wwPDB X-ray Structure Validation Summary 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 wwPDB X-ray Structure Validation Summary 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:

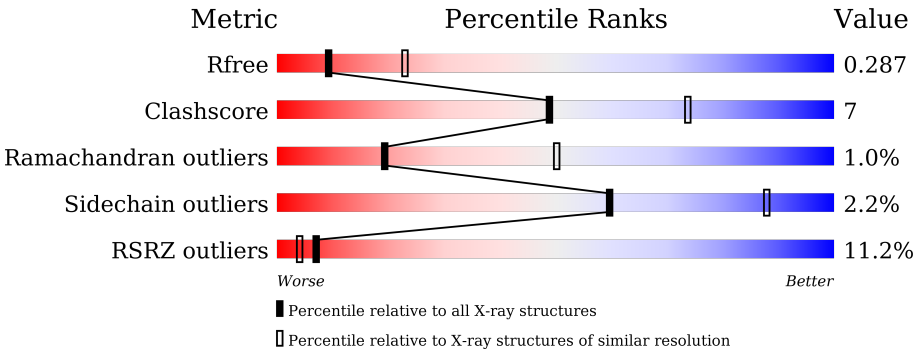
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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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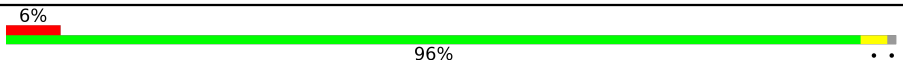
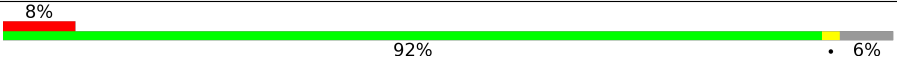
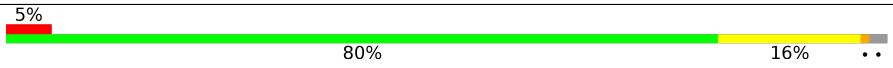
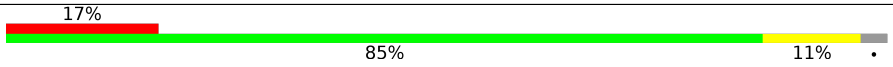
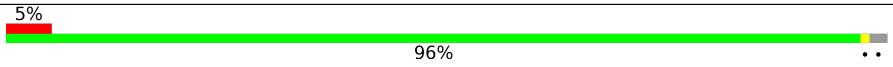
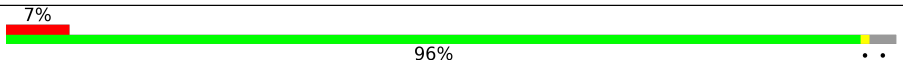
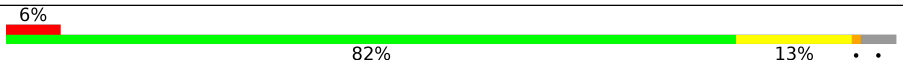
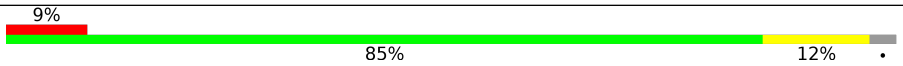
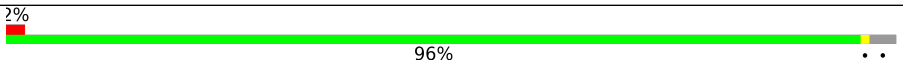
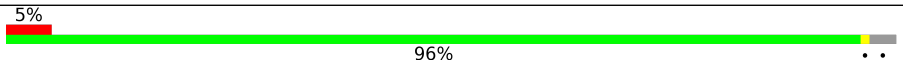
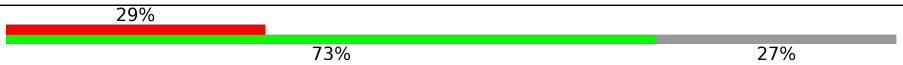
