	1,3,40	-	0/0/68/68	0/0/6/6
27	PHO	A1	408	-	-	0/53/103/103	0/1/6/6
29	LMG	A1	410	-	-	0/38/58/70	0/1/1/1
29	LMG	A1	412	-	-	0/36/56/70	0/1/1/1
31	BCT	A1	413	30	-	0/0/0/0	0/0/0/0
23	BCR	A2	401	-	-	0/29/63/63	0/2/2/2
25	CLA	A2	402	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	A2	403	-	3/3/19/25	0/33/131/135	0/0/9/9
25	CLA	A2	404	-	3/3/17/25	0/21/119/135	0/0/9/9
33	LHG	A2	405	-	-	0/37/37/53	0/0/0/0
26	OEX	A2	406	1,3,40	-	0/0/68/68	0/0/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PHO	A2	407	-	-	0/53/103/103	0/1/6/6
29	LMG	A2	412	-	-	0/23/43/70	0/1/1/1
31	BCT	A2	413	30	-	0/0/0/0	0/0/0/0
23	BCR	B1	601	-	-	0/29/63/63	0/2/2/2
23	BCR	B1	602	-	-	0/29/63/63	0/2/2/2
23	BCR	B1	603	-	-	0/29/63/63	0/2/2/2
25	CLA	B1	604	-	3/3/15/25	0/10/108/135	0/0/9/9
25	CLA	B1	605	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B1	606	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B1	607	-	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	B1	608	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B1	609	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B1	610	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B1	611	-	2/2/19/25	1/34/132/135	0/0/9/9
25	CLA	B1	612	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B1	613	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B1	614	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B1	615	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B1	616	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B1	617	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B1	618	-	3/3/18/25	0/29/127/135	0/0/9/9
25	CLA	B1	619	40	3/3/20/25	0/37/135/135	0/0/9/9
32	GOL	B1	620	-	-	0/4/4/4	0/0/0/0
33	LHG	B1	621	-	-	0/53/53/53	0/0/0/0
29	LMG	B1	622	-	-	0/26/46/70	0/1/1/1
29	LMG	B1	626	-	-	0/43/63/70	0/1/1/1
23	BCR	B2	601	-	-	0/29/63/63	0/2/2/2
23	BCR	B2	602	-	-	0/29/63/63	0/2/2/2
23	BCR	B2	603	-	-	0/29/63/63	0/2/2/2
25	CLA	B2	604	-	3/3/15/25	0/8/106/135	0/0/9/9
25	CLA	B2	605	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B2	606	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B2	607	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B2	608	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B2	609	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B2	610	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B2	611	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B2	612	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B2	613	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B2	614	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B2	615	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B2	616	-	3/3/17/25	0/24/122/135	0/0/9/9
25	CLA	B2	617	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B2	618	-	3/3/19/25	1/31/129/135	0/0/9/9
25	CLA	B2	619	-	3/3/20/25	0/37/135/135	0/0/9/9
29	LMG	B2	620	-	-	0/35/55/70	0/1/1/1
29	LMG	B2	621	-	-	0/31/51/70	0/1/1/1
37	SQD	B2	623	-	-	0/40/60/69	0/1/1/1
33	LHG	B2	627	-	-	0/46/46/53	0/0/0/0
23	BCR	C1	501	-	-	0/29/63/63	0/2/2/2
25	CLA	C1	502	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C1	503	-	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	C1	504	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C1	505	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C1	506	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C1	507	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C1	508	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C1	509	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C1	510	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C1	511	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C1	512	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C1	513	3	3/3/19/25	0/33/131/135	0/0/9/9
25	CLA	C1	514	-	3/3/16/25	0/11/111/135	0/0/9/9
34	DGD	C1	515	-	-	0/41/81/95	0/2/2/2
34	DGD	C1	516	-	-	0/51/91/95	0/2/2/2
34	DGD	C1	517	-	-	0/53/93/95	0/2/2/2
32	GOL	C1	518	-	-	0/4/4/4	0/0/0/0
35	LMT	C1	519	-	-	0/21/61/61	0/2/2/2
29	LMG	C1	520	-	-	0/43/63/70	0/1/1/1
23	BCR	C1	521	-	-	0/29/63/63	0/2/2/2
23	BCR	C2	502	-	-	0/29/63/63	0/2/2/2
25	CLA	C2	503	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C2	504	-	3/3/16/25	0/15/113/135	0/0/9/9
25	CLA	C2	505	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C2	506	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C2	507	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CLA	C2	508	-	3/3/17/25	0/19/117/135	0/0/9/9
25	CLA	C2	509	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C2	510	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CLA	C2	511	-	3/3/17/25	0/19/117/135	0/0/9/9
34	DGD	C2	512	-	-	0/20/60/95	0/2/2/2
25	CLA	C2	513	-	3/3/17/25	0/23/121/135	0/0/9/9
32	GOL	C2	514	-	-	0/4/4/4	0/0/0/0
29	LMG	C2	515	-	-	0/18/38/70	0/1/1/1
25	CLA	C2	516	-	3/3/16/25	0/15/113/135	0/0/9/9
25	CLA	C2	518	-	3/3/15/25	0/8/106/135	0/0/9/9
23	BCR	D1	401	-	-	0/29/63/63	0/2/2/2
25	CLA	D1	402	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	D1	403	-	3/3/17/25	0/21/119/135	0/0/9/9
33	LHG	D1	404	-	-	0/53/53/53	0/0/0/0
33	LHG	D1	405	-	-	0/53/53/53	0/0/0/0
29	LMG	D1	406	-	-	0/30/50/70	0/1/1/1
27	PHO	D1	407	-	-	0/51/101/103	0/1/6/6
36	PL9	D1	408	-	-	0/53/73/73	0/1/1/1
37	SQD	D1	409	-	-	0/29/49/69	0/1/1/1
25	CLA	D2	401	-	3/3/20/25	0/37/135/135	0/0/9/9
37	SQD	D2	402	-	-	0/18/38/69	0/1/1/1
33	LHG	D2	403	-	-	0/53/53/53	0/0/0/0
25	CLA	D2	404	-	3/3/19/25	0/33/131/135	0/0/9/9
33	LHG	D2	405	-	-	0/53/53/53	0/0/0/0
25	CLA	D2	406	-	3/3/20/25	0/37/135/135	0/0/9/9
27	PHO	D2	407	-	-	0/53/103/103	0/1/6/6
36	PL9	D2	408	-	-	0/53/73/73	0/1/1/1
38	HEM	E1	101	5,6	-	0/6/54/54	0/0/8/8
38	HEM	E2	101	5	-	0/6/54/54	0/0/8/8
23	BCR	F2	401	-	-	0/29/63/63	0/2/2/2
29	LMG	F2	402	-	-	0/30/50/70	0/1/1/1
34	DGD	H1	101	-	-	0/51/91/95	0/2/2/2
23	BCR	H1	102	-	-	0/15/32/63	0/1/1/2
34	DGD	H2	101	-	-	0/51/91/95	0/2/2/2
23	BCR	H2	103	-	-	0/17/34/63	0/1/1/2
29	LMG	I2	101	-	-	0/29/49/70	0/1/1/1
23	BCR	J1	101	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	K1	101	-	-	0/26/43/63	0/1/1/2
25	CLA	K2	101	-	3/3/18/25	0/25/123/135	0/0/9/9
23	BCR	K2	102	-	-	0/29/63/63	0/2/2/2
23	BCR	K2	104	-	-	0/12/46/63	0/2/2/2
33	LHG	L1	101	-	-	0/45/45/53	0/0/0/0
35	LMT	L1	102	-	-	0/9/9/61	0/0/0/2
33	LHG	L2	101	-	-	0/53/53/53	0/0/0/0
29	LMG	M1	101	-	-	0/31/31/70	0/0/0/1
35	LMT	M1	102	-	-	0/8/8/61	0/0/0/2
35	LMT	M1	103	-	-	0/15/35/61	0/1/1/2
35	LMT	T1	101	-	-	0/9/9/61	0/0/0/2
38	HEM	V1	201	16	-	0/6/54/54	0/0/8/8
38	HEM	V2	201	16	-	0/6/54/54	0/0/8/8
23	BCR	a1	401	-	-	0/29/63/63	0/2/2/2
25	CLA	a1	403	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	a1	404	-	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	a1	405	-	3/3/17/25	0/19/117/135	0/0/9/9
32	GOL	a1	406	-	-	0/4/4/4	0/0/0/0
33	LHG	a1	407	-	-	0/47/47/53	0/0/0/0
26	OEX	a1	408	1,3,40	-	0/0/68/68	0/0/6/6
27	PHO	a1	411	-	-	0/53/103/103	0/1/6/6
29	LMG	a1	412	-	-	0/46/66/70	0/1/1/1
31	BCT	a1	413	30	-	0/0/0/0	0/0/0/0
23	BCR	a2	402	-	-	0/29/63/63	0/2/2/2
25	CLA	a2	404	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	a2	405	-	3/3/20/25	0/37/135/135	0/0/9/9
35	LMT	a2	406	-	-	0/21/61/61	0/2/2/2
33	LHG	a2	407	-	-	0/33/33/53	0/0/0/0
26	OEX	a2	408	1,3,40	-	0/0/68/68	0/0/6/6
29	LMG	a2	412	-	-	0/39/59/70	0/1/1/1
25	CLA	a2	413	-	3/3/17/25	0/19/117/135	0/0/9/9
32	GOL	a2	415	-	-	0/4/4/4	0/0/0/0
27	PHO	a2	416	-	-	0/53/103/103	0/1/6/6
31	BCT	a2	417	30	-	0/0/0/0	0/0/0/0
23	BCR	b1	601	-	-	0/29/63/63	0/2/2/2
23	BCR	b1	602	-	-	0/29/63/63	0/2/2/2
23	BCR	b1	603	-	-	0/29/63/63	0/2/2/2
25	CLA	b1	604	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b1	605	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b1	606	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b1	607	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b1	608	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b1	609	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b1	610	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b1	611	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b1	612	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b1	613	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b1	614	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b1	615	-	3/3/18/25	0/30/128/135	0/0/9/9
25	CLA	b1	616	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b1	617	-	3/3/20/25	0/37/135/135	0/0/9/9
32	GOL	b1	618	-	-	0/4/4/4	0/0/0/0
25	CLA	b1	619	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b1	620	-	3/3/20/25	0/37/135/135	0/0/9/9
29	LMG	b1	621	-	-	0/33/53/70	0/1/1/1
33	LHG	b1	622	-	-	0/53/53/53	0/0/0/0
29	LMG	b1	624	-	-	0/34/54/70	0/1/1/1
29	LMG	b1	631	-	-	0/35/55/70	0/1/1/1
23	BCR	b2	601	-	-	0/29/63/63	0/2/2/2
23	BCR	b2	602	-	-	0/29/63/63	0/2/2/2
23	BCR	b2	603	-	-	0/29/63/63	0/2/2/2
25	CLA	b2	604	-	3/3/15/25	0/10/108/135	0/0/9/9
37	SQD	b2	605	-	-	0/40/60/69	0/1/1/1
25	CLA	b2	606	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b2	608	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b2	609	-	3/3/19/25	0/33/131/135	0/0/9/9
25	CLA	b2	610	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b2	611	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b2	612	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b2	613	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b2	614	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b2	615	-	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	b2	616	-	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	b2	617	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b2	618	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b2	619	-	3/3/18/25	0/30/128/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b2	620	40	3/3/20/25	0/37/135/135	0/0/9/9
35	LMT	b2	621	-	-	0/21/61/61	0/2/2/2
29	LMG	b2	622	-	-	0/34/54/70	0/1/1/1
35	LMT	b2	623	-	-	0/21/61/61	0/2/2/2
25	CLA	b2	624	-	3/3/20/25	0/37/135/135	0/0/9/9
33	LHG	b2	625	-	-	0/47/47/53	0/0/0/0
23	BCR	c1	501	-	-	0/29/63/63	0/2/2/2
23	BCR	c1	502	-	-	0/29/63/63	0/2/2/2
25	CLA	c1	503	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c1	504	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c1	505	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c1	506	40	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c1	507	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c1	508	-	3/3/17/25	0/19/117/135	0/0/9/9
25	CLA	c1	509	40	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c1	510	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c1	511	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c1	512	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c1	513	3	3/3/19/25	0/31/129/135	0/0/9/9
34	DGD	c1	514	-	-	0/40/80/95	0/2/2/2
25	CLA	c1	515	-	3/3/18/25	0/25/123/135	0/0/9/9
25	CLA	c1	516	-	3/3/20/25	0/37/135/135	0/0/9/9
35	LMT	c1	517	-	-	0/19/59/61	0/2/2/2
34	DGD	c1	518	-	-	0/51/91/95	0/2/2/2
29	LMG	c1	519	-	-	0/50/70/70	0/1/1/1
34	DGD	c1	520	-	-	0/51/91/95	0/2/2/2
32	GOL	c1	521	-	-	0/4/4/4	0/0/0/0
23	BCR	c2	501	-	-	0/29/63/63	0/2/2/2
25	CLA	c2	502	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c2	503	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c2	504	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c2	505	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c2	506	-	3/3/19/25	0/33/131/135	0/0/9/9
25	CLA	c2	507	-	3/3/17/25	0/24/122/135	0/0/9/9
25	CLA	c2	508	40	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c2	509	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c2	510	-	3/3/17/25	0/24/122/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c2	511	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c2	512	3	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c2	513	-	3/3/17/25	0/24/122/135	0/0/9/9
34	DGD	c2	514	-	-	0/51/91/95	0/2/2/2
25	CLA	c2	515	-	3/3/16/25	0/15/113/135	0/0/9/9
34	DGD	c2	516	-	-	0/41/81/95	0/2/2/2
34	DGD	c2	517	-	-	0/51/91/95	0/2/2/2
32	GOL	c2	518	-	-	0/4/4/4	0/0/0/0
29	LMG	c2	519	-	-	1/20/40/70	0/1/1/1
25	CLA	d1	401	-	3/3/20/25	0/37/135/135	0/0/9/9
33	LHG	d1	402	-	-	0/36/36/53	0/0/0/0
27	PHO	d1	403	-	-	0/53/103/103	0/1/6/6
25	CLA	d1	404	40	3/3/20/25	0/37/135/135	0/0/9/9
23	BCR	d1	405	-	-	0/29/63/63	0/2/2/2
25	CLA	d1	406	-	3/3/20/25	0/37/135/135	0/0/9/9
33	LHG	d1	407	-	-	0/53/53/53	0/0/0/0
29	LMG	d1	408	-	-	0/28/48/70	0/1/1/1
36	PL9	d1	409	-	-	0/53/73/73	0/1/1/1
29	LMG	d1	411	-	-	0/36/36/70	0/0/0/1
23	BCR	d2	401	-	-	0/29/63/63	0/2/2/2
25	CLA	d2	402	-	3/3/20/25	0/37/135/135	0/0/9/9
33	LHG	d2	403	-	-	0/53/53/53	0/0/0/0
25	CLA	d2	404	-	3/3/17/25	0/19/117/135	0/0/9/9
25	CLA	d2	405	-	3/3/20/25	0/37/135/135	0/0/9/9
33	LHG	d2	406	-	-	0/53/53/53	0/0/0/0
29	LMG	d2	407	-	-	0/21/41/70	0/1/1/1
27	PHO	d2	408	-	-	0/53/103/103	0/1/6/6
36	PL9	d2	409	-	-	0/53/73/73	0/1/1/1
38	HEM	e2	101	5,6	-	0/6/54/54	0/0/8/8
38	HEM	f1	101	6	-	0/6/54/54	0/0/8/8
34	DGD	h1	101	-	-	0/51/91/95	0/2/2/2
23	BCR	h1	102	-	-	0/29/63/63	0/2/2/2
23	BCR	h2	101	-	-	0/29/63/63	0/2/2/2
34	DGD	h2	102	-	-	0/51/91/95	0/2/2/2
32	GOL	i1	101	-	-	0/4/4/4	0/0/0/0
35	LMT	i2	102	-	-	0/4/4/61	0/0/0/2
29	LMG	j2	101	-	-	0/45/65/70	0/1/1/1
23	BCR	j2	102	-	-	0/29/63/63	0/2/2/2
23	BCR	k1	101	-	-	0/29/63/63	0/2/2/2
23	BCR	k2	501	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMT	l1	101	-	-	0/15/35/61	0/1/1/2
33	LHG	l1	102	-	-	0/53/53/53	0/0/0/0
33	LHG	l2	101	-	-	0/48/48/53	0/0/0/0
35	LMT	m1	101	-	-	0/21/61/61	0/2/2/2
35	LMT	m2	103	-	-	0/16/56/61	0/2/2/2
35	LMT	m2	104	-	-	0/15/55/61	0/2/2/2
38	HEM	v1	201	16	-	0/6/54/54	0/0/8/8
38	HEM	v2	201	16	-	0/6/54/54	0/0/8/8
23	BCR	z2	101	-	-	0/29/63/63	0/2/2/2

All (935) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	D1	409	SQD	C6-S	-9.31	1.66	1.77
37	B2	623	SQD	C6-S	-9.13	1.66	1.77
37	D2	402	SQD	C6-S	-9.11	1.66	1.77
37	b2	605	SQD	C6-S	-8.84	1.67	1.77
38	V2	201	HEM	C3B-C2B	-5.14	1.33	1.40
38	v2	201	HEM	C3C-C2C	-5.12	1.33	1.40
38	f1	101	HEM	C3B-C2B	-5.08	1.33	1.40
38	V1	201	HEM	C3C-C2C	-5.06	1.33	1.40
38	E2	101	HEM	C3B-C2B	-5.04	1.34	1.40
38	v1	201	HEM	C3C-C2C	-5.04	1.34	1.40
38	E1	101	HEM	C3B-C2B	-5.01	1.34	1.40
38	e2	101	HEM	C3B-C2B	-4.99	1.34	1.40
38	V2	201	HEM	C3C-C2C	-4.88	1.34	1.40
38	f1	101	HEM	C3C-C2C	-4.25	1.35	1.40
38	V1	201	HEM	C3B-C2B	-4.22	1.35	1.40
38	v1	201	HEM	C3B-C2B	-4.22	1.35	1.40
38	e2	101	HEM	C3C-C2C	-4.14	1.35	1.40
38	E1	101	HEM	C3C-C2C	-4.12	1.35	1.40
38	v2	201	HEM	C3B-C2B	-4.09	1.35	1.40
38	E2	101	HEM	C3C-C2C	-4.09	1.35	1.40
27	d1	403	PHO	C4A-NA	-3.56	1.26	1.35
27	a2	416	PHO	C4A-NA	-3.54	1.26	1.35
27	A1	408	PHO	C4A-NA	-3.52	1.26	1.35
27	d2	408	PHO	C4A-NA	-3.47	1.26	1.35
27	D2	407	PHO	C4A-NA	-3.46	1.26	1.35
27	A2	407	PHO	C4A-NA	-3.45	1.26	1.35
27	D1	407	PHO	C4A-NA	-3.44	1.26	1.35
27	a1	411	PHO	C4A-NA	-3.43	1.26	1.35
25	C1	509	CLA	CMB-C2B	-3.20	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b2	612	CLA	CMB-C2B	-3.17	1.45	1.51
25	b1	613	CLA	CMB-C2B	-3.03	1.45	1.51
25	B1	613	CLA	CMB-C2B	-3.01	1.45	1.51
25	B2	613	CLA	CMB-C2B	-2.87	1.45	1.51
27	a1	411	PHO	C3D-C4D	-2.85	1.34	1.43
27	d1	403	PHO	C3D-C4D	-2.84	1.34	1.43
25	b1	607	CLA	CMB-C2B	-2.80	1.45	1.51
27	A2	407	PHO	C3D-C4D	-2.80	1.34	1.43
27	A1	408	PHO	C3D-C4D	-2.74	1.34	1.43
25	C2	511	CLA	CMB-C2B	-2.74	1.46	1.51
27	d2	408	PHO	C3D-C4D	-2.73	1.34	1.43
27	D2	407	PHO	C3D-C4D	-2.72	1.34	1.43
25	c2	509	CLA	CMB-C2B	-2.72	1.46	1.51
27	a2	416	PHO	C3D-C4D	-2.70	1.34	1.43
25	c1	508	CLA	CMB-C2B	-2.69	1.46	1.51
25	b2	616	CLA	CMB-C2B	-2.68	1.46	1.51
27	D1	407	PHO	C3D-C4D	-2.68	1.34	1.43
25	B1	610	CLA	CMB-C2B	-2.63	1.46	1.51
25	c1	509	CLA	CMB-C2B	-2.62	1.46	1.51
25	A2	402	CLA	CMB-C2B	-2.62	1.46	1.51
25	A2	402	CLA	C3B-C2B	-2.61	1.37	1.40
25	c1	510	CLA	CMB-C2B	-2.59	1.46	1.51
25	B2	607	CLA	CMB-C2B	-2.58	1.46	1.51
25	c2	507	CLA	CMB-C2B	-2.58	1.46	1.51
25	A1	403	CLA	CMD-C2D	-2.57	1.46	1.51
25	B1	607	CLA	CMB-C2B	-2.57	1.46	1.51
25	b1	610	CLA	CMB-C2B	-2.56	1.46	1.51
25	A2	404	CLA	CMB-C2B	-2.56	1.46	1.51
25	A1	405	CLA	CMB-C2B	-2.56	1.46	1.51
25	A1	403	CLA	CMB-C2B	-2.55	1.46	1.51
25	C1	506	CLA	CMD-C2D	-2.55	1.46	1.51
25	b1	619	CLA	CMB-C2B	-2.54	1.46	1.51
25	d1	404	CLA	CMB-C2B	-2.54	1.46	1.51
25	c2	503	CLA	CMB-C2B	-2.54	1.46	1.51
25	d2	402	CLA	CMB-C2B	-2.54	1.46	1.51
25	B1	616	CLA	CMB-C2B	-2.54	1.46	1.51
25	C1	507	CLA	CMB-C2B	-2.53	1.46	1.51
25	b2	620	CLA	CMB-C2B	-2.53	1.46	1.51
25	a2	404	CLA	C3B-C2B	-2.52	1.37	1.40
25	C2	513	CLA	CMB-C2B	-2.52	1.46	1.51
25	B2	606	CLA	CMB-C2B	-2.52	1.46	1.51
25	b1	604	CLA	CMB-C2B	-2.52	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C2	509	CLA	CMB-C2B	-2.51	1.46	1.51
25	K2	101	CLA	CMB-C2B	-2.51	1.46	1.51
25	D2	404	CLA	CMB-C2B	-2.51	1.46	1.51
25	a1	404	CLA	CMB-C2B	-2.51	1.46	1.51
25	A1	406	CLA	CMB-C2B	-2.50	1.46	1.51
25	A1	405	CLA	C3B-C2B	-2.50	1.37	1.40
25	C1	504	CLA	CMB-C2B	-2.50	1.46	1.51
25	b2	614	CLA	CMD-C2D	-2.50	1.46	1.51
25	B2	617	CLA	CMB-C2B	-2.50	1.46	1.51
25	B1	606	CLA	CMB-C2B	-2.49	1.46	1.51
25	b2	611	CLA	CMB-C2B	-2.49	1.46	1.51
25	a2	413	CLA	CMD-C2D	-2.49	1.46	1.51
25	c1	507	CLA	CMB-C2B	-2.49	1.46	1.51
25	B1	614	CLA	CMB-C2B	-2.49	1.46	1.51
25	A1	403	CLA	C3B-C2B	-2.49	1.37	1.40
25	A2	403	CLA	CMB-C2B	-2.49	1.46	1.51
25	B2	616	CLA	CMB-C2B	-2.49	1.46	1.51
25	b2	618	CLA	CMB-C2B	-2.49	1.46	1.51
25	b1	606	CLA	CMB-C2B	-2.49	1.46	1.51
25	B1	619	CLA	CMB-C2B	-2.49	1.46	1.51
25	b1	609	CLA	CMB-C2B	-2.49	1.46	1.51
25	C2	516	CLA	CMB-C2B	-2.48	1.46	1.51
25	b1	611	CLA	CMB-C2B	-2.48	1.46	1.51
25	B1	612	CLA	CMB-C2B	-2.48	1.46	1.51
25	b1	614	CLA	CMD-C2D	-2.48	1.46	1.51
25	a2	405	CLA	CMB-C2B	-2.48	1.46	1.51
25	b1	616	CLA	CMB-C2B	-2.48	1.46	1.51
25	C1	510	CLA	CMB-C2B	-2.47	1.46	1.51
25	C1	506	CLA	CMB-C2B	-2.47	1.46	1.51
25	C2	506	CLA	CMB-C2B	-2.47	1.46	1.51
25	c2	512	CLA	CMB-C2B	-2.47	1.46	1.51
25	B2	618	CLA	CMB-C2B	-2.47	1.46	1.51
25	a2	413	CLA	CMB-C2B	-2.47	1.46	1.51
25	a2	404	CLA	CMB-C2B	-2.47	1.46	1.51
25	b2	609	CLA	CMB-C2B	-2.46	1.46	1.51
25	b1	620	CLA	CMB-C2B	-2.46	1.46	1.51
25	c2	504	CLA	CMB-C2B	-2.46	1.46	1.51
25	B1	611	CLA	CMB-C2B	-2.46	1.46	1.51
25	C2	508	CLA	CMB-C2B	-2.46	1.46	1.51
25	B1	609	CLA	CMB-C2B	-2.46	1.46	1.51
25	c1	507	CLA	CMD-C2D	-2.46	1.46	1.51
25	d2	404	CLA	CMB-C2B	-2.46	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c1	515	CLA	CMB-C2B	-2.46	1.46	1.51
25	b2	613	CLA	CMB-C2B	-2.46	1.46	1.51
25	D2	406	CLA	CMB-C2B	-2.46	1.46	1.51
25	C1	513	CLA	CMB-C2B	-2.46	1.46	1.51
25	B1	618	CLA	CMB-C2B	-2.46	1.46	1.51
25	C1	514	CLA	CMB-C2B	-2.45	1.46	1.51
25	b1	617	CLA	CMB-C2B	-2.45	1.46	1.51
25	c2	506	CLA	CMB-C2B	-2.45	1.46	1.51
25	c2	508	CLA	CMB-C2B	-2.45	1.46	1.51
25	B1	605	CLA	CMB-C2B	-2.45	1.46	1.51
25	a1	403	CLA	CMB-C2B	-2.45	1.46	1.51
25	C1	503	CLA	CMB-C2B	-2.44	1.46	1.51
25	c1	512	CLA	CMD-C2D	-2.44	1.46	1.51
25	b2	610	CLA	CMB-C2B	-2.44	1.46	1.51
25	B2	619	CLA	CMB-C2B	-2.44	1.46	1.51
25	D2	401	CLA	CMB-C2B	-2.44	1.46	1.51
25	B2	609	CLA	CMB-C2B	-2.44	1.46	1.51
25	B2	612	CLA	CMB-C2B	-2.44	1.46	1.51
25	c1	503	CLA	CMB-C2B	-2.44	1.46	1.51
25	c1	506	CLA	CMB-C2B	-2.44	1.46	1.51
25	c2	513	CLA	CMB-C2B	-2.44	1.46	1.51
25	C1	512	CLA	CMD-C2D	-2.44	1.46	1.51
25	b1	614	CLA	CMB-C2B	-2.44	1.46	1.51
25	b2	608	CLA	CMB-C2B	-2.44	1.46	1.51
25	b2	617	CLA	CMB-C2B	-2.44	1.46	1.51
25	C2	505	CLA	CMB-C2B	-2.43	1.46	1.51
25	c1	505	CLA	CMB-C2B	-2.43	1.46	1.51
25	a1	403	CLA	CMD-C2D	-2.43	1.46	1.51
25	c1	511	CLA	CMD-C2D	-2.43	1.46	1.51
25	a2	404	CLA	CMD-C2D	-2.43	1.46	1.51
25	K2	101	CLA	CMD-C2D	-2.43	1.46	1.51
25	B2	604	CLA	CMB-C2B	-2.43	1.46	1.51
25	C1	511	CLA	CMB-C2B	-2.43	1.46	1.51
25	b1	608	CLA	CMB-C2B	-2.43	1.46	1.51
25	c2	510	CLA	CMB-C2B	-2.43	1.46	1.51
25	B2	608	CLA	CMB-C2B	-2.43	1.46	1.51
25	B2	605	CLA	CMB-C2B	-2.43	1.46	1.51
25	b2	624	CLA	CMB-C2B	-2.42	1.46	1.51
25	C2	510	CLA	CMB-C2B	-2.42	1.46	1.51
25	C2	507	CLA	CMD-C2D	-2.42	1.46	1.51
25	c1	512	CLA	CMB-C2B	-2.42	1.46	1.51
25	C1	508	CLA	CMB-C2B	-2.42	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C2	518	CLA	CMB-C2B	-2.42	1.46	1.51
25	c2	505	CLA	CMB-C2B	-2.42	1.46	1.51
25	b2	615	CLA	CMB-C2B	-2.42	1.46	1.51
25	c2	511	CLA	CMB-C2B	-2.42	1.46	1.51
25	b1	612	CLA	CMB-C2B	-2.42	1.46	1.51
25	B2	614	CLA	CMB-C2B	-2.42	1.46	1.51
25	B1	604	CLA	CMB-C2B	-2.41	1.46	1.51
25	B1	608	CLA	CMB-C2B	-2.41	1.46	1.51
25	b2	606	CLA	CMB-C2B	-2.41	1.46	1.51
25	A1	404	CLA	CMB-C2B	-2.41	1.46	1.51
25	c2	506	CLA	CMD-C2D	-2.41	1.46	1.51
25	C1	512	CLA	CMB-C2B	-2.41	1.46	1.51
25	c1	513	CLA	CMB-C2B	-2.41	1.46	1.51
25	D1	403	CLA	CMB-C2B	-2.41	1.46	1.51
25	B2	607	CLA	CMD-C2D	-2.40	1.46	1.51
25	a1	405	CLA	CMB-C2B	-2.40	1.46	1.51
25	C2	503	CLA	CMB-C2B	-2.40	1.46	1.51
25	c1	516	CLA	CMB-C2B	-2.40	1.46	1.51
25	A1	404	CLA	CMD-C2D	-2.40	1.46	1.51
25	c1	513	CLA	CMD-C2D	-2.40	1.46	1.51
25	C2	507	CLA	CMB-C2B	-2.40	1.46	1.51
25	c2	502	CLA	CMB-C2B	-2.39	1.46	1.51
25	C1	505	CLA	CMB-C2B	-2.39	1.46	1.51
25	d1	406	CLA	CMB-C2B	-2.39	1.46	1.51
25	B2	614	CLA	CMD-C2D	-2.39	1.46	1.51
25	b1	605	CLA	CMB-C2B	-2.39	1.46	1.51
25	B1	614	CLA	CMD-C2D	-2.39	1.46	1.51
25	B1	613	CLA	CMD-C2D	-2.39	1.46	1.51
25	b2	619	CLA	CMB-C2B	-2.38	1.46	1.51
25	b2	604	CLA	CMB-C2B	-2.38	1.46	1.51
25	B1	617	CLA	CMB-C2B	-2.37	1.46	1.51
25	C2	504	CLA	CMB-C2B	-2.37	1.46	1.51
25	c2	515	CLA	CMB-C2B	-2.37	1.46	1.51
25	B1	613	CLA	C3B-C2B	-2.37	1.37	1.40
25	C1	511	CLA	CMD-C2D	-2.36	1.46	1.51
25	d2	405	CLA	CMB-C2B	-2.36	1.46	1.51
25	C1	510	CLA	CMD-C2D	-2.35	1.46	1.51
25	b2	612	CLA	C3B-C2B	-2.35	1.37	1.40
25	c1	511	CLA	CMB-C2B	-2.35	1.46	1.51
25	a1	403	CLA	C3B-C2B	-2.35	1.37	1.40
25	B2	613	CLA	CMD-C2D	-2.35	1.46	1.51
25	C1	502	CLA	CMB-C2B	-2.35	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c2	513	CLA	CMD-C2D	-2.34	1.46	1.51
25	B2	610	CLA	CMB-C2B	-2.34	1.46	1.51
25	c2	510	CLA	CMD-C2D	-2.34	1.46	1.51
25	B2	615	CLA	CMB-C2B	-2.34	1.46	1.51
25	B1	615	CLA	CMB-C2B	-2.34	1.46	1.51
25	a1	404	CLA	C3B-C2B	-2.33	1.37	1.40
25	b2	614	CLA	CMB-C2B	-2.33	1.46	1.51
25	B2	611	CLA	CMB-C2B	-2.33	1.46	1.51
25	b2	612	CLA	CMD-C2D	-2.33	1.46	1.51
25	c1	504	CLA	CMB-C2B	-2.33	1.46	1.51
25	D1	402	CLA	CMB-C2B	-2.33	1.46	1.51
25	d1	401	CLA	CMB-C2B	-2.33	1.46	1.51
25	B1	616	CLA	CMD-C2D	-2.32	1.46	1.51
25	D2	401	CLA	CMD-C2D	-2.32	1.46	1.51
25	b1	613	CLA	C3B-C2B	-2.32	1.37	1.40
25	C1	513	CLA	CMD-C2D	-2.31	1.46	1.51
25	B2	616	CLA	CMD-C2D	-2.31	1.46	1.51
25	b1	615	CLA	CMD-C2D	-2.31	1.46	1.51
25	b1	613	CLA	CMD-C2D	-2.31	1.46	1.51
25	A2	404	CLA	CMD-C2D	-2.31	1.46	1.51
25	b1	617	CLA	CMD-C2D	-2.30	1.46	1.51
25	b2	606	CLA	CMD-C2D	-2.30	1.46	1.51
25	b1	606	CLA	CMD-C2D	-2.30	1.46	1.51
25	b1	605	CLA	CMD-C2D	-2.30	1.46	1.51
25	B1	618	CLA	CMD-C2D	-2.30	1.46	1.51
25	B2	606	CLA	CMD-C2D	-2.30	1.46	1.51
25	c1	504	CLA	CMD-C2D	-2.30	1.46	1.51
25	C1	509	CLA	CMD-C2D	-2.29	1.46	1.51
25	b1	619	CLA	CMD-C2D	-2.29	1.46	1.51
25	B1	607	CLA	CMD-C2D	-2.29	1.46	1.51
25	d2	405	CLA	CMD-C2D	-2.29	1.46	1.51
25	b1	609	CLA	CMD-C2D	-2.29	1.46	1.51
25	C2	516	CLA	CMD-C2D	-2.29	1.46	1.51
25	c2	511	CLA	CMD-C2D	-2.29	1.46	1.51
25	b2	608	CLA	CMD-C2D	-2.29	1.46	1.51
25	c2	505	CLA	CMD-C2D	-2.29	1.46	1.51
25	a1	404	CLA	CMD-C2D	-2.29	1.46	1.51
25	C1	505	CLA	CMD-C2D	-2.29	1.46	1.51
25	c2	512	CLA	CMD-C2D	-2.28	1.46	1.51
25	C2	509	CLA	CMD-C2D	-2.28	1.46	1.51
25	b2	615	CLA	CMD-C2D	-2.28	1.46	1.51
25	b2	624	CLA	CMD-C2D	-2.28	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A1	405	CLA	CMD-C2D	-2.28	1.46	1.51
25	a1	405	CLA	CMD-C2D	-2.28	1.46	1.51
25	C2	518	CLA	CMD-C2D	-2.28	1.46	1.51
25	d1	401	CLA	CMD-C2D	-2.28	1.46	1.51
25	B1	604	CLA	CMD-C2D	-2.27	1.46	1.51
25	B2	608	CLA	CMD-C2D	-2.27	1.46	1.51
25	b2	619	CLA	CMD-C2D	-2.27	1.46	1.51
25	B1	606	CLA	CMD-C2D	-2.27	1.46	1.51
25	C2	506	CLA	CMD-C2D	-2.27	1.46	1.51
25	c1	506	CLA	CMD-C2D	-2.27	1.46	1.51
25	B1	609	CLA	CMD-C2D	-2.27	1.46	1.51
25	c2	508	CLA	CMD-C2D	-2.27	1.46	1.51
25	b1	607	CLA	CMD-C2D	-2.27	1.46	1.51
25	c1	515	CLA	CMD-C2D	-2.27	1.46	1.51
25	B1	612	CLA	CMD-C2D	-2.27	1.46	1.51
25	b1	615	CLA	CMB-C2B	-2.27	1.47	1.51
25	B2	617	CLA	CMD-C2D	-2.27	1.46	1.51
25	b2	611	CLA	CMD-C2D	-2.27	1.46	1.51
25	B2	618	CLA	CMD-C2D	-2.26	1.46	1.51
25	B1	608	CLA	CMD-C2D	-2.26	1.46	1.51
25	D1	402	CLA	CMD-C2D	-2.26	1.46	1.51
25	b2	613	CLA	CMD-C2D	-2.26	1.46	1.51
25	c1	509	CLA	CMD-C2D	-2.26	1.46	1.51
25	c2	509	CLA	CMD-C2D	-2.26	1.46	1.51
25	b2	620	CLA	CMD-C2D	-2.25	1.46	1.51
25	b1	612	CLA	CMD-C2D	-2.25	1.46	1.51
25	B2	605	CLA	CMD-C2D	-2.25	1.46	1.51
25	C1	508	CLA	CMD-C2D	-2.25	1.46	1.51
25	B2	615	CLA	CMD-C2D	-2.25	1.46	1.51
25	B1	610	CLA	CMD-C2D	-2.25	1.46	1.51
25	B2	610	CLA	CMD-C2D	-2.25	1.46	1.51
25	c1	503	CLA	CMD-C2D	-2.25	1.46	1.51
25	B2	612	CLA	CMD-C2D	-2.24	1.46	1.51
25	c2	504	CLA	CMD-C2D	-2.24	1.46	1.51
25	B2	611	CLA	CMD-C2D	-2.24	1.46	1.51
25	a2	405	CLA	CMD-C2D	-2.24	1.46	1.51
25	C2	504	CLA	CMD-C2D	-2.23	1.46	1.51
25	B1	615	CLA	CMD-C2D	-2.23	1.46	1.51
25	c1	508	CLA	CMD-C2D	-2.23	1.46	1.51
25	A2	403	CLA	CMD-C2D	-2.23	1.46	1.51
25	b2	618	CLA	CMD-C2D	-2.23	1.46	1.51
25	B2	609	CLA	CMD-C2D	-2.23	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C2	513	CLA	CMD-C2D	-2.23	1.46	1.51
25	c2	502	CLA	CMD-C2D	-2.23	1.46	1.51
25	b2	609	CLA	CMD-C2D	-2.23	1.46	1.51
25	b1	620	CLA	CMD-C2D	-2.23	1.46	1.51
25	C2	503	CLA	CMD-C2D	-2.23	1.46	1.51
25	B1	617	CLA	CMD-C2D	-2.23	1.46	1.51
25	d2	404	CLA	CMD-C2D	-2.23	1.46	1.51
25	c1	510	CLA	CMD-C2D	-2.22	1.46	1.51
25	b2	616	CLA	CMD-C2D	-2.22	1.46	1.51
25	C2	511	CLA	CMD-C2D	-2.22	1.46	1.51
25	c2	503	CLA	CMD-C2D	-2.22	1.46	1.51
25	b1	604	CLA	CMD-C2D	-2.22	1.46	1.51
25	C2	505	CLA	CMD-C2D	-2.22	1.46	1.51
25	b1	610	CLA	CMD-C2D	-2.21	1.46	1.51
25	D2	406	CLA	CMD-C2D	-2.21	1.46	1.51
25	c2	515	CLA	CMD-C2D	-2.21	1.46	1.51
25	C1	507	CLA	CMD-C2D	-2.21	1.46	1.51
25	C2	508	CLA	CMD-C2D	-2.21	1.46	1.51
25	A1	406	CLA	CMD-C2D	-2.21	1.46	1.51
25	b2	619	CLA	CMC-C2C	-2.21	1.46	1.50
25	c2	507	CLA	CMD-C2D	-2.21	1.46	1.51
25	b1	616	CLA	CMD-C2D	-2.21	1.46	1.51
25	b2	617	CLA	CMD-C2D	-2.21	1.46	1.51
25	b2	604	CLA	CMD-C2D	-2.21	1.46	1.51
25	b1	608	CLA	CMD-C2D	-2.20	1.46	1.51
25	d1	406	CLA	CMD-C2D	-2.20	1.46	1.51
25	d2	402	CLA	CMD-C2D	-2.20	1.46	1.51
25	b2	610	CLA	CMD-C2D	-2.20	1.46	1.51
25	A1	403	CLA	CMC-C2C	-2.20	1.46	1.50
25	C1	503	CLA	CMD-C2D	-2.20	1.46	1.51
25	B1	605	CLA	CMD-C2D	-2.20	1.46	1.51
25	C2	510	CLA	CMD-C2D	-2.20	1.46	1.51
25	b1	611	CLA	CMD-C2D	-2.19	1.46	1.51
25	A2	402	CLA	CMD-C2D	-2.19	1.46	1.51
25	B2	619	CLA	CMD-C2D	-2.19	1.46	1.51
25	c1	505	CLA	CMD-C2D	-2.19	1.46	1.51
25	C1	514	CLA	CMD-C2D	-2.19	1.46	1.51
25	B1	611	CLA	CMD-C2D	-2.18	1.46	1.51
25	b1	616	CLA	C3B-C2B	-2.18	1.37	1.40
25	C1	502	CLA	CMD-C2D	-2.17	1.46	1.51
25	B2	604	CLA	CMD-C2D	-2.17	1.46	1.51
25	C1	504	CLA	CMD-C2D	-2.17	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c1	516	CLA	CMD-C2D	-2.17	1.46	1.51
25	D1	403	CLA	CMD-C2D	-2.16	1.46	1.51
25	d1	404	CLA	CMD-C2D	-2.16	1.46	1.51
25	B2	618	CLA	CMC-C2C	-2.16	1.46	1.50
25	A2	402	CLA	CMC-C2C	-2.15	1.46	1.50
25	B1	619	CLA	CMD-C2D	-2.14	1.46	1.51
25	c1	508	CLA	C3B-C2B	-2.14	1.37	1.40
25	D2	404	CLA	CMD-C2D	-2.13	1.46	1.51
25	B1	616	CLA	C3B-C2B	-2.12	1.37	1.40
25	B1	618	CLA	CMC-C2C	-2.09	1.46	1.50
25	B2	609	CLA	CMC-C2C	-2.09	1.46	1.50
25	A2	403	CLA	C3B-C2B	-2.09	1.37	1.40
25	A1	406	CLA	C3B-C2B	-2.08	1.37	1.40
25	b1	619	CLA	CMC-C2C	-2.07	1.46	1.50
25	b2	609	CLA	CMC-C2C	-2.07	1.46	1.50
25	C2	511	CLA	CMC-C2C	-2.07	1.46	1.50
25	c1	510	CLA	CMC-C2C	-2.06	1.46	1.50
25	b1	607	CLA	C3B-C2B	-2.06	1.37	1.40
25	b1	613	CLA	CMC-C2C	-2.06	1.46	1.50
25	a1	403	CLA	CMC-C2C	-2.05	1.46	1.50
25	B2	616	CLA	C3B-C2B	-2.05	1.37	1.40
29	M1	101	LMG	O7-C8	-2.03	1.43	1.47
25	b2	612	CLA	CMC-C2C	-2.03	1.46	1.50
25	A2	404	CLA	C3B-C2B	-2.01	1.37	1.40
25	b1	616	CLA	CMC-C2C	-2.00	1.46	1.50
25	b1	614	CLA	CMC-C2C	-2.00	1.46	1.50
25	C2	506	CLA	CMC-C2C	-2.00	1.46	1.50
25	B2	607	CLA	C1D-ND	2.00	1.42	1.37
25	C1	502	CLA	C1D-ND	2.00	1.42	1.37
25	C2	504	CLA	C1D-ND	2.00	1.42	1.37
38	E2	101	HEM	CAD-C3D	2.00	1.54	1.52
25	B1	604	CLA	C1D-ND	2.00	1.42	1.37
38	V2	201	HEM	CAD-C3D	2.01	1.54	1.52
25	d1	404	CLA	C1D-ND	2.01	1.42	1.37
38	V1	201	HEM	CAD-C3D	2.02	1.54	1.52
36	d1	409	PL9	C2-C3	2.02	1.40	1.34
27	D2	407	PHO	C4C-C3C	2.02	1.49	1.45
25	c1	510	CLA	C1D-ND	2.02	1.42	1.37
25	B1	604	CLA	C4C-NC	2.02	1.40	1.37
25	B2	611	CLA	C1D-ND	2.03	1.42	1.37
25	B1	607	CLA	C4C-NC	2.03	1.40	1.37
25	c2	502	CLA	C1D-ND	2.03	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B1	616	CLA	C1D-ND	2.03	1.42	1.37
25	B1	611	CLA	C1D-ND	2.05	1.42	1.37
38	E1	101	HEM	CAD-C3D	2.05	1.54	1.52
36	D1	408	PL9	C2-C3	2.05	1.40	1.34
25	b1	605	CLA	C4C-NC	2.06	1.40	1.37
25	b1	608	CLA	C1D-ND	2.06	1.42	1.37
25	C1	507	CLA	C3C-C2C	2.08	1.41	1.36
27	a1	411	PHO	C1D-C2D	2.09	1.50	1.45
27	A1	408	PHO	C1D-C2D	2.10	1.50	1.45
27	A1	408	PHO	C4C-C3C	2.11	1.49	1.45
27	a1	411	PHO	C4C-C3C	2.11	1.49	1.45
27	a2	416	PHO	C1D-C2D	2.12	1.50	1.45
38	e2	101	HEM	CAD-C3D	2.13	1.55	1.52
27	A2	407	PHO	C1D-C2D	2.13	1.50	1.45
27	d1	403	PHO	C1D-C2D	2.14	1.50	1.45
25	A1	405	CLA	C4C-NC	2.14	1.40	1.37
27	D2	407	PHO	C1D-C2D	2.15	1.50	1.45
38	f1	101	HEM	CAD-C3D	2.16	1.55	1.52
27	D1	407	PHO	C1D-C2D	2.20	1.50	1.45
38	E2	101	HEM	C4D-ND	2.21	1.39	1.36
25	B1	609	CLA	C4C-NC	2.21	1.40	1.37
27	d2	408	PHO	C1D-C2D	2.22	1.50	1.45
38	f1	101	HEM	C4D-ND	2.27	1.39	1.36
23	c2	501	BCR	C19-C18	2.29	1.51	1.45
36	d2	409	PL9	C6-C5	2.29	1.48	1.35
36	d1	409	PL9	C6-C5	2.30	1.48	1.35
36	D1	408	PL9	C6-C5	2.31	1.48	1.35
38	E1	101	HEM	C4D-ND	2.33	1.39	1.36
36	D2	408	PL9	C6-C5	2.34	1.48	1.35
38	e2	101	HEM	C4D-ND	2.35	1.39	1.36
29	B2	621	LMG	O8-C28	2.40	1.45	1.33
38	V2	201	HEM	C4D-ND	2.40	1.40	1.36
29	A2	412	LMG	O8-C28	2.43	1.45	1.33
29	C2	515	LMG	O8-C28	2.43	1.45	1.33
27	A1	408	PHO	C3B-C4B	2.49	1.48	1.43
25	D1	402	CLA	CHC-C1C	2.50	1.42	1.35
38	V1	201	HEM	C4D-ND	2.51	1.40	1.36
25	d2	405	CLA	CHC-C1C	2.52	1.42	1.35
25	b2	614	CLA	CHC-C1C	2.52	1.42	1.35
25	C1	502	CLA	CHC-C1C	2.53	1.42	1.35
25	b1	613	CLA	CHC-C1C	2.53	1.42	1.35
25	C2	511	CLA	CHC-C1C	2.54	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b2	612	CLA	CHC-C1C	2.55	1.42	1.35
25	c1	503	CLA	CHC-C1C	2.55	1.42	1.35
25	C1	509	CLA	CHC-C1C	2.55	1.42	1.35
38	v1	201	HEM	C4D-ND	2.56	1.40	1.36
27	A2	407	PHO	C3B-C4B	2.57	1.48	1.43
25	C2	516	CLA	CHC-C1C	2.57	1.42	1.35
25	C1	513	CLA	CHC-C1C	2.58	1.42	1.35
25	B2	618	CLA	CHC-C1C	2.58	1.42	1.35
25	C2	509	CLA	CHC-C1C	2.58	1.42	1.35
25	a1	405	CLA	CHC-C1C	2.58	1.42	1.35
25	c2	512	CLA	CHC-C1C	2.58	1.42	1.35
25	B1	613	CLA	CHC-C1C	2.59	1.42	1.35
27	a1	411	PHO	C3B-C4B	2.59	1.48	1.43
25	B2	614	CLA	CHC-C1C	2.60	1.42	1.35
25	b2	609	CLA	CHC-C1C	2.60	1.42	1.35
25	c2	502	CLA	CHC-C1C	2.60	1.42	1.35
25	C1	505	CLA	CHC-C1C	2.61	1.43	1.35
25	B2	612	CLA	CHC-C1C	2.61	1.43	1.35
25	b2	610	CLA	CHC-C1C	2.61	1.43	1.35
25	c2	511	CLA	CHC-C1C	2.61	1.43	1.35
25	c1	509	CLA	CHC-C1C	2.62	1.43	1.35
25	a2	405	CLA	CHC-C1C	2.62	1.43	1.35
25	c1	510	CLA	CHC-C1C	2.62	1.43	1.35
25	c2	507	CLA	CHC-C1C	2.62	1.43	1.35
38	v2	201	HEM	C4D-ND	2.62	1.40	1.36
25	C1	503	CLA	CHC-C1C	2.62	1.43	1.35
25	B2	617	CLA	CHC-C1C	2.62	1.43	1.35
25	c2	505	CLA	CHC-C1C	2.62	1.43	1.35
25	C1	506	CLA	CHC-C1C	2.62	1.43	1.35
25	C2	510	CLA	CHC-C1C	2.62	1.43	1.35
25	C1	508	CLA	CHC-C1C	2.62	1.43	1.35
25	b1	614	CLA	CHC-C1C	2.62	1.43	1.35
25	b1	611	CLA	CHC-C1C	2.63	1.43	1.35
25	C1	512	CLA	CHC-C1C	2.63	1.43	1.35
25	c2	503	CLA	CHC-C1C	2.63	1.43	1.35
25	c1	516	CLA	CHC-C1C	2.63	1.43	1.35
25	B2	615	CLA	CHC-C1C	2.63	1.43	1.35
25	c2	513	CLA	CHC-C1C	2.64	1.43	1.35
25	D2	401	CLA	CHC-C1C	2.64	1.43	1.35
25	c1	511	CLA	CHC-C1C	2.64	1.43	1.35
25	B1	608	CLA	CHC-C1C	2.64	1.43	1.35
25	B2	613	CLA	CHC-C1C	2.64	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b1	617	CLA	CHC-C1C	2.64	1.43	1.35
25	b1	619	CLA	CHC-C1C	2.64	1.43	1.35
25	c2	509	CLA	CHC-C1C	2.64	1.43	1.35
25	b2	620	CLA	CHC-C1C	2.64	1.43	1.35
25	c2	504	CLA	CHC-C1C	2.65	1.43	1.35
25	B2	611	CLA	CHC-C1C	2.65	1.43	1.35
25	c2	508	CLA	CHC-C1C	2.65	1.43	1.35
25	b1	615	CLA	CHC-C1C	2.65	1.43	1.35
25	b2	619	CLA	CHC-C1C	2.65	1.43	1.35
25	b2	613	CLA	CHC-C1C	2.65	1.43	1.35
25	b2	618	CLA	CHC-C1C	2.65	1.43	1.35
25	C1	511	CLA	CHC-C1C	2.65	1.43	1.35
25	K2	101	CLA	CHC-C1C	2.65	1.43	1.35
25	b1	612	CLA	CHC-C1C	2.65	1.43	1.35
25	B2	608	CLA	CHC-C1C	2.65	1.43	1.35
25	B1	607	CLA	CHC-C1C	2.66	1.43	1.35
25	C2	505	CLA	CHC-C1C	2.66	1.43	1.35
25	b2	611	CLA	CHC-C1C	2.66	1.43	1.35
25	C2	518	CLA	CHC-C1C	2.66	1.43	1.35
25	c1	508	CLA	CHC-C1C	2.66	1.43	1.35
25	c1	512	CLA	CHC-C1C	2.66	1.43	1.35
25	C2	503	CLA	CHC-C1C	2.66	1.43	1.35
25	d1	401	CLA	CHC-C1C	2.66	1.43	1.35
25	B1	609	CLA	CHC-C1C	2.66	1.43	1.35
25	c1	507	CLA	CHC-C1C	2.67	1.43	1.35
25	c1	513	CLA	CHC-C1C	2.67	1.43	1.35
25	B1	611	CLA	CHC-C1C	2.67	1.43	1.35
27	d2	408	PHO	C3B-C4B	2.67	1.48	1.43
25	D2	406	CLA	CHC-C1C	2.67	1.43	1.35
25	B1	605	CLA	CHC-C1C	2.67	1.43	1.35
25	B1	614	CLA	CHC-C1C	2.67	1.43	1.35
25	C1	514	CLA	CHC-C1C	2.68	1.43	1.35
25	B2	605	CLA	CHC-C1C	2.68	1.43	1.35
25	b2	608	CLA	CHC-C1C	2.68	1.43	1.35
25	c1	505	CLA	CHC-C1C	2.68	1.43	1.35
25	B1	618	CLA	CHC-C1C	2.68	1.43	1.35
25	C2	508	CLA	CHC-C1C	2.68	1.43	1.35
25	b2	616	CLA	CHC-C1C	2.68	1.43	1.35
25	A1	406	CLA	CHC-C1C	2.68	1.43	1.35
25	c2	515	CLA	CHC-C1C	2.68	1.43	1.35
25	d2	402	CLA	CHC-C1C	2.68	1.43	1.35
25	B1	615	CLA	CHC-C1C	2.69	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a2	416	PHO	C3B-C4B	2.69	1.48	1.43
25	B1	617	CLA	CHC-C1C	2.69	1.43	1.35
25	D2	404	CLA	CHC-C1C	2.69	1.43	1.35
25	c2	510	CLA	CHC-C1C	2.69	1.43	1.35
25	d1	404	CLA	CHC-C1C	2.70	1.43	1.35
25	B1	604	CLA	CHC-C1C	2.70	1.43	1.35
27	D2	407	PHO	C3B-C4B	2.70	1.48	1.43
25	C2	504	CLA	CHC-C1C	2.70	1.43	1.35
25	c1	515	CLA	CHC-C1C	2.70	1.43	1.35
25	C2	506	CLA	CHC-C1C	2.70	1.43	1.35
25	c2	506	CLA	CHC-C1C	2.70	1.43	1.35
25	D1	403	CLA	CHC-C1C	2.70	1.43	1.35
25	b1	610	CLA	CHC-C1C	2.70	1.43	1.35
25	C1	504	CLA	CHC-C1C	2.70	1.43	1.35
25	C1	510	CLA	CHC-C1C	2.70	1.43	1.35
25	C2	507	CLA	CHC-C1C	2.70	1.43	1.35
25	b2	615	CLA	CHC-C1C	2.71	1.43	1.35
25	c1	504	CLA	CHC-C1C	2.71	1.43	1.35
25	b2	604	CLA	CHC-C1C	2.71	1.43	1.35
25	B2	609	CLA	CHC-C1C	2.71	1.43	1.35
25	A2	403	CLA	CHC-C1C	2.71	1.43	1.35
25	B1	610	CLA	CHC-C1C	2.71	1.43	1.35
25	B1	612	CLA	CHC-C1C	2.71	1.43	1.35
25	B2	604	CLA	CHC-C1C	2.72	1.43	1.35
25	b2	606	CLA	CHC-C1C	2.72	1.43	1.35
25	b1	606	CLA	CHC-C1C	2.73	1.43	1.35
25	B2	607	CLA	CHC-C1C	2.73	1.43	1.35
25	b1	609	CLA	CHC-C1C	2.73	1.43	1.35
25	b1	608	CLA	CHC-C1C	2.73	1.43	1.35
25	b1	616	CLA	CHC-C1C	2.74	1.43	1.35
25	A1	404	CLA	CHC-C1C	2.74	1.43	1.35
25	B2	619	CLA	CHC-C1C	2.74	1.43	1.35
27	d1	403	PHO	C3B-C4B	2.75	1.48	1.43
25	d1	406	CLA	CHC-C1C	2.75	1.43	1.35
25	b2	617	CLA	CHC-C1C	2.75	1.43	1.35
25	c1	506	CLA	CHC-C1C	2.75	1.43	1.35
25	B1	606	CLA	CHC-C1C	2.75	1.43	1.35
25	B2	616	CLA	CHC-C1C	2.75	1.43	1.35
27	D1	407	PHO	C3B-C4B	2.76	1.48	1.43
25	B2	606	CLA	CHC-C1C	2.76	1.43	1.35
25	B1	619	CLA	CHC-C1C	2.77	1.43	1.35
25	C2	513	CLA	CHC-C1C	2.77	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A2	404	CLA	CHC-C1C	2.78	1.43	1.35
25	C1	507	CLA	CHC-C1C	2.78	1.43	1.35
25	b2	624	CLA	CHC-C1C	2.79	1.43	1.35
25	b1	620	CLA	CHC-C1C	2.79	1.43	1.35
25	a2	413	CLA	CHC-C1C	2.79	1.43	1.35
25	a1	404	CLA	CHC-C1C	2.79	1.43	1.35
25	B1	616	CLA	CHC-C1C	2.79	1.43	1.35
27	A2	407	PHO	C3D-C2D	2.80	1.46	1.38
25	b1	605	CLA	CHC-C1C	2.80	1.43	1.35
25	B2	610	CLA	CHC-C1C	2.81	1.43	1.35
25	d2	404	CLA	CHC-C1C	2.81	1.43	1.35
25	b1	604	CLA	CHC-C1C	2.83	1.43	1.35
25	b1	607	CLA	CHC-C1C	2.85	1.43	1.35
27	a2	416	PHO	C3D-C2D	2.85	1.46	1.38
25	A1	405	CLA	CHC-C1C	2.87	1.43	1.35
27	A1	408	PHO	C3D-C2D	2.90	1.46	1.38
27	a1	411	PHO	C3D-C2D	2.92	1.46	1.38
27	d2	408	PHO	C3D-C2D	2.92	1.46	1.38
27	D2	407	PHO	C3D-C2D	2.94	1.46	1.38
25	a2	404	CLA	CHC-C1C	2.98	1.44	1.35
27	D1	407	PHO	C3D-C2D	3.00	1.47	1.38
27	d1	403	PHO	C3D-C2D	3.02	1.47	1.38
25	A1	403	CLA	CHC-C1C	3.03	1.44	1.35
27	a2	416	PHO	CHB-C4A	3.05	1.47	1.40
25	a1	403	CLA	CHC-C1C	3.07	1.44	1.35
27	d2	408	PHO	CHB-C4A	3.07	1.47	1.40
25	A2	402	CLA	CHC-C1C	3.08	1.44	1.35
27	d1	403	PHO	CHB-C4A	3.09	1.47	1.40
27	A1	408	PHO	CHB-C4A	3.10	1.47	1.40
27	D2	407	PHO	CHB-C4A	3.17	1.48	1.40
27	A1	408	PHO	CHD-C4C	3.18	1.48	1.40
27	D1	407	PHO	CHB-C4A	3.18	1.48	1.40
27	A2	407	PHO	CHB-C4A	3.19	1.48	1.40
25	A1	405	CLA	CHB-C4A	3.20	1.37	1.33
27	a2	416	PHO	CHD-C4C	3.23	1.48	1.40
27	a1	411	PHO	CHB-C4A	3.23	1.48	1.40
27	D1	407	PHO	CHD-C4C	3.26	1.48	1.40
27	d2	408	PHO	CHD-C4C	3.27	1.48	1.40
25	A2	402	CLA	CHB-C4A	3.30	1.38	1.33
27	A1	408	PHO	CHC-C4B	3.30	1.48	1.40
25	a2	404	CLA	CHB-C4A	3.31	1.38	1.33
27	d1	403	PHO	CHD-C4C	3.33	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D2	407	PHO	CHD-C4C	3.34	1.48	1.40
27	A2	407	PHO	CHD-C4C	3.34	1.48	1.40
27	D2	407	PHO	CHC-C4B	3.36	1.48	1.40
27	A2	407	PHO	CHC-C4B	3.37	1.48	1.40
25	B1	610	CLA	CHB-C4A	3.38	1.38	1.33
27	d2	408	PHO	CHC-C4B	3.40	1.48	1.40
25	a1	403	CLA	CHB-C4A	3.43	1.38	1.33
25	A1	403	CLA	CHB-C4A	3.43	1.38	1.33
27	a1	411	PHO	CHD-C4C	3.43	1.48	1.40
25	A1	406	CLA	CHB-C4A	3.43	1.38	1.33
27	d1	403	PHO	CHC-C4B	3.44	1.48	1.40
27	a1	411	PHO	CHC-C4B	3.45	1.48	1.40
25	b2	617	CLA	CHB-C4A	3.46	1.38	1.33
25	a1	404	CLA	CHB-C4A	3.47	1.38	1.33
38	V2	201	HEM	C3B-CAB	3.50	1.55	1.47
38	f1	101	HEM	C3B-CAB	3.51	1.55	1.47
25	a2	413	CLA	CHB-C4A	3.55	1.38	1.33
27	D1	407	PHO	CHC-C4B	3.55	1.49	1.40
25	d2	402	CLA	CHB-C4A	3.56	1.38	1.33
27	a2	416	PHO	CHC-C4B	3.56	1.49	1.40
25	d1	404	CLA	CHB-C4A	3.56	1.38	1.33
38	E2	101	HEM	C3B-CAB	3.57	1.55	1.47
25	A2	403	CLA	CHB-C4A	3.57	1.38	1.33
38	E1	101	HEM	C3B-CAB	3.59	1.55	1.47
25	c1	508	CLA	CHB-C4A	3.61	1.38	1.33
38	e2	101	HEM	C3B-CAB	3.63	1.55	1.47
27	a1	411	PHO	OBD-CAD	3.63	1.28	1.22
25	B2	613	CLA	CHB-C4A	3.64	1.38	1.33
25	B2	606	CLA	CHB-C4A	3.65	1.38	1.33
25	B1	606	CLA	CHB-C4A	3.66	1.38	1.33
25	b1	605	CLA	CHB-C4A	3.66	1.38	1.33
25	A1	404	CLA	CHB-C4A	3.66	1.38	1.33
25	d2	404	CLA	CHB-C4A	3.66	1.38	1.33
25	C1	509	CLA	CHB-C4A	3.67	1.38	1.33
25	c2	509	CLA	CHB-C4A	3.68	1.38	1.33
25	C1	507	CLA	CHB-C4A	3.69	1.38	1.33
25	b2	624	CLA	CHB-C4A	3.69	1.38	1.33
25	B1	618	CLA	CHB-C4A	3.69	1.38	1.33
25	B2	610	CLA	CHB-C4A	3.69	1.38	1.33
25	D1	403	CLA	CHB-C4A	3.70	1.38	1.33
38	V1	201	HEM	C3C-CAC	3.70	1.55	1.47
25	c2	505	CLA	CHB-C4A	3.71	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B1	611	CLA	CHB-C4A	3.71	1.38	1.33
25	d1	406	CLA	CHB-C4A	3.71	1.38	1.33
25	a2	405	CLA	CHB-C4A	3.72	1.38	1.33
25	B1	609	CLA	CHB-C4A	3.72	1.38	1.33
25	B2	619	CLA	CHB-C4A	3.72	1.38	1.33
25	B1	616	CLA	CHB-C4A	3.73	1.38	1.33
33	l1	102	LHG	O7-C7	3.73	1.45	1.34
25	b1	616	CLA	CHB-C4A	3.74	1.38	1.33
38	v1	201	HEM	C3B-CAB	3.74	1.55	1.47
25	C1	510	CLA	CHB-C4A	3.75	1.38	1.33
38	V2	201	HEM	C3C-CAC	3.75	1.55	1.47
25	B1	608	CLA	CHB-C4A	3.75	1.38	1.33
33	d2	406	LHG	O7-C7	3.75	1.45	1.34
25	C1	505	CLA	CHB-C4A	3.76	1.38	1.33
38	V1	201	HEM	C3B-CAB	3.76	1.55	1.47
38	f1	101	HEM	C3C-CAC	3.76	1.55	1.47
25	b1	620	CLA	CHB-C4A	3.76	1.38	1.33
33	D2	405	LHG	O7-C7	3.77	1.45	1.34
25	B2	616	CLA	CHB-C4A	3.77	1.38	1.33
27	A1	408	PHO	OBD-CAD	3.77	1.28	1.22
25	b2	611	CLA	CHB-C4A	3.77	1.38	1.33
38	v1	201	HEM	C3C-CAC	3.78	1.55	1.47
25	a1	405	CLA	CHB-C4A	3.78	1.38	1.33
33	B1	621	LHG	O7-C7	3.78	1.45	1.34
25	c1	516	CLA	CHB-C4A	3.78	1.38	1.33
29	d1	408	LMG	O7-C10	3.78	1.45	1.34
25	C2	513	CLA	CHB-C4A	3.79	1.38	1.33
25	C2	508	CLA	CHB-C4A	3.79	1.38	1.33
25	b1	610	CLA	CHB-C4A	3.79	1.38	1.33
25	b1	619	CLA	CHB-C4A	3.79	1.38	1.33
25	c1	510	CLA	CHB-C4A	3.79	1.38	1.33
33	d1	407	LHG	O7-C7	3.79	1.45	1.34
38	v2	201	HEM	C3C-CAC	3.79	1.55	1.47
25	B2	612	CLA	CHB-C4A	3.79	1.38	1.33
27	A2	407	PHO	OBD-CAD	3.80	1.28	1.22
25	b1	611	CLA	CHB-C4A	3.80	1.38	1.33
25	c1	506	CLA	CHB-C4A	3.81	1.38	1.33
25	b2	613	CLA	CHB-C4A	3.81	1.38	1.33
25	B1	612	CLA	CHB-C4A	3.81	1.38	1.33
33	L2	101	LHG	O7-C7	3.81	1.45	1.34
33	D2	403	LHG	O7-C7	3.81	1.45	1.34
25	A2	404	CLA	CHB-C4A	3.81	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a2	416	PHO	OBD-CAD	3.81	1.28	1.22
25	C2	506	CLA	CHB-C4A	3.81	1.38	1.33
25	c1	503	CLA	CHB-C4A	3.82	1.38	1.33
38	E1	101	HEM	C3C-CAC	3.82	1.55	1.47
25	b1	608	CLA	CHB-C4A	3.82	1.38	1.33
38	E2	101	HEM	C3C-CAC	3.83	1.55	1.47
38	v2	201	HEM	C3B-CAB	3.83	1.55	1.47
25	c2	515	CLA	CHB-C4A	3.84	1.38	1.33
25	b2	620	CLA	CHB-C4A	3.84	1.38	1.33
25	b1	613	CLA	CHB-C4A	3.84	1.38	1.33
25	b1	606	CLA	CHB-C4A	3.84	1.38	1.33
25	b2	612	CLA	CHB-C4A	3.84	1.38	1.33
25	B2	605	CLA	CHB-C4A	3.85	1.38	1.33
33	L1	101	LHG	O7-C7	3.85	1.45	1.34
38	e2	101	HEM	C3C-CAC	3.85	1.55	1.47
25	D2	406	CLA	CHB-C4A	3.85	1.38	1.33
25	b2	619	CLA	CHB-C4A	3.86	1.38	1.33
33	b1	622	LHG	O7-C7	3.86	1.45	1.34
25	b2	606	CLA	CHB-C4A	3.86	1.38	1.33
25	c2	507	CLA	CHB-C4A	3.86	1.38	1.33
27	d2	408	PHO	OBD-CAD	3.86	1.28	1.22
25	B1	619	CLA	CHB-C4A	3.86	1.38	1.33
33	D1	405	LHG	O7-C7	3.86	1.45	1.34
25	C2	509	CLA	CHB-C4A	3.87	1.38	1.33
25	B2	609	CLA	CHB-C4A	3.87	1.38	1.33
34	c1	520	DGD	O2G-C1B	3.87	1.45	1.34
25	b2	609	CLA	CHB-C4A	3.87	1.38	1.33
25	C1	512	CLA	CHB-C4A	3.87	1.38	1.33
25	B2	617	CLA	CHB-C4A	3.87	1.38	1.33
29	D1	406	LMG	O7-C10	3.88	1.45	1.34
25	b2	616	CLA	CHB-C4A	3.88	1.38	1.33
34	C1	516	DGD	O2G-C1B	3.88	1.45	1.34
25	B2	604	CLA	CHB-C4A	3.88	1.38	1.33
25	B1	604	CLA	CHB-C4A	3.89	1.38	1.33
25	C2	511	CLA	CHB-C4A	3.89	1.38	1.33
34	C1	517	DGD	O2G-C1B	3.89	1.45	1.34
33	d2	403	LHG	O7-C7	3.89	1.45	1.34
29	j2	101	LMG	O7-C10	3.90	1.45	1.34
25	C1	511	CLA	CHB-C4A	3.90	1.38	1.33
25	b2	608	CLA	CHB-C4A	3.90	1.38	1.33
25	c1	512	CLA	CHB-C4A	3.90	1.38	1.33
25	C1	513	CLA	CHB-C4A	3.91	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c2	511	CLA	CHB-C4A	3.91	1.38	1.33
25	B2	611	CLA	CHB-C4A	3.91	1.38	1.33
27	D1	407	PHO	OBD-CAD	3.91	1.28	1.22
33	D1	404	LHG	O7-C7	3.92	1.45	1.34
25	K2	101	CLA	CHB-C4A	3.92	1.38	1.33
29	B2	621	LMG	O7-C10	3.92	1.45	1.34
34	h1	101	DGD	O2G-C1B	3.92	1.45	1.34
34	C1	515	DGD	O2G-C1B	3.92	1.45	1.34
25	c2	506	CLA	CHB-C4A	3.92	1.38	1.33
34	c1	514	DGD	O2G-C1B	3.92	1.45	1.34
25	b1	607	CLA	CHB-C4A	3.92	1.38	1.33
25	C1	502	CLA	CHB-C4A	3.92	1.38	1.33
25	B2	607	CLA	CHB-C4A	3.93	1.38	1.33
25	C1	503	CLA	CHB-C4A	3.93	1.38	1.33
27	a1	411	PHO	O2A-CGA	3.93	1.45	1.33
25	B2	615	CLA	CHB-C4A	3.93	1.38	1.33
25	b2	610	CLA	CHB-C4A	3.93	1.38	1.33
25	B2	618	CLA	CHB-C4A	3.94	1.38	1.33
29	B1	622	LMG	O7-C10	3.94	1.45	1.34
25	C1	508	CLA	CHB-C4A	3.94	1.38	1.33
29	A1	412	LMG	O7-C10	3.94	1.45	1.34
34	c2	517	DGD	O2G-C1B	3.94	1.45	1.34
25	b1	604	CLA	CHB-C4A	3.94	1.38	1.33
29	b2	622	LMG	O7-C10	3.94	1.45	1.34
29	A1	410	LMG	O7-C10	3.94	1.45	1.34
25	b2	604	CLA	CHB-C4A	3.95	1.38	1.33
34	c1	518	DGD	O2G-C1B	3.95	1.45	1.34
25	D2	404	CLA	CHB-C4A	3.95	1.38	1.33
25	C2	505	CLA	CHB-C4A	3.95	1.38	1.33
25	C1	514	CLA	CHB-C4A	3.95	1.38	1.33
29	C1	520	LMG	O7-C10	3.95	1.45	1.34
33	B2	627	LHG	O7-C7	3.95	1.45	1.34
25	B1	615	CLA	CHB-C4A	3.95	1.38	1.33
25	B1	605	CLA	CHB-C4A	3.95	1.38	1.33
25	B1	617	CLA	CHB-C4A	3.96	1.38	1.33
25	b1	617	CLA	CHB-C4A	3.96	1.38	1.33
34	h2	102	DGD	O2G-C1B	3.96	1.45	1.34
34	c2	514	DGD	O2G-C1B	3.96	1.45	1.34
27	D2	407	PHO	O2A-CGA	3.96	1.45	1.33
25	c2	503	CLA	CHB-C4A	3.96	1.38	1.33
25	c2	508	CLA	CHB-C4A	3.96	1.38	1.33
37	B2	623	SQD	O47-C7	3.96	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D2	407	PHO	OBD-CAD	3.97	1.29	1.22
25	c2	504	CLA	CHB-C4A	3.97	1.38	1.33
33	l2	101	LHG	O7-C7	3.97	1.46	1.34
29	a2	412	LMG	O7-C10	3.97	1.46	1.34
27	A2	407	PHO	O2A-CGA	3.97	1.45	1.33
33	b2	625	LHG	O7-C7	3.97	1.46	1.34
25	b1	612	CLA	CHB-C4A	3.97	1.38	1.33
29	a1	412	LMG	O7-C10	3.98	1.46	1.34
25	C2	510	CLA	CHB-C4A	3.98	1.38	1.33
33	d1	402	LHG	O7-C7	3.98	1.46	1.34
25	c1	505	CLA	CHB-C4A	3.98	1.38	1.33
25	c2	502	CLA	CHB-C4A	3.98	1.38	1.33
25	d1	401	CLA	CHB-C4A	3.98	1.38	1.33
34	c2	516	DGD	O2G-C1B	3.98	1.46	1.34
25	d2	405	CLA	CHB-C4A	3.98	1.38	1.33
25	C2	518	CLA	CHB-C4A	3.98	1.38	1.33
25	C2	503	CLA	CHB-C4A	3.99	1.38	1.33
29	I2	101	LMG	O7-C10	3.99	1.46	1.34
25	B1	613	CLA	CHB-C4A	3.99	1.38	1.33
29	C2	515	LMG	O7-C10	4.00	1.46	1.34
33	b1	622	LHG	O8-C23	4.00	1.45	1.33
34	H2	101	DGD	O2G-C1B	4.00	1.46	1.34
25	C2	516	CLA	CHB-C4A	4.00	1.38	1.33
33	d1	407	LHG	O8-C23	4.00	1.45	1.33
27	d1	403	PHO	OBD-CAD	4.01	1.29	1.22
29	d1	411	LMG	O7-C10	4.01	1.46	1.34
29	F2	402	LMG	O7-C10	4.02	1.46	1.34
25	b1	614	CLA	CHB-C4A	4.02	1.38	1.33
25	c2	513	CLA	CHB-C4A	4.02	1.38	1.33
29	M1	101	LMG	O7-C10	4.02	1.46	1.34
27	A1	408	PHO	O2A-CGA	4.02	1.45	1.33
29	B2	620	LMG	O7-C10	4.02	1.46	1.34
29	A2	412	LMG	O7-C10	4.03	1.46	1.34
25	b2	618	CLA	CHB-C4A	4.03	1.38	1.33
34	H1	101	DGD	O2G-C1B	4.03	1.46	1.34
25	D1	402	CLA	CHB-C4A	4.03	1.38	1.33
25	c2	510	CLA	CHB-C4A	4.03	1.38	1.33
33	A2	405	LHG	O7-C7	4.04	1.46	1.34
25	C2	507	CLA	CHB-C4A	4.04	1.38	1.33
25	b2	615	CLA	CHB-C4A	4.05	1.38	1.33
25	c1	515	CLA	CHB-C4A	4.05	1.39	1.33
25	b2	614	CLA	CHB-C4A	4.05	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B1	626	LMG	O7-C10	4.06	1.46	1.34
33	D2	403	LHG	O8-C23	4.06	1.45	1.33
33	L1	101	LHG	O8-C23	4.06	1.45	1.33
25	c1	511	CLA	CHB-C4A	4.06	1.39	1.33
29	c1	519	LMG	O7-C10	4.06	1.46	1.34
33	a2	407	LHG	O7-C7	4.07	1.46	1.34
25	B1	607	CLA	CHB-C4A	4.07	1.39	1.33
25	c2	512	CLA	CHB-C4A	4.07	1.39	1.33
25	C1	504	CLA	CHB-C4A	4.07	1.39	1.33
33	A2	405	LHG	O8-C23	4.07	1.45	1.33
29	b1	624	LMG	O7-C10	4.07	1.46	1.34
33	D2	405	LHG	O8-C23	4.07	1.45	1.33
33	d2	406	LHG	O8-C23	4.07	1.45	1.33
33	a1	407	LHG	O7-C7	4.07	1.46	1.34
25	b1	609	CLA	CHB-C4A	4.08	1.39	1.33
34	C1	516	DGD	O1G-C1A	4.08	1.45	1.33
37	b2	605	SQD	O47-C7	4.09	1.46	1.34
25	b1	615	CLA	CHB-C4A	4.09	1.39	1.33
25	C2	504	CLA	CHB-C4A	4.09	1.39	1.33
33	l2	101	LHG	O8-C23	4.10	1.45	1.33
25	c1	504	CLA	CHB-C4A	4.10	1.39	1.33
33	B1	621	LHG	O8-C23	4.10	1.45	1.33
27	D1	407	PHO	O2A-CGA	4.11	1.45	1.33
29	b1	631	LMG	O7-C10	4.11	1.46	1.34
27	a2	416	PHO	O2A-CGA	4.12	1.45	1.33
29	a2	412	LMG	O8-C28	4.12	1.45	1.33
34	H1	101	DGD	O1G-C1A	4.13	1.45	1.33
25	C1	506	CLA	CHB-C4A	4.13	1.39	1.33
34	c1	518	DGD	O1G-C1A	4.13	1.45	1.33
25	B2	608	CLA	CHB-C4A	4.13	1.39	1.33
33	L2	101	LHG	O8-C23	4.13	1.45	1.33
25	c1	507	CLA	CHB-C4A	4.13	1.39	1.33
29	D1	406	LMG	O8-C28	4.13	1.45	1.33
33	D1	404	LHG	O8-C23	4.13	1.45	1.33
34	c2	514	DGD	O1G-C1A	4.14	1.45	1.33
29	B2	620	LMG	O8-C28	4.14	1.45	1.33
25	c1	509	CLA	CHB-C4A	4.14	1.39	1.33
27	d2	408	PHO	O2A-CGA	4.14	1.45	1.33
34	H2	101	DGD	O1G-C1A	4.14	1.45	1.33
33	D1	405	LHG	O8-C23	4.14	1.45	1.33
25	D2	401	CLA	CHB-C4A	4.14	1.39	1.33
34	h2	102	DGD	O1G-C1A	4.15	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	d2	403	LHG	O8-C23	4.16	1.45	1.33
34	C1	517	DGD	O1G-C1A	4.16	1.45	1.33
33	l1	102	LHG	O8-C23	4.16	1.45	1.33
34	c2	516	DGD	O1G-C1A	4.17	1.45	1.33
37	b2	605	SQD	O48-C23	4.17	1.45	1.33
37	D1	409	SQD	O48-C23	4.17	1.45	1.33
29	M1	101	LMG	O8-C28	4.17	1.45	1.33
29	B1	622	LMG	O8-C28	4.17	1.45	1.33
29	c1	519	LMG	O8-C28	4.18	1.45	1.33
33	d1	402	LHG	O8-C23	4.18	1.45	1.33
29	F2	402	LMG	O8-C28	4.18	1.45	1.33
33	a1	407	LHG	O8-C23	4.19	1.45	1.33
27	d1	403	PHO	O2A-CGA	4.19	1.45	1.33
33	b2	625	LHG	O8-C23	4.19	1.45	1.33
29	d1	411	LMG	O8-C28	4.19	1.45	1.33
29	C1	520	LMG	O8-C28	4.19	1.45	1.33
29	b1	621	LMG	O7-C10	4.19	1.46	1.34
29	c2	519	LMG	O8-C28	4.20	1.45	1.33
34	h1	101	DGD	O1G-C1A	4.21	1.45	1.33
29	d1	408	LMG	O8-C28	4.21	1.45	1.33
29	b1	631	LMG	O8-C28	4.21	1.45	1.33
29	j2	101	LMG	O8-C28	4.21	1.45	1.33
29	d2	407	LMG	O8-C28	4.21	1.45	1.33
37	B2	623	SQD	O48-C23	4.22	1.45	1.33
29	I2	101	LMG	O8-C28	4.23	1.45	1.33
29	b1	624	LMG	O8-C28	4.23	1.45	1.33
34	C1	515	DGD	O1G-C1A	4.23	1.45	1.33
34	c1	520	DGD	O1G-C1A	4.23	1.45	1.33
29	A1	410	LMG	O8-C28	4.24	1.45	1.33
25	B1	614	CLA	CHB-C4A	4.24	1.39	1.33
34	c2	517	DGD	O1G-C1A	4.25	1.46	1.33
25	c1	513	CLA	CHB-C4A	4.25	1.39	1.33
33	B2	627	LHG	O8-C23	4.26	1.46	1.33
29	b2	622	LMG	O8-C28	4.26	1.46	1.33
34	c1	514	DGD	O1G-C1A	4.30	1.46	1.33
29	b1	621	LMG	O8-C28	4.31	1.46	1.33
29	A1	412	LMG	O8-C28	4.31	1.46	1.33
29	B1	626	LMG	O8-C28	4.31	1.46	1.33
29	a1	412	LMG	O8-C28	4.32	1.46	1.33
25	B2	614	CLA	CHB-C4A	4.35	1.39	1.33
33	a2	407	LHG	O8-C23	4.53	1.45	1.32
37	D2	402	SQD	O48-C23	4.56	1.45	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C2	512	DGD	O1G-C1A	4.57	1.46	1.32
27	a2	416	PHO	CHD-C1D	4.64	1.47	1.38
27	A1	408	PHO	CHD-C1D	4.70	1.48	1.38
27	D1	407	PHO	CHD-C1D	4.71	1.48	1.38
37	D1	409	SQD	O47-C7	4.71	1.45	1.35
27	a1	411	PHO	CHD-C1D	4.73	1.48	1.38
37	D2	402	SQD	O47-C7	4.75	1.46	1.35
27	A1	408	PHO	O2D-CGD	4.76	1.45	1.33
27	d1	403	PHO	CHD-C1D	4.76	1.48	1.38
34	C2	512	DGD	O2G-C1B	4.78	1.46	1.35
27	d2	408	PHO	CHD-C1D	4.78	1.48	1.38
27	A2	407	PHO	CHD-C1D	4.82	1.48	1.38
29	d2	407	LMG	O7-C10	4.83	1.46	1.35
27	D2	407	PHO	CHD-C1D	4.85	1.48	1.38
27	A2	407	PHO	O2D-CGD	4.85	1.45	1.33
27	a1	411	PHO	O2D-CGD	4.87	1.45	1.33
37	b2	605	SQD	O8-S	4.89	1.63	1.47
27	a2	416	PHO	O2D-CGD	4.89	1.45	1.33
37	D1	409	SQD	O8-S	4.90	1.64	1.47
27	D2	407	PHO	O2D-CGD	4.90	1.45	1.33
37	B2	623	SQD	O8-S	4.93	1.64	1.47
27	D1	407	PHO	O2D-CGD	4.93	1.45	1.33
27	d1	403	PHO	O2D-CGD	4.94	1.45	1.33
27	A1	408	PHO	CHC-C1C	4.98	1.48	1.38
27	d1	403	PHO	CHB-C1B	4.99	1.48	1.38
27	d2	408	PHO	O2D-CGD	5.00	1.46	1.33
27	A2	407	PHO	CHC-C1C	5.03	1.48	1.38
27	d2	408	PHO	CHB-C1B	5.04	1.48	1.38
27	a1	411	PHO	CHC-C1C	5.06	1.48	1.38
27	D2	407	PHO	CHC-C1C	5.08	1.48	1.38
27	D2	407	PHO	CHB-C1B	5.11	1.48	1.38
27	D1	407	PHO	CHB-C1B	5.13	1.48	1.38
27	d2	408	PHO	CHC-C1C	5.13	1.48	1.38
27	A2	407	PHO	CHB-C1B	5.16	1.48	1.38
27	a2	416	PHO	CHB-C1B	5.16	1.48	1.38
27	A1	408	PHO	CHB-C1B	5.19	1.49	1.38
27	a1	411	PHO	CHB-C1B	5.21	1.49	1.38
27	d2	408	PHO	C3C-C2C	5.25	1.48	1.36
27	a2	416	PHO	CHC-C1C	5.25	1.49	1.38
27	d1	403	PHO	C3C-C2C	5.25	1.48	1.36
27	A2	407	PHO	C3C-C2C	5.26	1.48	1.36
27	A1	408	PHO	C3C-C2C	5.30	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d1	403	PHO	CHC-C1C	5.31	1.49	1.38
27	D1	407	PHO	CHC-C1C	5.32	1.49	1.38
27	D1	407	PHO	C3C-C2C	5.37	1.48	1.36
27	a2	416	PHO	C3C-C2C	5.38	1.48	1.36
27	a1	411	PHO	C3C-C2C	5.38	1.48	1.36
27	D2	407	PHO	C3C-C2C	5.39	1.48	1.36
29	c2	519	LMG	O7-C10	5.40	1.45	1.33
38	v2	201	HEM	C3D-C2D	5.42	1.53	1.37
38	v1	201	HEM	C3D-C2D	5.43	1.53	1.37
27	a2	416	PHO	C3B-C2B	5.44	1.47	1.37
38	f1	101	HEM	C3D-C2D	5.45	1.53	1.37
38	V2	201	HEM	C3D-C2D	5.45	1.53	1.37
27	A2	407	PHO	C3B-C2B	5.46	1.47	1.37
38	V1	201	HEM	C3D-C2D	5.46	1.53	1.37
38	E2	101	HEM	C3D-C2D	5.47	1.53	1.37
27	A1	408	PHO	C3B-C2B	5.47	1.47	1.37
38	e2	101	HEM	C3D-C2D	5.48	1.53	1.37
38	E1	101	HEM	C3D-C2D	5.48	1.53	1.37
27	a1	411	PHO	C3B-C2B	5.62	1.47	1.37
27	d2	408	PHO	C3B-C2B	5.68	1.47	1.37
27	D2	407	PHO	C3B-C2B	5.71	1.47	1.37
27	d1	403	PHO	C3B-C2B	5.71	1.47	1.37
27	D1	407	PHO	C3B-C2B	5.75	1.48	1.37
37	D2	402	SQD	O7-S	6.40	1.63	1.45