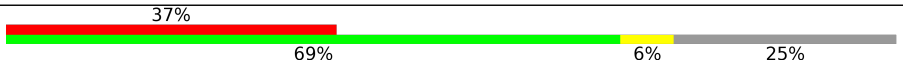
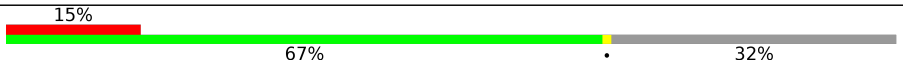
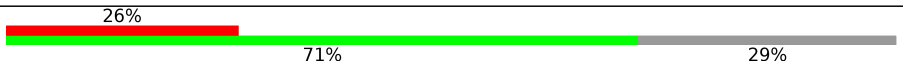
Mol	Chain	Length	Quality of chain
2	b1	509	
2	b2	509	
3	C1	460	
3	C2	460	
3	c1	460	
3	c2	460	
4	D1	351	
4	D2	351	
4	d1	351	
4	d2	351	
5	E1	84	
5	E2	84	
5	e1	84	
5	e2	84	
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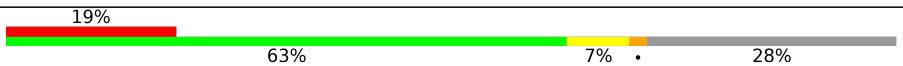
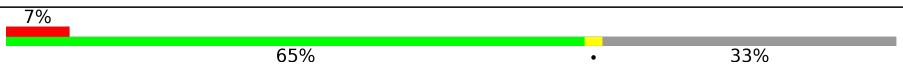
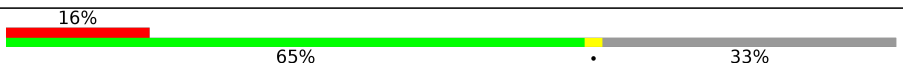
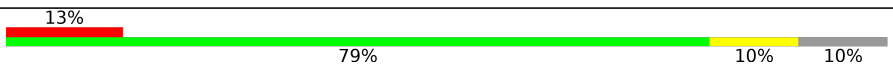
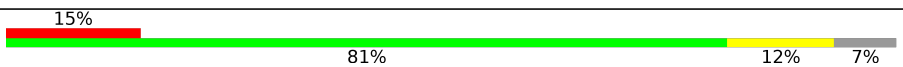
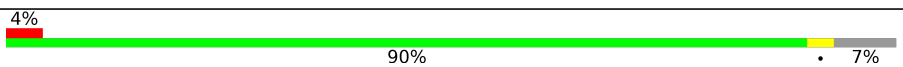
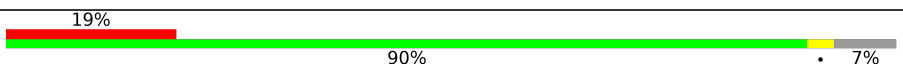
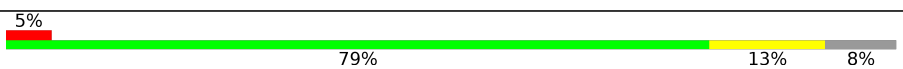
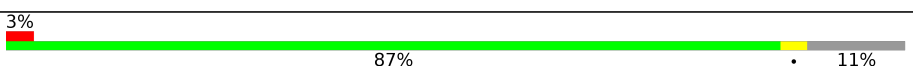
6	F2	43	
6	f1	43	
6	f2	43	
7	H1	67	
7	H2	67	
7	h1	67	
7	h2	67	
8	I1	38	
8	I2	38	
8	i1	38	