All (1905) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c2	501	BCR	C36-C18-C17	-10.45	107.70	122.89
23	c2	501	BCR	C24-C23-C22	-9.35	112.09	126.21
23	B2	602	BCR	C7-C8-C9	-6.72	116.06	126.21
23	c2	501	BCR	C16-C15-C14	-6.70	108.77	123.23
23	b2	602	BCR	C7-C8-C9	-6.44	116.48	126.21
23	b1	602	BCR	C7-C8-C9	-6.20	116.85	126.21
29	c2	519	LMG	O7-C10-O9	-6.08	118.62	125.61
23	j2	102	BCR	C33-C5-C6	-5.89	118.34	124.62
23	J1	101	BCR	C33-C5-C6	-5.72	118.53	124.62
23	B1	602	BCR	C7-C8-C9	-5.55	117.82	126.21
23	c2	501	BCR	C37-C22-C21	-5.51	114.88	122.89
23	k1	101	BCR	C33-C5-C6	-5.47	118.80	124.62
23	D1	401	BCR	C7-C8-C9	-5.45	117.97	126.21
23	J1	101	BCR	C20-C21-C22	-5.43	119.32	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	k1	101	BCR	C20-C21-C22	-5.38	119.40	127.22
23	B1	602	BCR	C11-C10-C9	-5.37	119.42	127.22
23	F2	401	BCR	C20-C21-C22	-5.31	119.51	127.22
23	K1	101	BCR	C15-C14-C13	-5.28	119.54	127.22
23	F2	401	BCR	C7-C8-C9	-5.24	118.28	126.21
23	B2	602	BCR	C11-C10-C9	-5.15	119.74	127.22
23	j2	102	BCR	C20-C21-C22	-5.13	119.76	127.22
23	d1	405	BCR	C7-C8-C9	-5.09	118.52	126.21
23	c1	502	BCR	C15-C14-C13	-5.05	119.88	127.22
23	c1	501	BCR	C11-C10-C9	-5.00	119.95	127.22
23	A2	401	BCR	C28-C27-C26	-4.95	105.66	113.87
23	c1	502	BCR	C24-C23-C22	-4.92	118.78	126.21
23	d2	401	BCR	C4-C5-C6	-4.87	117.38	122.73
23	c1	501	BCR	C15-C14-C13	-4.86	120.16	127.22
23	B2	601	BCR	C28-C27-C26	-4.83	105.86	113.87
23	c1	501	BCR	C16-C17-C18	-4.83	120.20	127.22
23	c2	501	BCR	C38-C26-C25	-4.82	119.48	124.62
23	b2	602	BCR	C20-C21-C22	-4.78	120.27	127.22
23	k2	501	BCR	C24-C23-C22	-4.76	119.01	126.21
23	d2	401	BCR	C16-C17-C18	-4.76	120.30	127.22
23	J1	101	BCR	C24-C23-C22	-4.75	119.03	126.21
23	K1	101	BCR	C33-C5-C6	-4.75	119.56	124.62
23	c1	502	BCR	C20-C21-C22	-4.74	120.32	127.22
23	b2	601	BCR	C28-C27-C26	-4.74	106.00	113.87
23	H1	102	BCR	C15-C14-C13	-4.74	120.33	127.22
23	D1	401	BCR	C11-C10-C9	-4.74	120.33	127.22
23	j2	102	BCR	C15-C14-C13	-4.73	120.35	127.22
23	C2	502	BCR	C15-C14-C13	-4.72	120.36	127.22
23	h2	101	BCR	C15-C14-C13	-4.71	120.38	127.22
23	B1	601	BCR	C28-C27-C26	-4.70	106.08	113.87
23	K2	102	BCR	C24-C23-C22	-4.66	119.16	126.21
23	D1	401	BCR	C16-C17-C18	-4.66	120.45	127.22
23	A2	401	BCR	C7-C8-C9	-4.61	119.25	126.21
23	K2	104	BCR	C28-C27-C26	-4.60	106.24	113.87
23	F2	401	BCR	C15-C14-C13	-4.56	120.60	127.22
23	k2	501	BCR	C20-C21-C22	-4.55	120.60	127.22
23	h1	102	BCR	C16-C17-C18	-4.55	120.61	127.22
23	K2	102	BCR	C20-C21-C22	-4.53	120.63	127.22
23	k2	501	BCR	C15-C14-C13	-4.53	120.64	127.22
23	C1	521	BCR	C11-C10-C9	-4.51	120.66	127.22
23	d2	401	BCR	C38-C26-C25	-4.51	119.82	124.62
23	c1	502	BCR	C33-C5-C6	-4.49	119.84	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	D1	408	PL9	C7-C8-C9	-4.48	119.08	126.70
23	A2	401	BCR	C16-C17-C18	-4.47	120.73	127.22
36	D2	408	PL9	C7-C8-C9	-4.46	119.10	126.70
23	c1	502	BCR	C7-C8-C9	-4.46	119.48	126.21
23	c1	501	BCR	C20-C21-C22	-4.45	120.75	127.22
23	C1	501	BCR	C15-C14-C13	-4.44	120.77	127.22
23	A2	401	BCR	C33-C5-C6	-4.43	119.90	124.62
23	j2	102	BCR	C24-C23-C22	-4.40	119.57	126.21
23	B2	601	BCR	C15-C14-C13	-4.39	120.84	127.22
23	c2	501	BCR	C7-C8-C9	-4.38	119.59	126.21
23	h1	102	BCR	C28-C27-C26	-4.37	106.62	113.87
23	b1	601	BCR	C28-C27-C26	-4.36	106.64	113.87
23	D1	401	BCR	C33-C5-C6	-4.35	119.98	124.62
36	d2	409	PL9	C7-C8-C9	-4.35	119.30	126.70
36	d1	409	PL9	C7-C8-C9	-4.35	119.30	126.70
23	B1	601	BCR	C7-C8-C9	-4.35	119.64	126.21
23	A2	401	BCR	C11-C10-C9	-4.35	120.90	127.22
23	h1	102	BCR	C20-C21-C22	-4.34	120.92	127.22
23	b2	601	BCR	C15-C14-C13	-4.32	120.95	127.22
23	b2	603	BCR	C7-C8-C9	-4.31	119.69	126.21
23	B1	602	BCR	C28-C27-C26	-4.30	106.75	113.87
23	a1	401	BCR	C33-C5-C6	-4.26	120.08	124.62
23	C2	502	BCR	C20-C21-C22	-4.26	121.03	127.22
23	K1	101	BCR	C16-C17-C18	-4.25	121.04	127.22
23	d1	405	BCR	C33-C5-C6	-4.24	120.11	124.62
36	d2	409	PL9	C22-C23-C24	-4.23	118.41	127.75
23	B2	603	BCR	C15-C14-C13	-4.23	121.07	127.22
23	k2	501	BCR	C16-C17-C18	-4.22	121.08	127.22
23	d2	401	BCR	C20-C21-C22	-4.22	121.09	127.22
23	C1	521	BCR	C15-C14-C13	-4.21	121.10	127.22
25	C1	509	CLA	CMB-C2B-C1B	-4.21	121.16	128.31
23	b2	603	BCR	C15-C14-C13	-4.20	121.12	127.22
36	D1	408	PL9	C22-C23-C24	-4.19	118.50	127.75
23	K1	101	BCR	C3-C4-C5	-4.18	106.94	113.87
23	k1	101	BCR	C24-C23-C22	-4.16	119.93	126.21
23	B2	602	BCR	C38-C26-C25	-4.15	120.20	124.62
25	B2	613	CLA	CMB-C2B-C1B	-4.14	121.27	128.31
23	a2	402	BCR	C38-C26-C25	-4.13	120.22	124.62
23	J1	101	BCR	C15-C14-C13	-4.11	121.24	127.22
23	K2	102	BCR	C15-C14-C13	-4.11	121.24	127.22
23	D1	401	BCR	C24-C23-C22	-4.11	120.00	126.21
23	c1	501	BCR	C24-C23-C22	-4.11	120.00	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b2	603	BCR	C11-C10-C9	-4.11	121.25	127.22
23	K2	104	BCR	C33-C5-C6	-4.09	120.26	124.62
23	b2	602	BCR	C15-C14-C13	-4.08	121.29	127.22
23	d2	401	BCR	C3-C4-C5	-4.06	107.14	113.87
36	d1	409	PL9	C22-C23-C24	-4.05	118.81	127.75
23	z2	101	BCR	C15-C14-C13	-4.05	121.33	127.22
23	b2	603	BCR	C38-C26-C25	-4.04	120.31	124.62
23	B2	603	BCR	C7-C8-C9	-4.04	120.10	126.21
23	a1	401	BCR	C38-C26-C25	-4.04	120.32	124.62
23	d2	401	BCR	C1-C6-C5	-4.03	117.11	122.50
36	d1	409	PL9	C42-C43-C44	-4.02	118.88	127.75
23	A1	401	BCR	C33-C5-C6	-4.02	120.34	124.62
23	d2	401	BCR	C11-C10-C9	-4.02	121.38	127.22
23	b2	602	BCR	C38-C26-C25	-4.01	120.34	124.62
23	b2	601	BCR	C7-C8-C9	-4.01	120.14	126.21
23	z2	101	BCR	C16-C17-C18	-4.01	121.39	127.22
23	c2	501	BCR	C33-C5-C6	-3.98	120.38	124.62
23	b2	602	BCR	C24-C23-C22	-3.97	120.21	126.21
25	B2	610	CLA	CMB-C2B-C1B	-3.97	121.56	128.31
36	D2	408	PL9	C42-C43-C44	-3.97	119.00	127.75
23	C1	521	BCR	C16-C17-C18	-3.96	121.46	127.22
23	d2	401	BCR	C24-C23-C22	-3.96	120.22	126.21
23	b2	603	BCR	C24-C23-C22	-3.96	120.23	126.21
23	B1	601	BCR	C33-C5-C6	-3.94	120.42	124.62
23	c2	501	BCR	C3-C4-C5	-3.94	107.34	113.87
23	b2	601	BCR	C33-C5-C6	-3.94	120.43	124.62
23	B2	602	BCR	C16-C17-C18	-3.94	121.50	127.22
23	B1	601	BCR	C24-C23-C22	-3.93	120.27	126.21
23	C2	502	BCR	C16-C17-C18	-3.93	121.50	127.22
23	A1	401	BCR	C38-C26-C25	-3.93	120.44	124.62
23	F2	401	BCR	C33-C5-C6	-3.91	120.46	124.62
36	D1	408	PL9	C37-C38-C39	-3.90	119.14	127.75
23	B2	603	BCR	C38-C26-C25	-3.90	120.46	124.62
23	B2	603	BCR	C11-C10-C9	-3.90	121.55	127.22
23	C1	521	BCR	C24-C23-C22	-3.89	120.33	126.21
23	b1	602	BCR	C28-C27-C26	-3.89	107.42	113.87
23	h1	102	BCR	C24-C23-C22	-3.88	120.34	126.21
25	c2	509	CLA	CMB-C2B-C1B	-3.87	121.73	128.31
25	b1	610	CLA	CMB-C2B-C1B	-3.87	121.73	128.31
23	B2	601	BCR	C33-C5-C6	-3.87	120.50	124.62
23	F2	401	BCR	C24-C23-C22	-3.86	120.37	126.21
27	d2	408	PHO	C3D-C2D-C1D	-3.86	99.43	105.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	h2	101	BCR	C11-C10-C9	-3.86	121.61	127.22
23	c2	501	BCR	C11-C10-C9	-3.85	121.63	127.22
23	b1	603	BCR	C7-C8-C9	-3.84	120.41	126.21
36	D2	408	PL9	C22-C23-C24	-3.84	119.28	127.75
23	k2	501	BCR	C11-C10-C9	-3.84	121.64	127.22
23	b2	601	BCR	C11-C10-C9	-3.82	121.66	127.22
23	A1	401	BCR	C7-C8-C9	-3.82	120.43	126.21
23	b1	601	BCR	C33-C5-C6	-3.82	120.55	124.62
23	k1	101	BCR	C15-C14-C13	-3.81	121.68	127.22
23	d1	405	BCR	C24-C23-C22	-3.81	120.45	126.21
23	K2	102	BCR	C3-C4-C5	-3.81	107.56	113.87
23	D1	401	BCR	C15-C14-C13	-3.81	121.69	127.22
23	d2	401	BCR	C15-C14-C13	-3.79	121.71	127.22
23	K1	101	BCR	C11-C10-C9	-3.79	121.71	127.22
23	b1	603	BCR	C15-C14-C13	-3.79	121.71	127.22
23	C1	521	BCR	C7-C8-C9	-3.79	120.49	126.21
23	C2	502	BCR	C7-C8-C9	-3.78	120.50	126.21
23	A1	401	BCR	C16-C17-C18	-3.78	121.73	127.22
25	b2	624	CLA	CMB-C2B-C1B	-3.78	121.88	128.31
23	c1	501	BCR	C7-C8-C9	-3.78	120.50	126.21
29	c2	519	LMG	C8-O7-C10	-3.77	111.79	117.29
27	D2	407	PHO	C3D-C2D-C1D	-3.77	99.59	105.76
23	F2	401	BCR	C11-C10-C9	-3.76	121.75	127.22
27	a1	411	PHO	C3D-C2D-C1D	-3.76	99.59	105.76
23	B1	603	BCR	C7-C8-C9	-3.76	120.53	126.21
23	b1	603	BCR	C11-C10-C9	-3.75	121.76	127.22
27	d2	408	PHO	C4C-C3C-C2C	-3.75	102.72	106.80
23	K2	102	BCR	C33-C5-C6	-3.74	120.63	124.62
27	D1	407	PHO	C3D-C2D-C1D	-3.74	99.62	105.76
27	d1	403	PHO	C3D-C2D-C1D	-3.74	99.63	105.76
25	c1	506	CLA	CMB-C2B-C1B	-3.74	121.95	128.31
27	A2	407	PHO	C3D-C2D-C1D	-3.74	99.63	105.76
27	a2	416	PHO	C3D-C2D-C1D	-3.73	99.64	105.76
23	c1	502	BCR	C11-C10-C9	-3.73	121.80	127.22
23	b1	601	BCR	C7-C8-C9	-3.73	120.58	126.21
25	b1	613	CLA	O2A-CGA-O1A	-3.72	113.77	123.51
23	b2	602	BCR	C16-C17-C18	-3.70	121.84	127.22
27	A1	408	PHO	C4C-C3C-C2C	-3.70	102.77	106.80
23	b2	603	BCR	C33-C5-C6	-3.70	120.68	124.62
27	D2	407	PHO	C4C-C3C-C2C	-3.70	102.78	106.80
23	a1	401	BCR	C7-C8-C9	-3.70	120.63	126.21
23	b1	603	BCR	C38-C26-C25	-3.69	120.69	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B1	603	BCR	C15-C14-C13	-3.69	121.86	127.22
23	C1	501	BCR	C7-C8-C9	-3.69	120.64	126.21
23	d1	405	BCR	C11-C10-C9	-3.69	121.86	127.22
23	a1	401	BCR	C11-C10-C9	-3.69	121.86	127.22
23	K2	104	BCR	C7-C8-C9	-3.68	120.65	126.21
23	b1	601	BCR	C15-C14-C13	-3.67	121.88	127.22
25	b1	615	CLA	CMB-C2B-C1B	-3.66	122.08	128.31
27	A1	408	PHO	C3D-C2D-C1D	-3.66	99.76	105.76
23	B2	601	BCR	C20-C21-C22	-3.66	121.91	127.22
25	b1	614	CLA	CMB-C2B-C1B	-3.65	122.11	128.31
27	d1	403	PHO	C4C-C3C-C2C	-3.64	102.84	106.80
23	z2	101	BCR	C33-C5-C6	-3.64	120.75	124.62
23	B1	601	BCR	C15-C14-C13	-3.62	121.95	127.22
27	a2	416	PHO	C4C-C3C-C2C	-3.62	102.86	106.80
23	k2	501	BCR	C3-C4-C5	-3.61	107.89	113.87
23	b2	602	BCR	C11-C10-C9	-3.60	121.99	127.22
23	k2	501	BCR	C7-C8-C9	-3.59	120.78	126.21
23	B2	603	BCR	C20-C21-C22	-3.59	122.00	127.22
23	B1	602	BCR	C16-C17-C18	-3.59	122.01	127.22
23	B2	603	BCR	C24-C23-C22	-3.58	120.79	126.21
25	c1	511	CLA	CMB-C2B-C1B	-3.57	122.23	128.31
23	A1	401	BCR	C15-C14-C13	-3.57	122.03	127.22
25	C2	506	CLA	CMB-C2B-C1B	-3.57	122.24	128.31
23	b2	603	BCR	C16-C17-C18	-3.57	122.03	127.22
23	J1	101	BCR	C11-C10-C9	-3.56	122.04	127.22
27	D1	407	PHO	C4C-C3C-C2C	-3.56	102.93	106.80
23	C1	521	BCR	C38-C26-C25	-3.56	120.83	124.62
25	B2	615	CLA	CMB-C2B-C1B	-3.55	122.27	128.31
23	C2	502	BCR	C38-C26-C25	-3.55	120.83	124.62
23	B2	602	BCR	C15-C14-C13	-3.55	122.06	127.22
23	d1	405	BCR	C16-C17-C18	-3.54	122.07	127.22
23	z2	101	BCR	C11-C10-C9	-3.54	122.08	127.22
25	B1	614	CLA	CMB-C2B-C1B	-3.53	122.30	128.31
23	K1	101	BCR	C7-C8-C9	-3.53	120.88	126.21
25	c1	504	CLA	CMB-C2B-C1B	-3.53	122.31	128.31
23	C2	502	BCR	C11-C10-C9	-3.53	122.10	127.22
36	d2	409	PL9	C25-C24-C23	-3.52	116.77	123.58
23	K2	102	BCR	C16-C17-C18	-3.52	122.10	127.22
23	b1	602	BCR	C16-C17-C18	-3.52	122.11	127.22
27	a2	416	PHO	CBA-CAA-C2A	-3.51	104.91	113.96
23	B1	603	BCR	C11-C10-C9	-3.51	122.12	127.22
23	c1	501	BCR	C33-C5-C6	-3.50	120.89	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c1	515	CLA	CMB-C2B-C1B	-3.50	122.36	128.31
27	a1	411	PHO	C4C-C3C-C2C	-3.49	103.00	106.80
23	B1	602	BCR	C24-C23-C22	-3.48	120.95	126.21
23	d1	405	BCR	C38-C26-C25	-3.48	120.92	124.62
23	B1	601	BCR	C11-C10-C9	-3.47	122.17	127.22
23	B2	601	BCR	C7-C8-C9	-3.47	120.96	126.21
25	C1	505	CLA	CMB-C2B-C1B	-3.47	122.41	128.31
25	c1	512	CLA	CMB-C2B-C1B	-3.47	122.41	128.31
23	b2	601	BCR	C16-C17-C18	-3.47	122.18	127.22
25	C2	508	CLA	CMB-C2B-C1B	-3.46	122.42	128.31
23	k1	101	BCR	C11-C10-C9	-3.46	122.19	127.22
25	B1	610	CLA	CMB-C2B-C1B	-3.46	122.42	128.31
27	D2	407	PHO	CHD-C1D-ND	-3.46	118.38	124.67
23	C2	502	BCR	C33-C5-C6	-3.46	120.93	124.62
25	c2	513	CLA	CMB-C2B-C1B	-3.46	122.43	128.31
23	B1	603	BCR	C16-C17-C18	-3.46	122.20	127.22
23	b2	602	BCR	C28-C27-C26	-3.45	108.14	113.87
36	D1	408	PL9	C25-C24-C23	-3.45	116.90	123.58
25	C1	511	CLA	CMB-C2B-C1B	-3.45	122.45	128.31
23	h2	101	BCR	C16-C17-C18	-3.45	122.21	127.22
23	k2	501	BCR	C38-C26-C25	-3.43	120.96	124.62
23	C2	502	BCR	C24-C23-C22	-3.43	121.02	126.21
23	h2	101	BCR	C3-C4-C5	-3.42	108.19	113.87
25	D1	403	CLA	CMB-C2B-C1B	-3.42	122.49	128.31
25	c2	507	CLA	CMB-C2B-C1B	-3.42	122.49	128.31
27	D1	407	PHO	CHD-C1D-ND	-3.42	118.46	124.67
36	d1	409	PL9	C27-C28-C29	-3.42	120.21	127.75
25	c1	513	CLA	CMB-C2B-C1B	-3.41	122.51	128.31
23	K2	102	BCR	C11-C10-C9	-3.41	122.27	127.22
25	b2	614	CLA	CMB-C2B-C1B	-3.41	122.52	128.31
25	d2	404	CLA	CMB-C2B-C1B	-3.41	122.52	128.31
25	c2	506	CLA	O2D-CGD-O1D	-3.39	116.62	123.77
25	d1	406	CLA	CMB-C2B-C1B	-3.39	122.54	128.31
36	d2	409	PL9	C17-C18-C19	-3.39	120.26	127.75
25	C2	511	CLA	CMB-C2B-C1B	-3.39	122.55	128.31
23	k2	501	BCR	C28-C27-C26	-3.39	108.25	113.87
23	b2	603	BCR	C20-C21-C22	-3.38	122.30	127.22
25	C2	507	CLA	CMB-C2B-C1B	-3.38	122.56	128.31
25	b2	615	CLA	CMB-C2B-C1B	-3.38	122.56	128.31
23	B2	602	BCR	C20-C21-C22	-3.38	122.31	127.22
36	D1	408	PL9	C32-C33-C34	-3.37	120.31	127.75
23	a2	402	BCR	C33-C5-C6	-3.37	121.03	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C1	501	BCR	C11-C10-C9	-3.37	122.32	127.22
25	B1	615	CLA	CMB-C2B-C1B	-3.37	122.58	128.31
25	B2	614	CLA	CMB-C2B-C1B	-3.37	122.58	128.31
25	B1	609	CLA	CAC-C3C-C2C	-3.37	121.72	127.51
27	A2	407	PHO	C4C-C3C-C2C	-3.36	103.14	106.80
23	B2	603	BCR	C16-C17-C18	-3.36	122.33	127.22
23	F2	401	BCR	C27-C26-C25	-3.36	119.04	122.73
25	b1	605	CLA	CMB-C2B-C1B	-3.36	122.60	128.31
23	k1	101	BCR	C38-C26-C25	-3.35	121.05	124.62
23	a2	402	BCR	C7-C8-C9	-3.35	121.15	126.21
23	A2	401	BCR	C27-C26-C25	-3.35	119.05	122.73
25	d1	404	CLA	CMB-C2B-C1B	-3.35	122.62	128.31
23	d1	405	BCR	C15-C14-C13	-3.35	122.36	127.22
36	d1	409	PL9	C17-C18-C19	-3.34	120.37	127.75
36	d2	409	PL9	C37-C38-C39	-3.34	120.37	127.75
23	k2	501	BCR	C33-C5-C6	-3.34	121.06	124.62
23	h2	101	BCR	C7-C8-C9	-3.34	121.16	126.21
23	h2	101	BCR	C33-C5-C6	-3.34	121.06	124.62
23	z2	101	BCR	C38-C26-C25	-3.34	121.06	124.62
25	C1	512	CLA	CMB-C2B-C1B	-3.34	122.63	128.31
23	B2	601	BCR	C16-C17-C18	-3.33	122.38	127.22
33	d1	402	LHG	C5-O7-C7	-3.33	109.67	117.91
23	C1	521	BCR	C20-C21-C22	-3.33	122.38	127.22
23	F2	401	BCR	C16-C17-C18	-3.33	122.39	127.22
23	b1	602	BCR	C20-C21-C22	-3.32	122.39	127.22
25	b2	612	CLA	CMB-C2B-C1B	-3.32	122.66	128.31
23	b1	601	BCR	C16-C17-C18	-3.32	122.40	127.22
25	a1	405	CLA	O2D-CGD-O1D	-3.32	116.79	123.77
25	b2	612	CLA	O2A-CGA-O1A	-3.32	114.82	123.51
25	B2	605	CLA	CMB-C2B-C1B	-3.31	122.68	128.31
23	b2	602	BCR	C4-C5-C6	-3.31	119.09	122.73
34	C1	516	DGD	C2G-O2G-C1B	-3.31	109.73	117.91
25	c1	516	CLA	CMB-C2B-C1B	-3.31	122.69	128.31
25	b1	613	CLA	CMB-C2B-C1B	-3.30	122.69	128.31
25	B2	609	CLA	CMB-C2B-C1B	-3.30	122.69	128.31
23	a1	401	BCR	C16-C17-C18	-3.30	122.42	127.22
25	c2	505	CLA	CMB-C2B-C1B	-3.30	122.70	128.31
36	D2	408	PL9	C37-C38-C39	-3.30	120.48	127.75
25	b2	613	CLA	CMB-C2B-C1B	-3.29	122.72	128.31
23	C1	521	BCR	C3-C4-C5	-3.28	108.44	113.87
23	a2	402	BCR	C11-C10-C9	-3.27	122.46	127.22
23	b1	603	BCR	C16-C17-C18	-3.27	122.46	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c2	515	CLA	CMB-C2B-C1B	-3.27	122.75	128.31
23	H1	102	BCR	C33-C5-C6	-3.27	121.14	124.62
25	b2	606	CLA	CMB-C2B-C1B	-3.27	122.75	128.31
23	c1	501	BCR	C38-C26-C25	-3.27	121.14	124.62
23	B1	603	BCR	C33-C5-C6	-3.26	121.15	124.62
23	B2	601	BCR	C24-C23-C22	-3.26	121.28	126.21
25	c2	506	CLA	CMB-C2B-C1B	-3.26	122.77	128.31
23	d2	401	BCR	C28-C27-C26	-3.26	108.47	113.87
25	B1	619	CLA	CMB-C2B-C1B	-3.25	122.78	128.31
36	D2	408	PL9	C27-C28-C29	-3.25	120.58	127.75
25	b2	611	CLA	CMB-C2B-C1B	-3.25	122.78	128.31
23	C1	501	BCR	C3-C4-C5	-3.25	108.49	113.87
25	b2	620	CLA	CMB-C2B-C1B	-3.24	122.80	128.31
25	B2	613	CLA	O2A-CGA-O1A	-3.22	115.07	123.51
25	B1	611	CLA	O2D-CGD-O1D	-3.22	116.99	123.77
23	K2	102	BCR	C38-C26-C25	-3.22	121.19	124.62
23	H2	103	BCR	C15-C14-C13	-3.22	122.55	127.22
25	c1	505	CLA	CMB-C2B-C1B	-3.21	122.84	128.31
25	B2	607	CLA	O2D-CGD-O1D	-3.21	117.00	123.77
23	z2	101	BCR	C7-C8-C9	-3.21	121.36	126.21
23	J1	101	BCR	C38-C26-C25	-3.21	121.20	124.62
23	b1	602	BCR	C33-C5-C6	-3.20	121.21	124.62
27	A2	407	PHO	CMD-C2D-C3D	-3.20	121.06	128.10
23	K2	102	BCR	C36-C18-C17	-3.20	118.23	122.89
25	b1	606	CLA	O2D-CGD-O1D	-3.20	117.03	123.77
25	C2	518	CLA	CMB-C2B-C1B	-3.20	122.87	128.31
23	B1	603	BCR	C38-C26-C25	-3.20	121.22	124.62
23	b1	601	BCR	C11-C10-C9	-3.19	122.58	127.22
23	B1	602	BCR	C20-C21-C22	-3.18	122.59	127.22
25	B1	612	CLA	CMB-C2B-C1B	-3.18	122.91	128.31
23	C1	501	BCR	C38-C26-C25	-3.18	121.24	124.62
36	d1	409	PL9	C25-C24-C23	-3.17	117.44	123.58
25	C1	509	CLA	O2D-CGD-O1D	-3.17	117.09	123.77
25	C2	503	CLA	CMB-C2B-C1B	-3.17	122.92	128.31
25	B2	611	CLA	CMB-C2B-C1B	-3.17	122.92	128.31
27	d1	403	PHO	CHD-C1D-ND	-3.17	118.92	124.67
25	c1	503	CLA	CMB-C2B-C1B	-3.16	122.93	128.31
36	d1	409	PL9	C32-C33-C34	-3.16	120.77	127.75
23	C1	521	BCR	C33-C5-C6	-3.16	121.26	124.62
23	C1	501	BCR	C33-C5-C6	-3.16	121.26	124.62
36	d2	409	PL9	C32-C33-C34	-3.16	120.78	127.75
23	c1	501	BCR	C3-C4-C5	-3.15	108.64	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A1	406	CLA	CMB-C2B-C1B	-3.15	122.95	128.31
27	d2	408	PHO	CHD-C1D-ND	-3.15	118.95	124.67
25	C1	507	CLA	CMB-C2B-C1B	-3.15	122.96	128.31
23	b2	601	BCR	C24-C23-C22	-3.14	121.46	126.21
25	b1	608	CLA	O2D-CGD-O1D	-3.14	117.16	123.77
25	B1	617	CLA	CMB-C2B-C1B	-3.14	122.98	128.31
25	c1	510	CLA	CMB-C2B-C1B	-3.14	122.98	128.31
23	b1	602	BCR	C24-C23-C22	-3.13	121.48	126.21
23	b1	601	BCR	C3-C4-C5	-3.13	108.68	113.87
33	l1	102	LHG	C5-O7-C7	-3.13	110.18	117.91
25	B1	609	CLA	CMB-C2B-C1B	-3.13	122.99	128.31
23	b2	601	BCR	C20-C21-C22	-3.12	122.68	127.22
23	A2	401	BCR	C15-C14-C13	-3.12	122.68	127.22
23	c1	502	BCR	C38-C26-C25	-3.12	121.30	124.62
23	b1	602	BCR	C35-C13-C14	-3.12	118.35	122.89
25	C2	504	CLA	CMB-C2B-C1B	-3.12	123.01	128.31
25	b1	609	CLA	CMB-C2B-C1B	-3.12	123.01	128.31
37	D2	402	SQD	C45-O47-C7	-3.12	112.06	117.93
23	B2	602	BCR	C24-C23-C22	-3.11	121.50	126.21
23	z2	101	BCR	C24-C23-C22	-3.11	121.51	126.21
25	B2	606	CLA	CMB-C2B-C1B	-3.11	123.03	128.31
33	L2	101	LHG	C5-O7-C7	-3.11	110.23	117.91
25	D2	404	CLA	CMB-C2B-C1B	-3.10	123.03	128.31
27	D2	407	PHO	CMD-C2D-C3D	-3.10	121.28	128.10
23	j2	102	BCR	C38-C26-C25	-3.10	121.32	124.62
25	C1	514	CLA	CMB-C2B-C1B	-3.10	123.04	128.31
23	B2	601	BCR	C11-C10-C9	-3.09	122.72	127.22
23	h1	102	BCR	C15-C14-C13	-3.09	122.72	127.22
23	A1	401	BCR	C11-C10-C9	-3.09	122.73	127.22
25	B2	619	CLA	CMB-C2B-C1B	-3.09	123.06	128.31
23	B1	601	BCR	C16-C17-C18	-3.08	122.74	127.22
23	F2	401	BCR	C28-C27-C26	-3.08	108.76	113.87
25	C2	505	CLA	CMB-C2B-C1B	-3.08	123.08	128.31
25	B1	613	CLA	O2A-CGA-O1A	-3.08	115.45	123.51
25	b2	608	CLA	CMB-C2B-C1B	-3.08	123.08	128.31
25	C2	513	CLA	CMB-C2B-C1B	-3.07	123.08	128.31
25	B1	619	CLA	O2D-CGD-O1D	-3.07	117.30	123.77
25	B2	605	CLA	O2D-CGD-O1D	-3.07	117.30	123.77
25	B1	605	CLA	CMB-C2B-C1B	-3.07	123.09	128.31
23	B1	602	BCR	C15-C14-C13	-3.07	122.76	127.22
25	C1	503	CLA	CMB-C2B-C1B	-3.07	123.09	128.31
25	b1	614	CLA	O2D-CGD-O1D	-3.07	117.31	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B2	617	CLA	CMB-C2B-C1B	-3.07	123.09	128.31
25	B2	608	CLA	CMB-C2B-C1B	-3.07	123.09	128.31
25	B2	612	CLA	CMB-C2B-C1B	-3.07	123.10	128.31
23	J1	101	BCR	C16-C17-C18	-3.06	122.77	127.22
25	A1	406	CLA	O2D-CGD-O1D	-3.06	117.33	123.77
23	b2	601	BCR	C38-C26-C25	-3.06	121.36	124.62
25	C1	504	CLA	CMB-C2B-C1B	-3.05	123.12	128.31
25	D2	401	CLA	CMB-C2B-C1B	-3.05	123.12	128.31
25	A1	404	CLA	CMB-C2B-C1B	-3.04	123.14	128.31
25	C1	502	CLA	CMB-C2B-C1B	-3.04	123.14	128.31
25	C2	509	CLA	CMB-C2B-C1B	-3.04	123.14	128.31
23	j2	102	BCR	C30-C25-C26	-3.04	118.43	122.50
23	K2	104	BCR	C3-C4-C5	-3.04	108.83	113.87
23	B1	603	BCR	C28-C27-C26	-3.04	108.83	113.87
23	z2	101	BCR	C20-C21-C22	-3.03	122.81	127.22
23	a1	401	BCR	C24-C23-C22	-3.03	121.63	126.21
25	c1	507	CLA	O2D-CGD-O1D	-3.03	117.39	123.77
25	D2	404	CLA	O2D-CGD-O1D	-3.03	117.39	123.77
23	C1	501	BCR	C24-C23-C22	-3.03	121.64	126.21
25	B1	606	CLA	CMB-C2B-C1B	-3.03	123.17	128.31
25	C2	518	CLA	O2D-CGD-O1D	-3.02	117.40	123.77
23	a2	402	BCR	C15-C14-C13	-3.02	122.83	127.22
23	a2	402	BCR	C16-C17-C18	-3.02	122.83	127.22
25	B1	611	CLA	CMB-C2B-C1B	-3.02	123.18	128.31
36	D1	408	PL9	C27-C28-C29	-3.02	121.09	127.75
25	c1	510	CLA	O2D-CGD-O1D	-3.01	117.42	123.77
25	c1	508	CLA	CMB-C2B-C1B	-3.01	123.19	128.31
25	A2	404	CLA	CMB-C2B-C1B	-3.01	123.19	128.31
25	C1	508	CLA	CMB-C2B-C1B	-3.01	123.19	128.31
27	A1	408	PHO	CBA-CAA-C2A	-3.01	106.20	113.96
23	B2	603	BCR	C33-C5-C6	-3.01	121.42	124.62
25	a2	405	CLA	CMB-C2B-C1B	-3.01	123.19	128.31
25	c2	505	CLA	O2D-CGD-O1D	-3.01	117.44	123.77
25	b1	619	CLA	CMB-C2B-C1B	-3.01	123.20	128.31
25	B1	610	CLA	O2D-CGD-O1D	-3.00	117.45	123.77
27	a1	411	PHO	CMD-C2D-C3D	-3.00	121.50	128.10
23	h2	101	BCR	C38-C26-C25	-3.00	121.43	124.62
25	d1	401	CLA	O2D-CGD-O1D	-3.00	117.46	123.77
25	a2	413	CLA	CMB-C2B-C1B	-3.00	123.22	128.31
27	A1	408	PHO	CMD-C2D-C3D	-2.99	121.52	128.10
27	D1	407	PHO	CMD-C2D-C3D	-2.99	121.52	128.10
25	B1	618	CLA	CMB-C2B-C1B	-2.99	123.22	128.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a2	416	PHO	O1D-CGD-CBD	-2.99	119.98	124.64
23	b1	603	BCR	C24-C23-C22	-2.99	121.69	126.21
25	d2	402	CLA	CMB-C2B-C1B	-2.99	123.22	128.31
25	B2	616	CLA	O2D-CGD-O1D	-2.99	117.47	123.77
23	F2	401	BCR	C36-C18-C17	-2.98	118.55	122.89
25	C2	510	CLA	CMB-C2B-C1B	-2.98	123.24	128.31
34	c1	518	DGD	C2G-O2G-C1B	-2.98	110.54	117.91
36	D1	408	PL9	C17-C18-C19	-2.98	121.18	127.75
25	d2	402	CLA	O2D-CGD-O1D	-2.98	117.50	123.77
23	b1	603	BCR	C28-C27-C26	-2.98	108.93	113.87
25	b2	612	CLA	O2D-CGD-O1D	-2.98	117.50	123.77
25	d1	406	CLA	O2D-CGD-O1D	-2.97	117.51	123.77
25	c2	511	CLA	CMB-C2B-C1B	-2.97	123.25	128.31
25	c2	509	CLA	O2D-CGD-O1D	-2.97	117.52	123.77
38	v1	201	HEM	CBD-CAD-C3D	-2.97	107.26	112.47
25	d1	401	CLA	CMB-C2B-C1B	-2.97	123.26	128.31
25	B2	609	CLA	O2D-CGD-O1D	-2.97	117.52	123.77
25	B2	604	CLA	CMB-C2B-C1B	-2.97	123.27	128.31
23	C1	501	BCR	C16-C17-C18	-2.97	122.91	127.22
25	b1	605	CLA	O2D-CGD-O1D	-2.96	117.53	123.77
25	b1	609	CLA	O2D-CGD-O1D	-2.96	117.53	123.77
25	B1	613	CLA	CMB-C2B-C1B	-2.96	123.27	128.31
36	D2	408	PL9	C32-C33-C34	-2.96	121.22	127.75
25	A2	402	CLA	CMB-C2B-C1B	-2.96	123.28	128.31
25	b1	607	CLA	CMB-C2B-C1B	-2.96	123.28	128.31
27	a2	416	PHO	CMD-C2D-C3D	-2.96	121.59	128.10
25	C2	516	CLA	CMB-C2B-C1B	-2.96	123.28	128.31
25	B2	619	CLA	O2D-CGD-O1D	-2.95	117.55	123.77
36	d1	409	PL9	C37-C38-C39	-2.95	121.24	127.75
25	C1	510	CLA	CMB-C2B-C1B	-2.95	123.30	128.31
25	C2	511	CLA	O2D-CGD-O1D	-2.95	117.57	123.77
25	c1	509	CLA	CMB-C2B-C1B	-2.94	123.30	128.31
23	c1	501	BCR	C4-C5-C6	-2.94	119.50	122.73
23	b2	602	BCR	C1-C6-C5	-2.94	118.57	122.50
25	B1	618	CLA	O2D-CGD-O1D	-2.94	117.58	123.77
25	b1	617	CLA	CMB-C2B-C1B	-2.94	123.31	128.31
25	b2	609	CLA	CMB-C2B-C1B	-2.94	123.31	128.31
27	A2	407	PHO	CBA-CAA-C2A	-2.94	106.39	113.96
25	c1	507	CLA	CMB-C2B-C1B	-2.94	123.32	128.31
23	k1	101	BCR	C16-C17-C18	-2.93	122.96	127.22
25	b2	610	CLA	CMB-C2B-C1B	-2.93	123.32	128.31
25	b1	612	CLA	CMB-C2B-C1B	-2.93	123.33	128.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b2	604	CLA	CMB-C2B-C1B	-2.93	123.33	128.31
25	b2	617	CLA	CMB-C2B-C1B	-2.92	123.35	128.31
23	h1	102	BCR	C33-C5-C6	-2.91	121.52	124.62
23	j2	102	BCR	C11-C10-C9	-2.91	122.99	127.22
23	b1	601	BCR	C38-C26-C25	-2.91	121.52	124.62
25	a1	405	CLA	CMB-C2B-C1B	-2.91	123.36	128.31
27	d1	403	PHO	CMD-C2D-C3D	-2.91	121.71	128.10
25	c2	502	CLA	CMB-C2B-C1B	-2.90	123.37	128.31
27	d2	408	PHO	CMD-C2D-C3D	-2.90	121.72	128.10
25	A1	403	CLA	CMB-C2B-C1B	-2.90	123.38	128.31
29	B1	622	LMG	C8-O7-C10	-2.90	110.74	117.91
25	b1	606	CLA	CMB-C2B-C1B	-2.90	123.38	128.31
25	b2	620	CLA	O2D-CGD-O1D	-2.90	117.67	123.77
34	C2	512	DGD	C2G-O2G-C1B	-2.90	112.47	117.93
25	C2	507	CLA	O2D-CGD-O1D	-2.90	117.67	123.77
25	B2	618	CLA	O2D-CGD-O1D	-2.90	117.67	123.77
25	c1	508	CLA	O2D-CGD-O1D	-2.90	117.67	123.77
29	A1	410	LMG	C8-O7-C10	-2.89	110.75	117.91
25	C1	513	CLA	CMB-C2B-C1B	-2.89	123.39	128.31
25	B1	608	CLA	O2D-CGD-O1D	-2.89	117.68	123.77
23	b1	602	BCR	C15-C14-C13	-2.89	123.02	127.22
25	A1	405	CLA	CMB-C2B-C1B	-2.88	123.41	128.31
25	b2	618	CLA	CMB-C2B-C1B	-2.88	123.42	128.31
23	B1	602	BCR	C38-C26-C25	-2.87	121.56	124.62
25	b1	608	CLA	CMB-C2B-C1B	-2.87	123.43	128.31
25	a1	403	CLA	CMB-C2B-C1B	-2.87	123.43	128.31
25	b1	616	CLA	O2D-CGD-O1D	-2.87	117.73	123.77
23	b2	602	BCR	C3-C4-C5	-2.87	109.11	113.87
23	b1	602	BCR	C34-C9-C10	-2.86	118.72	122.89
27	A2	407	PHO	C1C-C2C-C3C	-2.86	103.12	106.43
25	b1	604	CLA	CMB-C2B-C1B	-2.86	123.44	128.31
25	B1	604	CLA	CMB-C2B-C1B	-2.86	123.44	128.31
25	c1	515	CLA	O2D-CGD-O1D	-2.86	117.74	123.77
25	D2	406	CLA	CMB-C2B-C1B	-2.86	123.44	128.31
25	C1	506	CLA	O2D-CGD-O1D	-2.86	117.75	123.77
25	C2	503	CLA	O2D-CGD-O1D	-2.86	117.75	123.77
23	D1	401	BCR	C38-C26-C25	-2.86	121.58	124.62
25	c1	506	CLA	O2D-CGD-O1D	-2.85	117.76	123.77
25	C1	509	CLA	O2A-CGA-O1A	-2.85	116.03	123.51
23	B1	601	BCR	C27-C26-C25	-2.85	119.60	122.73
25	d2	405	CLA	CMB-C2B-C1B	-2.85	123.46	128.31
25	B1	607	CLA	O2D-CGD-O1D	-2.85	117.77	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	H2	103	BCR	C33-C5-C6	-2.85	121.59	124.62
25	B2	618	CLA	CMB-C2B-C1B	-2.85	123.47	128.31
25	D2	406	CLA	O2D-CGD-O1D	-2.84	117.78	123.77
23	B1	601	BCR	C38-C26-C25	-2.84	121.60	124.62
25	B2	616	CLA	CMB-C2B-C1B	-2.84	123.49	128.31
25	d2	404	CLA	O2D-CGD-O1D	-2.84	117.80	123.77
23	B1	603	BCR	C20-C21-C22	-2.83	123.10	127.22
23	b2	603	BCR	C28-C27-C26	-2.83	109.17	113.87
25	c2	504	CLA	CMB-C2B-C1B	-2.83	123.50	128.31
25	b1	607	CLA	O2D-CGD-O1D	-2.83	117.81	123.77
25	b2	616	CLA	CMB-C2B-C1B	-2.82	123.51	128.31
29	d2	407	LMG	C8-O7-C10	-2.82	112.62	117.93
25	b2	617	CLA	O2D-CGD-O1D	-2.82	117.83	123.77
23	a1	401	BCR	C15-C14-C13	-2.82	123.12	127.22
25	c1	503	CLA	O2D-CGD-O1D	-2.82	117.83	123.77
23	a1	401	BCR	C40-C30-C25	-2.82	106.03	110.33
23	c2	501	BCR	C34-C9-C10	-2.81	118.80	122.89
25	c2	502	CLA	O2D-CGD-O1D	-2.81	117.85	123.77
25	d1	404	CLA	O2D-CGD-O1D	-2.81	117.85	123.77
25	B1	616	CLA	O2D-CGD-O1D	-2.81	117.85	123.77
25	A2	403	CLA	CMB-C2B-C1B	-2.81	123.53	128.31
23	K2	104	BCR	C27-C26-C25	-2.81	119.64	122.73
25	D1	402	CLA	CMB-C2B-C1B	-2.81	123.53	128.31
25	c2	503	CLA	O2D-CGD-O1D	-2.81	117.86	123.77
25	C1	507	CLA	O2D-CGD-O1D	-2.81	117.86	123.77
36	d2	409	PL9	C27-C28-C29	-2.81	121.56	127.75
23	A2	401	BCR	C23-C24-C25	-2.81	119.10	127.24
25	c2	510	CLA	CMB-C2B-C1B	-2.80	123.54	128.31
27	D2	407	PHO	CAA-CBA-CGA	-2.80	105.17	113.28
25	C1	502	CLA	O2D-CGD-O1D	-2.80	117.87	123.77
25	c2	512	CLA	CMB-C2B-C1B	-2.80	123.55	128.31
25	b2	619	CLA	CMB-C2B-C1B	-2.80	123.55	128.31
23	c1	502	BCR	C15-C16-C17	-2.79	117.21	123.23
25	C2	506	CLA	O2D-CGD-O1D	-2.79	117.89	123.77
36	D2	408	PL9	C25-C24-C23	-2.79	118.19	123.58
23	b1	602	BCR	C3-C4-C5	-2.78	109.25	113.87
25	B2	604	CLA	CAA-C2A-C3A	-2.78	110.28	116.22
25	b2	606	CLA	O2D-CGD-O1D	-2.78	117.92	123.77
29	b1	624	LMG	C8-O7-C10	-2.78	111.03	117.91
27	a2	416	PHO	CHD-C1D-ND	-2.78	119.63	124.67
23	F2	401	BCR	C38-C26-C25	-2.78	121.66	124.62
25	D1	402	CLA	O2D-CGD-O1D	-2.78	117.92	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A2	407	PHO	CHD-C1D-ND	-2.78	119.63	124.67
25	B1	616	CLA	CMB-C2B-C1B	-2.77	123.59	128.31
23	A1	401	BCR	C20-C21-C22	-2.77	123.19	127.22
23	A2	401	BCR	C38-C26-C25	-2.77	121.67	124.62
25	B1	609	CLA	O2D-CGD-O1D	-2.77	117.93	123.77
25	C2	508	CLA	O2D-CGD-O1D	-2.77	117.93	123.77
23	H2	103	BCR	C19-C18-C17	-2.77	120.70	125.83
25	C1	508	CLA	O2D-CGD-O1D	-2.77	117.94	123.77
25	a2	404	CLA	CMB-C2B-C1B	-2.77	123.60	128.31
23	k1	101	BCR	C7-C8-C9	-2.76	122.03	126.21
25	C1	514	CLA	O2D-CGD-O1D	-2.76	117.95	123.77
37	D1	409	SQD	C45-O47-C7	-2.76	112.73	117.93
25	D1	403	CLA	O2D-CGD-O1D	-2.76	117.95	123.77
23	b2	601	BCR	C27-C26-C25	-2.76	119.70	122.73
25	B1	614	CLA	O2D-CGD-O1D	-2.76	117.96	123.77
25	B2	607	CLA	CMB-C2B-C1B	-2.76	123.63	128.31
25	b1	611	CLA	CMB-C2B-C1B	-2.75	123.63	128.31
25	C2	504	CLA	O2D-CGD-O1D	-2.75	117.97	123.77
25	c2	508	CLA	CMB-C2B-C1B	-2.75	123.63	128.31
25	C2	505	CLA	O2D-CGD-O1D	-2.75	117.99	123.77
27	D2	407	PHO	O1D-CGD-CBD	-2.74	120.37	124.64
25	B1	606	CLA	O2D-CGD-O1D	-2.74	118.00	123.77
23	H2	103	BCR	C11-C10-C9	-2.74	123.24	127.22
25	A2	404	CLA	O2D-CGD-O1D	-2.74	118.00	123.77
25	b1	620	CLA	O2D-CGD-O1D	-2.74	118.01	123.77
33	d1	407	LHG	C5-O7-C7	-2.74	111.14	117.91
25	B1	617	CLA	O2D-CGD-O1D	-2.73	118.01	123.77
23	b1	601	BCR	C24-C23-C22	-2.73	122.09	126.21
25	b1	604	CLA	O2D-CGD-O1D	-2.73	118.03	123.77
25	b1	612	CLA	O2D-CGD-O1D	-2.73	118.03	123.77
25	B2	617	CLA	O2D-CGD-O1D	-2.73	118.03	123.77
23	A2	401	BCR	C20-C21-C22	-2.72	123.26	127.22
25	b2	611	CLA	O2D-CGD-O1D	-2.72	118.05	123.77
27	A1	408	PHO	C1C-C2C-C3C	-2.72	103.29	106.43
25	B2	613	CLA	O2D-CGD-O1D	-2.72	118.05	123.77
25	c2	504	CLA	O2D-CGD-O1D	-2.72	118.05	123.77
23	h1	102	BCR	C38-C26-C25	-2.72	121.73	124.62
25	c2	508	CLA	O2D-CGD-O1D	-2.71	118.06	123.77
25	C1	505	CLA	O2D-CGD-O1D	-2.71	118.06	123.77
36	d1	409	PL9	C12-C13-C14	-2.71	121.77	127.75
25	C1	506	CLA	CMB-C2B-C1B	-2.71	123.71	128.31
25	K2	101	CLA	CMB-C2B-C1B	-2.71	123.71	128.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c2	515	CLA	O2D-CGD-O1D	-2.70	118.08	123.77
23	b1	602	BCR	C38-C26-C25	-2.70	121.74	124.62
25	B1	608	CLA	CMB-C2B-C1B	-2.70	123.72	128.31
27	a2	416	PHO	C4D-ND-C1D	-2.70	102.04	106.99
29	B1	626	LMG	C8-O7-C10	-2.69	111.25	117.91
25	C1	513	CLA	O2D-CGD-O1D	-2.69	118.10	123.77
25	c1	516	CLA	O2D-CGD-O1D	-2.69	118.11	123.77
25	A2	403	CLA	O2D-CGD-O1D	-2.68	118.12	123.77
36	D2	408	PL9	C17-C18-C19	-2.68	121.83	127.75
23	b1	603	BCR	C20-C21-C22	-2.68	123.33	127.22
29	B2	620	LMG	C8-O7-C10	-2.68	111.28	117.91
25	c2	503	CLA	CMB-C2B-C1B	-2.68	123.76	128.31
25	b2	610	CLA	O2D-CGD-O1D	-2.68	118.14	123.77
34	c2	514	DGD	C2G-O2G-C1B	-2.68	111.29	117.91
25	b1	620	CLA	CMB-C2B-C1B	-2.67	123.76	128.31
25	B2	611	CLA	O2D-CGD-O1D	-2.67	118.14	123.77
25	B1	612	CLA	O2D-CGD-O1D	-2.67	118.15	123.77
23	K1	101	BCR	C20-C21-C22	-2.67	123.34	127.22
25	c2	512	CLA	O2D-CGD-O1D	-2.67	118.15	123.77
25	B1	613	CLA	O2D-CGD-O1D	-2.67	118.15	123.77
27	a1	411	PHO	C1C-C2C-C3C	-2.67	103.36	106.43
27	A1	408	PHO	C4D-ND-C1D	-2.66	102.12	106.99
25	B2	608	CLA	O2D-CGD-O1D	-2.66	118.17	123.77
25	C1	503	CLA	O2D-CGD-O1D	-2.66	118.17	123.77
25	a2	413	CLA	O2D-CGD-O1D	-2.66	118.17	123.77
25	d2	405	CLA	O2D-CGD-O1D	-2.66	118.17	123.77
25	b1	610	CLA	O2D-CGD-O1D	-2.66	118.18	123.77
23	B2	601	BCR	C27-C26-C25	-2.65	119.81	122.73
23	A1	401	BCR	C3-C4-C5	-2.65	109.47	113.87
23	b1	603	BCR	C1-C6-C5	-2.65	118.95	122.50
23	b1	602	BCR	C11-C10-C9	-2.65	123.37	127.22
25	a2	405	CLA	O2D-CGD-O1D	-2.65	118.20	123.77
27	a1	411	PHO	CHD-C1D-ND	-2.64	119.87	124.67
25	B1	605	CLA	O2D-CGD-O1D	-2.64	118.20	123.77
33	D2	405	LHG	C5-O7-C7	-2.64	111.37	117.91
25	b2	604	CLA	O2D-CGD-O1D	-2.64	118.21	123.77
25	b2	618	CLA	O2D-CGD-O1D	-2.64	118.21	123.77
27	D1	407	PHO	O1D-CGD-CBD	-2.64	120.53	124.64
25	B1	604	CLA	O2D-CGD-O1D	-2.64	118.22	123.77
29	b1	631	LMG	C8-O7-C10	-2.64	111.39	117.91
25	b2	608	CLA	O2D-CGD-O1D	-2.63	118.23	123.77
25	a1	404	CLA	O2D-CGD-O1D	-2.63	118.23	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A2	407	PHO	O1D-CGD-CBD	-2.63	120.55	124.64
25	D2	401	CLA	O2D-CGD-O1D	-2.62	118.24	123.77
27	d1	403	PHO	O2D-CGD-O1D	-2.62	118.24	123.77
25	A1	403	CLA	O2D-CGD-O1D	-2.62	118.25	123.77
23	H1	102	BCR	C17-C16-C15	-2.62	120.98	125.83
37	B2	623	SQD	C45-O47-C7	-2.62	111.43	117.91
25	C2	513	CLA	O2D-CGD-O1D	-2.62	118.26	123.77
25	b2	613	CLA	O2D-CGD-O1D	-2.61	118.27	123.77
23	h2	101	BCR	C21-C20-C19	-2.61	115.06	123.11
25	c2	511	CLA	O2D-CGD-O1D	-2.60	118.30	123.77
25	b2	609	CLA	O2D-CGD-O1D	-2.60	118.30	123.77
27	A2	407	PHO	C4D-ND-C1D	-2.60	102.23	106.99
27	D1	407	PHO	C1C-C2C-C3C	-2.60	103.43	106.43
23	C1	501	BCR	C15-C16-C17	-2.60	117.63	123.23
25	c2	507	CLA	O2D-CGD-O1D	-2.59	118.31	123.77
25	A1	405	CLA	O2D-CGD-O1D	-2.59	118.31	123.77
25	b2	616	CLA	O2D-CGD-O1D	-2.59	118.31	123.77
23	c1	502	BCR	C37-C22-C21	-2.59	119.12	122.89
27	d2	408	PHO	C4D-ND-C1D	-2.59	102.25	106.99
27	a2	416	PHO	C1C-C2C-C3C	-2.59	103.44	106.43
27	d2	408	PHO	C1C-C2C-C3C	-2.59	103.44	106.43
33	l2	101	LHG	C5-O7-C7	-2.59	111.51	117.91
25	b1	619	CLA	O2D-CGD-O1D	-2.59	118.33	123.77
25	b1	616	CLA	CMB-C2B-C1B	-2.59	123.91	128.31
23	A1	401	BCR	C24-C23-C22	-2.58	122.30	126.21
25	c2	513	CLA	O2D-CGD-O1D	-2.58	118.33	123.77
23	B2	602	BCR	C28-C27-C26	-2.58	109.59	113.87
25	b2	614	CLA	O2D-CGD-O1D	-2.58	118.33	123.77
27	d1	403	PHO	C4D-ND-C1D	-2.58	102.26	106.99
23	b1	601	BCR	C20-C21-C22	-2.58	123.47	127.22
29	a1	412	LMG	C8-O7-C10	-2.58	111.53	117.91
25	B2	606	CLA	O2D-CGD-O1D	-2.58	118.34	123.77
23	a2	402	BCR	C23-C24-C25	-2.58	119.76	127.24
25	A1	404	CLA	O2D-CGD-O1D	-2.58	118.34	123.77
23	h1	102	BCR	C10-C11-C12	-2.57	115.16	123.11
29	a2	412	LMG	C8-O7-C10	-2.57	111.56	117.91
25	c2	509	CLA	O2A-CGA-O1A	-2.56	116.79	123.51
33	L1	101	LHG	C5-O7-C7	-2.56	111.57	117.91
23	c1	502	BCR	C36-C18-C17	-2.56	119.16	122.89
23	J1	101	BCR	C7-C8-C9	-2.56	122.34	126.21
25	a2	404	CLA	OBD-CAD-CBD	-2.56	122.08	125.94
25	C2	516	CLA	O2D-CGD-O1D	-2.55	118.39	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	D1	407	PHO	C4D-ND-C1D	-2.55	102.31	106.99
25	C2	510	CLA	O2D-CGD-O1D	-2.55	118.39	123.77
23	h1	102	BCR	C3-C4-C5	-2.55	109.64	113.87
23	H2	103	BCR	C7-C8-C9	-2.55	122.36	126.21
23	A2	401	BCR	C24-C23-C22	-2.54	122.37	126.21
25	A2	402	CLA	C2C-C1C-NC	-2.54	108.48	110.22
25	b1	613	CLA	O2D-CGD-O1D	-2.54	118.42	123.77
27	D2	407	PHO	C1C-C2C-C3C	-2.54	103.50	106.43
23	D1	401	BCR	C28-C27-C26	-2.54	109.66	113.87
25	b1	615	CLA	O2D-CGD-O1D	-2.54	118.43	123.77
25	B2	610	CLA	O2D-CGD-O1D	-2.54	118.43	123.77
23	c1	501	BCR	C8-C7-C6	-2.53	119.89	127.24
23	j2	102	BCR	C37-C22-C21	-2.53	119.20	122.89
23	C1	521	BCR	C4-C5-C6	-2.53	119.95	122.73
25	c1	513	CLA	O2D-CGD-O1D	-2.53	118.44	123.77
23	J1	101	BCR	C36-C18-C17	-2.53	119.21	122.89
23	h1	102	BCR	C11-C10-C9	-2.53	123.55	127.22
25	B2	614	CLA	O2D-CGD-O1D	-2.52	118.46	123.77
29	I2	101	LMG	C8-O7-C10	-2.52	111.67	117.91
23	C2	502	BCR	C3-C4-C5	-2.52	109.69	113.87
25	B1	615	CLA	O2D-CGD-O1D	-2.52	118.47	123.77
27	d1	403	PHO	C1C-C2C-C3C	-2.52	103.53	106.43
23	a2	402	BCR	C3-C4-C5	-2.52	109.70	113.87
27	D2	407	PHO	C4D-ND-C1D	-2.52	102.38	106.99
25	C1	512	CLA	O2D-CGD-O1D	-2.52	118.47	123.77
38	V2	201	HEM	CBA-CAA-C2A	-2.51	108.07	112.49
27	a1	411	PHO	O2D-CGD-O1D	-2.51	118.48	123.77
23	a1	401	BCR	C20-C21-C22	-2.51	123.57	127.22
27	D2	407	PHO	C4-C3-C2	-2.51	118.73	123.58
25	c1	504	CLA	O2D-CGD-O1D	-2.51	118.49	123.77
23	C1	501	BCR	C21-C20-C19	-2.51	115.36	123.11
23	j2	102	BCR	C16-C17-C18	-2.50	123.58	127.22
25	B1	607	CLA	CMB-C2B-C1B	-2.50	124.06	128.31
23	a1	401	BCR	C28-C27-C26	-2.50	109.73	113.87
23	c2	501	BCR	C28-C27-C26	-2.50	109.73	113.87
23	F2	401	BCR	C30-C25-C26	-2.50	119.16	122.50
25	b2	615	CLA	O2D-CGD-O1D	-2.49	118.52	123.77
25	C2	518	CLA	CAA-C2A-C3A	-2.49	110.90	116.22
36	d2	409	PL9	C35-C34-C33	-2.49	118.76	123.58
23	J1	101	BCR	C8-C7-C6	-2.49	120.01	127.24
27	a1	411	PHO	C4D-ND-C1D	-2.49	102.43	106.99
25	c2	510	CLA	O2D-CGD-O1D	-2.49	118.53	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a2	402	BCR	C20-C21-C22	-2.49	123.60	127.22
25	a1	404	CLA	CMB-C2B-C1B	-2.49	124.08	128.31
29	B2	621	LMG	C7-O1-C1	-2.48	108.63	113.81
23	B2	603	BCR	C28-C27-C26	-2.48	109.76	113.87
27	A1	408	PHO	O2D-CGD-O1D	-2.48	118.56	123.77
27	A1	408	PHO	CHD-C1D-ND	-2.48	120.18	124.67
23	H1	102	BCR	C7-C8-C9	-2.47	122.47	126.21
25	K2	101	CLA	O2D-CGD-O1D	-2.47	118.57	123.77
29	M1	101	LMG	C8-O7-C10	-2.47	114.61	117.79
25	C1	510	CLA	O2D-CGD-O1D	-2.47	118.57	123.77
29	A2	412	LMG	C8-O7-C10	-2.47	111.81	117.91
25	A2	402	CLA	O2D-CGD-O1D	-2.47	118.58	123.77
34	h1	101	DGD	C2G-O2G-C1B	-2.46	111.82	117.91
25	b2	619	CLA	O2D-CGD-O1D	-2.46	118.58	123.77
23	K2	102	BCR	C37-C22-C21	-2.46	119.30	122.89
36	d1	409	PL9	C45-C44-C43	-2.46	118.82	123.58
23	a2	402	BCR	C24-C23-C22	-2.46	122.49	126.21
23	B1	603	BCR	C24-C23-C22	-2.46	122.50	126.21
25	c1	510	CLA	O2A-CGA-O1A	-2.46	117.07	123.51
25	b1	617	CLA	O2D-CGD-O1D	-2.45	118.61	123.77
23	b2	601	BCR	C3-C4-C5	-2.45	109.80	113.87
25	C2	511	CLA	O2A-CGA-O1A	-2.45	117.09	123.51
23	H2	103	BCR	C3-C4-C5	-2.45	109.81	113.87
29	b1	631	LMG	C7-O1-C1	-2.44	108.70	113.81
23	B1	601	BCR	C20-C21-C22	-2.44	123.67	127.22
23	B1	602	BCR	C34-C9-C10	-2.44	119.33	122.89
25	B2	612	CLA	O2D-CGD-O1D	-2.44	118.63	123.77
25	a1	403	CLA	O2D-CGD-O1D	-2.44	118.64	123.77
23	b1	603	BCR	C33-C5-C6	-2.44	122.02	124.62
23	k1	101	BCR	C37-C22-C21	-2.44	119.34	122.89
25	c1	511	CLA	O2D-CGD-O1D	-2.43	118.65	123.77
25	c1	512	CLA	O2D-CGD-O1D	-2.43	118.65	123.77
25	B2	609	CLA	O2A-CGA-O1A	-2.43	117.13	123.51
23	A1	401	BCR	C23-C24-C25	-2.43	120.18	127.24
25	C2	509	CLA	O2D-CGD-O1D	-2.43	118.66	123.77
25	c1	505	CLA	O2D-CGD-O1D	-2.43	118.66	123.77
33	D1	405	LHG	C5-O7-C7	-2.42	111.91	117.91
23	B1	601	BCR	C3-C4-C5	-2.42	109.85	113.87
23	d2	401	BCR	C16-C15-C14	-2.42	118.01	123.23
25	b2	624	CLA	O2D-CGD-O1D	-2.42	118.67	123.77
27	d2	408	PHO	C3B-C2B-C1B	-2.42	100.99	106.36
36	D2	408	PL9	C12-C13-C14	-2.42	122.42	127.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	D1	408	PL9	C42-C43-C44	-2.42	122.42	127.75
23	b2	602	BCR	C33-C5-C6	-2.41	122.05	124.62
33	B2	627	LHG	C5-O7-C7	-2.41	111.95	117.91
25	B2	615	CLA	O2D-CGD-O1D	-2.41	118.71	123.77
35	c1	517	LMT	C1B-O1B-C4'	-2.40	111.61	118.00
23	B2	602	BCR	C34-C9-C10	-2.40	119.39	122.89
34	C1	515	DGD	C2G-O2G-C1B	-2.39	111.99	117.91
23	B2	602	BCR	C3-C4-C5	-2.39	109.90	113.87
23	K1	101	BCR	C7-C6-C5	-2.39	115.82	121.36
27	a2	416	PHO	C3B-C2B-C1B	-2.39	101.07	106.36
23	A2	401	BCR	C16-C15-C14	-2.38	118.09	123.23
27	D2	407	PHO	C3B-C2B-C1B	-2.38	101.08	106.36
27	d1	403	PHO	C3B-C2B-C1B	-2.37	101.10	106.36
29	d1	408	LMG	C8-O7-C10	-2.37	112.05	117.91
23	h1	102	BCR	C7-C8-C9	-2.37	122.63	126.21
23	k1	101	BCR	C36-C18-C17	-2.37	119.45	122.89
23	h1	102	BCR	C39-C30-C25	-2.36	106.72	110.33
25	C1	511	CLA	O2D-CGD-O1D	-2.36	118.80	123.77
25	b1	609	CLA	O2A-CGA-O1A	-2.36	117.33	123.51
35	C1	519	LMT	C1B-O1B-C4'	-2.35	111.74	118.00
25	B2	604	CLA	O2D-CGD-O1D	-2.35	118.82	123.77
27	d2	408	PHO	O1D-CGD-CBD	-2.35	120.99	124.64
33	b1	622	LHG	C5-O7-C7	-2.34	112.12	117.91
23	B2	601	BCR	C38-C26-C25	-2.33	122.14	124.62
25	a2	413	CLA	O2A-CGA-O1A	-2.33	117.39	123.51
27	D1	407	PHO	C3B-C2B-C1B	-2.33	101.19	106.36
23	d2	401	BCR	C8-C7-C6	-2.33	120.48	127.24
23	B1	602	BCR	C27-C26-C25	-2.32	120.18	122.73
25	A2	404	CLA	O2A-CGA-O1A	-2.32	117.43	123.51
35	m2	103	LMT	C1B-O5B-C5B	-2.32	109.19	113.74
23	a2	402	BCR	C21-C20-C19	-2.32	115.95	123.11
29	F2	402	LMG	C8-O7-C10	-2.32	112.18	117.91
23	K2	102	BCR	C7-C8-C9	-2.31	122.71	126.21
23	d1	405	BCR	C20-C21-C22	-2.31	123.86	127.22
23	B2	601	BCR	C3-C4-C5	-2.31	110.04	113.87
27	a1	411	PHO	C3B-C2B-C1B	-2.31	101.23	106.36
27	A2	407	PHO	C3B-C2B-C1B	-2.30	101.25	106.36
36	D2	408	PL9	C45-C44-C43	-2.30	119.13	123.58
23	c2	501	BCR	C4-C5-C6	-2.30	120.20	122.73
29	C2	515	LMG	C8-O7-C10	-2.30	112.23	117.91
25	c1	515	CLA	O2A-CGA-O1A	-2.29	117.50	123.51
33	d2	403	LHG	C5-O7-C7	-2.29	112.25	117.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A1	412	LMG	C8-O7-C10	-2.29	112.25	117.91
23	B1	602	BCR	C1-C6-C5	-2.29	119.44	122.50
25	a2	404	CLA	O2D-CGD-O1D	-2.28	118.96	123.77
27	A1	408	PHO	C3B-C2B-C1B	-2.28	101.30	106.36
27	d2	408	PHO	C6-C5-C3	-2.28	108.67	112.76
36	D1	408	PL9	C40-C39-C38	-2.28	119.17	123.58
25	b1	615	CLA	O2A-CGA-O1A	-2.28	117.54	123.51
23	z2	101	BCR	C28-C27-C26	-2.28	110.09	113.87
23	h2	101	BCR	C23-C24-C25	-2.27	120.64	127.24
23	J1	101	BCR	C37-C22-C21	-2.27	119.58	122.89
23	D1	401	BCR	C16-C15-C14	-2.27	118.33	123.23
27	D1	407	PHO	C6-C5-C3	-2.27	108.70	112.76
25	a1	405	CLA	C1-C2-C3	-2.26	122.78	126.64
23	D1	401	BCR	C21-C20-C19	-2.26	116.12	123.11
25	b1	611	CLA	O2D-CGD-O1D	-2.26	119.00	123.77
23	H2	103	BCR	C16-C17-C18	-2.25	120.73	125.07
29	d1	411	LMG	C8-O7-C10	-2.25	112.34	117.91
23	B2	603	BCR	C3-C4-C5	-2.25	110.14	113.87
23	H1	102	BCR	C11-C10-C9	-2.25	123.95	127.22
23	C1	501	BCR	C23-C24-C25	-2.24	120.73	127.24
23	b1	602	BCR	C27-C26-C25	-2.24	120.27	122.73
25	A1	406	CLA	O2A-CGA-O1A	-2.24	117.65	123.51
23	b2	601	BCR	C23-C24-C25	-2.23	120.76	127.24
23	k1	101	BCR	C8-C7-C6	-2.23	120.76	127.24
25	d1	401	CLA	O2A-CGA-O1A	-2.23	117.66	123.51
23	a1	401	BCR	C23-C24-C25	-2.23	120.78	127.24
23	j2	102	BCR	C36-C18-C17	-2.23	119.65	122.89
38	V1	201	HEM	CAD-CBD-CGD	-2.23	108.45	112.78
23	C2	502	BCR	C28-C27-C26	-2.22	110.19	113.87
23	K2	104	BCR	C38-C26-C25	-2.22	122.26	124.62
34	H1	101	DGD	C2G-O2G-C1B	-2.22	112.43	117.91
25	B1	617	CLA	O2A-CGA-O1A	-2.22	117.70	123.51
25	b1	616	CLA	O2A-CGA-O1A	-2.22	117.70	123.51
25	B2	614	CLA	O2A-CGA-O1A	-2.22	117.70	123.51
23	H1	102	BCR	C3-C4-C5	-2.22	110.20	113.87
25	c1	508	CLA	C1-C2-C3	-2.21	122.87	126.64
29	D1	406	LMG	C8-O7-C10	-2.21	112.44	117.91
35	a2	406	LMT	C1B-O1B-C4'	-2.21	112.12	118.00
33	D1	404	LHG	C5-O7-C7	-2.21	112.44	117.91
23	h1	102	BCR	C27-C26-C25	-2.21	120.31	122.73
33	d2	406	LHG	C5-O7-C7	-2.20	112.46	117.91
27	A1	408	PHO	O1D-CGD-CBD	-2.20	121.21	124.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	C1	517	DGD	C2G-O2G-C1B	-2.20	112.46	117.91
25	B1	606	CLA	O2A-CGA-O1A	-2.20	117.74	123.51
25	C1	504	CLA	O2D-CGD-O1D	-2.20	119.13	123.77
25	b1	606	CLA	O2A-CGA-O1A	-2.20	117.75	123.51
29	b2	622	LMG	C8-O7-C10	-2.20	112.48	117.91
23	b2	602	BCR	C37-C22-C21	-2.20	119.69	122.89
36	d2	409	PL9	C42-C43-C44	-2.20	122.91	127.75
23	B2	602	BCR	C23-C24-C25	-2.19	120.88	127.24
23	J1	101	BCR	C28-C27-C26	-2.19	110.24	113.87
38	V2	201	HEM	CAD-CBD-CGD	-2.19	108.53	112.78
23	K2	102	BCR	C4-C5-C6	-2.18	120.33	122.73
27	d1	403	PHO	CBA-CAA-C2A	-2.18	108.33	113.96
25	B2	607	CLA	O2A-CGA-O1A	-2.18	117.80	123.51
27	a1	411	PHO	O1D-CGD-CBD	-2.18	121.25	124.64
23	k2	501	BCR	C8-C7-C6	-2.18	120.92	127.24
25	b2	616	CLA	O2A-CGA-O1A	-2.17	117.81	123.51
25	A1	404	CLA	O2A-CGA-O1A	-2.17	117.81	123.51
23	d1	405	BCR	C16-C15-C14	-2.17	118.55	123.23
25	b1	610	CLA	O2A-CGA-O1A	-2.17	117.82	123.51
23	c1	502	BCR	C16-C17-C18	-2.17	124.06	127.22
25	B2	616	CLA	O2A-CGA-O1A	-2.17	117.83	123.51
23	h2	101	BCR	C28-C27-C26	-2.17	110.28	113.87
23	j2	102	BCR	C8-C7-C6	-2.16	120.96	127.24
27	a1	411	PHO	CBA-CAA-C2A	-2.16	108.38	113.96
25	a1	405	CLA	O2A-CGA-O1A	-2.16	117.85	123.51
25	C2	508	CLA	C1-C2-C3	-2.16	122.96	126.64
23	C1	521	BCR	C28-C27-C26	-2.16	110.29	113.87
27	D1	407	PHO	O2D-CGD-O1D	-2.16	119.23	123.77
25	c1	509	CLA	O2D-CGD-O1D	-2.15	119.23	123.77
25	C1	504	CLA	O2A-CGA-O1A	-2.15	117.86	123.51
25	d2	404	CLA	C1-C2-C3	-2.15	122.97	126.64
23	b1	602	BCR	C39-C30-C25	-2.15	107.05	110.33
23	C1	521	BCR	C15-C16-C17	-2.14	118.61	123.23
23	A2	401	BCR	C3-C4-C5	-2.14	110.32	113.87
25	b2	615	CLA	O2A-CGA-O1A	-2.14	117.91	123.51
23	a1	401	BCR	C21-C20-C19	-2.13	116.52	123.11
23	j2	102	BCR	C27-C26-C25	-2.13	120.39	122.73
23	F2	401	BCR	C3-C4-C5	-2.13	110.33	113.87
25	C1	503	CLA	OBD-CAD-CBD	-2.13	122.72	125.94
23	d1	405	BCR	C3-C4-C5	-2.13	110.34	113.87
25	a2	413	CLA	C1-C2-C3	-2.13	123.01	126.64
25	c2	503	CLA	OBD-CAD-CBD	-2.13	122.72	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C1	521	BCR	C8-C7-C6	-2.13	121.07	127.24
23	k1	101	BCR	C28-C27-C26	-2.13	110.34	113.87
23	D1	401	BCR	C3-C4-C5	-2.12	110.35	113.87
25	b2	618	CLA	O2A-CGA-O1A	-2.12	117.96	123.51
25	C1	506	CLA	O2A-CGA-O1A	-2.12	117.96	123.51
25	B2	615	CLA	O2A-CGA-O1A	-2.11	117.97	123.51
23	j2	102	BCR	C7-C8-C9	-2.11	123.02	126.21
25	B2	611	CLA	O2A-CGA-O1A	-2.11	117.97	123.51
23	h1	102	BCR	C16-C15-C14	-2.11	118.68	123.23
25	B1	607	CLA	O2A-CGA-O1A	-2.11	117.98	123.51
33	B1	621	LHG	C5-O7-C7	-2.11	112.69	117.91
27	A1	408	PHO	CHD-C4C-NC	-2.11	120.95	124.89
23	K2	104	BCR	C8-C7-C6	-2.11	121.12	127.24
25	c1	505	CLA	O2A-CGA-O1A	-2.11	117.99	123.51
27	d2	408	PHO	CHD-C4C-NC	-2.10	120.96	124.89
23	K2	102	BCR	C28-C27-C26	-2.10	110.38	113.87
25	B1	616	CLA	O2A-CGA-O1A	-2.10	118.00	123.51
23	K2	102	BCR	C8-C7-C6	-2.10	121.14	127.24
25	b2	624	CLA	O2A-CGA-O1A	-2.10	118.00	123.51
25	B1	615	CLA	O2A-CGA-O1A	-2.10	118.00	123.51
23	H2	103	BCR	C10-C11-C12	-2.10	116.62	123.11
25	A1	403	CLA	O2A-CGA-O1A	-2.10	118.01	123.51
34	c1	514	DGD	C1E-O6E-C5E	-2.10	109.63	113.74
33	b1	622	LHG	O8-C23-O10	-2.10	118.02	123.51
36	D1	408	PL9	C35-C34-C33	-2.09	119.53	123.58
25	A1	403	CLA	C2C-C1C-NC	-2.09	108.79	110.22
23	b2	602	BCR	C10-C11-C12	-2.09	116.64	123.11
25	B1	609	CLA	O2A-CGA-O1A	-2.09	118.02	123.51
27	A2	407	PHO	O2D-CGD-O1D	-2.09	119.37	123.77
23	B2	602	BCR	C33-C5-C6	-2.09	122.39	124.62
25	a2	404	CLA	O2A-CGA-O1A	-2.09	118.03	123.51
25	d1	404	CLA	OBD-CAD-CBD	-2.08	122.79	125.94
23	B1	603	BCR	C3-C4-C5	-2.08	110.42	113.87
25	c1	508	CLA	O2A-CGA-O1A	-2.08	118.05	123.51
25	b1	610	CLA	OBD-CAD-CBD	-2.08	122.80	125.94
25	b2	606	CLA	O2A-CGA-O1A	-2.08	118.06	123.51
25	a1	403	CLA	OBD-CAD-CBD	-2.08	122.80	125.94
23	d1	405	BCR	C40-C30-C25	-2.08	107.16	110.33
23	d1	405	BCR	C21-C20-C19	-2.08	116.69	123.11
23	K1	101	BCR	C35-C13-C14	-2.08	119.86	122.89
23	B1	601	BCR	C21-C20-C19	-2.08	116.69	123.11
23	C1	501	BCR	C20-C21-C22	-2.07	124.21	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b2	603	BCR	C3-C4-C5	-2.07	110.44	113.87
36	d2	409	PL9	C40-C39-C38	-2.07	119.58	123.58
23	h1	102	BCR	C36-C18-C17	-2.07	119.88	122.89
27	D2	407	PHO	O2D-CGD-O1D	-2.07	119.42	123.77
29	C1	520	LMG	C8-O7-C10	-2.06	112.81	117.91
25	b2	609	CLA	O2A-CGA-O1A	-2.06	118.10	123.51
27	D2	407	PHO	CHD-C4C-NC	-2.06	121.04	124.89
37	D2	402	SQD	C1-C2-C3	-2.06	105.89	109.98
25	b1	604	CLA	O2A-CGA-O1A	-2.06	118.11	123.51
33	b2	625	LHG	C5-O7-C7	-2.06	112.82	117.91
29	a2	412	LMG	C7-O1-C1	-2.06	109.52	113.81
23	c1	502	BCR	C19-C18-C17	-2.05	115.64	118.95
23	h1	102	BCR	C8-C7-C6	-2.05	121.28	127.24
25	C2	518	CLA	CMA-C3A-C2A	-2.05	111.84	116.22
23	h2	101	BCR	C8-C7-C6	-2.05	121.29	127.24
23	b2	603	BCR	C34-C9-C10	-2.05	119.91	122.89
23	B1	602	BCR	C4-C5-C6	-2.05	120.48	122.73
25	A2	402	CLA	O2A-CGA-O1A	-2.05	118.14	123.51
35	l1	101	LMT	C1-O1'-C1'	-2.04	110.43	114.00
25	b1	611	CLA	O2A-CGA-O1A	-2.04	118.16	123.51
25	b1	607	CLA	O2A-CGA-O1A	-2.04	118.16	123.51
25	b1	619	CLA	O2A-CGA-O1A	-2.04	118.17	123.51
25	D2	406	CLA	OBD-CAD-CBD	-2.04	122.86	125.94
33	D2	403	LHG	C5-O7-C7	-2.03	112.88	117.91
25	a2	405	CLA	O2A-CGA-O1A	-2.03	118.18	123.51
27	d2	408	PHO	O2D-CGD-O1D	-2.03	119.49	123.77
23	k2	501	BCR	C11-C12-C13	-2.03	120.38	126.34
33	a1	407	LHG	O8-C23-O10	-2.03	118.19	123.51
25	b2	610	CLA	O2A-CGA-O1A	-2.03	118.19	123.51
25	C1	512	CLA	O2A-CGA-O1A	-2.03	118.19	123.51
25	b1	607	CLA	CAA-CBA-CGA	-2.02	107.42	113.28
25	B2	617	CLA	O2A-CGA-O1A	-2.02	118.20	123.51
25	C1	507	CLA	O2A-CGA-O1A	-2.02	118.20	123.51
23	h2	101	BCR	C15-C16-C17	-2.02	118.87	123.23
25	b2	608	CLA	O2A-CGA-O1A	-2.02	118.21	123.51
25	b2	612	CLA	C4B-CHC-C1C	-2.02	125.33	129.34
25	c1	503	CLA	O2A-CGA-O1A	-2.02	118.22	123.51
23	F2	401	BCR	C23-C24-C25	-2.01	121.39	127.24
23	b2	601	BCR	C15-C16-C17	-2.01	118.90	123.23
25	c1	510	CLA	OBD-CAD-CBD	-2.01	122.90	125.94
34	c2	516	DGD	C2G-O2G-C1B	-2.01	112.94	117.91
23	b1	601	BCR	C39-C30-C25	-2.01	107.26	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B2	612	CLA	O2A-CGA-O1A	-2.01	118.25	123.51
23	B2	601	BCR	C15-C16-C17	-2.01	118.90	123.23
23	B1	601	BCR	C39-C30-C25	-2.01	107.27	110.33
25	C2	505	CLA	O2A-CGA-O1A	-2.01	118.25	123.51
25	b1	612	CLA	O2A-CGA-O1A	-2.01	118.25	123.51
25	D2	401	CLA	O2A-CGA-O1A	-2.01	118.25	123.51
36	d1	409	PL9	C12-C11-C9	-2.01	105.98	112.61
37	D1	409	SQD	O48-C23-O10	-2.01	118.25	123.51
23	j2	102	BCR	C10-C11-C12	-2.00	116.92	123.11
33	l2	101	LHG	O8-C23-O10	-2.00	118.26	123.51
23	F2	401	BCR	C15-C16-C17	-2.00	118.91	123.23
23	B2	601	BCR	C39-C30-C25	-2.00	107.27	110.33
25	B2	610	CLA	O2A-CGA-O1A	-2.00	118.26	123.51
25	C1	509	CLA	CAA-C2A-C3A	-2.00	107.35	112.79
25	d2	405	CLA	O2A-CGA-O1A	-2.00	118.27	123.51
27	a1	411	PHO	CMC-C2C-C1C	2.00	128.26	125.06
34	C1	515	DGD	O5D-C1E-C2E	2.00	110.46	108.00
25	C2	507	CLA	O1D-CGD-CBD	2.00	127.75	124.64
25	C2	506	CLA	O1D-CGD-CBD	2.01	127.76	124.64
25	B2	609	CLA	O1D-CGD-CBD	2.01	127.76	124.64
25	c2	511	CLA	CMD-C2D-C3D	2.01	129.01	125.09
29	F2	402	LMG	C9-O8-C28	2.01	122.98	117.00
25	c1	515	CLA	O1D-CGD-CBD	2.01	127.76	124.64
25	C2	504	CLA	O1D-CGD-CBD	2.01	127.76	124.64
25	C2	516	CLA	CMD-C2D-C3D	2.01	129.02	125.09
25	a1	404	CLA	O1D-CGD-CBD	2.01	127.77	124.64
25	b1	614	CLA	C2A-C3A-C4A	2.01	103.90	101.84
25	C2	510	CLA	O1D-CGD-CBD	2.01	127.77	124.64
36	d1	409	PL9	C51-C49-C50	2.01	119.50	114.61
25	b2	612	CLA	O1D-CGD-CBD	2.02	127.77	124.64
25	B1	619	CLA	O1D-CGD-CBD	2.02	127.77	124.64
25	c2	515	CLA	O2D-CGD-CBD	2.02	114.13	111.22
25	c1	505	CLA	O2D-CGD-CBD	2.02	114.13	111.22
25	b1	617	CLA	O2D-CGD-CBD	2.02	114.13	111.22
34	c2	514	DGD	O6D-C5D-C6D	2.02	110.79	106.61
25	c1	512	CLA	CMD-C2D-C3D	2.02	129.04	125.09
25	b1	608	CLA	CMD-C2D-C3D	2.02	129.05	125.09
23	a2	402	BCR	C2-C1-C6	2.03	113.49	110.48
25	c1	513	CLA	O1D-CGD-CBD	2.03	127.79	124.64
25	b1	620	CLA	C4-C3-C5	2.03	118.46	115.37
25	C2	503	CLA	CMD-C2D-C3D	2.03	129.06	125.09
25	c2	515	CLA	O1D-CGD-CBD	2.03	127.80	124.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C1	507	CLA	O2D-CGD-CBD	2.03	114.15	111.22
25	c1	503	CLA	CMD-C2D-C3D	2.03	129.06	125.09
25	b2	606	CLA	O2D-CGD-CBD	2.03	114.15	111.22
27	a2	416	PHO	CED-O2D-CGD	2.03	120.80	115.97
23	C1	521	BCR	C38-C26-C27	2.04	117.42	113.47
25	c1	509	CLA	C2A-C1A-CHA	2.04	127.08	123.80
29	j2	101	LMG	O1-C1-C2	2.04	110.51	108.00
25	C1	506	CLA	C4-C3-C5	2.04	118.48	115.37
25	C2	508	CLA	O1D-CGD-CBD	2.04	127.82	124.64
25	B1	605	CLA	CMD-C2D-C3D	2.04	129.09	125.09
25	c1	508	CLA	O2D-CGD-CBD	2.04	114.17	111.22
23	D1	401	BCR	C38-C26-C27	2.05	117.43	113.47
25	b2	615	CLA	O1D-CGD-CBD	2.05	127.82	124.64
25	C2	509	CLA	C2A-C1A-CHA	2.05	127.10	123.80
25	c2	515	CLA	CMD-C2D-C3D	2.05	129.10	125.09
25	D2	404	CLA	O1D-CGD-CBD	2.05	127.83	124.64
25	b2	613	CLA	O2D-CGD-CBD	2.05	114.17	111.22
37	D2	402	SQD	O8-S-C6	2.05	109.25	104.99
25	b1	620	CLA	C6-C5-C3	2.05	116.44	112.76
25	A1	403	CLA	O1D-CGD-CBD	2.05	127.83	124.64
25	a2	404	CLA	C4A-NA-C1A	2.05	108.98	106.38
25	B2	617	CLA	CMD-C2D-C3D	2.05	129.10	125.09
25	d1	404	CLA	CMD-C2D-C3D	2.05	129.10	125.09
25	C1	513	CLA	O1D-CGD-CBD	2.05	127.83	124.64
25	c1	504	CLA	O1D-CGD-CBD	2.05	127.83	124.64
25	B1	604	CLA	CMD-C2D-C3D	2.06	129.11	125.09
25	B1	604	CLA	O2D-CGD-CBD	2.06	114.18	111.22
36	d1	409	PL9	C35-C34-C36	2.06	118.50	115.37
25	b2	619	CLA	CMD-C2D-C3D	2.06	129.11	125.09
25	a1	404	CLA	C4A-NA-C1A	2.06	108.99	106.38
27	a2	416	PHO	O2A-CGA-CBA	2.06	118.19	111.85
25	C1	512	CLA	C2A-C3A-C4A	2.06	103.95	101.84
25	b2	613	CLA	CMD-C2D-C3D	2.06	129.12	125.09
25	C1	514	CLA	O1D-CGD-CBD	2.06	127.84	124.64
36	D1	408	PL9	C35-C34-C36	2.06	118.51	115.37
25	C1	512	CLA	CMD-C2D-C3D	2.06	129.12	125.09
25	b1	615	CLA	O1D-CGD-CBD	2.06	127.85	124.64
23	C1	501	BCR	C2-C1-C6	2.07	113.55	110.48
25	b2	604	CLA	O1D-CGD-CBD	2.07	127.85	124.64
25	d2	402	CLA	CMD-C2D-C3D	2.07	129.13	125.09
25	C2	513	CLA	CMD-C2D-C3D	2.07	129.14	125.09
23	D1	401	BCR	C33-C5-C4	2.07	117.47	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d2	405	CLA	CMD-C2D-C3D	2.07	129.14	125.09
25	c2	511	CLA	O1D-CGD-CBD	2.07	127.86	124.64
25	C1	514	CLA	O2D-CGD-CBD	2.07	114.20	111.22
25	d1	406	CLA	CMD-C2D-C3D	2.07	129.14	125.09
25	b1	616	CLA	O2D-CGD-CBD	2.07	114.21	111.22
25	c2	503	CLA	O1D-CGD-CBD	2.07	127.86	124.64
25	C1	514	CLA	CMD-C2D-C3D	2.07	129.15	125.09
25	c2	502	CLA	CMD-C2D-C3D	2.08	129.15	125.09
25	b2	611	CLA	CMD-C2D-C3D	2.08	129.15	125.09
34	H2	101	DGD	O6D-C5D-C6D	2.08	110.90	106.61
25	A1	405	CLA	C4A-NA-C1A	2.08	109.01	106.38
25	B2	616	CLA	O1D-CGD-CBD	2.08	127.87	124.64
25	A2	403	CLA	O2D-CGD-CBD	2.08	114.22	111.22
25	B2	618	CLA	CMB-C2B-C3B	2.08	129.16	125.09
25	b1	614	CLA	CMD-C2D-C3D	2.08	129.16	125.09
25	B1	616	CLA	O2D-CGD-CBD	2.09	114.22	111.22
25	B1	614	CLA	C2A-C3A-C4A	2.09	103.97	101.84
25	B1	608	CLA	CMD-C2D-C3D	2.09	129.17	125.09
25	B2	607	CLA	CMD-C2D-C3D	2.09	129.18	125.09
23	B2	603	BCR	C33-C5-C4	2.09	117.52	113.47
25	c2	503	CLA	C2A-C1A-CHA	2.09	127.17	123.80
25	C2	507	CLA	CMD-C2D-C3D	2.10	129.19	125.09
25	C1	510	CLA	C2A-C3A-C4A	2.10	103.99	101.84
23	A1	401	BCR	C33-C5-C4	2.10	117.53	113.47
25	B2	607	CLA	CGD-CBD-CHA	2.10	118.08	110.88
25	B2	607	CLA	CMB-C2B-C3B	2.10	129.19	125.09
25	C2	508	CLA	O2D-CGD-CBD	2.10	114.25	111.22
25	b2	620	CLA	CMD-C2D-C3D	2.10	129.20	125.09
25	b1	610	CLA	CMD-C2D-C3D	2.10	129.20	125.09
25	b1	615	CLA	CMD-C2D-C3D	2.11	129.21	125.09
25	B1	605	CLA	O2D-CGD-CBD	2.11	114.26	111.22
25	C1	505	CLA	CMD-C2D-C3D	2.11	129.21	125.09
25	b2	606	CLA	O1D-CGD-CBD	2.11	127.92	124.64
25	c2	510	CLA	C2A-C3A-C4A	2.11	104.00	101.84
25	B1	617	CLA	CMD-C2D-C3D	2.11	129.21	125.09
25	C2	504	CLA	O2D-CGD-CBD	2.11	114.26	111.22
25	B1	610	CLA	O1D-CGD-CBD	2.11	127.92	124.64
23	c1	502	BCR	C20-C19-C18	2.11	132.53	126.34
25	b1	607	CLA	CMB-C2B-C3B	2.11	129.22	125.09
25	B2	604	CLA	CMD-C2D-C3D	2.11	129.22	125.09
25	C2	509	CLA	CMD-C2D-C3D	2.11	129.22	125.09
25	B1	616	CLA	O1D-CGD-CBD	2.11	127.92	124.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b2	615	CLA	CMD-C2D-C3D	2.12	129.23	125.09
25	C2	511	CLA	CMD-C2D-C3D	2.12	129.23	125.09
25	b2	610	CLA	CMD-C2D-C3D	2.12	129.24	125.09
27	D1	407	PHO	CMB-C2B-C1B	2.12	128.45	125.06
25	c2	503	CLA	O2D-CGD-CBD	2.12	114.28	111.22
25	b1	613	CLA	O2D-CGD-CBD	2.12	114.28	111.22
25	b2	610	CLA	O1D-CGD-CBD	2.12	127.94	124.64
25	b1	608	CLA	O2D-CGD-CBD	2.12	114.28	111.22
36	d2	409	PL9	C51-C49-C50	2.13	119.78	114.61
25	b2	611	CLA	O1D-CGD-CBD	2.13	127.95	124.64
25	c2	513	CLA	O1D-CGD-CBD	2.13	127.95	124.64
23	K1	101	BCR	C1-C6-C7	2.13	122.04	115.96
25	c2	510	CLA	CMB-C2B-C3B	2.13	129.26	125.09
25	c1	509	CLA	CMD-C2D-C3D	2.13	129.26	125.09
25	A2	403	CLA	CMD-C2D-C3D	2.13	129.26	125.09
25	A2	404	CLA	CMB-C2B-C3B	2.13	129.26	125.09
25	B1	608	CLA	O2D-CGD-CBD	2.13	114.30	111.22
25	C1	505	CLA	O1D-CGD-CBD	2.13	127.96	124.64
25	b1	604	CLA	O2D-CGD-CBD	2.13	114.30	111.22
25	B1	612	CLA	CMD-C2D-C3D	2.14	129.26	125.09
25	B2	610	CLA	CMD-C2D-C3D	2.14	129.27	125.09
25	b1	619	CLA	O1D-CGD-CBD	2.14	127.96	124.64
23	B1	601	BCR	C33-C5-C4	2.14	117.60	113.47
25	B2	611	CLA	CMD-C2D-C3D	2.14	129.27	125.09
25	C1	510	CLA	O1D-CGD-CBD	2.14	127.97	124.64
25	A2	403	CLA	CMB-C2B-C3B	2.14	129.28	125.09
25	b2	612	CLA	CMB-C2B-C3B	2.14	129.28	125.09
25	D1	402	CLA	CMD-C2D-C3D	2.14	129.28	125.09
25	B1	611	CLA	CMD-C2D-C3D	2.14	129.28	125.09
34	c1	514	DGD	O3G-C1D-C2D	2.14	110.64	108.00
25	b1	605	CLA	O2D-CGD-CBD	2.14	114.31	111.22
29	F2	402	LMG	O8-C28-C29	2.14	118.45	111.85
25	C2	508	CLA	CMD-C2D-C3D	2.15	129.28	125.09
25	C1	504	CLA	CMD-C2D-C3D	2.15	129.28	125.09
25	B2	614	CLA	C2A-C3A-C4A	2.15	104.04	101.84
25	b2	614	CLA	C2A-C3A-C4A	2.15	104.04	101.84
25	C2	513	CLA	O1D-CGD-CBD	2.15	127.98	124.64
25	b1	606	CLA	CMD-C2D-C3D	2.15	129.29	125.09
36	d1	409	PL9	C10-C9-C11	2.15	118.65	115.37
25	A1	403	CLA	C4A-NA-C1A	2.15	109.11	106.38
25	C1	508	CLA	CMD-C2D-C3D	2.15	129.29	125.09
25	b1	620	CLA	CMB-C2B-C3B	2.15	129.30	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C2	502	BCR	C33-C5-C4	2.15	117.63	113.47
25	C2	510	CLA	CMD-C2D-C3D	2.15	129.30	125.09
25	C1	507	CLA	O1D-CGD-CBD	2.16	127.99	124.64
25	C1	502	CLA	CMD-C2D-C3D	2.16	129.31	125.09
25	b2	614	CLA	O1D-CGD-CBD	2.17	128.01	124.64
25	b1	616	CLA	CMD-C2D-C3D	2.17	129.33	125.09
25	a2	413	CLA	C4A-NA-C1A	2.17	109.13	106.38
25	b2	624	CLA	CMD-C2D-C3D	2.17	129.33	125.09
25	C2	506	CLA	O2D-CGD-CBD	2.17	114.35	111.22
25	B1	608	CLA	O1D-CGD-CBD	2.17	128.02	124.64
25	c2	503	CLA	CMB-C2B-C3B	2.17	129.34	125.09
25	a2	405	CLA	O2D-CGD-CBD	2.18	114.36	111.22
25	b2	604	CLA	CMD-C2D-C3D	2.18	129.34	125.09
25	b1	604	CLA	CMD-C2D-C3D	2.18	129.34	125.09
25	D2	401	CLA	CMD-C2D-C3D	2.18	129.35	125.09
25	b2	616	CLA	CMB-C2B-C3B	2.18	129.35	125.09
23	C1	501	BCR	C33-C5-C4	2.18	117.68	113.47
23	K2	102	BCR	C38-C26-C27	2.18	117.68	113.47
25	c2	506	CLA	CMD-C2D-C3D	2.18	129.35	125.09
25	a1	404	CLA	CAC-C3C-C4C	2.18	128.04	124.82
25	b1	613	CLA	CMB-C2B-C3B	2.18	129.35	125.09
25	d2	404	CLA	CMD-C2D-C3D	2.18	129.35	125.09
25	A2	402	CLA	CMD-C2D-C3D	2.18	129.35	125.09
23	b1	601	BCR	C33-C5-C4	2.18	117.69	113.47
25	B2	605	CLA	CMD-C2D-C3D	2.18	129.36	125.09
25	c2	513	CLA	CMD-C2D-C3D	2.18	129.36	125.09
25	b1	606	CLA	O1D-CGD-CBD	2.19	128.04	124.64
25	c2	508	CLA	CMD-C2D-C3D	2.19	129.37	125.09
29	d2	407	LMG	O8-C28-C29	2.19	118.58	111.85
25	B1	606	CLA	O1D-CGD-CBD	2.19	128.04	124.64
23	a1	401	BCR	C38-C26-C27	2.19	117.71	113.47
25	B1	610	CLA	C4A-NA-C1A	2.19	109.16	106.38
29	b1	624	LMG	O8-C28-C29	2.20	118.61	111.85
25	C1	507	CLA	CMD-C2D-C3D	2.20	129.38	125.09
25	b1	616	CLA	CMB-C2B-C3B	2.20	129.38	125.09
23	b2	603	BCR	C38-C26-C27	2.20	117.73	113.47
25	c1	505	CLA	CMD-C2D-C3D	2.20	129.39	125.09
25	D1	403	CLA	CMD-C2D-C3D	2.20	129.40	125.09
25	b1	616	CLA	O1D-CGD-CBD	2.20	128.06	124.64
25	A2	402	CLA	C4A-NA-C1A	2.20	109.17	106.38
25	b1	609	CLA	CMD-C2D-C3D	2.20	129.40	125.09
25	C2	505	CLA	CMD-C2D-C3D	2.20	129.40	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b1	605	CLA	CMD-C2D-C3D	2.20	129.40	125.09
25	b1	614	CLA	O2D-CGD-CBD	2.21	114.40	111.22
25	A2	402	CLA	CMB-C2B-C3B	2.21	129.41	125.09
25	b2	619	CLA	CMB-C2B-C3B	2.21	129.41	125.09
25	c2	512	CLA	O1D-CGD-CBD	2.21	128.08	124.64
25	b2	618	CLA	CMD-C2D-C3D	2.21	129.42	125.09
34	c1	518	DGD	O6D-C5D-C6D	2.21	111.19	106.61
36	d2	409	PL9	C45-C44-C46	2.21	118.74	115.37
25	a2	413	CLA	O2D-CGD-CBD	2.22	114.41	111.22
25	c2	508	CLA	O1D-CGD-CBD	2.22	128.08	124.64
23	B2	602	BCR	C2-C1-C6	2.22	113.78	110.48
25	B1	614	CLA	CMD-C2D-C3D	2.22	129.43	125.09
25	C1	507	CLA	C4A-NA-C1A	2.22	109.19	106.38
23	B2	601	BCR	C33-C5-C4	2.22	117.77	113.47
25	c1	511	CLA	C2A-C3A-C4A	2.22	104.12	101.84
25	B1	609	CLA	CMD-C2D-C3D	2.22	129.44	125.09
27	a2	416	PHO	CAC-C3C-C4C	2.23	127.78	125.21
25	D2	404	CLA	CMD-C2D-C3D	2.23	129.44	125.09
25	C1	506	CLA	CMB-C2B-C3B	2.23	129.44	125.09
25	B1	616	CLA	CMB-C2B-C3B	2.23	129.44	125.09
23	B1	602	BCR	C29-C30-C25	2.23	113.79	110.48
25	B1	612	CLA	O1D-CGD-CBD	2.23	128.10	124.64
23	F2	401	BCR	C33-C5-C4	2.23	117.78	113.47
25	C2	506	CLA	CMD-C2D-C3D	2.23	129.45	125.09
25	c2	504	CLA	CMD-C2D-C3D	2.23	129.45	125.09
25	c1	516	CLA	O2D-CGD-CBD	2.23	114.44	111.22
25	A1	406	CLA	CMD-C2D-C3D	2.23	129.46	125.09
25	K2	101	CLA	CMB-C2B-C3B	2.23	129.46	125.09
23	B2	602	BCR	C38-C26-C27	2.24	117.80	113.47
34	C1	517	DGD	O1G-C1A-C2A	2.24	118.74	111.85
25	C1	503	CLA	CMD-C2D-C3D	2.24	129.47	125.09
25	C1	503	CLA	O1D-CGD-CBD	2.24	128.12	124.64
25	c2	509	CLA	CMD-C2D-C3D	2.24	129.47	125.09
36	d2	409	PL9	C35-C34-C36	2.24	118.79	115.37
27	a2	416	PHO	CMB-C2B-C1B	2.25	128.65	125.06
25	b1	613	CLA	C4A-NA-C1A	2.25	109.23	106.38
25	C1	508	CLA	O2D-CGD-CBD	2.25	114.46	111.22
25	b2	609	CLA	CMD-C2D-C3D	2.25	129.49	125.09
25	B1	618	CLA	CMD-C2D-C3D	2.25	129.49	125.09
25	b2	614	CLA	CMD-C2D-C3D	2.25	129.49	125.09
25	A2	403	CLA	C4A-NA-C1A	2.25	109.23	106.38
23	J1	101	BCR	C38-C26-C27	2.25	117.82	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c1	515	CLA	CMD-C2D-C3D	2.25	129.49	125.09
25	c1	507	CLA	CMD-C2D-C3D	2.25	129.49	125.09
25	B2	614	CLA	O1D-CGD-CBD	2.25	128.14	124.64
25	A1	405	CLA	CAC-C3C-C4C	2.25	128.15	124.82
25	c2	510	CLA	O1D-CGD-CBD	2.25	128.14	124.64
25	b1	619	CLA	CMD-C2D-C3D	2.25	129.50	125.09
25	B1	615	CLA	CMD-C2D-C3D	2.25	129.50	125.09
34	h1	101	DGD	O3G-C1D-C2D	2.26	110.78	108.00
25	c2	507	CLA	CMD-C2D-C3D	2.26	129.50	125.09
23	b2	603	BCR	C33-C5-C4	2.26	117.84	113.47
25	b2	606	CLA	CMD-C2D-C3D	2.26	129.51	125.09
23	j2	102	BCR	C33-C5-C4	2.26	117.84	113.47
25	D1	402	CLA	O2D-CGD-CBD	2.26	114.48	111.22
33	d1	407	LHG	O8-C23-C24	2.26	118.81	111.85
25	C2	518	CLA	CMD-C2D-C3D	2.26	129.51	125.09
25	B1	607	CLA	O1D-CGD-CBD	2.26	128.16	124.64
25	b1	605	CLA	O1D-CGD-CBD	2.26	128.16	124.64
25	b2	617	CLA	O2D-CGD-CBD	2.26	114.48	111.22
25	c2	507	CLA	O1D-CGD-CBD	2.26	128.16	124.64
25	c1	504	CLA	CMD-C2D-C3D	2.27	129.52	125.09
25	c1	508	CLA	O1D-CGD-CBD	2.27	128.16	124.64
23	b1	601	BCR	C38-C26-C27	2.27	117.85	113.47
25	c1	508	CLA	C4A-NA-C1A	2.27	109.25	106.38
25	A1	405	CLA	O2D-CGD-CBD	2.27	114.49	111.22
25	c2	508	CLA	CMB-C2B-C3B	2.27	129.52	125.09
25	B1	606	CLA	CMD-C2D-C3D	2.27	129.53	125.09
25	c1	515	CLA	O2D-CGD-CBD	2.27	114.49	111.22
23	k2	501	BCR	C33-C5-C4	2.27	117.86	113.47
27	d2	408	PHO	CMB-C2B-C1B	2.27	128.70	125.06
36	D1	408	PL9	C51-C49-C50	2.27	120.14	114.61
25	b1	610	CLA	O1D-CGD-CBD	2.28	128.18	124.64
34	C1	516	DGD	O1G-C1A-C2A	2.28	118.86	111.85
23	h2	101	BCR	C33-C5-C4	2.28	117.87	113.47
25	D2	406	CLA	CMB-C2B-C3B	2.28	129.54	125.09
25	b1	604	CLA	CMB-C2B-C3B	2.28	129.55	125.09
25	c2	512	CLA	CMB-C2B-C3B	2.29	129.56	125.09
25	B2	618	CLA	CMD-C2D-C3D	2.29	129.56	125.09
25	b1	612	CLA	O2D-CGD-CBD	2.29	114.52	111.22
34	c2	516	DGD	O5D-C1E-C2E	2.29	110.82	108.00
29	D1	406	LMG	O8-C28-C29	2.29	118.91	111.85
25	b2	608	CLA	O1D-CGD-CBD	2.30	128.22	124.64
25	B1	608	CLA	CMB-C2B-C3B	2.30	129.59	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A1	403	CLA	CMB-C2B-C3B	2.30	129.59	125.09
25	b1	611	CLA	C4A-NA-C1A	2.30	109.30	106.38
27	A1	408	PHO	O2A-CGA-CBA	2.31	118.95	111.85
25	B1	609	CLA	O2D-CGD-CBD	2.31	114.55	111.22
25	A1	405	CLA	CMB-C2B-C3B	2.31	129.60	125.09
25	c1	506	CLA	O1D-CGD-CBD	2.31	128.23	124.64
25	B2	611	CLA	C4A-NA-C1A	2.31	109.31	106.38
25	B2	616	CLA	CMB-C2B-C3B	2.31	129.62	125.09
25	b1	612	CLA	CMD-C2D-C3D	2.32	129.62	125.09
25	B2	610	CLA	C4A-NA-C1A	2.32	109.32	106.38
25	C1	511	CLA	O1D-CGD-CBD	2.32	128.24	124.64
23	h1	102	BCR	C38-C26-C27	2.32	117.97	113.47
25	C2	507	CLA	O2D-CGD-CBD	2.33	114.57	111.22
27	D1	407	PHO	CAC-C3C-C4C	2.33	127.90	125.21
25	C1	509	CLA	CMD-C2D-C3D	2.33	129.65	125.09
25	d2	404	CLA	C4A-NA-C1A	2.33	109.34	106.38
37	D1	409	SQD	O7-S-C6	2.33	108.57	106.92
23	b1	602	BCR	C38-C26-C27	2.33	117.98	113.47
25	C1	506	CLA	CMD-C2D-C3D	2.33	129.65	125.09
25	C1	510	CLA	CMB-C2B-C3B	2.33	129.65	125.09
23	b2	601	BCR	C33-C5-C4	2.34	117.99	113.47
25	b1	619	CLA	CMB-C2B-C3B	2.34	129.66	125.09
25	c2	504	CLA	O2D-CGD-CBD	2.34	114.59	111.22
34	c1	520	DGD	O1G-C1A-C2A	2.34	119.05	111.85
25	C1	509	CLA	C4A-NA-C1A	2.35	109.35	106.38
25	D1	403	CLA	C4A-NA-C1A	2.35	109.35	106.38
25	a2	404	CLA	O1D-CGD-CBD	2.35	128.29	124.64
25	B1	604	CLA	CMB-C2B-C3B	2.35	129.68	125.09
25	b1	614	CLA	O1D-CGD-CBD	2.35	128.29	124.64
25	B1	613	CLA	O2D-CGD-CBD	2.35	114.61	111.22
34	c1	514	DGD	O5D-C1E-C2E	2.35	110.89	108.00
27	A2	407	PHO	O2A-CGA-CBA	2.35	119.09	111.85
25	C2	516	CLA	O1D-CGD-CBD	2.35	128.30	124.64
25	a2	404	CLA	CMB-C2B-C3B	2.36	129.70	125.09
25	b1	611	CLA	CMB-C2B-C3B	2.36	129.70	125.09
23	B1	603	BCR	C29-C30-C25	2.36	113.99	110.48
25	b1	612	CLA	CMB-C2B-C3B	2.36	129.70	125.09
25	B1	611	CLA	C4A-NA-C1A	2.36	109.37	106.38
23	B2	601	BCR	C38-C26-C27	2.36	118.03	113.47
34	c2	517	DGD	O1G-C1A-C2A	2.36	119.11	111.85
25	b1	611	CLA	O1D-CGD-CBD	2.36	128.31	124.64
25	b1	604	CLA	C4A-NA-C1A	2.36	109.38	106.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B1	612	CLA	C4A-NA-C1A	2.36	109.38	106.38
25	B2	611	CLA	O1D-CGD-CBD	2.36	128.31	124.64
25	B1	610	CLA	O2D-CGD-CBD	2.36	114.63	111.22
25	B2	614	CLA	CMD-C2D-C3D	2.37	129.72	125.09
25	D1	403	CLA	O2D-CGD-CBD	2.37	114.63	111.22
25	a2	405	CLA	C4A-NA-C1A	2.37	109.39	106.38
25	d2	404	CLA	O2D-CGD-CBD	2.37	114.64	111.22
29	d1	408	LMG	O8-C28-C29	2.37	119.15	111.85
25	C2	503	CLA	O2D-CGD-CBD	2.37	114.64	111.22
25	b1	610	CLA	C4A-NA-C1A	2.38	109.39	106.38
35	b2	623	LMT	O1'-C1'-C2'	2.38	110.92	108.00
25	D2	401	CLA	O2D-CGD-CBD	2.38	114.64	111.22
25	C2	513	CLA	C4A-NA-C1A	2.38	109.39	106.38
25	B1	618	CLA	O1D-CGD-CBD	2.38	128.34	124.64
25	B2	616	CLA	O2D-CGD-CBD	2.38	114.65	111.22
25	b2	618	CLA	CMB-C2B-C3B	2.38	129.75	125.09
25	b2	624	CLA	C4A-NA-C1A	2.38	109.40	106.38
25	d2	405	CLA	O2D-CGD-CBD	2.39	114.66	111.22
29	B2	620	LMG	O1-C1-C2	2.39	110.94	108.00
25	c2	502	CLA	CMB-C2B-C3B	2.39	129.76	125.09
25	B2	606	CLA	O1D-CGD-CBD	2.39	128.35	124.64
25	B2	609	CLA	CMD-C2D-C3D	2.39	129.76	125.09
23	K2	104	BCR	C38-C26-C27	2.39	118.10	113.47
25	a1	405	CLA	CMB-C2B-C3B	2.39	129.77	125.09
25	B1	614	CLA	O1D-CGD-CBD	2.40	128.36	124.64
29	B1	622	LMG	O1-C1-C2	2.40	110.95	108.00
25	a1	403	CLA	CMB-C2B-C3B	2.40	129.78	125.09
25	c1	508	CLA	CMB-C2B-C3B	2.40	129.78	125.09
29	B1	626	LMG	O1-C1-C2	2.40	110.95	108.00
25	c1	510	CLA	CMD-C2D-C3D	2.40	129.78	125.09
25	B1	617	CLA	C4A-NA-C1A	2.40	109.43	106.38
25	d2	402	CLA	CMB-C2B-C3B	2.40	129.79	125.09
25	B2	605	CLA	C4A-NA-C1A	2.41	109.43	106.38
25	c2	512	CLA	C4A-NA-C1A	2.41	109.43	106.38
25	b1	611	CLA	CMD-C2D-C3D	2.41	129.80	125.09
25	b2	608	CLA	C4A-NA-C1A	2.41	109.44	106.38
25	c2	503	CLA	CMD-C2D-C3D	2.41	129.81	125.09
25	d1	404	CLA	C4A-NA-C1A	2.41	109.44	106.38
25	c2	504	CLA	CMB-C2B-C3B	2.41	129.81	125.09
25	B1	611	CLA	CMB-C2B-C3B	2.41	129.81	125.09
34	c1	520	DGD	O5D-C1E-C2E	2.41	110.97	108.00
25	C2	516	CLA	CMB-C2B-C3B	2.41	129.81	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b1	608	CLA	CMB-C2B-C3B	2.42	129.82	125.09
25	D1	402	CLA	CMB-C2B-C3B	2.42	129.82	125.09
33	D1	405	LHG	O8-C23-C24	2.42	119.30	111.85
25	B1	618	CLA	C4A-NA-C1A	2.42	109.45	106.38
25	B1	617	CLA	O2D-CGD-CBD	2.42	114.71	111.22
23	c2	501	BCR	C38-C26-C27	2.42	118.16	113.47
25	B1	616	CLA	C4A-NA-C1A	2.43	109.46	106.38
25	B2	609	CLA	O2D-CGD-CBD	2.43	114.72	111.22
25	b2	611	CLA	C4A-NA-C1A	2.43	109.46	106.38
25	B1	609	CLA	C4A-NA-C1A	2.43	109.46	106.38
25	b2	612	CLA	C4A-NA-C1A	2.43	109.46	106.38
25	b2	612	CLA	O2D-CGD-CBD	2.43	114.72	111.22
25	B1	618	CLA	CMB-C2B-C3B	2.43	129.85	125.09
23	k2	501	BCR	C38-C26-C27	2.43	118.18	113.47
25	C1	513	CLA	CMB-C2B-C3B	2.44	129.85	125.09
25	C2	506	CLA	C4A-NA-C1A	2.44	109.47	106.38
37	D1	409	SQD	O8-S-C6	2.44	110.06	104.99
25	b1	617	CLA	CMB-C2B-C3B	2.44	129.86	125.09
25	c1	507	CLA	CMB-C2B-C3B	2.44	129.86	125.09
25	c1	509	CLA	CMB-C2B-C3B	2.44	129.86	125.09
33	A2	405	LHG	O7-C7-C8	2.44	119.53	110.82
25	B2	612	CLA	C4A-NA-C1A	2.44	109.48	106.38
25	b2	610	CLA	C4A-NA-C1A	2.45	109.48	106.38
25	B1	619	CLA	CMD-C2D-C3D	2.45	129.88	125.09
25	b2	604	CLA	CMB-C2B-C3B	2.45	129.88	125.09
36	D2	408	PL9	C35-C34-C36	2.45	119.11	115.37
25	b2	618	CLA	O2D-CGD-CBD	2.45	114.76	111.22
25	B1	605	CLA	C4A-NA-C1A	2.46	109.49	106.38
25	c2	509	CLA	C4A-NA-C1A	2.46	109.49	106.38
25	c1	503	CLA	O1D-CGD-CBD	2.46	128.46	124.64
25	B1	607	CLA	C4A-NA-C1A	2.46	109.50	106.38
25	b1	605	CLA	C4A-NA-C1A	2.46	109.50	106.38
25	d2	405	CLA	CMB-C2B-C3B	2.46	129.90	125.09
25	b2	609	CLA	CMB-C2B-C3B	2.46	129.90	125.09
29	A1	410	LMG	O1-C1-C2	2.46	111.03	108.00
25	b2	613	CLA	C4A-NA-C1A	2.46	109.50	106.38
25	D2	404	CLA	C4A-NA-C1A	2.46	109.50	106.38
25	C1	514	CLA	C4A-NA-C1A	2.46	109.50	106.38
37	D1	409	SQD	O6-C1-C2	2.46	111.03	108.00
25	d1	406	CLA	C4A-NA-C1A	2.47	109.51	106.38
25	B2	617	CLA	O2D-CGD-CBD	2.47	114.78	111.22
25	B2	615	CLA	CMD-C2D-C3D	2.47	129.92	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	D2	404	CLA	O2D-CGD-CBD	2.47	114.78	111.22
25	b1	611	CLA	C6-C5-C3	2.47	117.20	112.76
23	j2	102	BCR	C38-C26-C27	2.47	118.25	113.47
25	b1	606	CLA	CMB-C2B-C3B	2.47	129.92	125.09
25	C2	505	CLA	O2D-CGD-CBD	2.47	114.78	111.22
25	C2	513	CLA	CMB-C2B-C3B	2.47	129.93	125.09
25	A2	404	CLA	C4A-NA-C1A	2.47	109.52	106.38
25	b2	609	CLA	O1D-CGD-CBD	2.48	128.49	124.64
23	B1	602	BCR	C38-C26-C27	2.48	118.26	113.47
25	c2	502	CLA	O2D-CGD-CBD	2.48	114.79	111.22
25	c2	507	CLA	C4A-NA-C1A	2.48	109.52	106.38
25	c2	510	CLA	C4A-NA-C1A	2.48	109.52	106.38
25	b2	617	CLA	C4A-NA-C1A	2.48	109.52	106.38
25	c1	516	CLA	C4A-NA-C1A	2.48	109.52	106.38
25	C1	510	CLA	C4A-NA-C1A	2.48	109.53	106.38
25	B2	607	CLA	C4A-NA-C1A	2.48	109.53	106.38
25	d2	405	CLA	C4A-NA-C1A	2.48	109.53	106.38
25	C1	513	CLA	C4A-NA-C1A	2.48	109.53	106.38
25	A1	404	CLA	O2D-CGD-CBD	2.49	114.81	111.22
25	C2	504	CLA	C4A-NA-C1A	2.49	109.54	106.38
25	c2	511	CLA	CMB-C2B-C3B	2.49	129.96	125.09
36	d1	409	PL9	C45-C44-C46	2.49	119.17	115.37
25	C1	511	CLA	C4A-NA-C1A	2.49	109.54	106.38
25	A1	406	CLA	CMB-C2B-C3B	2.50	129.97	125.09
25	d1	404	CLA	CMB-C2B-C3B	2.50	129.97	125.09
25	c1	504	CLA	C4A-NA-C1A	2.50	109.55	106.38
25	b1	612	CLA	C4A-NA-C1A	2.50	109.55	106.38
23	J1	101	BCR	C33-C5-C4	2.50	118.31	113.47
25	B2	619	CLA	C4A-NA-C1A	2.50	109.55	106.38
25	b2	610	CLA	CMB-C2B-C3B	2.50	129.99	125.09
25	B2	617	CLA	C4A-NA-C1A	2.50	109.56	106.38
25	B2	608	CLA	O1D-CGD-CBD	2.51	128.53	124.64
25	b1	615	CLA	C4A-NA-C1A	2.51	109.56	106.38
25	b1	608	CLA	C4A-NA-C1A	2.51	109.56	106.38
27	A1	408	PHO	CMB-C2B-C1B	2.51	129.07	125.06
25	B2	613	CLA	C4A-NA-C1A	2.51	109.56	106.38
27	a1	411	PHO	CMB-C2B-C1B	2.51	129.08	125.06
25	B2	604	CLA	CMB-C2B-C3B	2.52	130.01	125.09
25	b1	607	CLA	C4A-NA-C1A	2.52	109.57	106.38
25	B2	613	CLA	CMD-C2D-C3D	2.52	130.01	125.09
36	D1	408	PL9	C45-C44-C46	2.52	119.21	115.37
25	b1	619	CLA	C4A-NA-C1A	2.52	109.57	106.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b1	608	CLA	O1D-CGD-CBD	2.52	128.56	124.64
25	C1	503	CLA	C4A-NA-C1A	2.52	109.58	106.38
25	B2	604	CLA	C4A-NA-C1A	2.52	109.58	106.38
25	c2	505	CLA	C4A-NA-C1A	2.53	109.58	106.38
25	b1	614	CLA	C4A-NA-C1A	2.53	109.58	106.38
25	c2	511	CLA	C4A-NA-C1A	2.53	109.59	106.38
25	C1	504	CLA	CMB-C2B-C3B	2.53	130.03	125.09
25	b2	604	CLA	C4A-NA-C1A	2.53	109.59	106.38
25	C1	508	CLA	C4A-NA-C1A	2.53	109.59	106.38
27	D2	407	PHO	CMB-C2B-C1B	2.53	129.11	125.06
25	c2	505	CLA	O2D-CGD-CBD	2.53	114.87	111.22
25	a2	413	CLA	CMB-C2B-C3B	2.53	130.04	125.09
25	B2	612	CLA	CMB-C2B-C3B	2.53	130.05	125.09
25	c2	515	CLA	C4A-NA-C1A	2.54	109.59	106.38
29	b1	621	LMG	O8-C28-C29	2.54	119.65	111.85
27	A2	407	PHO	CAC-C3C-C4C	2.54	128.14	125.21
25	b2	612	CLA	CMD-C2D-C3D	2.54	130.05	125.09
25	C2	508	CLA	C4A-NA-C1A	2.54	109.60	106.38
27	a1	411	PHO	O2A-CGA-CBA	2.54	119.66	111.85
25	b1	609	CLA	C4A-NA-C1A	2.54	109.60	106.38
37	b2	605	SQD	O48-C23-C24	2.54	119.67	111.85
29	c1	519	LMG	O8-C28-C29	2.54	119.67	111.85
25	A1	404	CLA	C4A-NA-C1A	2.54	109.60	106.38
25	B1	613	CLA	C4A-NA-C1A	2.54	109.61	106.38
25	c1	510	CLA	CMB-C2B-C3B	2.55	130.07	125.09
25	c1	512	CLA	C4A-NA-C1A	2.55	109.61	106.38
25	C1	504	CLA	C4A-NA-C1A	2.55	109.61	106.38
25	b1	609	CLA	CMB-C2B-C3B	2.55	130.07	125.09
25	d1	401	CLA	CMB-C2B-C3B	2.55	130.07	125.09
25	C2	510	CLA	CMB-C2B-C3B	2.55	130.07	125.09
25	C2	509	CLA	CMB-C2B-C3B	2.55	130.07	125.09
25	b1	606	CLA	O2D-CGD-CBD	2.55	114.90	111.22
25	B1	619	CLA	O2D-CGD-CBD	2.55	114.90	111.22
25	B1	612	CLA	CMB-C2B-C3B	2.55	130.08	125.09
25	B1	604	CLA	C4A-NA-C1A	2.55	109.62	106.38
25	b1	609	CLA	O2D-CGD-CBD	2.56	114.90	111.22
29	A1	412	LMG	O8-C28-C29	2.56	119.72	111.85
25	D2	401	CLA	CMB-C2B-C3B	2.56	130.09	125.09
25	d1	406	CLA	O2D-CGD-CBD	2.56	114.91	111.22
25	b2	620	CLA	C4A-NA-C1A	2.56	109.63	106.38
25	D2	404	CLA	CMB-C2B-C3B	2.56	130.10	125.09
25	b1	613	CLA	CMD-C2D-C3D	2.56	130.10	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c1	511	CLA	C4A-NA-C1A	2.57	109.63	106.38
25	b2	608	CLA	CMB-C2B-C3B	2.57	130.11	125.09
25	C2	511	CLA	O2D-CGD-CBD	2.57	114.92	111.22
25	B2	617	CLA	CMB-C2B-C3B	2.57	130.12	125.09
29	b1	631	LMG	O8-C28-C29	2.57	119.76	111.85
25	b1	620	CLA	C4A-NA-C1A	2.57	109.64	106.38
25	B1	609	CLA	CBC-CAC-C3C	2.57	120.19	112.38
23	k1	101	BCR	C33-C5-C4	2.57	118.44	113.47
25	B1	619	CLA	C4A-NA-C1A	2.57	109.64	106.38
25	B1	614	CLA	C4A-NA-C1A	2.57	109.64	106.38
25	B2	606	CLA	C4A-NA-C1A	2.57	109.64	106.38
25	A1	404	CLA	CMB-C2B-C3B	2.57	130.12	125.09
25	b1	617	CLA	C4A-NA-C1A	2.58	109.65	106.38
25	B1	615	CLA	C4A-NA-C1A	2.58	109.65	106.38
25	B2	606	CLA	CMB-C2B-C3B	2.58	130.13	125.09
25	b2	616	CLA	O2D-CGD-CBD	2.58	114.94	111.22
25	B1	606	CLA	CMB-C2B-C3B	2.58	130.13	125.09
25	b2	617	CLA	CMB-C2B-C3B	2.58	130.14	125.09
25	b2	614	CLA	C4A-NA-C1A	2.58	109.65	106.38
25	C2	505	CLA	CMB-C2B-C3B	2.58	130.14	125.09
37	B2	623	SQD	O48-C23-C24	2.58	119.80	111.85
25	c2	506	CLA	C4A-NA-C1A	2.58	109.66	106.38
25	B2	608	CLA	CMB-C2B-C3B	2.58	130.14	125.09
25	a1	405	CLA	C4A-NA-C1A	2.58	109.66	106.38
25	C1	502	CLA	O2D-CGD-CBD	2.59	114.95	111.22
25	b2	618	CLA	C4A-NA-C1A	2.59	109.66	106.38
25	a2	405	CLA	CMB-C2B-C3B	2.59	130.15	125.09
25	C2	511	CLA	CMB-C2B-C3B	2.59	130.16	125.09
25	C1	508	CLA	CMB-C2B-C3B	2.59	130.16	125.09
25	c2	513	CLA	C4A-NA-C1A	2.59	109.67	106.38
27	D1	407	PHO	O2A-CGA-CBA	2.59	119.83	111.85
25	D2	406	CLA	C4A-NA-C1A	2.60	109.67	106.38
23	b2	602	BCR	C38-C26-C27	2.60	118.50	113.47
23	b1	602	BCR	C29-C30-C25	2.60	114.35	110.48
25	B2	615	CLA	C4A-NA-C1A	2.60	109.68	106.38
29	C2	515	LMG	O7-C10-C11	2.60	120.11	110.82
25	b1	606	CLA	C4A-NA-C1A	2.60	109.68	106.38
29	C1	520	LMG	O8-C28-C29	2.60	119.87	111.85
34	c1	518	DGD	O1G-C1A-C2A	2.61	119.87	111.85
25	c1	515	CLA	C4A-NA-C1A	2.61	109.69	106.38
25	c1	505	CLA	C4A-NA-C1A	2.61	109.69	106.38
36	D2	408	PL9	C45-C44-C46	2.61	119.35	115.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c2	508	CLA	C4A-NA-C1A	2.61	109.69	106.38
35	m2	104	LMT	O1B-C1B-C2B	2.61	114.61	108.12
25	B2	605	CLA	O1D-CGD-CBD	2.61	128.70	124.64
25	c1	510	CLA	C4A-NA-C1A	2.61	109.69	106.38
25	A1	406	CLA	C4A-NA-C1A	2.61	109.70	106.38
25	c1	506	CLA	C4A-NA-C1A	2.61	109.70	106.38
23	b1	602	BCR	C8-C9-C10	2.62	123.17	118.95
25	C1	502	CLA	CMB-C2B-C3B	2.62	130.21	125.09
27	A2	407	PHO	CMB-C2B-C1B	2.62	129.25	125.06
25	c1	503	CLA	C4A-NA-C1A	2.62	109.70	106.38
33	D2	405	LHG	O8-C23-C24	2.62	119.91	111.85
25	B1	609	CLA	CMB-C2B-C3B	2.62	130.21	125.09
25	c1	513	CLA	C4A-NA-C1A	2.62	109.70	106.38
25	B2	609	CLA	C4A-NA-C1A	2.62	109.70	106.38
34	c1	514	DGD	O1G-C1A-C2A	2.62	119.92	111.85
34	H2	101	DGD	O1G-C1A-C2A	2.62	119.92	111.85
25	c2	502	CLA	C4A-NA-C1A	2.62	109.71	106.38
25	K2	101	CLA	C4A-NA-C1A	2.62	109.71	106.38
25	b2	615	CLA	C4A-NA-C1A	2.62	109.71	106.38
25	C1	507	CLA	CMB-C2B-C3B	2.63	130.23	125.09
25	b2	619	CLA	C4A-NA-C1A	2.63	109.72	106.38
25	C2	518	CLA	C4A-NA-C1A	2.63	109.72	106.38
23	d2	401	BCR	C38-C26-C27	2.63	118.56	113.47
34	c2	514	DGD	O1G-C1A-C2A	2.63	119.95	111.85
25	B2	616	CLA	C4A-NA-C1A	2.63	109.72	106.38
25	C1	503	CLA	CMB-C2B-C3B	2.63	130.24	125.09
25	A2	404	CLA	O2D-CGD-CBD	2.63	115.02	111.22
25	C2	507	CLA	C4A-NA-C1A	2.64	109.72	106.38
27	d1	403	PHO	CAC-C3C-C4C	2.64	128.25	125.21
25	C1	514	CLA	CMB-C2B-C3B	2.64	130.25	125.09
25	d2	402	CLA	C4A-NA-C1A	2.64	109.72	106.38
25	c2	503	CLA	C4A-NA-C1A	2.64	109.73	106.38
36	D2	408	PL9	C10-C9-C11	2.64	119.39	115.37
27	a1	411	PHO	C3C-C4C-NC	2.64	114.47	110.31
25	C2	509	CLA	C4A-NA-C1A	2.64	109.73	106.38
25	B1	617	CLA	CMB-C2B-C3B	2.64	130.25	125.09
25	B1	608	CLA	C4A-NA-C1A	2.64	109.73	106.38
33	A2	405	LHG	O8-C23-C24	2.64	119.98	111.85
25	b1	616	CLA	C4A-NA-C1A	2.64	109.73	106.38
25	C2	516	CLA	C4A-NA-C1A	2.64	109.73	106.38
25	B1	610	CLA	CMB-C2B-C3B	2.65	130.27	125.09
25	C2	511	CLA	C4A-NA-C1A	2.65	109.74	106.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C2	505	CLA	C4A-NA-C1A	2.65	109.74	106.38
25	b1	620	CLA	O2D-CGD-CBD	2.66	115.05	111.22
25	C1	505	CLA	C4A-NA-C1A	2.66	109.75	106.38
33	L1	101	LHG	O8-C23-C24	2.66	120.02	111.85
27	D2	407	PHO	CAC-C3C-C4C	2.66	128.28	125.21
25	C2	503	CLA	C4A-NA-C1A	2.66	109.75	106.38
25	B1	619	CLA	CMB-C2B-C3B	2.66	130.29	125.09
25	c2	504	CLA	C4A-NA-C1A	2.66	109.76	106.38
23	A2	401	BCR	C33-C5-C4	2.66	118.62	113.47
23	K1	101	BCR	C33-C5-C4	2.66	118.62	113.47
25	C2	504	CLA	CMB-C2B-C3B	2.67	130.30	125.09
29	I2	101	LMG	O8-C28-C29	2.67	120.06	111.85
29	b2	622	LMG	O8-C28-C29	2.67	120.07	111.85
33	B1	621	LHG	O8-C23-C24	2.67	120.08	111.85
25	C2	510	CLA	C4A-NA-C1A	2.68	109.77	106.38
34	C1	515	DGD	O1G-C1A-C2A	2.68	120.09	111.85
33	d2	403	LHG	O8-C23-C24	2.68	120.09	111.85
25	B2	614	CLA	C4A-NA-C1A	2.68	109.78	106.38
25	B1	605	CLA	CMB-C2B-C3B	2.68	130.33	125.09
25	B2	618	CLA	C4A-NA-C1A	2.68	109.78	106.38
25	d1	401	CLA	C4A-NA-C1A	2.68	109.78	106.38
25	C2	503	CLA	CMB-C2B-C3B	2.69	130.35	125.09
25	B2	619	CLA	CMB-C2B-C3B	2.69	130.35	125.09
25	D2	401	CLA	C4A-NA-C1A	2.69	109.79	106.38
25	b2	611	CLA	CMB-C2B-C3B	2.69	130.35	125.09
25	b2	616	CLA	C4A-NA-C1A	2.70	109.80	106.38
25	C2	518	CLA	CMB-C2B-C3B	2.70	130.37	125.09
25	b2	606	CLA	C4A-NA-C1A	2.70	109.81	106.38
25	D1	402	CLA	C4A-NA-C1A	2.71	109.81	106.38
35	m2	103	LMT	O1'-C1'-C2'	2.71	111.33	108.00
25	B2	608	CLA	C4A-NA-C1A	2.71	109.82	106.38
25	B1	606	CLA	C4A-NA-C1A	2.71	109.82	106.38
29	j2	101	LMG	O8-C28-C29	2.72	120.21	111.85
25	b2	620	CLA	CMB-C2B-C3B	2.72	130.40	125.09
25	c1	507	CLA	C4A-NA-C1A	2.72	109.83	106.38
25	C1	502	CLA	C4A-NA-C1A	2.72	109.83	106.38
25	c1	505	CLA	CMB-C2B-C3B	2.72	130.41	125.09
27	d2	408	PHO	O2A-CGA-CBA	2.72	120.23	111.85
27	d1	403	PHO	O2A-CGA-CBA	2.72	120.23	111.85
25	B2	611	CLA	CMB-C2B-C3B	2.72	130.42	125.09
33	l2	101	LHG	O8-C23-C24	2.73	120.24	111.85
36	D1	408	PL9	C53-C6-C1	2.73	120.46	114.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	d2	406	LHG	O8-C23-C24	2.73	120.25	111.85
27	A2	407	PHO	C3C-C4C-NC	2.73	114.61	110.31
25	C1	512	CLA	C4A-NA-C1A	2.73	109.84	106.38
25	b2	609	CLA	C4A-NA-C1A	2.73	109.84	106.38
25	B2	613	CLA	O2D-CGD-CBD	2.73	115.16	111.22
33	l1	102	LHG	O8-C23-C24	2.74	120.28	111.85
27	D2	407	PHO	C3C-C4C-NC	2.74	114.63	110.31
36	D2	408	PL9	C53-C6-C1	2.74	120.50	114.66
27	a1	411	PHO	C4-C3-C5	2.74	119.55	115.37
23	C1	521	BCR	C33-C5-C4	2.75	118.78	113.47
23	b2	602	BCR	C33-C5-C4	2.75	118.78	113.47
23	B1	601	BCR	C38-C26-C27	2.75	118.78	113.47
29	c2	519	LMG	O8-C28-C29	2.75	120.30	111.85
29	A1	410	LMG	O8-C28-C29	2.75	120.31	111.85
33	L2	101	LHG	O8-C23-C24	2.75	120.31	111.85
36	d2	409	PL9	C10-C9-C11	2.75	119.56	115.37
27	a1	411	PHO	CAC-C3C-C4C	2.76	128.39	125.21
25	C1	506	CLA	C4A-NA-C1A	2.76	109.88	106.38
25	B1	613	CLA	CMD-C2D-C3D	2.76	130.49	125.09
34	H1	101	DGD	O1G-C1A-C2A	2.76	120.34	111.85
27	d1	403	PHO	C3C-C4C-NC	2.76	114.66	110.31
23	h1	102	BCR	C29-C30-C25	2.77	114.59	110.48
23	K2	104	BCR	C29-C30-C25	2.77	114.59	110.48
33	D1	404	LHG	O8-C23-C24	2.77	120.37	111.85
25	c1	516	CLA	CMB-C2B-C3B	2.77	130.51	125.09
25	c2	506	CLA	CMB-C2B-C3B	2.77	130.51	125.09
25	c1	509	CLA	C4A-NA-C1A	2.77	109.90	106.38
25	c2	507	CLA	CMB-C2B-C3B	2.78	130.52	125.09
34	h1	101	DGD	O1G-C1A-C2A	2.78	120.41	111.85
25	c2	505	CLA	CMB-C2B-C3B	2.78	130.53	125.09
25	c1	503	CLA	CMB-C2B-C3B	2.78	130.53	125.09
27	d1	403	PHO	C4D-C3D-CAD	2.78	110.77	105.61
25	B2	614	CLA	CMB-C2B-C3B	2.79	130.54	125.09
29	d1	411	LMG	O8-C28-C29	2.79	120.43	111.85
27	D1	407	PHO	C4D-C3D-CAD	2.79	110.78	105.61
27	d2	408	PHO	C4D-C3D-CAD	2.79	110.78	105.61
25	C1	512	CLA	CMB-C2B-C3B	2.79	130.55	125.09
25	c1	507	CLA	O2D-CGD-CBD	2.80	115.25	111.22
33	b1	622	LHG	O8-C23-C24	2.80	120.47	111.85
25	c2	515	CLA	CMB-C2B-C3B	2.80	130.57	125.09
27	D1	407	PHO	C3C-C4C-NC	2.80	114.73	110.31
23	K2	104	BCR	C33-C5-C4	2.80	118.89	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b2	606	CLA	CMB-C2B-C3B	2.81	130.57	125.09
34	h2	102	DGD	O1G-C1A-C2A	2.81	120.48	111.85
36	d1	409	PL9	C40-C39-C41	2.81	119.65	115.37
25	B2	609	CLA	CMB-C2B-C3B	2.81	130.58	125.09
25	b1	607	CLA	O2D-CGD-CBD	2.81	115.27	111.22
25	C1	506	CLA	O2D-CGD-CBD	2.81	115.28	111.22
23	b2	601	BCR	C38-C26-C27	2.81	118.91	113.47
25	B2	618	CLA	O2D-CGD-CBD	2.82	115.28	111.22
25	C2	507	CLA	CMB-C2B-C3B	2.82	130.60	125.09
25	b2	615	CLA	CMB-C2B-C3B	2.82	130.60	125.09
36	d1	409	PL9	C25-C24-C26	2.82	119.67	115.37
23	b2	601	BCR	C29-C30-C25	2.82	114.68	110.48
27	D1	407	PHO	C2C-C1C-NC	2.83	114.02	109.81
36	d1	409	PL9	C30-C29-C31	2.83	119.68	115.37
36	D1	408	PL9	C10-C9-C11	2.84	119.69	115.37
27	d2	408	PHO	CAC-C3C-C4C	2.85	128.50	125.21
25	d2	404	CLA	CMB-C2B-C3B	2.85	130.65	125.09
27	a1	411	PHO	C2D-C1D-ND	2.85	114.05	109.81
27	d2	408	PHO	C3C-C4C-NC	2.85	114.80	110.31
33	d1	402	LHG	O8-C23-C24	2.85	119.65	111.16
27	D2	407	PHO	C4D-C3D-CAD	2.85	110.89	105.61
25	b2	613	CLA	CMB-C2B-C3B	2.85	130.67	125.09
25	D2	406	CLA	O2D-CGD-CBD	2.85	115.34	111.22
25	B1	614	CLA	CMB-C2B-C3B	2.85	130.67	125.09
37	D1	409	SQD	O48-C23-C24	2.86	120.64	111.85
25	c1	513	CLA	CMB-C2B-C3B	2.86	130.68	125.09
25	d1	406	CLA	CMB-C2B-C3B	2.86	130.68	125.09
37	B2	623	SQD	O6-C1-C2	2.86	111.52	108.00
27	d1	403	PHO	C4-C3-C5	2.86	119.73	115.37
25	B1	615	CLA	CMB-C2B-C3B	2.86	130.68	125.09
29	M1	101	LMG	O8-C28-C29	2.87	120.67	111.85
27	a1	411	PHO	C4D-C3D-CAD	2.87	110.93	105.61
27	a2	416	PHO	C3C-C4C-NC	2.87	114.84	110.31
25	C1	509	CLA	O2D-CGD-CBD	2.87	115.36	111.22
33	B2	627	LHG	O8-C23-C24	2.88	120.70	111.85
23	K2	102	BCR	C33-C5-C4	2.88	119.03	113.47
27	a2	416	PHO	C2C-C1C-NC	2.88	114.09	109.81
25	C2	518	CLA	O2D-CGD-CBD	2.88	115.37	111.22
27	D2	407	PHO	C4-C3-C5	2.88	119.76	115.37
25	B2	605	CLA	CMB-C2B-C3B	2.89	130.73	125.09
36	d2	409	PL9	C53-C6-C1	2.89	120.81	114.66
25	C1	511	CLA	CMB-C2B-C3B	2.90	130.75	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	D2	408	PL9	C25-C24-C26	2.90	119.78	115.37
25	c1	512	CLA	CMB-C2B-C3B	2.90	130.76	125.09
25	c1	515	CLA	CMB-C2B-C3B	2.90	130.76	125.09
23	B1	601	BCR	C29-C30-C25	2.90	114.80	110.48
27	d1	403	PHO	C2D-C1D-ND	2.90	114.13	109.81
33	a1	407	LHG	O8-C23-C24	2.90	120.79	111.85
29	B2	620	LMG	O8-C28-C29	2.91	120.79	111.85
27	D2	407	PHO	O2A-CGA-CBA	2.91	120.80	111.85
27	A2	407	PHO	C2D-C1D-ND	2.91	114.14	109.81
25	b2	614	CLA	CMB-C2B-C3B	2.91	130.78	125.09
27	A1	408	PHO	C3C-C4C-NC	2.91	114.90	110.31
25	c2	513	CLA	CMB-C2B-C3B	2.91	130.78	125.09
27	d1	403	PHO	C2C-C1C-NC	2.92	114.15	109.81
33	b2	625	LHG	O8-C23-C24	2.92	120.83	111.85
27	D2	407	PHO	C2D-C1D-ND	2.92	114.15	109.81
36	d1	409	PL9	C53-C6-C1	2.92	120.87	114.66
25	C1	505	CLA	CMB-C2B-C3B	2.92	130.81	125.09
29	a2	412	LMG	O8-C28-C29	2.93	120.87	111.85
33	D2	403	LHG	O8-C23-C24	2.93	120.87	111.85
25	d1	401	CLA	O2D-CGD-CBD	2.94	115.45	111.22
25	c2	509	CLA	O2D-CGD-CBD	2.94	115.45	111.22
34	c2	516	DGD	O1G-C1A-C2A	2.94	120.89	111.85
27	d2	408	PHO	C4-C3-C5	2.94	119.85	115.37
23	A2	401	BCR	C29-C30-C25	2.94	114.86	110.48
25	C2	508	CLA	CMB-C2B-C3B	2.94	130.85	125.09
25	b2	620	CLA	O2D-CGD-CBD	2.95	115.47	111.22
27	a2	416	PHO	C4A-NA-C1A	2.95	110.44	108.22
27	A1	408	PHO	C2D-C1D-ND	2.96	114.21	109.81
27	a2	416	PHO	C4D-C3D-CAD	2.96	111.09	105.61
25	C1	509	CLA	CMB-C2B-C3B	2.96	130.88	125.09
36	D2	408	PL9	C30-C29-C31	2.97	119.89	115.37
27	A1	408	PHO	C4D-C3D-CAD	2.97	111.11	105.61
25	D1	403	CLA	CMB-C2B-C3B	2.97	130.90	125.09
27	D1	407	PHO	C2D-C1D-ND	2.97	114.23	109.81
25	b2	620	CLA	C6-C5-C3	2.97	118.10	112.76
27	d1	403	PHO	C4A-NA-C1A	2.99	110.47	108.22
25	b1	605	CLA	CMB-C2B-C3B	2.99	130.93	125.09
25	c1	511	CLA	CMB-C2B-C3B	2.99	130.93	125.09
27	a2	416	PHO	C4-C3-C5	2.99	119.92	115.37
25	B2	615	CLA	CMB-C2B-C3B	3.00	130.95	125.09
23	A2	401	BCR	C38-C26-C27	3.00	119.27	113.47
23	F2	401	BCR	C38-C26-C27	3.01	119.28	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	d2	408	PHO	C2D-C1D-ND	3.01	114.28	109.81
36	d2	409	PL9	C20-C19-C21	3.02	119.97	115.37
25	C2	506	CLA	CMB-C2B-C3B	3.02	130.99	125.09
27	D2	407	PHO	C2C-C1C-NC	3.03	114.31	109.81
25	B2	619	CLA	O2D-CGD-CBD	3.03	115.58	111.22
23	b1	601	BCR	C29-C30-C25	3.04	115.00	110.48
29	a1	412	LMG	O1-C1-C2	3.04	111.74	108.00
36	D2	408	PL9	C40-C39-C41	3.04	120.00	115.37
25	c1	510	CLA	O2D-CGD-CBD	3.04	115.61	111.22
27	a2	416	PHO	C2D-C1D-ND	3.04	114.34	109.81
29	a1	412	LMG	O8-C28-C29	3.05	121.22	111.85
23	B2	601	BCR	C29-C30-C25	3.05	115.01	110.48
36	d2	409	PL9	C15-C14-C16	3.05	120.02	115.37
27	A2	407	PHO	C4D-C3D-CAD	3.05	111.27	105.61
27	a1	411	PHO	C2C-C1C-NC	3.05	114.36	109.81
27	d2	408	PHO	C2C-C1C-NC	3.06	114.36	109.81
27	a1	411	PHO	C4A-NA-C1A	3.06	110.52	108.22
25	c2	509	CLA	CMB-C2B-C3B	3.07	131.09	125.09
23	c2	501	BCR	C33-C5-C4	3.07	119.41	113.47
25	b1	614	CLA	CMB-C2B-C3B	3.07	131.10	125.09
25	c1	504	CLA	CMB-C2B-C3B	3.07	131.10	125.09
27	A1	408	PHO	CAC-C3C-C4C	3.09	128.77	125.21
25	c2	506	CLA	O2D-CGD-CBD	3.10	115.69	111.22
25	B2	613	CLA	CMB-C2B-C3B	3.10	131.16	125.09
29	B1	622	LMG	O8-C28-C29	3.11	121.41	111.85
27	A1	408	PHO	C4-C3-C5	3.13	120.13	115.37
36	D1	408	PL9	C20-C19-C21	3.13	120.14	115.37
25	d1	404	CLA	O2D-CGD-CBD	3.13	115.74	111.22
25	b1	615	CLA	CMB-C2B-C3B	3.14	131.23	125.09
27	A2	407	PHO	C4-C3-C5	3.14	120.16	115.37
36	D2	408	PL9	C20-C19-C21	3.14	120.16	115.37
25	b1	610	CLA	CMB-C2B-C3B	3.16	131.28	125.09
23	c1	501	BCR	C33-C5-C4	3.17	119.60	113.47
25	c1	506	CLA	CMB-C2B-C3B	3.19	131.32	125.09
25	a1	405	CLA	O2D-CGD-CBD	3.19	115.82	111.22
37	D2	402	SQD	O6-C1-C2	3.19	111.93	108.00
27	A1	408	PHO	C2C-C1C-NC	3.21	114.58	109.81
27	A2	407	PHO	C2C-C1C-NC	3.22	114.60	109.81
25	b2	624	CLA	CMB-C2B-C3B	3.23	131.41	125.09
25	B1	611	CLA	O2D-CGD-CBD	3.24	115.89	111.22
29	B1	626	LMG	O8-C28-C29	3.29	121.97	111.85
35	l1	101	LMT	O1'-C1'-C2'	3.29	112.05	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	d2	408	PHO	C4A-NA-C1A	3.29	110.70	108.22
37	B2	623	SQD	O7-S-C6	3.31	109.25	106.92
36	D2	408	PL9	C15-C14-C16	3.31	120.42	115.37
27	A1	408	PHO	C4A-NA-C1A	3.32	110.72	108.22
27	D1	407	PHO	C4A-NA-C1A	3.32	110.72	108.22
23	d2	401	BCR	C33-C5-C4	3.33	119.91	113.47
27	D1	407	PHO	C4-C3-C5	3.33	120.45	115.37
25	d2	402	CLA	O2D-CGD-CBD	3.34	116.04	111.22
25	B2	607	CLA	O2D-CGD-CBD	3.36	116.07	111.22
27	a1	411	PHO	C2B-C1B-NB	3.38	114.84	109.81
36	D1	408	PL9	C25-C24-C26	3.40	120.55	115.37
36	d1	409	PL9	C15-C14-C16	3.41	120.57	115.37
25	B2	610	CLA	CMB-C2B-C3B	3.41	131.76	125.09
27	A1	408	PHO	C2B-C1B-NB	3.44	114.92	109.81
27	A2	407	PHO	C4A-NA-C1A	3.44	110.81	108.22
27	A2	407	PHO	C2B-C1B-NB	3.49	115.01	109.81
27	D2	407	PHO	C2B-C1B-NB	3.51	115.03	109.81
36	d2	409	PL9	C25-C24-C26	3.52	120.73	115.37
25	A1	406	CLA	O2D-CGD-CBD	3.53	116.31	111.22
34	c1	520	DGD	O2G-C1B-C2B	3.53	118.97	111.53
33	B1	621	LHG	O7-C7-C8	3.54	118.99	111.53
37	D1	409	SQD	O9-S-C6	3.54	109.42	106.92
29	a2	412	LMG	O1-C1-C2	3.55	112.36	108.00
36	D1	408	PL9	C30-C29-C31	3.56	120.79	115.37
27	D1	407	PHO	C2B-C1B-NB	3.56	115.11	109.81
29	B2	621	LMG	O1-C1-C2	3.57	112.39	108.00
37	D2	402	SQD	O7-S-C6	3.58	109.44	106.92
36	d1	409	PL9	C20-C19-C21	3.59	120.84	115.37
27	a2	416	PHO	C2B-C1B-NB	3.59	115.15	109.81
27	d2	408	PHO	C2B-C1B-NB	3.62	115.20	109.81
36	D1	408	PL9	C15-C14-C16	3.63	120.91	115.37
27	d1	403	PHO	C2B-C1B-NB	3.65	115.25	109.81
33	D2	403	LHG	O7-C7-C8	3.68	119.27	111.53
34	c2	517	DGD	O2G-C1B-C2B	3.69	119.29	111.53
34	h2	102	DGD	O2G-C1B-C2B	3.69	119.30	111.53
29	b2	622	LMG	O7-C10-C11	3.70	119.33	111.53
36	d2	409	PL9	C30-C29-C31	3.71	121.02	115.37
29	B2	620	LMG	O7-C10-C11	3.74	119.40	111.53
33	d2	403	LHG	O7-C7-C8	3.75	119.42	111.53
29	c1	519	LMG	O7-C10-C11	3.75	119.43	111.53
33	d2	406	LHG	O7-C7-C8	3.79	119.51	111.53
29	a1	412	LMG	O7-C10-C11	3.83	119.60	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B1	622	LMG	O7-C10-C11	3.86	119.66	111.53
33	D1	405	LHG	O7-C7-C8	3.89	119.73	111.53
34	H2	101	DGD	O2G-C1B-C2B	3.90	119.74	111.53
29	d1	411	LMG	O7-C10-C11	3.90	119.74	111.53
29	b1	631	LMG	O1-C1-C2	3.90	112.80	108.00
34	C1	517	DGD	O2G-C1B-C2B	3.91	119.76	111.53
29	D1	406	LMG	O7-C10-C11	3.91	119.77	111.53
33	b1	622	LHG	O7-C7-C8	3.92	119.78	111.53
23	j2	102	BCR	C36-C18-C19	3.92	124.49	118.08
23	k1	101	BCR	C36-C18-C19	3.93	124.50	118.08
33	L1	101	LHG	O7-C7-C8	3.93	119.81	111.53
29	A1	410	LMG	O7-C10-C11	3.93	119.82	111.53
33	D2	405	LHG	O7-C7-C8	3.95	119.85	111.53
29	a2	412	LMG	O7-C10-C11	3.95	119.85	111.53
33	D1	404	LHG	O7-C7-C8	3.97	119.88	111.53
27	D2	407	PHO	C4A-NA-C1A	3.99	111.23	108.22
33	d1	407	LHG	O7-C7-C8	4.01	119.97	111.53
37	b2	605	SQD	O7-S-C6	4.02	109.75	106.92
29	B2	621	LMG	O7-C10-C11	4.02	120.00	111.53
33	a1	407	LHG	O7-C7-C8	4.03	120.02	111.53
37	b2	605	SQD	O9-S-C6	4.04	109.76	106.92
29	A1	412	LMG	O7-C10-C11	4.05	120.06	111.53
29	F2	402	LMG	O7-C10-C11	4.06	120.09	111.53
23	J1	101	BCR	C36-C18-C19	4.07	124.73	118.08
33	b2	625	LHG	O7-C7-C8	4.07	120.10	111.53
33	l1	102	LHG	O7-C7-C8	4.08	120.12	111.53
34	h1	101	DGD	O2G-C1B-C2B	4.10	120.16	111.53
33	B2	627	LHG	O7-C7-C8	4.10	120.17	111.53
23	b1	602	BCR	C35-C13-C12	4.11	124.80	118.08
33	a2	407	LHG	O7-C7-C8	4.12	120.21	111.53
29	d1	408	LMG	O7-C10-C11	4.14	120.26	111.53
33	l2	101	LHG	O7-C7-C8	4.14	120.26	111.53
29	C1	520	LMG	O7-C10-C11	4.15	120.27	111.53
23	K2	102	BCR	C36-C18-C19	4.17	124.90	118.08
34	c2	514	DGD	O2G-C1B-C2B	4.20	120.37	111.53
29	I2	101	LMG	O7-C10-C11	4.21	120.39	111.53
34	C1	516	DGD	O2G-C1B-C2B	4.21	120.40	111.53
33	L2	101	LHG	O7-C7-C8	4.22	120.41	111.53
29	j2	101	LMG	O7-C10-C11	4.23	120.44	111.53
34	H1	101	DGD	O2G-C1B-C2B	4.23	120.44	111.53
23	c2	501	BCR	C36-C18-C19	4.24	125.00	118.08
37	D2	402	SQD	O9-S-C6	4.27	109.93	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	C1	515	DGD	O2G-C1B-C2B	4.28	120.55	111.53
34	c1	514	DGD	O2G-C1B-C2B	4.29	120.56	111.53
29	A2	412	LMG	O7-C10-C11	4.30	120.59	111.53
37	B2	623	SQD	O47-C7-C8	4.32	120.62	111.53
23	F2	401	BCR	C36-C18-C19	4.32	125.14	118.08
23	c1	502	BCR	C36-C18-C19	4.35	125.19	118.08
37	B2	623	SQD	O9-S-C6	4.36	109.99	106.92
29	b1	631	LMG	O7-C10-C11	4.38	120.77	111.53
29	b1	621	LMG	O7-C10-C11	4.41	120.82	111.53
29	B1	626	LMG	O7-C10-C11	4.46	120.92	111.53
34	c1	518	DGD	O2G-C1B-C2B	4.47	120.95	111.53
34	c2	516	DGD	O2G-C1B-C2B	4.51	121.02	111.53
29	M1	101	LMG	O7-C10-C11	4.51	121.03	111.53
37	b2	605	SQD	O47-C7-C8	4.61	121.23	111.53
34	C2	512	DGD	O2G-C1B-C2B	4.72	120.07	111.09
33	d1	402	LHG	O7-C7-C8	4.73	121.50	111.53
29	d2	407	LMG	O7-C10-C11	4.75	120.12	111.09
37	D2	402	SQD	O47-C7-C8	4.83	120.28	111.09
37	D1	409	SQD	O47-C7-C8	4.83	120.29	111.09
29	b1	624	LMG	O7-C10-C11	5.02	122.10	111.53
25	B1	609	CLA	CAC-C3C-C4C	5.03	132.25	124.82
29	b1	624	LMG	O1-C1-C2	5.10	114.28	108.00
23	c2	501	BCR	C19-C18-C17	5.16	127.28	118.95
23	c2	501	BCR	C15-C16-C17	5.34	134.76	123.23
27	d2	408	PHO	O2D-CGD-CBD	5.75	119.52	111.22
23	c2	501	BCR	C20-C21-C22	5.85	135.72	127.22
27	a2	416	PHO	O2D-CGD-CBD	6.12	120.06	111.22
27	A2	407	PHO	O2D-CGD-CBD	6.14	120.08	111.22
27	D2	407	PHO	O2D-CGD-CBD	6.23	120.21	111.22
27	d1	403	PHO	O2D-CGD-CBD	6.23	120.21	111.22
27	D1	407	PHO	O2D-CGD-CBD	6.25	120.23	111.22
27	A1	408	PHO	O2D-CGD-CBD	6.25	120.24	111.22
27	a1	411	PHO	O2D-CGD-CBD	6.27	120.27	111.22
23	c2	501	BCR	C23-C22-C21	6.40	129.27	118.95
27	d1	403	PHO	CMD-C2D-C1D	8.51	138.66	125.06
27	A1	408	PHO	CMD-C2D-C1D	8.55	138.72	125.06
27	a2	416	PHO	CMD-C2D-C1D	8.57	138.77	125.06
27	d2	408	PHO	CMD-C2D-C1D	8.62	138.84	125.06
27	D1	407	PHO	CMD-C2D-C1D	8.63	138.85	125.06
27	a1	411	PHO	CMD-C2D-C1D	8.66	138.91	125.06
27	D2	407	PHO	CMD-C2D-C1D	8.80	139.13	125.06
23	c2	501	BCR	C16-C17-C18	8.90	140.16	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A2	407	PHO	CMD-C2D-C1D	8.91	139.31	125.06