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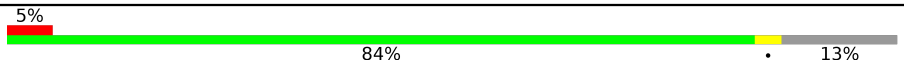
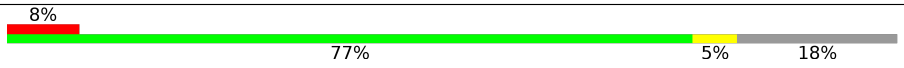
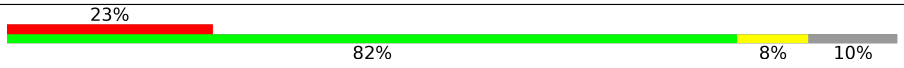
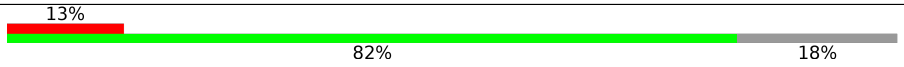
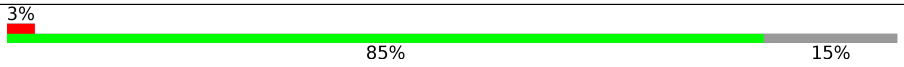
Mol	Chain	Length	Quality of chain
8	i2	38	
9	J1	39	
9	J2	39	
9	j1	39	
9	j2	39	
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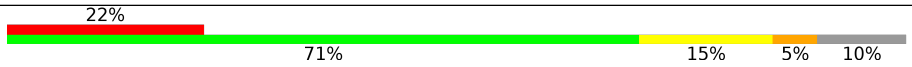
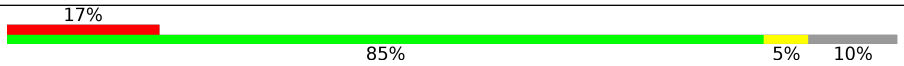
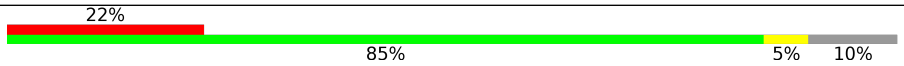
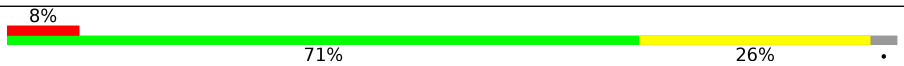
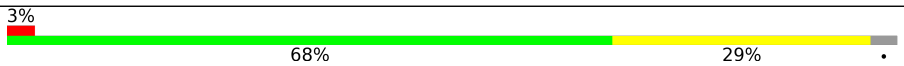
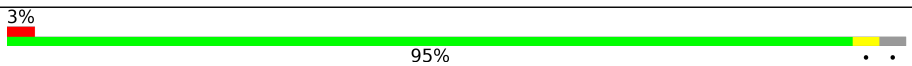
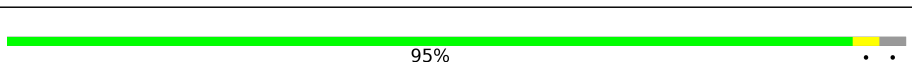
10	K2	41	
10	k1	41	
10	k2	41	
11	L1	38	
11	L2	38	
11	l1	38	
11	l2	38	
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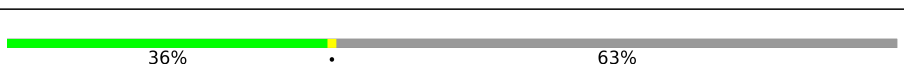
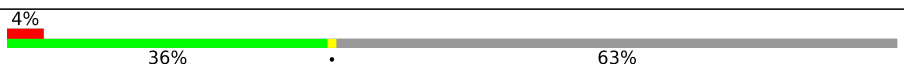
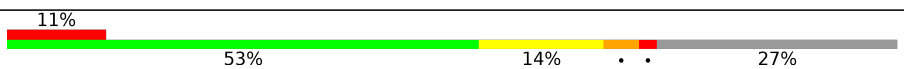
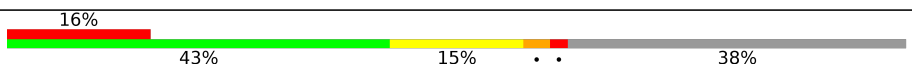
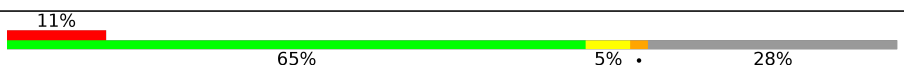
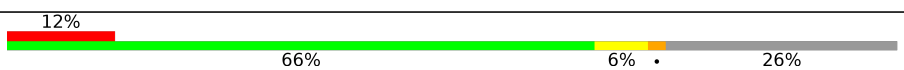
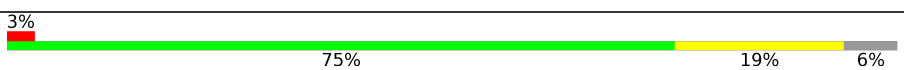
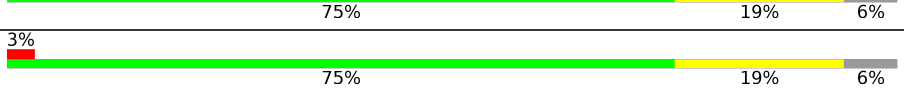
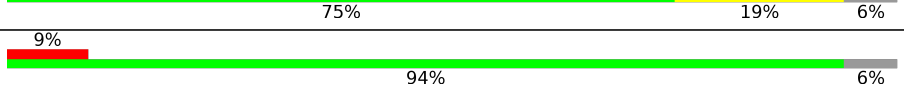
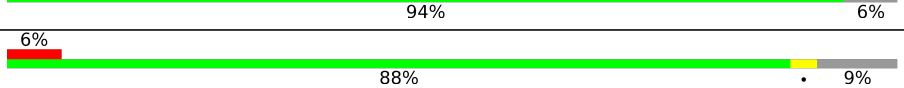
12	m1	108	
12	m2	108	
13	O1	329	
13	O2	329	
13	o1	329	
13	o2	329	
14	T1	32	
14	T2	32	
14	t1	32	
14	t2	32	

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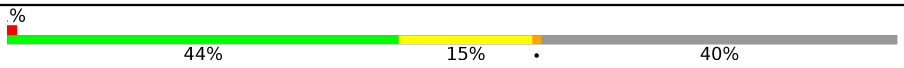
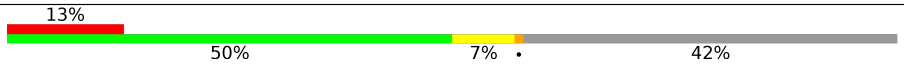
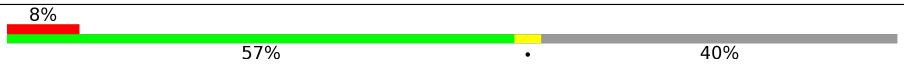
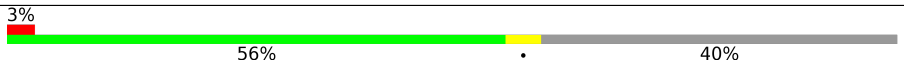
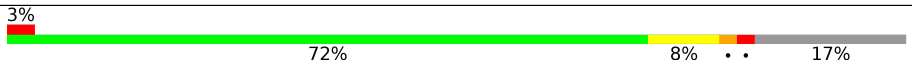
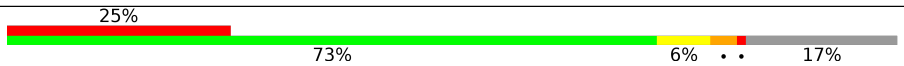
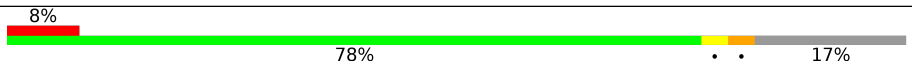
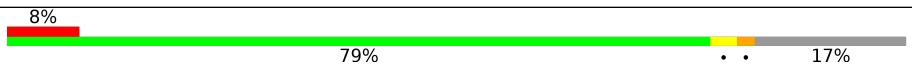
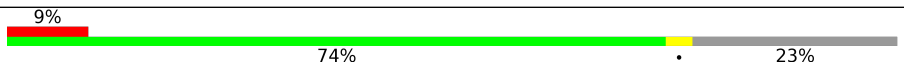
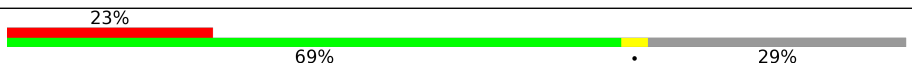
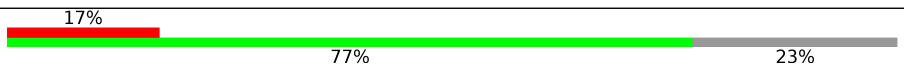
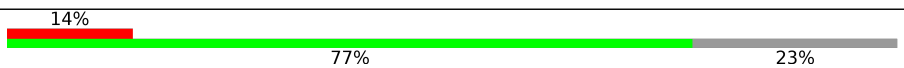
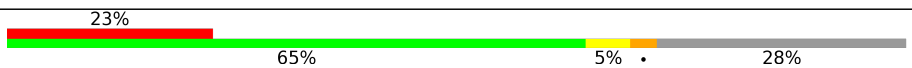
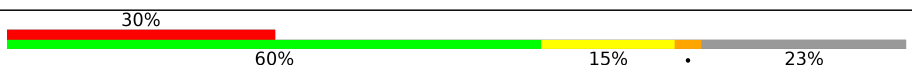
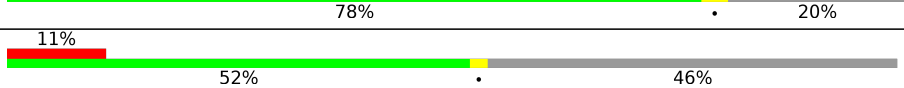
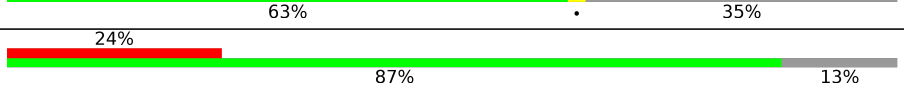
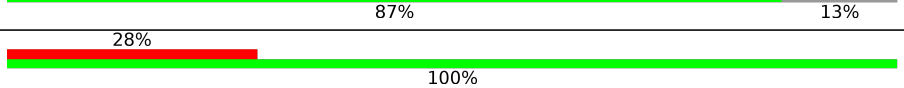
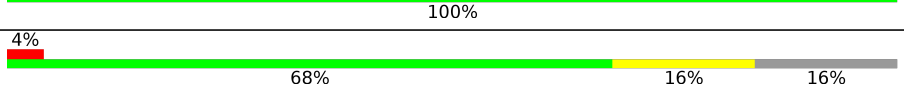
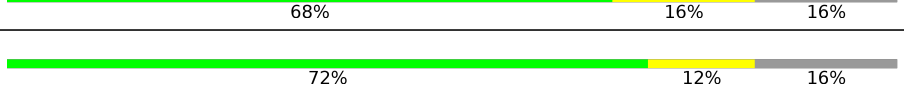
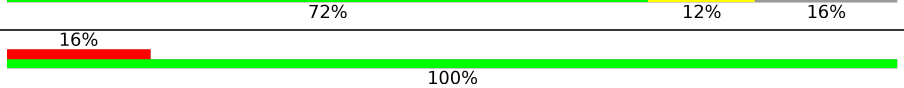
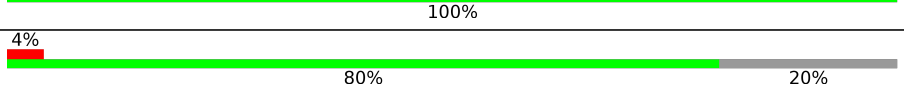
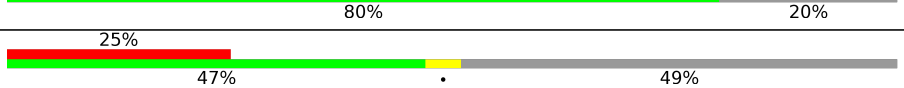
Mol	Chain	Length	Quality of chain
15	U1	155	
15	U2	155	
15	u1	155	
15	u2	155	
16	V1	155	
16	V2	155	
16	v1	155	
16	v2	155	
17	Y1	35	
17	Y2	35	
17	y1	35	
17	y2	35	
18	X1	40	
18	X2	40	
18	x1	40	
18	x2	40	
19	S1	46	
19	S2	46	
19	s1	46	
19	s2	46	
20	W1	25	
20	W2	25	
20	w1	25	
20	w2	25	
21	Q2	218	