All (419) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	D2	404	CLA	NC
25	D2	404	CLA	ND
25	D2	404	CLA	NA
25	B1	608	CLA	NC
25	B1	608	CLA	ND
25	B1	608	CLA	NA
25	b2	613	CLA	NC
25	b2	613	CLA	ND
25	b2	613	CLA	NA
25	b2	620	CLA	NC
25	b2	620	CLA	ND
25	b2	620	CLA	NA
25	a1	405	CLA	NC
25	a1	405	CLA	ND
25	a1	405	CLA	NA
25	B2	619	CLA	NC
25	B2	619	CLA	ND
25	B2	619	CLA	NA
25	B2	616	CLA	NC
25	B2	616	CLA	ND
25	B2	616	CLA	NA
25	c2	510	CLA	NC
25	c2	510	CLA	ND
25	c2	510	CLA	NA
25	b2	606	CLA	NC
25	b2	606	CLA	ND
25	b2	606	CLA	NA
25	b1	608	CLA	NC
25	b1	608	CLA	ND
25	b1	608	CLA	NA
25	b1	606	CLA	NC
25	b1	606	CLA	ND
25	b1	606	CLA	NA
25	D2	401	CLA	NC
25	D2	401	CLA	ND
25	D2	401	CLA	NA
25	C1	511	CLA	NC

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Mol	Chain	Res	Type	Atom
25	C1	511	CLA	ND
25	C1	511	CLA	NA
25	b2	619	CLA	NC
25	b2	619	CLA	ND
25	b2	619	CLA	NA
25	C2	504	CLA	NC
25	C2	504	CLA	ND
25	C2	504	CLA	NA
25	b2	624	CLA	NC
25	b2	624	CLA	ND
25	b2	624	CLA	NA
25	c2	503	CLA	NC
25	c2	503	CLA	ND
25	c2	503	CLA	NA
25	b2	604	CLA	NC
25	b2	604	CLA	ND
25	b2	604	CLA	NA
25	d2	405	CLA	NC
25	d2	405	CLA	ND
25	d2	405	CLA	NA
25	c1	516	CLA	NC
25	c1	516	CLA	ND
25	c1	516	CLA	NA
25	b1	604	CLA	NC
25	b1	604	CLA	ND
25	b1	604	CLA	NA
25	B2	607	CLA	NC
25	B2	607	CLA	ND
25	B2	607	CLA	NA
25	b2	611	CLA	NC
25	b2	611	CLA	ND
25	b2	611	CLA	NA
25	b1	616	CLA	NC
25	b1	616	CLA	ND
25	b1	616	CLA	NA
25	B2	613	CLA	NC
25	B2	613	CLA	ND
25	B2	613	CLA	NA
25	b1	619	CLA	NC
25	b1	619	CLA	ND
25	b1	619	CLA	NA
25	A2	404	CLA	NC