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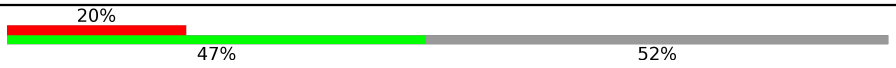
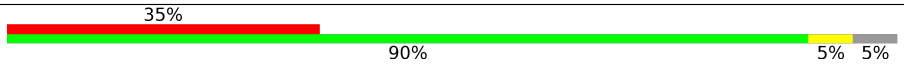
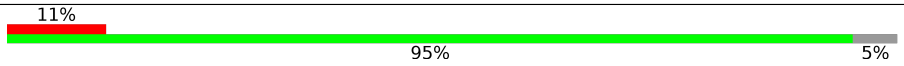
Mol	Chain	Length	Quality of chain
21	q1	218	
22	Z2	62	
22	z2	62	

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 292	C 197	N 46	O 49	0	0	0
11	l1	37	Total 299	C 203	N 47	O 49	0	0	0
11	L2	37	Total 299	C 202	N 46	O 51	0	0	0
11	l2	37	Total 299	C 202	N 46	O 51	0	0	0

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

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

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

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

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

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

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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

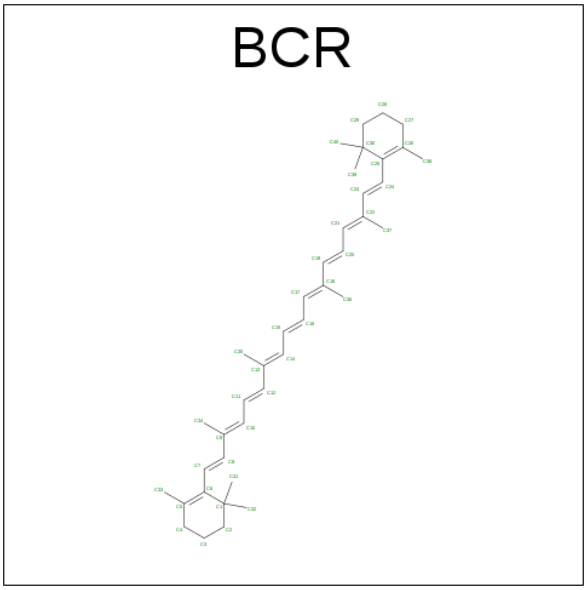
- Molecule 21 is a protein called Extrinsic protein in photosystem II.