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Mol	Chain	Res	Type	Atom
25	A2	404	CLA	ND
25	A2	404	CLA	NA
25	C1	508	CLA	NC
25	C1	508	CLA	ND
25	C1	508	CLA	NA
25	C2	510	CLA	NC
25	C2	510	CLA	ND
25	C2	510	CLA	NA
25	b1	609	CLA	NC
25	b1	609	CLA	ND
25	b1	609	CLA	NA
25	b2	617	CLA	NC
25	b2	617	CLA	ND
25	b2	617	CLA	NA
25	B1	607	CLA	NC
25	B1	607	CLA	ND
25	B1	607	CLA	NA
25	B2	604	CLA	NC
25	B2	604	CLA	ND
25	B2	604	CLA	NA
25	C1	505	CLA	NC
25	C1	505	CLA	ND
25	C1	505	CLA	NA
25	b1	614	CLA	NC
25	b1	614	CLA	ND
25	b1	614	CLA	NA
25	B1	613	CLA	NC
25	B1	613	CLA	ND
25	B1	613	CLA	NA
25	C1	506	CLA	NC
25	C1	506	CLA	ND
25	C1	506	CLA	NA
25	c2	506	CLA	NC
25	c2	506	CLA	ND
25	c2	506	CLA	NA
25	C2	505	CLA	NC
25	C2	505	CLA	ND
25	C2	505	CLA	NA
25	A1	406	CLA	NC
25	A1	406	CLA	ND
25	A1	406	CLA	NA
25	c1	506	CLA	NC

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Mol	Chain	Res	Type	Atom
25	c1	506	CLA	ND
25	c1	506	CLA	NA
25	a2	404	CLA	NC
25	a2	404	CLA	ND
25	a2	404	CLA	NA
25	C2	503	CLA	NC
25	C2	503	CLA	ND
25	C2	503	CLA	NA
25	C1	509	CLA	NC
25	C1	509	CLA	ND
25	C1	509	CLA	NA
25	b1	613	CLA	NC
25	b1	613	CLA	ND
25	b1	613	CLA	NA
25	B2	610	CLA	NC
25	B2	610	CLA	ND
25	B2	610	CLA	NA
25	c2	515	CLA	NC
25	c2	515	CLA	ND
25	c2	515	CLA	NA
25	d2	404	CLA	NC
25	d2	404	CLA	ND
25	d2	404	CLA	NA
25	c1	515	CLA	NC
25	c1	515	CLA	ND
25	c1	515	CLA	NA
25	B2	615	CLA	NC
25	B2	615	CLA	ND
25	B2	615	CLA	NA
25	B1	609	CLA	NC
25	B1	609	CLA	ND
25	B1	609	CLA	NA
25	c1	513	CLA	NC
25	c1	513	CLA	ND
25	c1	513	CLA	NA
25	b2	615	CLA	NC
25	b2	615	CLA	ND
25	b2	615	CLA	NA
25	C2	518	CLA	NC
25	C2	518	CLA	ND
25	C2	518	CLA	NA
25	b1	620	CLA	NC

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Mol	Chain	Res	Type	Atom
25	b1	620	CLA	ND
25	b1	620	CLA	NA
25	C2	509	CLA	NC
25	C2	509	CLA	ND
25	C2	509	CLA	NA
25	C2	506	CLA	NC
25	C2	506	CLA	ND
25	C2	506	CLA	NA
25	c2	508	CLA	NC
25	c2	508	CLA	ND
25	c2	508	CLA	NA
25	C1	510	CLA	NC
25	C1	510	CLA	ND
25	C1	510	CLA	NA
25	B2	617	CLA	NC
25	B2	617	CLA	ND
25	B2	617	CLA	NA
25	c2	505	CLA	NC
25	c2	505	CLA	ND
25	c2	505	CLA	NA
25	c1	510	CLA	NC
25	c1	510	CLA	ND
25	c1	510	CLA	NA
25	c1	509	CLA	NC
25	c1	509	CLA	ND
25	c1	509	CLA	NA
25	B1	606	CLA	NC
25	B1	606	CLA	ND
25	B1	606	CLA	NA
25	B2	612	CLA	NC
25	B2	612	CLA	ND
25	B2	612	CLA	NA
25	B2	609	CLA	NC
25	B2	609	CLA	ND
25	B2	609	CLA	NA
25	c1	507	CLA	NC
25	c1	507	CLA	ND
25	c1	507	CLA	NA
25	C1	513	CLA	NC
25	C1	513	CLA	ND
25	C1	513	CLA	NA
25	A2	403	CLA	NC

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Mol	Chain	Res	Type	Atom
25	A2	403	CLA	ND
25	A2	403	CLA	NA
25	b1	612	CLA	NC
25	b1	612	CLA	ND
25	b1	612	CLA	NA
25	b1	605	CLA	NC
25	b1	605	CLA	ND
25	b1	605	CLA	NA
25	d1	406	CLA	NC
25	d1	406	CLA	ND
25	d1	406	CLA	NA
25	b2	610	CLA	NC
25	b2	610	CLA	ND
25	b2	610	CLA	NA
25	B1	610	CLA	NC
25	B1	610	CLA	ND
25	B1	610	CLA	NA
25	c2	512	CLA	NC
25	c2	512	CLA	ND
25	c2	512	CLA	NA
25	B2	614	CLA	NC
25	B2	614	CLA	ND
25	B2	614	CLA	NA
25	C2	508	CLA	NC
25	C2	508	CLA	ND
25	C2	508	CLA	NA
25	C2	513	CLA	NC
25	C2	513	CLA	ND
25	C2	513	CLA	NA
25	c2	507	CLA	NC
25	c2	507	CLA	ND
25	c2	507	CLA	NA
25	A1	405	CLA	NC
25	A1	405	CLA	ND
25	A1	405	CLA	NA
25	b2	609	CLA	NC
25	b2	609	CLA	ND
25	b2	609	CLA	NA
25	C1	507	CLA	NC
25	C1	507	CLA	ND
25	C1	507	CLA	NA
25	B1	611	CLA	NC

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Mol	Chain	Res	Type	Atom
25	B1	611	CLA	NA
25	b1	610	CLA	NC
25	b1	610	CLA	ND
25	b1	610	CLA	NA
25	c2	502	CLA	NC
25	c2	502	CLA	ND
25	c2	502	CLA	NA
25	b1	611	CLA	NC
25	b1	611	CLA	ND
25	b1	611	CLA	NA
25	B1	615	CLA	NC
25	B1	615	CLA	ND
25	B1	615	CLA	NA
25	B1	618	CLA	NC
25	B1	618	CLA	ND
25	B1	618	CLA	NA
25	c1	511	CLA	NC
25	c1	511	CLA	ND
25	c1	511	CLA	NA
25	B1	605	CLA	NC
25	B1	605	CLA	ND
25	B1	605	CLA	NA
25	c2	509	CLA	NC
25	c2	509	CLA	ND
25	c2	509	CLA	NA
25	B1	617	CLA	NC
25	B1	617	CLA	ND
25	B1	617	CLA	NA
25	a1	403	CLA	NC
25	a1	403	CLA	ND
25	a1	403	CLA	NA
25	b1	607	CLA	NC
25	b1	607	CLA	ND
25	b1	607	CLA	NA
25	c1	512	CLA	NC
25	c1	512	CLA	ND
25	c1	512	CLA	NA
25	B1	604	CLA	NC
25	B1	604	CLA	ND
25	B1	604	CLA	NA
25	b1	615	CLA	NC
25	b1	615	CLA	ND

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Mol	Chain	Res	Type	Atom
25	b1	615	CLA	NA
25	C1	512	CLA	NC
25	C1	512	CLA	ND
25	C1	512	CLA	NA
25	C2	507	CLA	NC
25	C2	507	CLA	ND
25	C2	507	CLA	NA
25	D1	403	CLA	NC
25	D1	403	CLA	ND
25	D1	403	CLA	NA
25	d1	404	CLA	NC
25	d1	404	CLA	ND
25	d1	404	CLA	NA
25	C2	511	CLA	NC
25	C2	511	CLA	ND
25	C2	511	CLA	NA
25	A1	403	CLA	NC
25	A1	403	CLA	ND
25	A1	403	CLA	NA
25	d2	402	CLA	NC
25	d2	402	CLA	ND
25	d2	402	CLA	NA
25	K2	101	CLA	NC
25	K2	101	CLA	ND
25	K2	101	CLA	NA
25	C2	516	CLA	NC
25	C2	516	CLA	ND
25	C2	516	CLA	NA
25	B1	616	CLA	NC
25	B1	616	CLA	ND
25	B1	616	CLA	NA
25	c1	504	CLA	NC
25	c1	504	CLA	ND
25	c1	504	CLA	NA
25	B1	619	CLA	NC
25	B1	619	CLA	ND
25	B1	619	CLA	NA
25	C1	502	CLA	NC
25	C1	502	CLA	ND
25	C1	502	CLA	NA
25	b1	617	CLA	NC
25	b1	617	CLA	ND

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Mol	Chain	Res	Type	Atom
25	b1	617	CLA	NA
25	c1	503	CLA	NC
25	c1	503	CLA	ND
25	c1	503	CLA	NA
25	b2	614	CLA	NC
25	b2	614	CLA	ND
25	b2	614	CLA	NA
25	B1	612	CLA	NC
25	B1	612	CLA	ND
25	B1	612	CLA	NA
25	d1	401	CLA	NC
25	d1	401	CLA	ND
25	d1	401	CLA	NA
25	B2	611	CLA	NC
25	B2	611	CLA	ND
25	B2	611	CLA	NA
25	D2	406	CLA	NC
25	D2	406	CLA	ND
25	D2	406	CLA	NA
25	c2	504	CLA	NC
25	c2	504	CLA	ND
25	c2	504	CLA	NA
25	a1	404	CLA	NC
25	a1	404	CLA	ND
25	a1	404	CLA	NA
25	c2	511	CLA	NC
25	c2	511	CLA	ND
25	c2	511	CLA	NA
25	b2	616	CLA	NC
25	b2	616	CLA	ND
25	b2	616	CLA	NA
25	c1	505	CLA	NC
25	c1	505	CLA	ND
25	c1	505	CLA	NA
25	b2	612	CLA	NC
25	b2	612	CLA	ND
25	b2	612	CLA	NA
25	C1	514	CLA	NC
25	C1	514	CLA	ND
25	C1	514	CLA	NA
25	B2	608	CLA	NC
25	B2	608	CLA	ND

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Mol	Chain	Res	Type	Atom
25	B2	608	CLA	NA
25	B1	614	CLA	NC
25	B1	614	CLA	ND
25	B1	614	CLA	NA
25	a2	405	CLA	NC
25	a2	405	CLA	ND
25	a2	405	CLA	NA
25	C1	504	CLA	NC
25	C1	504	CLA	ND
25	C1	504	CLA	NA
25	b2	608	CLA	NC
25	b2	608	CLA	ND
25	b2	608	CLA	NA
25	A2	402	CLA	NC
25	A2	402	CLA	ND
25	A2	402	CLA	NA
25	C1	503	CLA	NC
25	C1	503	CLA	ND
25	C1	503	CLA	NA
25	A1	404	CLA	NC
25	A1	404	CLA	ND
25	A1	404	CLA	NA
25	B2	618	CLA	NC
25	B2	618	CLA	ND
25	B2	618	CLA	NA
25	D1	402	CLA	NC
25	D1	402	CLA	ND
25	D1	402	CLA	NA
25	c2	513	CLA	NC
25	c2	513	CLA	ND
25	c2	513	CLA	NA
25	a2	413	CLA	NC
25	a2	413	CLA	ND
25	a2	413	CLA	NA
25	b2	618	CLA	NC
25	b2	618	CLA	ND
25	b2	618	CLA	NA
25	B2	605	CLA	NC
25	B2	605	CLA	ND
25	B2	605	CLA	NA
25	B2	606	CLA	NC
25	B2	606	CLA	ND

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Mol	Chain	Res	Type	Atom
25	B2	606	CLA	NA
25	c1	508	CLA	NC
25	c1	508	CLA	ND
25	c1	508	CLA	NA

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	B2	618	CLA	CED-O2D-CGD-CBD
25	B1	611	CLA	CED-O2D-CGD-CBD
29	c2	519	LMG	C8-O7-C10-O9

There are no ring outliers.