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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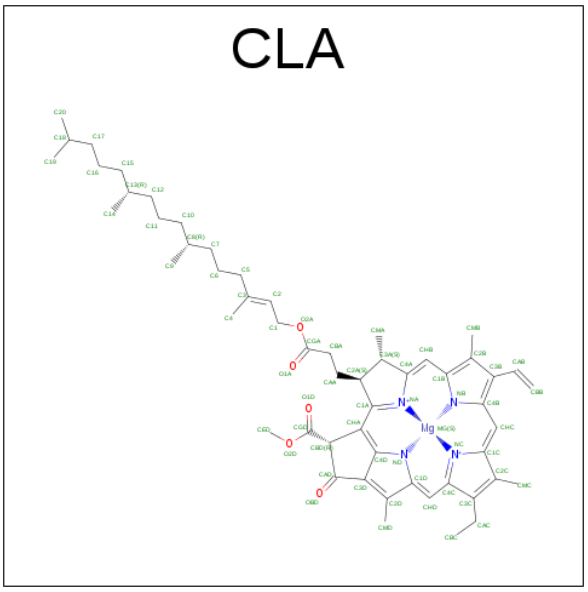
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	K2	1	Total C 29 29	0	0
23	a2	1	Total C 40 40	0	0
23	b2	1	Total C 40 40	0	0
23	b2	1	Total C 40 40	0	0
23	b2	1	Total C 40 40	0	0
23	c2	1	Total C 40 40	0	0
23	d2	1	Total C 40 40	0	0
23	h2	1	Total C 40 40	0	0
23	j2	1	Total C 40 40	0	0
23	k2	1	Total C 40 40	0	0
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 65	C 55	Mg 1	N 4	O 5	0	0
25	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B1	1	Total 58	C 48	Mg 1	N 4	O 5	0	0
25	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C1	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
25	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C1	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
25	C1	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
25	D1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D1	1	Total 51	C 41	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	a1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a1	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
25	a1	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 59	C 49	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c1	1	Total 65	C 55	Mg 1	N 4	O 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 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B2	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
25	B2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C2	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
25	C2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C2	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
25	C2	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
25	C2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C2	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
25	C2	1	Total 50	C 40	Mg 1	N 4	O 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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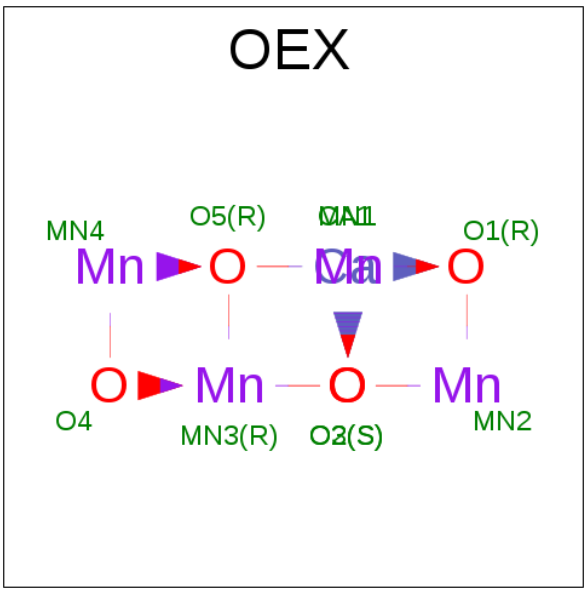
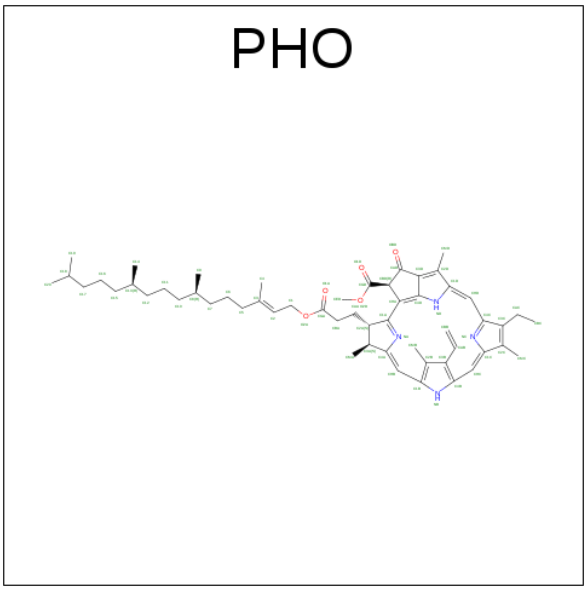
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b2	1	Total 59	C 49	Mg 1	N 4	O 5	0	0
25	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
25	c2	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
25	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
25	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c2	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
25	c2	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
25	d2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	d2	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
25	d2	1	Total 65	C 55	Mg 1	N 4	O 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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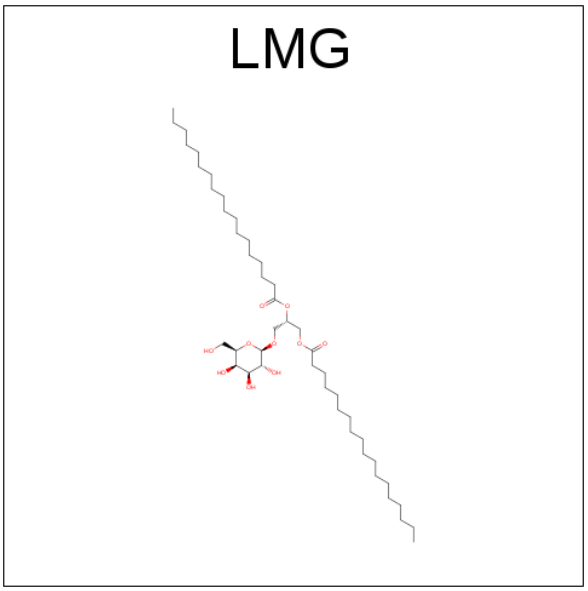
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	b1	7	Total C 92 92	0	0
28	t1	2	Total C 27 27	0	0
28	m1	1	Total C 6 6	0	0
28	a2	4	Total C 55 55	0	0
28	K2	1	Total C 5 5	0	0
28	A1	1	Total C 14 14	0	0
28	l1	1	Total C 12 12	0	0
28	b2	1	Total C 12 12	0	0
28	x1	1	Total C 15 15	0	0
28	X2	1	Total C 7 7	0	0
28	k2	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 C O 43 33 10	0	0
29	A1	1	Total C O 41 31 10	0	0
29	B1	1	Total C O 31 21 10	0	0
29	B1	1	Total C O 48 38 10	0	0
29	C1	1	Total C O 48 38 10	0	0
29	D1	1	Total C O 35 25 10	0	0
29	M1	1	Total C O 31 27 4	0	0
29	a1	1	Total C O 51 41 10	0	0
29	b1	1	Total C O 38 28 10	0	0
29	b1	1	Total C O 39 29 10	0	0
29	b1	1	Total C O 40 30 10	0	0
29	c1	1	Total C O 55 45 10	0	0
29	d1	1	Total C O 33 23 10	0	0
29	d1	1	Total C O 35 30 5	0	0

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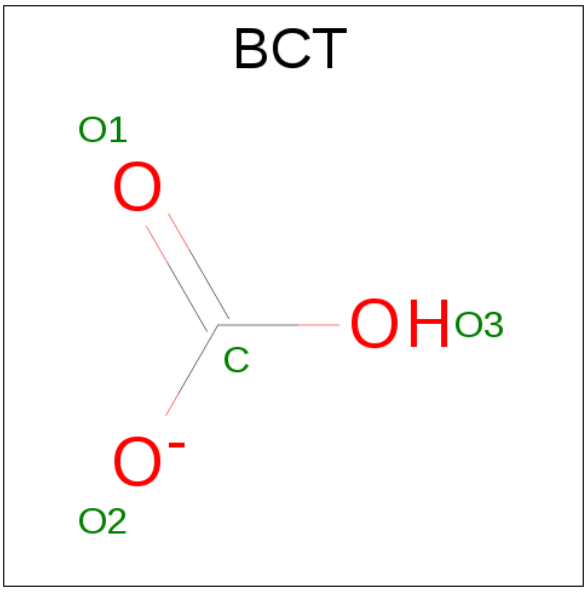
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A2	1	Total C O 29 19 10	0	0
29	B2	1	Total C O 40 30 10	0	0
29	B2	1	Total C O 37 27 10	0	0
29	C2	1	Total C O 24 14 10	0	0
29	F2	1	Total C O 35 25 10	0	0
29	I2	1	Total C O 34 24 10	0	0
29	a2	1	Total C O 44 34 10	0	0
29	b2	1	Total C O 39 29 10	0	0
29	c2	1	Total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

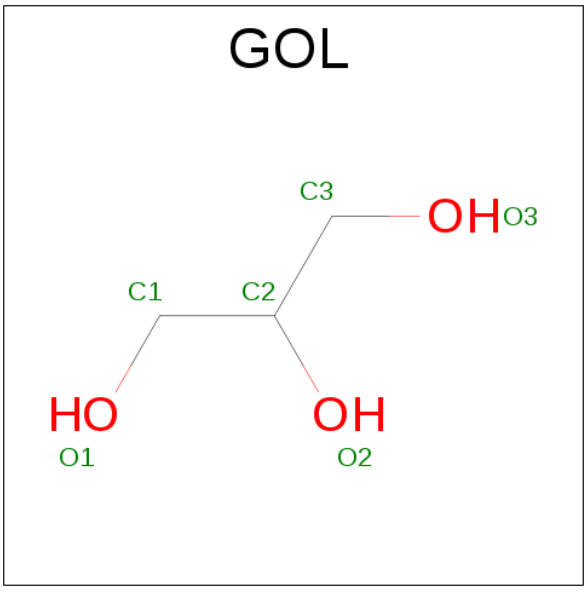
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	a1	1	Total Fe 1 1	0	0
30	A2	1	Total Fe 1 1	0	0
30	A1	1	Total Fe 1 1	0	0
30	a2	1	Total Fe 1 1	0	0

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



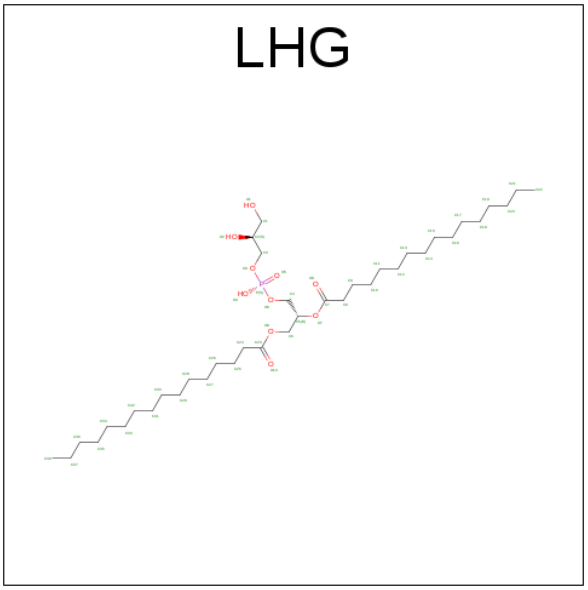
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A1	1	Total C O 4 1 3	0	0
31	a1	1	Total C O 4 1 3	0	0
31	A2	1	Total C O 4 1 3	0	0
31	a2	1	Total C O 4 1 3	0	0