127 monomers are involved in 501 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A1	401	BCR	9	0
25	A1	403	CLA	8	0
25	A1	404	CLA	9	0
25	A1	405	CLA	6	0
25	A1	406	CLA	5	0
27	A1	408	PHO	2	0
29	A1	410	LMG	3	0
29	A1	412	LMG	3	0
23	A2	401	BCR	6	0
25	A2	402	CLA	6	0
25	A2	403	CLA	10	0
25	A2	404	CLA	4	0
33	A2	405	LHG	3	0
27	A2	407	PHO	4	0
29	A2	412	LMG	1	0
23	B1	601	BCR	9	0
23	B1	602	BCR	8	0
23	B1	603	BCR	6	0
25	B1	604	CLA	2	0
25	B1	605	CLA	3	0
25	B1	606	CLA	10	0
25	B1	607	CLA	4	0
25	B1	608	CLA	5	0
25	B1	609	CLA	6	0
25	B1	610	CLA	6	0
25	B1	611	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B1	612	CLA	6	0
25	B1	613	CLA	6	0
25	B1	614	CLA	6	0
25	B1	615	CLA	5	0
25	B1	616	CLA	7	0
25	B1	617	CLA	6	0
25	B1	618	CLA	1	0
25	B1	619	CLA	6	0
33	B1	621	LHG	9	0
29	B1	622	LMG	1	0
29	B1	626	LMG	2	0
23	B2	601	BCR	5	0
23	B2	602	BCR	7	0
23	B2	603	BCR	9	0
25	B2	604	CLA	2	0
25	B2	605	CLA	2	0
25	B2	606	CLA	10	0
25	B2	607	CLA	2	0
25	B2	608	CLA	9	0
25	B2	609	CLA	6	0
25	B2	610	CLA	8	0
25	B2	611	CLA	6	0
25	B2	612	CLA	7	0
25	B2	613	CLA	5	0
25	B2	614	CLA	5	0
25	B2	615	CLA	6	0
25	B2	616	CLA	5	0
25	B2	617	CLA	4	0
25	B2	618	CLA	2	0
25	B2	619	CLA	3	0
29	B2	620	LMG	1	0
29	B2	621	LMG	2	0
37	B2	623	SQD	1	0
33	B2	627	LHG	2	0
23	C1	501	BCR	9	0
25	C1	502	CLA	3	0
25	C1	503	CLA	4	0
25	C1	504	CLA	10	0
25	C1	505	CLA	3	0
25	C1	506	CLA	6	0
25	C1	507	CLA	6	0
25	C1	508	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C1	509	CLA	10	0
25	C1	510	CLA	8	0
25	C1	511	CLA	7	0
25	C1	512	CLA	11	0
25	C1	513	CLA	5	0
25	C1	514	CLA	2	0
34	C1	515	DGD	2	0
34	C1	516	DGD	7	0
34	C1	517	DGD	1	0
35	C1	519	LMT	3	0
29	C1	520	LMG	1	0
23	C1	521	BCR	3	0
23	C2	502	BCR	4	0
25	C2	503	CLA	7	0
25	C2	504	CLA	1	0
25	C2	505	CLA	6	0
25	C2	506	CLA	6	0
25	C2	507	CLA	3	0
25	C2	508	CLA	1	0
25	C2	509	CLA	4	0
25	C2	510	CLA	3	0
25	C2	511	CLA	3	0
25	C2	513	CLA	1	0
23	D1	401	BCR	3	0
25	D1	402	CLA	2	0
33	D1	404	LHG	5	0
33	D1	405	LHG	6	0
29	D1	406	LMG	1	0
27	D1	407	PHO	1	0
36	D1	408	PL9	10	0
37	D1	409	SQD	1	0
25	D2	401	CLA	3	0
33	D2	403	LHG	12	0
25	D2	404	CLA	3	0
33	D2	405	LHG	7	0
25	D2	406	CLA	6	0
27	D2	407	PHO	3	0
36	D2	408	PL9	11	0
38	E1	101	HEM	3	0
38	E2	101	HEM	4	0
23	F2	401	BCR	4	0
29	F2	402	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	H1	101	DGD	4	0
23	H1	102	BCR	5	0
34	H2	101	DGD	3	0
23	H2	103	BCR	4	0
29	I2	101	LMG	2	0
23	J1	101	BCR	6	0
23	K1	101	BCR	5	0
25	K2	101	CLA	5	0
23	K2	102	BCR	5	0
23	K2	104	BCR	3	0
33	L1	101	LHG	1	0
35	L1	102	LMT	1	0
33	L2	101	LHG	10	0
29	M1	101	LMG	2	0
35	M1	102	LMT	1	0
38	V1	201	HEM	5	0
38	V2	201	HEM	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	344/344 (100%)	0.10	12 (3%) 48 40	31, 48, 79, 104	0
1	A2	332/344 (96%)	0.49	23 (6%) 20 13	51, 75, 91, 112	0
1	a1	334/344 (97%)	-0.00	12 (3%) 46 39	36, 48, 68, 105	0
1	a2	334/344 (97%)	0.03	16 (4%) 34 26	34, 50, 83, 107	0
2	B1	483/509 (94%)	0.30	30 (6%) 24 17	40, 63, 93, 108	0
2	B2	503/509 (98%)	0.51	53 (10%) 8 5	46, 65, 93, 112	0
2	b1	503/509 (98%)	0.22	28 (5%) 28 20	36, 53, 80, 99	0
2	b2	481/509 (94%)	0.46	39 (8%) 15 9	43, 70, 99, 115	0
3	C1	449/460 (97%)	0.14	25 (5%) 28 20	33, 59, 78, 93	0
3	C2	444/460 (96%)	0.99	78 (17%) 2 1	73, 97, 117, 128	0
3	c1	449/460 (97%)	0.28	24 (5%) 30 22	41, 62, 85, 101	0
3	c2	448/460 (97%)	0.41	30 (6%) 21 14	39, 70, 93, 110	0
4	D1	337/351 (96%)	0.38	21 (6%) 24 17	36, 56, 88, 94	0
4	D2	340/351 (96%)	0.61	33 (9%) 10 6	51, 69, 85, 96	0
4	d1	339/351 (96%)	0.09	7 (2%) 67 60	34, 45, 65, 94	0
4	d2	340/351 (96%)	0.26	17 (5%) 32 24	36, 56, 88, 118	0
5	E1	61/84 (72%)	1.60	24 (39%) 0 0	64, 87, 141, 158	0
5	E2	63/84 (75%)	2.52	31 (49%) 0 0	77, 98, 131, 144	0
5	e1	57/84 (67%)	1.03	13 (22%) 1 1	49, 65, 87, 91	0
5	e2	60/84 (71%)	1.87	22 (36%) 0 0	59, 80, 144, 159	0
6	F1	28/43 (65%)	0.32	2 (7%) 19 12	62, 75, 123, 131	0
6	F2	31/43 (72%)	1.53	8 (25%) 1 0	81, 92, 144, 146	0
6	f1	29/43 (67%)	0.29	3 (10%) 9 5	50, 60, 95, 108	0
6	f2	29/43 (67%)	0.93	7 (24%) 1 1	64, 73, 128, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
7	H1	60/67 (89%)	0.52	9 (15%) 3 2	70, 84, 93, 101	0
7	H2	62/67 (92%)	0.74	10 (16%) 3 1	63, 75, 92, 124	0
7	h1	62/67 (92%)	0.31	3 (4%) 34 26	47, 67, 78, 84	0
7	h2	62/67 (92%)	1.14	13 (20%) 1 1	72, 87, 98, 122	0
8	I1	34/38 (89%)	0.06	1 (2%) 55 47	53, 61, 70, 71	0
8	I2	35/38 (92%)	0.50	2 (5%) 27 20	82, 93, 105, 109	0
8	i1	34/38 (89%)	0.04	1 (2%) 55 47	54, 61, 71, 76	0
8	i2	33/38 (86%)	0.18	2 (6%) 25 17	60, 67, 75, 77	0
9	J1	32/39 (82%)	0.21	3 (9%) 11 6	51, 65, 89, 105	0
9	J2	35/39 (89%)	1.27	9 (25%) 1 0	75, 87, 125, 136	0
9	j1	32/39 (82%)	0.27	5 (15%) 3 2	49, 63, 74, 81	0
9	j2	33/39 (84%)	0.10	1 (3%) 54 46	54, 70, 88, 110	0
10	K1	37/41 (90%)	0.68	3 (8%) 15 9	56, 66, 78, 79	0
10	K2	37/41 (90%)	1.05	9 (24%) 1 0	86, 96, 111, 117	0
10	k1	37/41 (90%)	0.77	7 (18%) 2 1	56, 67, 81, 81	0
10	k2	37/41 (90%)	1.27	9 (24%) 1 0	67, 76, 89, 92	0
11	L1	37/38 (97%)	-0.01	3 (8%) 15 9	39, 43, 67, 77	0
11	L2	37/38 (97%)	-0.04	1 (2%) 58 50	49, 56, 61, 73	0
11	l1	37/38 (97%)	-0.08	1 (2%) 58 50	36, 43, 63, 73	0
11	l2	37/38 (97%)	0.15	0 100 100	43, 47, 73, 79	0
12	M1	40/108 (37%)	0.01	1 (2%) 61 53	32, 46, 62, 67	0
12	M2	40/108 (37%)	0.03	0 100 100	45, 54, 67, 69	0
12	m1	40/108 (37%)	-0.05	0 100 100	34, 44, 65, 67	0
12	m2	40/108 (37%)	0.24	4 (10%) 9 5	44, 51, 65, 71	0
13	O1	240/329 (72%)	0.56	35 (14%) 3 2	38, 61, 96, 107	0
13	O2	205/329 (62%)	1.53	54 (26%) 1 0	54, 91, 119, 151	0
13	o1	238/329 (72%)	0.71	35 (14%) 3 2	38, 76, 121, 145	0
13	o2	245/329 (74%)	0.67	40 (16%) 2 1	41, 64, 103, 127	0
14	T1	30/32 (93%)	-0.20	1 (3%) 50 42	37, 44, 60, 68	0
14	T2	30/32 (93%)	0.08	1 (3%) 50 42	54, 63, 76, 82	0
14	t1	30/32 (93%)	-0.04	3 (10%) 9 5	40, 46, 60, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
14	t2	29/32 (90%)	-0.23	2 (6%) 20 13	38, 48, 68, 84	0
15	U1	93/155 (60%)	0.24	2 (2%) 65 58	44, 59, 75, 104	0
15	U2	90/155 (58%)	1.14	20 (22%) 1 1	74, 91, 104, 115	0
15	u1	93/155 (60%)	0.59	13 (13%) 4 2	53, 68, 88, 95	0
15	u2	93/155 (60%)	0.31	4 (4%) 39 31	44, 58, 71, 86	0
16	V1	129/155 (83%)	0.22	5 (3%) 43 35	47, 62, 87, 93	0
16	V2	129/155 (83%)	1.54	39 (30%) 1 0	75, 96, 114, 127	0
16	v1	129/155 (83%)	0.59	12 (9%) 11 7	47, 69, 108, 124	0
16	v2	129/155 (83%)	0.40	12 (9%) 11 7	47, 63, 90, 105	0
17	Y1	27/35 (77%)	0.08	3 (11%) 7 4	64, 74, 103, 118	0
17	Y2	25/35 (71%)	1.40	8 (32%) 1 0	96, 100, 107, 109	0
17	y1	27/35 (77%)	0.93	6 (22%) 1 1	64, 71, 105, 107	0
17	y2	27/35 (77%)	0.61	5 (18%) 2 1	72, 79, 92, 106	0
18	X1	29/40 (72%)	1.87	9 (31%) 1 0	98, 113, 130, 135	0
18	X2	31/40 (77%)	1.69	12 (38%) 0 0	83, 101, 115, 121	0
18	x1	36/40 (90%)	0.75	6 (16%) 2 1	61, 83, 96, 102	0
18	x2	32/40 (80%)	1.61	13 (40%) 0 0	83, 104, 122, 126	0
19	S1	25/46 (54%)	0.92	5 (20%) 1 1	73, 79, 85, 98	0
19	S2	30/46 (65%)	2.25	16 (53%) 0 0	98, 114, 120, 122	0
19	s1	40/46 (86%)	1.28	11 (27%) 1 0	54, 78, 94, 95	0
19	s2	46/46 (100%)	1.55	13 (28%) 1 0	75, 90, 106, 112	0
20	W1	21/25 (84%)	-0.35	1 (4%) 34 26	71, 79, 86, 90	0
20	W2	21/25 (84%)	-0.73	0 100 100	66, 76, 84, 89	0
20	w1	25/25 (100%)	0.26	4 (16%) 3 1	73, 79, 96, 101	0
20	w2	20/25 (80%)	-0.15	1 (5%) 32 24	91, 96, 103, 111	0
21	Q2	111/218 (50%)	1.90	55 (49%) 0 0	122, 132, 145, 151	0
21	q1	105/218 (48%)	1.93	43 (40%) 0 0	103, 125, 138, 144	0
22	Z2	59/62 (95%)	1.60	22 (37%) 0 0	108, 121, 134, 140	0
22	z2	59/62 (95%)	0.51	7 (11%) 6 3	83, 101, 116, 127	0
All	All	10516/12316 (85%)	0.52	1173 (11%) 7 4	31, 66, 113, 159	0

All (1173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	e2	21	VAL	13.5
13	O2	194	SER	10.3
6	F2	15	ILE	9.3
9	J2	7	ARG	9.1
13	O2	195	GLY	8.6
7	h2	2	ALA	8.4
18	X1	33	SER	8.3
5	E1	78	ASP	8.2
21	q1	172	ILE	8.2
5	E2	80	THR	8.1
13	O2	193	THR	8.0
13	O2	15	LEU	7.7
13	o1	22	VAL	7.7
5	e2	25	ILE	7.5
3	C2	181	PHE	7.5
10	K2	15	TYR	7.3
5	E2	23	HIS	7.2
2	B1	86	SER	7.1
13	O2	14	GLY	7.1
13	O2	214	VAL	7.1
19	s2	36	ALA	7.1
5	E2	58	GLU	6.9
16	V2	78	ASN	6.9
21	Q2	175	ALA	6.9
3	C2	77	PRO	6.9
22	z2	34	SER	6.9
5	E2	57	SER	6.9
1	A1	10	SER	6.8
5	e2	19	TYR	6.8
3	C2	144	PHE	6.7
16	v1	15	ASN	6.7
5	e2	22	ILE	6.6
13	o2	195	GLY	6.6
1	A1	227	THR	6.6
4	d2	228	ALA	6.6
3	C2	183	GLY	6.5
3	C2	182	ILE	6.5
13	O2	220	LEU	6.5
15	U2	76	LYS	6.5
21	q1	149	LEU	6.4
2	B2	82	GLY	6.4
13	O2	211	ILE	6.3
19	S2	15	LEU	6.3

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Mol	Chain	Res	Type	RSRZ
5	E2	72	ALA	6.3
5	e2	78	ASP	6.2
13	o1	178(E)	VAL	6.2
21	Q2	156	VAL	6.2
17	y1	41	THR	6.1
13	o1	220	LEU	6.1
6	f2	17	THR	6.1
13	O2	23	VAL	6.1
13	o2	87	VAL	6.0
2	B1	352	HIS	6.0
2	b2	301	ALA	5.9
5	e1	23	HIS	5.9
13	O1	220	LEU	5.8
19	S1	8	LEU	5.8
19	s2	37	ALA	5.8
13	o1	133	ASP	5.8
21	Q2	160	ALA	5.8
9	J2	9	PRO	5.8
18	x2	32	VAL	5.8
19	s1	29	ALA	5.7
21	q1	215	VAL	5.7
3	C2	357	ARG	5.6
4	d1	14	TRP	5.6
2	B2	492	PHE	5.6
9	J1	9	PRO	5.5
13	O2	191	GLN	5.5
3	C2	392	ALA	5.5
9	J2	40	LEU	5.5
13	o1	195	GLY	5.5
21	q1	141	ALA	5.5
5	E2	25	ILE	5.5
2	B2	413	ASP	5.4
18	X1	32	VAL	5.4
5	E2	76	LEU	5.4
22	Z2	4	ILE	5.4
3	C2	263	ALA	5.4
1	A1	12	SER	5.4
3	c2	249	ILE	5.4
18	X2	12	TRP	5.4
7	H2	4	LYS	5.3
2	b1	86	SER	5.3
7	h2	22	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
3	C2	184	GLY	5.3
17	y1	18	VAL	5.3
2	B2	352	HIS	5.3
6	F2	33	PHE	5.3
21	Q2	153	CYS	5.3
3	C2	258	SER	5.3
21	q1	159	TYR	5.2
22	Z2	57	LEU	5.2
3	C2	250	TRP	5.2
21	q1	216	VAL	5.2
5	E1	22	ILE	5.2
5	E1	25	ILE	5.2
5	e2	23	HIS	5.2
3	C2	207	ALA	5.2
1	A2	12	SER	5.2
13	O2	209	ASN	5.2
21	Q2	192	MET	5.1
9	J2	6	GLY	5.1
3	c2	200	THR	5.1
5	E2	38	VAL	5.1
3	C2	146	PHE	5.1
5	E2	79	LEU	5.1
21	Q2	210	ASP	5.1
16	V2	16	GLY	5.1
6	f2	18	PHE	5.0
5	E2	22	ILE	5.0
5	E2	75	GLU	5.0
16	V2	15	ASN	5.0
1	A2	228	THR	5.0
13	O2	178(D)	ALA	5.0
15	U2	86	PRO	5.0
21	q1	168	GLU	5.0
22	z2	33	TRP	4.9
4	D2	97	ALA	4.9
3	C2	319	VAL	4.9
2	B1	484	ALA	4.9
4	D1	28	VAL	4.9
3	c1	249	ILE	4.9
7	h2	23	PRO	4.9
17	y1	16	TRP	4.8
5	E1	70	PHE	4.8
3	C2	25	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
16	V2	85	SER	4.8
3	C2	206	PRO	4.8
18	x1	26	THR	4.8
13	o1	178(D)	ALA	4.8
19	S2	11	ALA	4.8
17	y2	16	TRP	4.8
8	I2	2	PHE	4.8
3	c2	201	ASN	4.8
3	C2	254	THR	4.8
13	o2	220	LEU	4.8
13	o1	90	ASN	4.8
21	q1	144	LEU	4.8
21	Q2	214	SER	4.8
17	Y2	18	VAL	4.7
5	E1	59	ASN	4.7
3	c2	147	PHE	4.7
21	q1	112	TYR	4.7
2	B2	339	ALA	4.7
4	D1	79	SER	4.7
2	b2	88	PRO	4.7
13	o2	178(E)	VAL	4.6
18	X2	16	TRP	4.6
13	O2	90	ASN	4.6
6	F2	17	THR	4.6
22	Z2	34	SER	4.6
13	O2	2	VAL	4.6
18	X1	30	ILE	4.6
2	B2	126	PRO	4.6
21	Q2	165	THR	4.6
5	E1	41	GLY	4.6
3	C2	177	ILE	4.6
7	h2	26	GLY	4.6
17	y2	41	THR	4.6
21	Q2	182	ARG	4.6
4	D2	14	TRP	4.6
13	O2	200	ALA	4.6
7	H1	25	TRP	4.5
16	V2	18	ILE	4.5
1	a1	344	ALA	4.5
15	U2	84	ALA	4.5
5	E1	19	TYR	4.5
7	h2	25	TRP	4.5

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Mol	Chain	Res	Type	RSRZ
16	V2	94	SER	4.5
15	U2	79	MET	4.5
19	s2	38	ALA	4.5
20	w1	1	ALA	4.5
13	O1	182	LEU	4.5
13	o2	92	THR	4.5
17	Y2	16	TRP	4.5
6	F2	16	PHE	4.5
13	O1	23	VAL	4.5
16	V2	14	THR	4.5
16	V2	107	LEU	4.5
19	S2	29	ALA	4.5
7	H1	63	THR	4.5
21	Q2	186	MET	4.5
10	k2	44	GLY	4.4
3	c1	144	PHE	4.4
21	q1	173	GLU	4.4
21	Q2	159	TYR	4.4
2	b2	77	GLY	4.4
19	s2	8	LEU	4.4
2	B2	301	ALA	4.4
10	K1	42	ALA	4.4
19	s2	4	ALA	4.4
21	q1	165	THR	4.4
7	H1	22	ALA	4.4
16	v1	14	THR	4.4
17	Y2	17	GLN	4.4
7	h2	24	GLY	4.4
2	b2	128	THR	4.4
5	E2	56	PHE	4.4
13	o2	90	ASN	4.3
2	B2	295	GLY	4.3
3	C2	143	SER	4.3
19	S2	7	ALA	4.3
5	e2	20	TRP	4.3
4	D2	27	PHE	4.3
10	k2	45	PHE	4.3
16	V2	99	ASP	4.3
3	c1	254	THR	4.3
5	e2	24	SER	4.3
13	O1	5	LEU	4.3
3	c1	143	SER	4.3

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Mol	Chain	Res	Type	RSRZ
3	C1	140	LEU	4.3
18	x1	32	VAL	4.3
19	S1	9	LEU	4.3
16	V2	132	GLY	4.3
3	c1	181	PHE	4.3
10	k2	14	THR	4.2
13	O2	18	ARG	4.2
3	c1	253	LEU	4.2
13	O2	51	LEU	4.2
16	V2	19	LEU	4.2
19	S2	13	LEU	4.2
5	E2	78	ASP	4.2
3	C2	262	ARG	4.2
21	q1	145	ALA	4.2
21	q1	148	THR	4.2
13	o2	93	TRP	4.2
18	x2	33	SER	4.2
13	O2	87	VAL	4.2
5	e2	58	GLU	4.2
16	V2	104	MET	4.2
2	B1	339	ALA	4.2
19	s1	33	ALA	4.2
1	a2	240	GLY	4.1
3	C2	325	GLY	4.1
21	Q2	196	ASP	4.1
6	f2	21	LEU	4.1
13	O2	41	VAL	4.1
2	b2	376	ILE	4.1
17	Y2	19	ILE	4.1
1	A2	262	TYR	4.1
7	h2	18	TYR	4.1
21	q1	160	ALA	4.1
5	E2	77	ASP	4.1
3	c2	28	ILE	4.1
5	E1	74	GLU	4.1
9	j1	10	LEU	4.1
15	U2	75	ILE	4.1
1	a2	263	ALA	4.1
16	v2	107	LEU	4.1
13	O1	26	SER	4.1
13	O2	237	GLY	4.1
13	o2	207	THR	4.0

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Mol	Chain	Res	Type	RSRZ
9	J2	35	GLY	4.0
16	v2	113	TYR	4.0
4	d2	27	PHE	4.0
5	E2	43	ALA	4.0
15	u1	59	ASP	4.0
6	F1	20	TRP	4.0
16	v1	18	ILE	4.0
2	B1	85	VAL	4.0
4	D2	218	VAL	4.0
2	b2	431	GLU	4.0
21	q1	214	SER	4.0
22	Z2	45	ILE	4.0
1	a2	11	THR	4.0
16	v2	16	GLY	4.0
2	B2	406	LEU	4.0
6	F2	18	PHE	4.0
16	V2	20	ASN	3.9
21	Q2	194	ASP	3.9
6	F2	34	PHE	3.9
19	s1	8	LEU	3.9
3	c2	144	PHE	3.9
3	c2	194	GLY	3.9
16	V2	133	GLY	3.9
19	s1	10	ALA	3.9
18	x2	31	TRP	3.9
3	C2	185	ILE	3.9
10	k2	42	ALA	3.9
16	V2	76	MET	3.9
19	S2	30	TRP	3.9
8	i2	1	MET	3.9
1	A1	262	TYR	3.9
13	O2	22	VAL	3.9
1	A1	13	LEU	3.9
13	O2	-2	THR	3.9
15	U2	92	PHE	3.9
14	T1	30	ALA	3.8
5	E1	24	SER	3.8
8	i2	2	PHE	3.8
13	O1	93	TRP	3.8
15	U2	78	TYR	3.8
2	B1	262	SER	3.8
21	Q2	109	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
3	c2	191	PRO	3.8
15	U2	66	GLU	3.8
16	v2	15	ASN	3.8
13	o1	89	GLU	3.8
9	J2	11	TRP	3.8
5	e2	27	ILE	3.8
15	U2	85	LEU	3.8
21	q1	147	GLY	3.8
22	Z2	35	LYS	3.8
1	a1	261	GLN	3.8
21	q1	140	SER	3.8
13	o1	132	ALA	3.8
5	E2	59	ASN	3.8
17	y2	38	TYR	3.8
2	B2	379	ALA	3.8
3	c2	471	PRO	3.8
1	A1	242	GLU	3.7
7	H2	5	THR	3.7
4	D1	27	PHE	3.7
5	E2	45	ASP	3.7
19	S2	10	ALA	3.7
21	q1	114	ALA	3.7
22	Z2	58	ASN	3.7
4	d1	237	PRO	3.7
7	h1	23	PRO	3.7
21	Q2	212	TRP	3.7
3	c2	204	LEU	3.7
4	d1	97	ALA	3.7
13	o2	35	THR	3.7
22	Z2	59	SER	3.7
3	C2	106	VAL	3.7
5	e2	59	ASN	3.7
5	E1	18	ARG	3.7
21	q1	167	GLN	3.7
14	t1	30	ALA	3.7
2	B1	408	ASN	3.7
5	e1	27	ILE	3.7
3	c2	254	THR	3.7
2	b2	482	ILE	3.6
1	A2	136	ARG	3.6
13	O2	85	LEU	3.6
16	V2	77	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
22	Z2	3	ILE	3.6
13	o2	84	GLU	3.6
15	U2	15	GLU	3.6
3	C2	75	PHE	3.6
3	C2	205	ASN	3.6
13	o1	28	GLY	3.6
2	B1	436	ILE	3.6
3	C2	76	ILE	3.6
2	b2	83	GLU	3.6
2	b2	130	GLU	3.6
22	Z2	55	GLY	3.6
7	H2	54	ILE	3.6
14	T2	29	ILE	3.6
5	e2	30	LEU	3.6
3	c2	145	SER	3.6
4	d2	13	GLY	3.6
5	e2	56	PHE	3.6
1	A2	336	ALA	3.6
15	U2	48	LYS	3.6
16	V2	96	ALA	3.6
3	c2	203	THR	3.6
5	E1	73	ARG	3.6
13	O2	207	THR	3.6
5	E2	44	TYR	3.6
21	Q2	195	GLN	3.6
2	b2	161	LEU	3.6
13	O2	101	MET	3.5
2	B2	284	ILE	3.5
18	x2	4	THR	3.5
2	B1	224	ARG	3.5
13	O2	21	GLU	3.5
3	C2	204	LEU	3.5
3	C2	372	SER	3.5
16	V2	97	SER	3.5
2	B1	126	PRO	3.5
6	f1	45	ARG	3.5
18	x2	30	ILE	3.5
15	U2	87	PRO	3.5
21	q1	156	VAL	3.5
3	C1	200	THR	3.5
7	H2	63	THR	3.5
13	O2	223	THR	3.5

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Mol	Chain	Res	Type	RSRZ
2	b2	298	LEU	3.5
15	U2	55	TYR	3.5
2	b2	86	SER	3.5
19	s2	40	ALA	3.5
13	O2	10	VAL	3.5
2	B1	128	THR	3.5
15	U1	62	LEU	3.5
21	Q2	149	LEU	3.5
3	C2	137	PRO	3.4
3	C2	384	ILE	3.4
5	e1	32	ILE	3.4
13	o2	5	LEU	3.4
10	k1	12	PRO	3.4
13	O1	4	GLN	3.4
5	E2	42	LEU	3.4
19	s1	30	TRP	3.4
4	D2	331	ALA	3.4
1	a1	11	THR	3.4
4	D2	92	LEU	3.4
5	E1	26	THR	3.4
3	c2	32	GLY	3.4
17	y1	40	SER	3.4
2	b1	496	GLN	3.4
2	b2	402	TYR	3.4
3	C2	95	LEU	3.4
5	E1	76	LEU	3.4
2	b2	156	PHE	3.4
5	E1	77	ASP	3.4
2	B2	273	TYR	3.4
5	E2	19	TYR	3.4
15	u2	62	LEU	3.4
13	O2	88	ASN	3.4
21	Q2	171	ASN	3.4
5	e1	36	LEU	3.4
13	O2	178(E)	VAL	3.4
21	Q2	168	GLU	3.4
21	Q2	199	GLU	3.4
9	j1	11	TRP	3.4
21	Q2	167	GLN	3.4
2	B2	416	THR	3.3
13	o1	202	ASN	3.3
18	X2	17	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
21	q1	192	MET	3.3
2	b2	186	GLY	3.3
3	c1	109	TYR	3.3
6	f1	44	GLN	3.3
13	o2	38	TYR	3.3
21	Q2	176	TYR	3.3
2	b1	352	HIS	3.3
17	Y1	16	TRP	3.3
18	X1	31	TRP	3.3
5	E2	41	GLY	3.3
17	Y2	39	LEU	3.3
1	A1	260	PHE	3.3
13	O2	139	SER	3.3
2	b1	504	LYS	3.3
2	B2	378	ARG	3.3
1	A1	249	VAL	3.3
13	o2	208	SER	3.3
3	C1	148	GLY	3.3
2	B2	296	LEU	3.3
3	C2	253	LEU	3.3
4	D1	18	LEU	3.3
21	Q2	188	PHE	3.3
13	o2	0	GLN	3.3
2	B1	481	GLY	3.3
19	s1	9	LEU	3.3
5	e2	61	GLN	3.3
13	O1	195	GLY	3.3
13	O1	200	ALA	3.3
13	O2	206	PRO	3.3
16	V2	136	TYR	3.3
4	D2	64	ALA	3.3
17	y2	40	SER	3.2
3	C2	111	TYR	3.2
10	k1	15	TYR	3.2
21	q1	138	VAL	3.2
9	J1	10	LEU	3.2
4	D1	57	SER	3.2
21	Q2	110	ASN	3.2
21	q1	121	LYS	3.2
3	C2	80	PRO	3.2
3	C2	352	GLY	3.2
21	Q2	105	THR	3.2

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Mol	Chain	Res	Type	RSRZ
4	D2	341	PHE	3.2
10	K2	36	ALA	3.2
13	o2	200	ALA	3.2
19	s1	41	ALA	3.2
16	V1	85	SER	3.2
21	Q2	117	ASN	3.2
5	E2	27	ILE	3.2
2	B2	500	ASP	3.2
13	o1	187	ASP	3.2
21	Q2	204	ALA	3.2
13	o2	218	GLU	3.2
1	A1	309	SER	3.2
5	e2	29	SER	3.2
2	b1	85	VAL	3.2
16	V2	124	GLN	3.2
5	e1	45	ASP	3.2
16	V2	21	ILE	3.2
18	x1	30	ILE	3.2
10	K2	42	ALA	3.2
13	O2	181	VAL	3.2
2	b2	377	ILE	3.2
5	E2	32	ILE	3.2
16	V2	135	ILE	3.2
15	u1	84	ALA	3.2
13	o2	4	GLN	3.2
17	Y2	21	GLN	3.2
13	o1	201	VAL	3.2
21	Q2	116	ILE	3.2
21	Q2	126	ALA	3.2
7	H2	3	LEU	3.2
13	O1	1	ASP	3.1
2	b1	408	ASN	3.1
3	C2	378	ASN	3.1
16	V1	126	GLN	3.1
22	z2	42	THR	3.1
2	B2	375	GLY	3.1
19	s2	3	ALA	3.1
4	D2	352	LEU	3.1
13	O1	246	SER	3.1
16	v2	98	SER	3.1
13	O2	210	GLU	3.1
15	u1	58	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
16	v1	97	SER	3.1
18	x1	38	LEU	3.1
2	b2	126	PRO	3.1
22	Z2	36	SER	3.1
21	q1	155	LYS	3.1
3	c2	250	TRP	3.1
2	b2	339	ALA	3.1
19	s2	41	ALA	3.1
21	q1	190	ALA	3.1
15	U2	18(A)	TYR	3.1
21	Q2	148	THR	3.1
13	o1	245	PRO	3.1
14	t2	29	ILE	3.1
18	x1	36	ASP	3.1
19	s2	34	PHE	3.1
2	B2	129	LEU	3.1
19	S2	21	ALA	3.1
19	s2	35	ALA	3.1
16	V2	91	ILE	3.1
18	X2	26	THR	3.1
19	S2	26	LEU	3.1
5	E2	60	ARG	3.1
2	b1	375	GLY	3.0
13	O1	28	GLY	3.0
3	C1	31	THR	3.0
5	e2	53	ASN	3.0
2	b2	84	SER	3.0
5	E1	58	GLU	3.0
19	s1	7	ALA	3.0
16	V2	131	GLY	3.0
1	a2	264	SER	3.0
15	U2	45	ALA	3.0
20	w2	5	ALA	3.0
21	Q2	198	ALA	3.0
1	a1	337	HIS	3.0
1	A2	230	ASN	3.0
13	o1	216	VAL	3.0
4	D1	95	PRO	3.0
2	B1	483	GLY	3.0
5	E1	32	ILE	3.0
7	h2	19	GLY	3.0
22	Z2	40	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	a2	262	TYR	3.0
13	o1	131	ASN	3.0
4	D2	50	THR	3.0
4	D1	21	TRP	3.0
19	S2	9	LEU	3.0
5	e2	32	ILE	3.0
16	V2	25	GLN	3.0
2	b2	129	LEU	3.0
13	O1	234	LEU	3.0
19	S2	5	ALA	3.0
19	s2	1	ALA	3.0
4	D2	215	GLY	3.0
10	k2	28	ILE	3.0
1	a1	252	HIS	3.0
3	c2	146	PHE	3.0
13	o2	50	PHE	3.0
7	H2	55	LEU	3.0
13	O1	244	LEU	3.0
13	o2	201	VAL	3.0
21	q1	217	GLY	3.0
22	Z2	30	ALA	3.0
3	C2	368	PRO	3.0
10	k1	29	PRO	3.0
16	V2	93	PRO	3.0
13	O1	90	ASN	3.0
21	Q2	132	LYS	3.0
4	D1	66	SER	3.0
17	Y2	38	TYR	3.0
19	S2	18	VAL	3.0
7	h1	26	GLY	3.0
4	D2	327	ALA	3.0
16	V1	13	ASP	2.9
3	c1	137	PRO	2.9
16	V2	100	ILE	2.9
4	D2	15	PHE	2.9
3	C2	82	TYR	2.9
2	B2	219	VAL	2.9
3	c1	207	ALA	2.9
16	V2	86	GLU	2.9
21	q1	110	ASN	2.9
4	d2	226	GLY	2.9
13	O1	181	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
6	f2	20	TRP	2.9
21	Q2	185	ASP	2.9
1	A2	337	HIS	2.9
8	I2	6	ILE	2.9
13	o2	196	ARG	2.9
18	X1	11	PHE	2.9
2	B2	502	THR	2.9
5	e2	26	THR	2.9
16	v1	80	THR	2.9
20	w1	6	VAL	2.9
1	A2	99	ALA	2.9
3	C2	110	PRO	2.9
3	C2	189	TRP	2.9
7	H1	59	ASP	2.9
16	V2	51	ASN	2.9
16	v2	99	ASP	2.9
13	O2	39	LYS	2.9
15	u1	61	ILE	2.9
1	a1	12	SER	2.9
11	l1	2	GLY	2.9
21	Q2	158	SER	2.9
21	q1	153	CYS	2.9
2	B2	85	VAL	2.9
3	C2	78	GLU	2.9
13	O2	171	ALA	2.9
16	V2	127	ALA	2.9
3	C2	150	ASP	2.9
21	q1	120	LYS	2.9
16	v2	105	ARG	2.9
2	B2	179	GLN	2.9
3	C2	247	GLY	2.9
3	c2	184	GLY	2.9
5	e1	22	ILE	2.9
13	O1	91	GLY	2.9
21	Q2	104	ILE	2.9
21	Q2	154	SER	2.9
3	C2	141	GLU	2.9
13	o2	1	ASP	2.9
19	S1	32	ALA	2.9
22	Z2	11	ALA	2.9
3	C2	362	ARG	2.9
5	E2	61	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A1	248	ILE	2.9
13	O1	25	SER	2.9
3	C1	55	ALA	2.9
16	v1	19	LEU	2.8
3	C1	26	ARG	2.8
3	c2	26	ARG	2.8
2	B2	394	GLN	2.8
1	a1	262	TYR	2.8
4	D1	14	TRP	2.8
6	f2	23	ILE	2.8
3	C2	473	ASP	2.8
4	D2	230	ASP	2.8
13	O1	0	GLN	2.8
3	C2	149	TYR	2.8
2	b1	262	SER	2.8
4	D2	26	ARG	2.8
1	a2	228	THR	2.8
10	K2	14	THR	2.8
2	B2	218	ASN	2.8
10	k2	46	ARG	2.8
4	D1	15	PHE	2.8
13	O2	9	GLN	2.8
2	B2	350	GLU	2.8
10	K2	44	GLY	2.8
3	C1	199	ILE	2.8
3	C2	142	ASP	2.8
15	u1	60	ASP	2.8
19	s2	39	PHE	2.8
3	c1	465	PRO	2.8
13	o1	214	VAL	2.8
5	e1	24	SER	2.8
16	v1	39	SER	2.8
13	o1	93	TRP	2.8
3	C1	127	PHE	2.8
4	D1	65	SER	2.8
3	c1	82	TYR	2.8
5	E2	20	TRP	2.8
2	b1	492	PHE	2.8
3	C2	373	ASN	2.8
2	B1	252	VAL	2.7
16	V2	126	GLN	2.7
21	q1	194	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
13	O2	5	LEU	2.7
3	C2	382	ASN	2.7
13	O1	136	ILE	2.7
18	X1	15	ILE	2.7
10	k2	29	PRO	2.7
3	c2	143	SER	2.7
13	o1	194	SER	2.7
5	e2	77	ASP	2.7
2	B2	420	TYR	2.7
6	F1	34	PHE	2.7
3	c1	463	ASN	2.7
2	B1	295	GLY	2.7
5	e1	59	ASN	2.7
3	C1	28	ILE	2.7
17	y1	36	ILE	2.7
1	A2	316	THR	2.7
9	j2	9	PRO	2.7
7	h2	21	VAL	2.7
22	z2	31	SER	2.7
7	h2	55	LEU	2.7
16	V1	14	THR	2.7
9	J2	39	SER	2.7
22	Z2	22	ALA	2.7
1	A1	9	GLU	2.7
2	B1	285	GLU	2.7
4	d2	227	GLU	2.7
4	d2	93	TRP	2.7
2	B2	293	SER	2.7
5	e1	33	ALA	2.7
2	B1	437	LEU	2.7
3	C2	435	PHE	2.7
4	D2	59	TYR	2.7
9	J1	32	SER	2.7
16	V2	38	SER	2.7
13	o2	214	VAL	2.7
16	v2	42	VAL	2.7
18	x2	3	MET	2.7
21	q1	117	ASN	2.7
13	o1	234	LEU	2.7
3	C2	302	TYR	2.7
4	d1	227	GLU	2.7
15	u1	69	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	B2	168	ILE	2.7
5	E1	69	ARG	2.7
2	b2	180	SER	2.7
3	c1	114	THR	2.7
7	H1	23	PRO	2.6
7	h1	2	ALA	2.6
4	D2	54	PHE	2.6
1	A2	306	ILE	2.6
11	L1	3	ILE	2.6
3	C2	108	THR	2.6
1	a2	100	ALA	2.6
3	C1	191	PRO	2.6
22	Z2	48	VAL	2.6
13	o2	32	LEU	2.6
3	C1	143	SER	2.6
18	X1	6	SER	2.6
13	O2	20	PRO	2.6
2	B2	288	VAL	2.6
13	o1	210	GLU	2.6
13	o2	65	PHE	2.6
2	b1	164	PRO	2.6
3	C2	180	LEU	2.6
10	K1	11	LEU	2.6
15	U1	63	LYS	2.6
2	B2	376	ILE	2.6
3	c1	208	ILE	2.6
3	C2	36	TRP	2.6
3	C1	137	PRO	2.6
4	d2	236	THR	2.6
13	O2	13	THR	2.6
18	x2	5	PRO	2.6
3	C2	155	ASN	2.6
13	o2	63	ARG	2.6
2	B1	288	VAL	2.6
3	c1	142	ASP	2.6
6	F2	40	MET	2.6
21	q1	109	LEU	2.6
13	O2	137	SER	2.6
13	o1	230	PRO	2.6
2	B1	2	ALA	2.6
13	o1	165	ALA	2.6
13	O2	241	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
21	Q2	138	VAL	2.6
1	a2	242	GLU	2.6
1	a2	243	GLU	2.6
2	b2	375	GLY	2.6
5	E1	56	PHE	2.6
7	H2	8	GLY	2.6
21	Q2	179	PHE	2.6
3	C1	73	SER	2.6
2	b1	126	PRO	2.6
5	e1	40	THR	2.6
12	m2	33	ASN	2.6
13	O2	111	PRO	2.6
18	X1	16	TRP	2.6
4	D2	332	GLN	2.6
21	Q2	170	GLN	2.6
3	c2	135	VAL	2.6
4	D2	339	PHE	2.6
10	k1	18	PHE	2.6
13	O1	202	ASN	2.5
17	Y1	17	GLN	2.5
13	o2	91	GLY	2.5
2	B2	434	ARG	2.5
18	X2	3	MET	2.5
19	s1	34	PHE	2.5
4	D2	66	SER	2.5
2	B2	501	LYS	2.5
7	h2	4	LYS	2.5
2	b2	338	GLU	2.5
4	D2	107	ILE	2.5
10	K1	13	GLU	2.5
21	Q2	131	ALA	2.5
18	X2	27	GLY	2.5
18	X2	32	VAL	2.5
2	b2	220	ARG	2.5
2	B2	491	GLU	2.5
13	O2	192	GLU	2.5
15	U2	29	ASN	2.5
16	v1	20	ASN	2.5
14	t2	27	PRO	2.5
3	c1	57	ALA	2.5
16	V2	71	ALA	2.5
19	s2	25	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
3	c2	472	LEU	2.5
13	O1	22	VAL	2.5
13	O1	65	PHE	2.5
13	O2	120	PHE	2.5
16	v1	101	PHE	2.5
1	A2	111	PRO	2.5
2	B1	435	THR	2.5
3	C2	53	HIS	2.5
13	O2	136	ILE	2.5
13	O2	138	THR	2.5
13	o2	227	ALA	2.5
21	q1	119	ALA	2.5
15	U2	56	GLY	2.5
1	a2	246	TYR	2.5
5	e2	55	TYR	2.5
2	B1	347	GLN	2.5
4	D2	217	THR	2.5
9	j1	9	PRO	2.5
4	D2	68	LEU	2.5
18	x2	12	TRP	2.5
4	D1	78	VAL	2.5
13	o1	87	VAL	2.5
21	q1	146	VAL	2.5
4	d2	15	PHE	2.5
13	O1	94	LYS	2.5
16	v2	20	ASN	2.5
3	c1	473	ASP	2.5
13	o1	134	ASP	2.5
18	X1	28	ALA	2.5
21	q1	183	ILE	2.5
2	B2	490	VAL	2.5
13	o2	194	SER	2.5
17	y1	38	TYR	2.5
1	A2	266	ASN	2.5
1	A2	229	GLU	2.5
2	B2	289	GLU	2.5
15	U2	65	PRO	2.5
4	D1	60	THR	2.5
3	c2	252	ILE	2.5
7	H2	25	TRP	2.5
2	B2	294	ASN	2.5
7	H2	24	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	a1	343	LEU	2.4
2	B2	225	LEU	2.4
4	D1	107	ILE	2.4
16	V2	98	SER	2.4
18	x2	16	TRP	2.4
21	Q2	215	VAL	2.4
21	Q2	216	VAL	2.4
22	Z2	31	SER	2.4
15	u1	82	PHE	2.4
10	k2	13	GLU	2.4
21	Q2	183	ILE	2.4
13	o2	66	VAL	2.4
2	B2	191	ASN	2.4
3	C1	144	PHE	2.4
15	u2	21	GLY	2.4
3	c2	206	PRO	2.4
18	x2	26	THR	2.4
20	w1	2	ALA	2.4
1	A2	300	LEU	2.4
3	C1	253	LEU	2.4
4	d2	26	ARG	2.4
16	V2	32	LEU	2.4
18	X2	23	LEU	2.4
21	Q2	172	ILE	2.4
4	D2	172	SER	2.4
1	A2	205	VAL	2.4
5	E2	74	GLU	2.4
6	f2	16	PHE	2.4
15	u1	86	PRO	2.4
2	b2	296	LEU	2.4
6	f2	22	ALA	2.4
13	O1	142	LEU	2.4
3	C1	60	ILE	2.4
2	B2	121	ASP	2.4
3	C1	142	ASP	2.4
21	q1	170	GLN	2.4
1	a2	236	GLY	2.4
2	b1	351	GLY	2.4
15	u1	55	TYR	2.4
21	q1	176	TYR	2.4
22	z2	15	TYR	2.4
17	y2	42	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	a1	336	ALA	2.4
2	B1	255	THR	2.4
3	c1	45	LEU	2.4
16	v2	19	LEU	2.4
7	h2	43	ILE	2.4
9	J2	8	ILE	2.4
13	o1	49	GLN	2.4
18	x1	33	SER	2.4
1	a2	255	PHE	2.4
3	c1	147	PHE	2.4
15	u2	78	TYR	2.4
13	O1	245	PRO	2.4
2	B2	298	LEU	2.4
2	B2	309	LEU	2.4
13	o1	193	THR	2.4
22	Z2	51	VAL	2.4
16	V2	134	LYS	2.4
21	q1	143	ARG	2.4
3	C2	322	GLN	2.4
4	D2	216	ALA	2.4
5	e2	33	ALA	2.4
13	o2	182	LEU	2.4
15	u2	67	LEU	2.4
17	Y2	40	SER	2.4
19	S1	29	ALA	2.4
21	Q2	129	ALA	2.4
4	D2	25	ASP	2.4
3	C1	252	ILE	2.4
5	E2	71	ASN	2.4
13	o2	88	ASN	2.4
13	o2	94	LYS	2.4
13	o2	96	ILE	2.4
1	A2	14	TRP	2.4
5	E1	60	ARG	2.4
18	x2	19	VAL	2.4
3	C1	159	THR	2.3
5	E2	26	THR	2.3
18	X2	20	LEU	2.3
20	w1	5	ALA	2.3
3	C2	294	ASN	2.3
3	C2	249	ILE	2.3
3	c1	62	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
13	o2	146	PHE	2.3
2	b1	185	TRP	2.3
2	B1	480	ALA	2.3
3	C1	467	LEU	2.3
3	C2	333	GLY	2.3
4	D1	77	ALA	2.3
4	d1	226	GLY	2.3
2	b2	162	PHE	2.3
18	x2	34	GLN	2.3
1	a2	252	HIS	2.3
3	C2	81	LEU	2.3
10	k1	11	LEU	2.3
13	O1	226	GLY	2.3
13	O1	227	ALA	2.3
13	O2	142	LEU	2.3
16	V2	34	ASN	2.3
2	b1	376	ILE	2.3
13	O1	201	VAL	2.3
4	D2	96	GLU	2.3
19	S2	8	LEU	2.3
3	C1	181	PHE	2.3
10	k2	27	VAL	2.3
3	c2	141	GLU	2.3
2	b2	69	LEU	2.3
4	D1	80	SER	2.3
4	D2	65	SER	2.3
5	E2	24	SER	2.3
2	B2	349	LYS	2.3
2	b2	408	ASN	2.3
11	L1	4	ASN	2.3
13	o1	138	THR	2.3
20	W1	20	ALA	2.3
21	Q2	189	ALA	2.3
10	k1	28	ILE	2.3
1	A2	16	ARG	2.3
4	D2	233	ARG	2.3
2	b2	82	GLY	2.3
3	C2	387	TRP	2.3
4	D1	226	GLY	2.3
4	D2	13	GLY	2.3
3	C2	145	SER	2.3
5	e2	39	SER	2.3

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Mol	Chain	Res	Type	RSRZ
13	o2	36	LYS	2.3
16	v2	39	SER	2.3
22	Z2	44	SER	2.3
1	A2	135	TYR	2.3
2	b2	155	ALA	2.3
10	K2	19	ALA	2.3
18	x2	17	ALA	2.3
21	Q2	141	ALA	2.3
2	B1	431	GLU	2.3
1	A2	143	ILE	2.3
4	D2	73	PHE	2.3
13	o1	66	VAL	2.3
18	X2	19	VAL	2.3
3	C2	232	ASP	2.3
3	C2	35	TRP	2.3
4	d2	21	TRP	2.3
1	A2	296	ASN	2.3
3	C1	59	LEU	2.3
7	H1	2	ALA	2.3
2	B1	430	PHE	2.3
2	B2	348	ASP	2.3
2	B2	405	LYS	2.3
8	I1	2	PHE	2.3
2	b2	119	ASP	2.3
21	Q2	123	ILE	2.3
4	D2	247	VAL	2.3
15	u1	83	VAL	2.3
13	O1	45	LEU	2.2
21	q1	198	ALA	2.2
15	u1	57	THR	2.2
21	q1	191	ARG	2.2
1	A2	77	ILE	2.2
2	b1	369	ILE	2.2
16	v1	13	ASP	2.2
19	S2	22	VAL	2.2
1	a2	12	SER	2.2
13	O1	85	LEU	2.2
13	o1	45	LEU	2.2
16	V2	50	PRO	2.2
3	C2	55	ALA	2.2
12	m2	36	MET	2.2
16	v1	104	MET	2.2

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Mol	Chain	Res	Type	RSRZ
6	F2	45	ARG	2.2
14	t1	28	ARG	2.2
19	s1	36	ALA	2.2
19	S2	14	ALA	2.2
2	B2	172	TYR	2.2
2	b1	495	PHE	2.2
2	b1	377	ILE	2.2
14	t1	29	ILE	2.2
16	V1	40	CYS	2.2
22	z2	46	GLY	2.2
4	D1	267	LEU	2.2
5	e1	30	LEU	2.2
3	C2	331	THR	2.2
2	b1	151	PHE	2.2
4	D1	341	PHE	2.2
12	m2	38	GLU	2.2
21	q1	116	ILE	2.2
5	E1	57	SER	2.2
1	A2	312	ARG	2.2
4	D1	63	LEU	2.2
2	B2	302	TRP	2.2
3	C2	321	ASP	2.2
2	b1	411	PHE	2.2
2	b2	426	PHE	2.2
3	c1	212	TYR	2.2
10	K2	22	ILE	2.2
12	M1	33	ASN	2.2
21	Q2	113	ARG	2.2
3	C2	101	PRO	2.2
5	E1	30	LEU	2.2
5	E2	28	PRO	2.2
2	B1	405	LYS	2.2
2	b1	438	ASP	2.2
12	m2	39	ALA	2.2
11	L1	2	GLY	2.2
13	o1	180	GLU	2.2
3	c2	109	TYR	2.2
4	d2	235	PHE	2.2
2	B2	498	VAL	2.2
3	c2	152	ARG	2.2
13	o1	51	LEU	2.2
2	b2	197	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
3	C1	57	ALA	2.2
3	C2	452	ALA	2.2
19	S1	30	TRP	2.2
11	L2	2	GLY	2.2
2	B1	284	ILE	2.2
17	Y1	40	SER	2.2
22	z2	38	SER	2.2
5	e1	42	LEU	2.2
3	C2	356	MET	2.2
21	q1	126	ALA	2.2
13	O1	-2	THR	2.2
21	Q2	203	THR	2.2
4	d2	54	PHE	2.2
6	f1	18	PHE	2.2
3	C2	465	PRO	2.1
2	b2	378	ARG	2.1
13	o2	178(D)	ALA	2.1
2	B1	423	LYS	2.1
5	E1	75	GLU	2.1
13	o2	130	ASN	2.1
7	H1	60	ILE	2.1
13	O2	238	VAL	2.1
2	B2	299	PRO	2.1
13	O1	78	LEU	2.1
15	U2	54	PRO	2.1
2	b1	260	ALA	2.1
13	O1	165	ALA	2.1
19	S2	12	ALA	2.1
4	d2	238	THR	2.1
13	O2	77	THR	2.1
4	D2	169	PHE	2.1
10	K2	18	PHE	2.1
13	O2	208	SER	2.1
16	v2	38	SER	2.1
22	Z2	28	SER	2.1
2	b2	120	LEU	2.1
3	C2	208	ILE	2.1
3	C1	473	ASP	2.1
2	B2	224	ARG	2.1
3	C2	79	LYS	2.1
13	O2	11	LYS	2.1
5	e1	75	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
7	H1	5	THR	2.1
1	a1	260	PHE	2.1
1	a1	216	GLY	2.1
4	d2	24	ARG	2.1
3	c1	77	PRO	2.1
5	E1	23	HIS	2.1
19	s1	40	ALA	2.1
1	A1	266	ASN	2.1
2	b1	162	PHE	2.1
2	B1	125	ASP	2.1
16	V2	66	ARG	2.1
1	a2	235	TYR	2.1
2	b1	174	LEU	2.1
3	C2	227	VAL	2.1
13	o1	244	LEU	2.1
4	d2	112	THR	2.1
7	h2	27	THR	2.1
1	a1	16	ARG	2.1
2	b2	297	SER	2.1
22	Z2	17	PHE	2.1
4	d2	25	ASP	2.1
1	a2	249	VAL	2.1
2	b1	436	ILE	2.1
3	c1	53	HIS	2.1
9	J2	14	VAL	2.1
3	c1	471	PRO	2.1
2	B2	2	ALA	2.1
2	B2	182	ALA	2.1
2	b2	260	ALA	2.1
5	E1	72	ALA	2.1
21	Q2	174	LYS	2.1
13	o2	26	SER	2.1
2	b1	498	VAL	2.1
7	H1	3	LEU	2.1
4	d1	98	GLN	2.1
2	B1	402	TYR	2.1
21	q1	166	LYS	2.1
1	A2	305	SER	2.1
3	C2	335	THR	2.1
4	d2	240	SER	2.1
13	O1	138	THR	2.1
8	i1	2	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
21	Q2	142	LEU	2.0
18	X2	21	VAL	2.0
21	Q2	107	GLU	2.0
2	b1	503	THR	2.0
13	o2	31	SER	2.0
3	C1	257	PHE	2.0
13	o1	50	PHE	2.0
9	j1	40	LEU	2.0
22	Z2	41	VAL	2.0
3	c2	208	ILE	2.0
2	b2	350	GLU	2.0
2	b1	484	ALA	2.0
2	B2	480	ALA	2.0
16	v1	116	ALA	2.0
2	B2	396	GLY	2.0
4	D1	240	SER	2.0
9	j1	32	SER	2.0
10	K2	23	ASP	2.0
15	U2	23	ASP	2.0
22	Z2	47	TRP	2.0
3	c2	119	LEU	2.0
3	c2	253	LEU	2.0
15	u1	62	LEU	2.0
2	b1	142	HIS	2.0
10	k1	46	ARG	2.0
2	b2	436	ILE	2.0
3	c2	107	ASN	2.0
21	Q2	211	ASN	2.0
4	d1	56	SER	2.0
13	O2	144	GLY	2.0
18	X2	13	SER	2.0
13	o2	68	THR	2.0
15	u1	38	PHE	2.0
3	C2	318	LEU	2.0
13	o1	192	GLU	2.0
21	Q2	150	ARG	2.0
7	H2	23	PRO	2.0
13	O2	48	LYS	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
28	UNL	l1	103	12/-	0.87	0.35	10.49	35,47,53,55	0
28	UNL	b1	630	17/-	0.78	0.41	8.63	48,57,74,75	0
28	UNL	B1	623	16/-	0.74	0.28	7.57	53,68,72,74	0
23	BCR	K1	101	31/40	0.58	0.54	7.40	64,82,93,96	0
28	UNL	m2	101	18/-	0.82	0.33	6.95	44,57,79,85	0
35	LMT	a2	406	35/35	0.61	0.36	6.60	43,80,92,94	0
23	BCR	c2	501	40/40	0.77	0.36	6.27	66,82,89,92	0
32	GOL	a2	415	6/6	0.92	0.46	5.85	47,55,59,63	0
23	BCR	H2	103	24/40	0.81	0.30	5.57	65,76,82,85	0
28	UNL	b2	607	12/-	0.73	0.36	5.50	64,75,80,87	0
28	UNL	b1	629	15/-	0.74	0.29	5.47	46,59,71,83	0
29	LMG	j2	101	50/55	0.72	0.41	5.43	60,78,97,107	0
28	UNL	B2	625	18/-	0.77	0.34	5.32	37,56,68,68	0
28	UNL	d2	411	12/-	0.86	0.41	5.32	55,67,73,79	0
28	UNL	J2	101	10/-	0.42	0.86	5.15	71,82,86,88	0
32	GOL	B1	620	6/6	0.81	0.31	4.86	63,75,81,82	0
28	UNL	m2	102	18/-	0.70	0.38	4.81	46,65,79,79	0
28	UNL	a2	401	18/-	0.79	0.30	4.78	46,56,70,86	0
29	LMG	b2	622	39/55	0.78	0.30	4.76	47,60,85,90	0
28	UNL	C2	517	18/-	0.63	0.44	4.73	74,83,87,89	0
35	LMT	m2	103	30/35	0.74	0.29	4.38	52,89,111,113	0
28	UNL	a2	409	18/-	0.63	0.34	4.29	61,74,86,90	0
31	BCT	a1	413	4/4	0.96	0.37	4.01	43,48,48,50	0
29	LMG	B2	621	37/55	0.85	0.25	3.84	53,68,80,96	0
23	BCR	H1	102	22/40	0.86	0.23	3.82	75,88,95,100	0
37	SQD	B2	623	45/54	0.79	0.34	3.71	58,79,89,96	0
28	UNL	B2	622	17/-	0.73	0.29	3.69	57,71,76,78	0
23	BCR	b1	602	40/40	0.84	0.25	3.53	35,57,65,73	0
32	GOL	c2	518	6/6	0.75	0.35	3.52	50,55,59,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	BCR	B1	602	40/40	0.86	0.21	3.46	49,62,74,78	0
25	CLA	C2	506	65/65	0.85	0.33	3.45	78,90,97,100	0
28	UNL	t1	101	18/-	0.70	0.40	3.44	43,60,66,67	0
28	UNL	a2	411	11/-	0.82	0.30	3.42	51,55,65,67	0
28	UNL	A2	408	18/-	0.69	0.38	3.35	62,83,92,93	0
28	UNL	B1	625	7/-	0.88	0.27	3.33	45,52,55,63	0
29	LMG	d1	411	35/55	0.70	0.34	3.31	58,76,94,99	0
35	LMT	l1	101	24/35	0.80	0.28	3.29	42,55,89,90	0
37	SQD	b2	605	45/54	0.82	0.31	3.26	54,83,114,124	0
35	LMT	b2	621	35/35	0.65	0.35	3.16	69,110,123,123	0
29	LMG	M1	101	31/55	0.89	0.24	3.09	41,52,63,70	0
23	BCR	K2	102	40/40	0.65	0.45	2.94	84,99,113,115	0
23	BCR	k1	101	40/40	0.80	0.43	2.88	56,70,82,85	0
28	UNL	A1	409	14/-	0.89	0.21	2.83	44,48,57,68	0
33	LHG	B2	627	42/49	0.74	0.32	2.68	67,88,120,132	0
33	LHG	b2	625	43/49	0.60	0.41	2.59	62,87,109,126	0
28	UNL	x1	101	15/-	0.77	0.39	2.56	55,73,79,82	0
35	LMT	c1	517	33/35	0.64	0.43	2.48	63,100,117,119	0
32	GOL	i1	101	6/6	0.87	0.49	2.47	55,57,60,64	0
28	UNL	B2	624	8/-	0.86	0.24	2.44	46,51,54,55	0
28	UNL	a1	409	11/-	0.87	0.23	2.37	43,51,60,63	0
23	BCR	b2	603	40/40	0.81	0.26	2.29	60,74,102,104	0
23	BCR	c1	502	40/40	0.79	0.33	2.29	57,66,72,72	0
35	LMT	m1	101	35/35	0.81	0.24	2.27	44,80,103,112	0
28	UNL	d1	410	12/-	0.68	0.31	2.20	49,72,77,79	0
35	LMT	m2	104	29/35	0.76	0.27	2.17	49,104,119,122	0
23	BCR	J1	101	40/40	0.86	0.33	2.13	50,70,86,88	0
28	UNL	j1	101	17/-	0.59	0.46	2.13	60,69,71,77	0
25	CLA	C1	502	65/65	0.89	0.23	2.13	51,63,68,70	0
36	PL9	d2	409	55/55	0.88	0.28	2.07	33,44,56,57	0
25	CLA	B1	604	42/65	0.77	0.31	2.05	83,98,107,113	0
28	UNL	B1	624	18/-	0.83	0.27	2.04	43,71,79,81	0
25	CLA	B2	606	65/65	0.90	0.25	2.02	53,67,75,78	0
37	SQD	D1	409	35/54	0.85	0.35	2.01	61,75,92,97	0
33	LHG	a2	407	30/49	0.55	0.37	1.94	55,75,94,102	0
35	LMT	b2	623	35/35	0.80	0.30	1.92	63,90,98,101	0
29	LMG	c1	519	55/55	0.87	0.26	1.89	47,70,84,91	0
23	BCR	z2	101	40/40	0.80	0.41	1.88	80,95,100,101	0
25	CLA	b2	611	65/65	0.92	0.29	1.86	66,72,80,83	0
23	BCR	b2	602	40/40	0.87	0.20	1.84	51,70,78,82	0
23	BCR	B1	601	40/40	0.92	0.20	1.83	41,55,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	BCR	B2	603	40/40	0.90	0.25	1.83	46,59,76,81	0
38	HEM	E1	101	43/43	0.90	0.43	1.80	108,134,152,155	0
23	BCR	b2	601	40/40	0.91	0.22	1.79	51,61,69,72	0
23	BCR	k2	501	40/40	0.86	0.29	1.76	61,84,95,98	0
33	LHG	A2	405	33/49	0.81	0.34	1.72	70,80,90,97	0
25	CLA	b2	618	65/65	0.88	0.25	1.66	68,82,90,92	0
25	CLA	a2	405	65/65	0.91	0.20	1.65	51,60,81,87	0
25	CLA	B1	615	65/65	0.95	0.18	1.65	35,47,73,80	0
28	UNL	b1	627	16/-	0.76	0.27	1.65	42,56,75,77	0
28	UNL	d2	410	13/-	0.55	0.59	1.63	74,92,108,111	0
23	BCR	h2	101	40/40	0.76	0.36	1.60	71,85,107,109	0
25	CLA	d1	406	65/65	0.87	0.23	1.52	44,58,94,99	0
29	LMG	C1	520	48/55	0.82	0.26	1.50	59,69,78,86	0
35	LMT	L1	102	12/35	0.91	0.21	1.46	35,45,59,62	0
33	LHG	D1	404	49/49	0.88	0.26	1.44	48,60,84,90	0
25	CLA	B1	619	65/65	0.93	0.20	1.36	32,50,57,73	0
28	UNL	b1	626	13/-	0.70	0.29	1.34	53,64,83,86	0
25	CLA	b1	619	65/65	0.89	0.21	1.31	48,62,81,85	0
25	CLA	b2	620	65/65	0.94	0.21	1.26	42,56,63,72	0
23	BCR	B2	602	40/40	0.87	0.20	1.26	47,59,80,86	0
25	CLA	a1	404	60/65	0.91	0.19	1.25	49,57,82,89	0
25	CLA	c2	508	65/65	0.91	0.22	1.24	68,78,84,88	0
25	CLA	B2	604	41/65	0.90	0.32	1.23	68,79,92,97	0
29	LMG	b1	624	39/55	0.83	0.36	1.19	58,73,84,87	0
25	CLA	B2	612	65/65	0.91	0.23	1.18	58,64,71,83	0
25	CLA	B1	617	65/65	0.90	0.24	1.17	59,67,74,75	0
23	BCR	C1	521	40/40	0.78	0.29	1.16	59,68,80,84	0
23	BCR	j2	102	40/40	0.81	0.28	1.15	59,75,86,87	0
25	CLA	c2	503	65/65	0.93	0.22	1.12	53,62,83,89	0
36	PL9	D1	408	55/55	0.93	0.25	1.11	28,42,52,63	0
25	CLA	c1	503	65/65	0.91	0.22	1.09	55,66,71,75	0
23	BCR	K2	104	29/40	0.74	0.38	1.08	92,100,109,112	0
25	CLA	b1	604	65/65	0.86	0.26	1.05	52,78,110,115	0
33	LHG	d2	406	49/49	0.93	0.20	1.05	36,50,59,66	0
25	CLA	C2	503	65/65	0.85	0.28	1.04	94,104,112,116	0
25	CLA	c2	502	65/65	0.89	0.22	1.03	60,78,85,90	0
28	UNL	B2	626	15/-	0.65	0.36	1.02	79,83,92,95	0
25	CLA	B2	608	65/65	0.94	0.21	1.00	43,53,70,76	0
25	CLA	b2	619	59/65	0.87	0.23	1.00	71,80,106,109	0
34	DGD	H2	101	62/66	0.83	0.26	1.00	51,74,83,85	0
33	LHG	d1	402	32/49	0.82	0.27	1.00	45,63,76,86	0
25	CLA	C1	513	61/65	0.84	0.28	0.98	49,68,74,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
25	CLA	B2	610	65/65	0.93	0.20	0.96	44,59,82,86	0
25	CLA	b2	606	65/65	0.91	0.26	0.95	68,77,84,90	0
29	LMG	B2	620	40/55	0.87	0.26	0.95	62,74,97,98	0
25	CLA	B2	614	65/65	0.91	0.23	0.94	46,58,66,68	0
23	BCR	a2	402	40/40	0.94	0.19	0.94	33,51,62,67	0
25	CLA	B1	618	58/65	0.85	0.25	0.93	53,64,80,86	0
29	LMG	a1	412	51/55	0.81	0.26	0.92	54,67,77,91	0
23	BCR	a1	401	40/40	0.93	0.20	0.92	47,56,64,65	0
25	CLA	C1	506	65/65	0.91	0.21	0.92	49,62,70,73	0
28	UNL	W2	101	9/-	0.85	0.21	0.92	64,77,83,87	0
25	CLA	C2	509	65/65	0.84	0.25	0.91	90,101,106,108	0
27	PHO	a2	416	64/64	0.92	0.20	0.90	35,46,53,62	0
25	CLA	b1	605	65/65	0.94	0.24	0.89	38,52,60,66	0
29	LMG	F2	402	35/55	0.79	0.29	0.87	68,81,91,92	0
25	CLA	B2	607	65/65	0.91	0.20	0.86	49,59,73,78	0
25	CLA	c2	510	54/65	0.91	0.23	0.86	64,69,77,79	0
31	BCT	A1	413	4/4	0.96	0.27	0.85	54,60,62,63	0
36	PL9	d1	409	55/55	0.91	0.24	0.85	28,41,50,61	0
29	LMG	b1	631	40/55	0.84	0.23	0.84	29,52,85,92	0
25	CLA	B1	611	62/65	0.85	0.25	0.84	58,78,87,89	0
25	CLA	A2	403	61/65	0.88	0.26	0.84	80,89,98,102	0
25	CLA	C1	503	60/65	0.93	0.21	0.83	38,53,67,73	0
35	LMT	C1	519	35/35	0.86	0.24	0.81	57,76,85,93	0
23	BCR	d1	405	40/40	0.89	0.18	0.80	38,51,94,99	0
25	CLA	c1	507	65/65	0.93	0.21	0.80	49,62,72,80	0
25	CLA	C1	505	65/65	0.89	0.20	0.79	43,55,64,68	0
25	CLA	b1	614	65/65	0.95	0.20	0.79	35,45,54,56	0
23	BCR	b1	603	40/40	0.93	0.18	0.78	40,58,69,77	0
34	DGD	c1	520	62/66	0.91	0.22	0.78	36,59,73,87	0
25	CLA	c1	511	65/65	0.94	0.23	0.77	38,53,71,78	0
25	CLA	C2	513	53/65	0.84	0.26	0.76	78,91,106,110	0
38	HEM	f1	101	43/43	0.93	0.38	0.76	62,82,124,136	0
25	CLA	C1	510	65/65	0.93	0.23	0.75	47,59,77,82	0
25	CLA	B1	610	65/65	0.94	0.19	0.75	46,58,73,76	0
31	BCT	a2	417	4/4	0.98	0.27	0.75	59,65,67,73	0
33	LHG	D1	405	49/49	0.95	0.18	0.74	35,45,54,56	0
25	CLA	c2	512	65/65	0.87	0.26	0.73	61,76,86,93	0
34	DGD	h2	102	62/66	0.88	0.22	0.72	47,67,82,96	0
25	CLA	d1	401	65/65	0.93	0.19	0.71	30,36,44,47	0
25	CLA	B1	612	65/65	0.92	0.21	0.70	52,66,71,77	0
33	LHG	B1	621	49/49	0.92	0.22	0.69	41,57,67,73	0
34	DGD	C1	515	52/66	0.89	0.19	0.67	36,58,67,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	BCR	b1	601	40/40	0.94	0.17	0.67	36,47,56,57	0
25	CLA	B1	609	65/65	0.90	0.23	0.66	54,71,81,90	0
38	HEM	e2	101	43/43	0.90	0.47	0.65	126,145,163,171	0
25	CLA	c1	509	65/65	0.90	0.20	0.65	51,62,68,72	0
25	CLA	b1	617	65/65	0.94	0.23	0.65	47,56,65,68	0
36	PL9	D2	408	55/55	0.89	0.26	0.64	43,59,64,74	0
25	CLA	c2	506	61/65	0.92	0.21	0.64	55,70,77,83	0
25	CLA	D2	401	65/65	0.89	0.24	0.63	43,53,71,76	0
33	LHG	b1	622	49/49	0.93	0.22	0.63	36,49,57,69	0
23	BCR	C1	501	40/40	0.85	0.24	0.60	47,61,72,75	0
27	PHO	A2	407	64/64	0.92	0.23	0.60	53,64,72,80	0
34	DGD	c2	516	52/66	0.88	0.20	0.59	37,63,71,75	0
25	CLA	c1	516	65/65	0.81	0.32	0.58	66,82,104,109	0
23	BCR	h1	102	40/40	0.92	0.21	0.58	53,60,67,69	0
23	BCR	B1	603	40/40	0.93	0.17	0.58	45,56,78,85	0
23	BCR	A1	401	40/40	0.94	0.17	0.58	36,48,54,58	0
25	CLA	C2	508	50/65	0.83	0.32	0.57	87,103,112,115	0
33	LHG	L2	101	49/49	0.92	0.21	0.57	42,57,70,78	0
29	LMG	b1	621	38/55	0.81	0.24	0.56	52,63,76,82	0
25	CLA	b1	606	65/65	0.94	0.23	0.56	44,53,61,63	0
25	CLA	C2	507	45/65	0.88	0.23	0.55	73,93,102,113	0
25	CLA	A1	406	65/65	0.95	0.19	0.55	28,37,46,55	0
29	LMG	I2	101	34/55	0.74	0.26	0.55	82,103,109,114	0
23	BCR	A2	401	40/40	0.91	0.22	0.54	58,84,90,91	0
33	LHG	d1	407	49/49	0.95	0.18	0.54	34,44,53,67	0
25	CLA	C1	514	45/65	0.81	0.30	0.53	73,84,92,96	0
34	DGD	c1	518	62/66	0.93	0.19	0.53	41,61,69,79	0
29	LMG	A1	412	41/55	0.80	0.24	0.53	50,75,96,100	0
25	CLA	c2	513	54/65	0.82	0.29	0.51	75,94,102,105	0
25	CLA	d1	404	65/65	0.93	0.19	0.51	31,43,49,51	0
26	OEX	A1	407	10/10	0.97	0.19	0.51	45,49,63,68	0
23	BCR	d2	401	40/40	0.86	0.22	0.50	48,67,81,85	0
34	DGD	H1	101	62/66	0.85	0.23	0.49	50,71,84,89	0
25	CLA	b1	608	65/65	0.95	0.20	0.49	37,48,58,63	0
25	CLA	C2	510	45/65	0.80	0.34	0.48	107,116,121,126	0
32	GOL	c1	521	6/6	0.91	0.20	0.47	54,56,60,65	0
38	HEM	V1	201	43/43	0.95	0.21	0.47	35,61,66,71	0
25	CLA	A1	405	55/65	0.93	0.17	0.46	38,46,59,65	0
25	CLA	A1	403	65/65	0.96	0.18	0.46	27,37,49,54	0
34	DGD	h1	101	62/66	0.90	0.19	0.46	37,48,59,65	0
23	BCR	B2	601	40/40	0.94	0.18	0.45	41,56,66,68	0
27	PHO	D2	407	64/64	0.90	0.21	0.44	58,68,81,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	BCR	D1	401	40/40	0.85	0.23	0.44	54,67,89,95	0
33	LHG	D2	405	49/49	0.93	0.20	0.44	52,60,66,68	0
25	CLA	c1	512	65/65	0.94	0.24	0.43	36,50,57,60	0
25	CLA	b1	615	59/65	0.95	0.16	0.43	31,43,58,64	0
25	CLA	b1	620	65/65	0.94	0.18	0.43	31,43,56,60	0
25	CLA	C1	509	65/65	0.92	0.20	0.42	48,59,71,80	0
29	LMG	a2	412	44/55	0.83	0.26	0.42	55,70,78,93	0
38	HEM	E2	101	43/43	0.91	0.35	0.42	116,132,146,152	0
25	CLA	D2	404	61/65	0.79	0.26	0.41	67,87,113,120	0
25	CLA	b1	609	65/65	0.89	0.21	0.41	42,58,84,104	0
27	PHO	D1	407	63/64	0.91	0.20	0.41	40,56,63,67	0
23	BCR	c1	501	40/40	0.84	0.24	0.40	56,66,79,82	0
25	CLA	C1	512	65/65	0.85	0.24	0.39	63,82,102,121	0
25	CLA	B2	618	60/65	0.89	0.22	0.38	59,65,80,85	0
29	LMG	B1	626	48/55	0.82	0.24	0.38	55,70,89,94	0
33	LHG	d2	403	49/49	0.92	0.21	0.37	42,59,69,73	0
25	CLA	b1	616	65/65	0.93	0.18	0.37	39,46,57,69	0
25	CLA	B2	617	65/65	0.94	0.20	0.37	52,63,70,74	0
34	DGD	c2	514	62/66	0.93	0.20	0.37	47,59,67,69	0
23	BCR	C2	502	40/40	0.78	0.35	0.35	95,106,118,120	0
25	CLA	d2	405	65/65	0.92	0.20	0.33	34,44,61,77	0
35	LMT	M1	103	24/35	0.83	0.21	0.33	42,68,97,101	0
25	CLA	c1	515	55/65	0.86	0.25	0.32	69,82,90,94	0
25	CLA	b2	608	65/65	0.93	0.20	0.31	65,77,85,86	0
25	CLA	K2	101	55/65	0.83	0.28	0.30	86,98,104,109	0
38	HEM	v1	201	43/43	0.93	0.24	0.30	60,66,72,75	0
25	CLA	B1	605	65/65	0.93	0.21	0.29	60,75,87,88	0
25	CLA	c1	504	65/65	0.93	0.21	0.28	36,53,83,98	0
25	CLA	B1	613	65/65	0.95	0.18	0.27	38,49,57,64	0
27	PHO	d2	408	64/64	0.92	0.19	0.27	45,56,62,64	0
25	CLA	b2	613	65/65	0.87	0.23	0.27	59,84,96,99	0
25	CLA	d2	402	65/65	0.94	0.18	0.26	24,37,48,52	0
25	CLA	C2	518	41/65	0.83	0.29	0.26	105,121,127,134	0
25	CLA	b1	607	65/65	0.95	0.19	0.26	33,46,69,76	0
33	LHG	a1	407	43/49	0.93	0.20	0.25	36,52,66,70	0
25	CLA	B1	606	65/65	0.91	0.25	0.25	60,71,77,82	0
25	CLA	C2	505	65/65	0.84	0.23	0.25	78,100,112,118	0
25	CLA	B1	614	65/65	0.95	0.19	0.24	43,55,62,67	0
25	CLA	b2	604	42/65	0.88	0.29	0.23	82,109,116,127	0
25	CLA	c1	508	50/65	0.86	0.22	0.22	57,66,77,81	0
25	CLA	b2	614	65/65	0.94	0.18	0.21	51,66,73,75	0
25	CLA	d2	404	50/65	0.83	0.23	0.21	57,74,83,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
25	CLA	c2	511	65/65	0.92	0.22	0.20	54,65,72,75	0
29	LMG	d1	408	33/55	0.91	0.19	0.19	41,50,61,63	0
25	CLA	b2	624	65/65	0.93	0.21	0.19	47,60,75,82	0
25	CLA	b2	617	65/65	0.92	0.19	0.17	47,58,65,72	0
33	LHG	l1	102	49/49	0.96	0.18	0.17	25,43,67,75	0
25	CLA	B1	607	60/65	0.92	0.20	0.17	45,56,68,72	0
25	CLA	b2	616	60/65	0.94	0.20	0.16	51,64,82,82	0
34	DGD	c1	514	51/66	0.91	0.20	0.15	46,54,62,64	0
25	CLA	B2	609	65/65	0.91	0.19	0.15	51,67,76,82	0
25	CLA	a1	403	65/65	0.94	0.18	0.14	29,37,48,51	0
33	LHG	D2	403	49/49	0.93	0.19	0.14	45,60,68,73	0
38	HEM	v2	201	43/43	0.94	0.21	0.13	47,60,66,78	0
32	GOL	a1	406	6/6	0.63	0.29	0.11	68,75,86,90	0
27	PHO	A1	408	64/64	0.95	0.18	0.11	30,42,50,56	0
25	CLA	C1	511	65/65	0.91	0.23	0.10	45,56,62,68	0
34	DGD	c2	517	62/66	0.92	0.16	0.09	45,57,70,75	0
25	CLA	D1	403	51/65	0.87	0.21	0.09	64,74,88,90	0
25	CLA	c2	515	46/65	0.86	0.27	0.09	81,100,104,109	0
29	LMG	D1	406	35/55	0.91	0.22	0.09	50,57,71,74	0
25	CLA	c2	504	65/65	0.93	0.21	0.09	46,78,92,100	0
31	BCT	A2	413	4/4	0.97	0.26	0.07	65,69,71,72	0
34	DGD	C1	517	64/66	0.92	0.17	0.07	38,55,75,92	0
25	CLA	c2	507	54/65	0.90	0.22	0.06	76,81,86,92	0
25	CLA	C1	508	65/65	0.91	0.18	0.06	47,66,76,80	0
34	DGD	C1	516	62/66	0.93	0.17	0.04	44,53,60,61	0
29	LMG	B1	622	31/55	0.87	0.18	0.04	66,74,81,83	0
25	CLA	D2	406	65/65	0.93	0.20	0.03	45,57,65,67	0
25	CLA	A2	402	65/65	0.93	0.20	0.02	47,57,69,77	0
25	CLA	b1	611	65/65	0.92	0.17	0.01	37,59,68,73	0
25	CLA	B2	615	65/65	0.93	0.16	0.01	44,56,73,86	0
25	CLA	b1	612	65/65	0.95	0.21	0.00	45,54,60,68	0
25	CLA	C1	507	65/65	0.91	0.19	-0.01	46,67,86,105	0
25	CLA	b2	615	60/65	0.96	0.15	-0.02	45,54,67,74	0
25	CLA	c2	505	65/65	0.92	0.18	-0.06	48,61,71,80	0
25	CLA	b2	609	61/65	0.91	0.20	-0.06	77,89,95,100	0
25	CLA	c1	506	65/65	0.91	0.18	-0.07	40,54,68,73	0
38	HEM	V2	201	43/43	0.89	0.25	-0.08	83,98,102,107	0
29	LMG	A2	412	29/55	0.84	0.22	-0.08	86,94,100,102	0
25	CLA	c1	513	60/65	0.92	0.20	-0.08	49,59,71,72	0
27	PHO	a1	411	64/64	0.95	0.17	-0.09	33,41,47,50	0
25	CLA	B1	608	65/65	0.95	0.18	-0.10	46,58,71,81	0
25	CLA	B2	611	65/65	0.89	0.21	-0.10	51,73,81,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	BCR	F2	401	40/40	0.81	0.23	-0.12	67,81,107,113	0
25	CLA	A1	404	51/65	0.94	0.16	-0.13	37,48,58,70	0
25	CLA	B2	605	65/65	0.91	0.18	-0.13	63,71,77,82	0
25	CLA	b1	610	65/65	0.95	0.16	-0.14	37,47,56,63	0
29	LMG	A1	410	43/55	0.89	0.18	-0.14	52,59,65,76	0
25	CLA	D1	402	65/65	0.94	0.17	-0.15	31,40,58,63	0
25	CLA	b2	610	65/65	0.87	0.21	-0.15	60,82,90,92	0
25	CLA	a2	404	65/65	0.95	0.17	-0.19	30,42,52,53	0
25	CLA	c1	505	65/65	0.92	0.21	-0.24	47,70,79,88	0
25	CLA	C1	504	65/65	0.93	0.19	-0.24	49,64,74,77	0
27	PHO	d1	403	64/64	0.94	0.16	-0.24	32,41,50,54	0
25	CLA	B2	619	65/65	0.92	0.17	-0.26	46,55,63,71	0
25	CLA	b2	612	65/65	0.92	0.17	-0.28	39,54,64,70	0
25	CLA	B2	616	54/65	0.93	0.18	-0.28	43,51,57,59	0
37	SQD	D2	402	25/54	0.90	0.25	-0.28	85,90,96,98	0
25	CLA	B2	613	65/65	0.95	0.16	-0.28	41,52,68,70	0
33	LHG	L1	101	41/49	0.94	0.16	-0.29	30,46,61,85	0
25	CLA	b1	613	65/65	0.94	0.16	-0.33	36,44,54,68	0
29	LMG	d2	407	27/55	0.92	0.16	-0.33	49,60,64,70	0
33	LHG	l2	101	44/49	0.95	0.16	-0.45	36,53,66,72	0
25	CLA	B1	616	65/65	0.94	0.16	-0.50	39,49,58,66	0
25	CLA	c2	509	65/65	0.91	0.18	-0.53	54,70,82,85	0
29	LMG	c2	519	26/55	0.86	0.21	-0.54	58,67,73,74	0
24	CL	A1	402	1/1	0.89	0.15	-0.58	39,39,39,39	0
32	GOL	C2	514	6/6	0.85	0.22	-0.59	87,93,100,101	0
25	CLA	C2	504	46/65	0.89	0.18	-0.60	72,88,95,96	0
25	CLA	a2	413	50/65	0.94	0.14	-0.61	33,46,57,66	0
30	FE	a1	410	1/1	0.98	0.19	-0.64	49,49,49,49	0
25	CLA	C2	516	46/65	0.89	0.18	-0.64	70,92,97,100	0
25	CLA	A2	404	51/65	0.92	0.16	-0.66	47,58,70,73	0
26	OEX	a1	408	10/10	0.98	0.15	-0.76	39,49,62,70	0
25	CLA	C2	511	50/65	0.90	0.18	-0.79	85,93,100,104	0
26	OEX	a2	408	10/10	0.98	0.15	-0.80	42,49,58,61	0
34	DGD	C2	512	33/66	0.87	0.20	-0.85	63,77,83,93	0
25	CLA	a1	405	50/65	0.95	0.14	-0.89	25,33,49,55	0
24	CL	A2	410	1/1	0.80	0.18	-1.05	87,87,87,87	0
26	OEX	A2	406	10/10	0.93	0.10	-1.24	68,84,93,94	0
28	UNL	F2	403	16/-	0.68	0.19	-1.53	51,76,86,89	0
25	CLA	c1	510	65/65	0.91	0.16	-1.55	41,54,62,72	0
24	CL	a1	402	1/1	0.96	0.08	-1.57	49,49,49,49	0
30	FE	A2	411	1/1	0.99	0.18	-1.96	63,63,63,63	0
24	CL	a2	403	1/1	0.98	0.06	-3.31	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
28	UNL	i2	101	14/-	0.87	0.21	-	62,66,73,75	0
28	UNL	a2	410	8/-	0.81	0.26	-	61,68,70,76	0
28	UNL	k2	503	6/-	0.81	0.46	-	67,76,79,80	0
28	UNL	I2	102	17/-	0.62	0.36	-	80,92,102,103	0
30	FE	A1	411	1/1	0.96	0.12	-	52,52,52,52	0
35	LMT	T1	101	12/35	0.87	0.28	-	46,51,54,56	0
28	UNL	m1	102	6/-	0.81	0.32	-	54,55,63,66	0
28	UNL	I2	103	14/-	0.55	0.38	-	62,93,102,104	0
28	UNL	k2	504	9/-	0.74	0.36	-	66,74,80,88	0
28	UNL	k2	505	6/-	0.69	0.22	-	70,80,84,87	0
32	GOL	b1	618	6/6	0.84	0.24	-	60,69,80,80	0
30	FE	a2	414	1/1	0.99	0.15	-	57,57,57,57	0
28	UNL	A2	409	10/-	0.67	0.38	-	72,82,85,87	0
28	UNL	t1	102	9/-	0.90	0.26	-	45,57,68,69	0
29	LMG	C2	515	24/55	0.70	0.60	-	82,97,104,105	0
28	UNL	b1	625	10/-	0.83	0.42	-	50,62,68,69	0
28	UNL	M2	101	11/-	0.80	0.30	-	59,68,73,74	0
32	GOL	C1	518	6/6	0.69	0.44	-	65,73,77,81	0
28	UNL	H2	102	5/-	0.77	0.55	-	72,81,84,85	0
28	UNL	k2	502	9/-	0.77	0.39	-	72,78,84,86	0
28	UNL	D1	410	6/-	0.68	0.49	-	59,62,66,66	0
28	UNL	K2	103	5/-	0.89	0.40	-	79,83,88,90	0
35	LMT	i2	102	7/35	0.82	0.28	-	68,71,76,79	0
28	UNL	c2	520	15/-	0.45	0.32	-	86,97,106,108	0
39	CA	o2	401	1/1	0.61	0.34	-	101,101,101,101	0
28	UNL	C2	501	6/-	0.72	0.43	-	72,74,78,87	0
35	LMT	M1	102	11/35	0.92	0.26	-	47,52,56,58	0
39	CA	O1	401	1/1	0.84	0.07	-	82,82,82,82	0
28	UNL	b1	623	11/-	0.70	0.42	-	59,74,83,84	0
28	UNL	X2	101	7/-	0.66	0.43	-	83,85,91,93	0
28	UNL	b1	628	10/-	0.88	0.35	-	51,57,61,67	0

6.5 Other polymers (i)

There are no such residues in this entry.