- 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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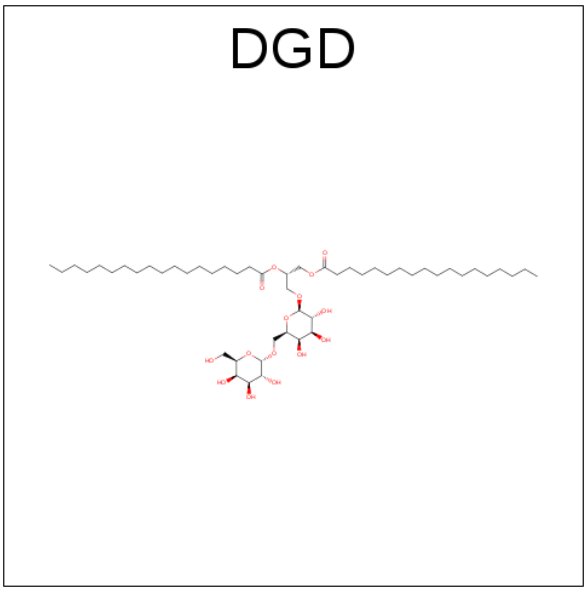
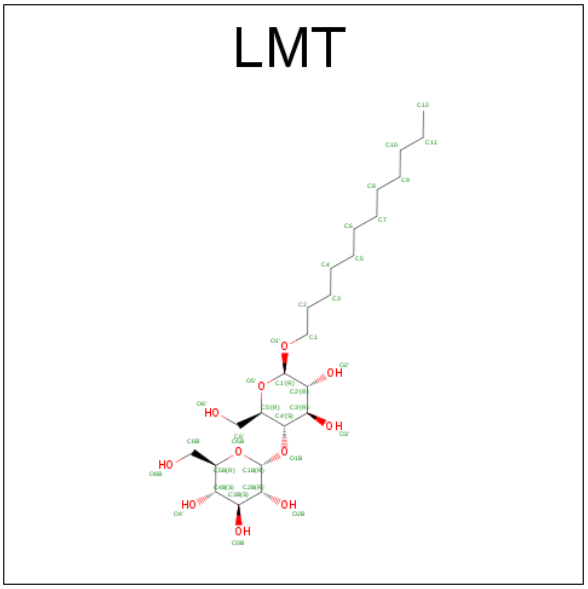
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	D1	1	Total	C	O	P	0	0
			49	38	10	1		
33	L1	1	Total	C	O	P	0	0
			41	30	10	1		
33	a1	1	Total	C	O	P	0	0
			43	32	10	1		
33	b1	1	Total	C	O	P	0	0
			49	38	10	1		
33	d1	1	Total	C	O	P	0	0
			32	21	10	1		
33	d1	1	Total	C	O	P	0	0
			49	38	10	1		
33	l1	1	Total	C	O	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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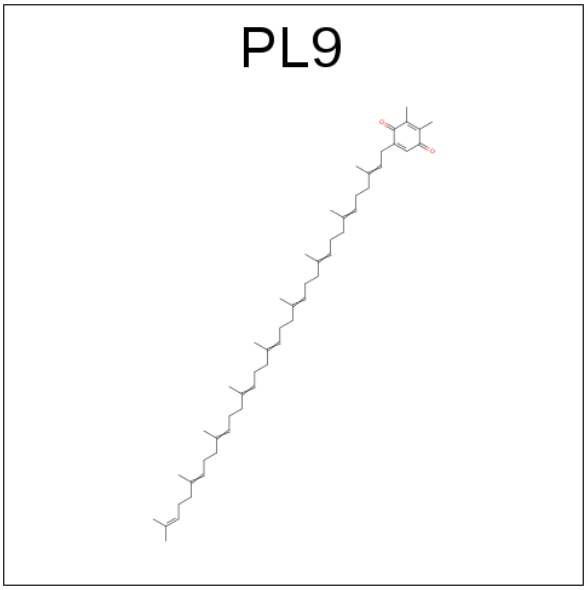
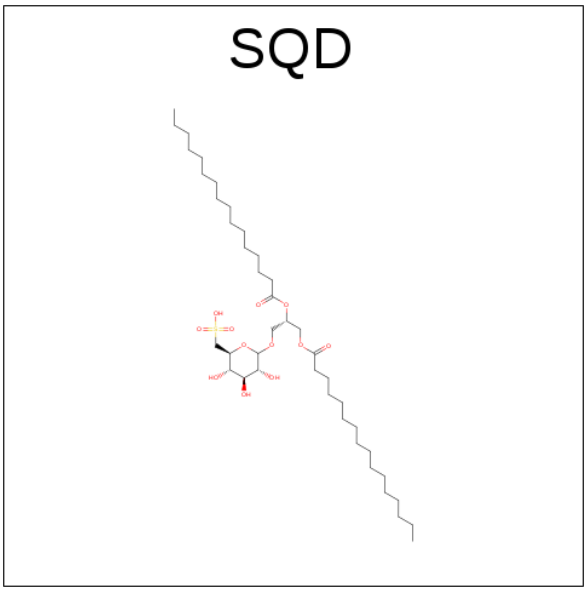
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	m2	1	Total C O 30 19 11	0	0
35	m2	1	Total C O 29 18 11	0	0

- 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: $C_{53}H_{80}O_2$).



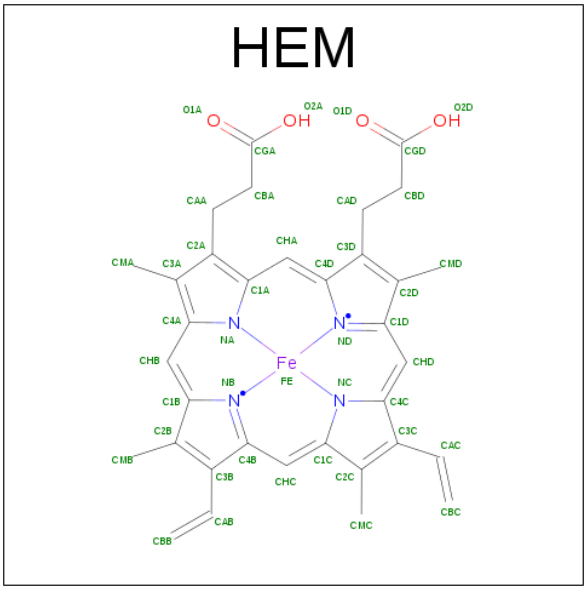
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	D1	1	Total C O 55 53 2	0	0
36	d1	1	Total C O 55 53 2	0	0
36	D2	1	Total C O 55 53 2	0	0
36	d2	1	Total C O 55 53 2	0	0

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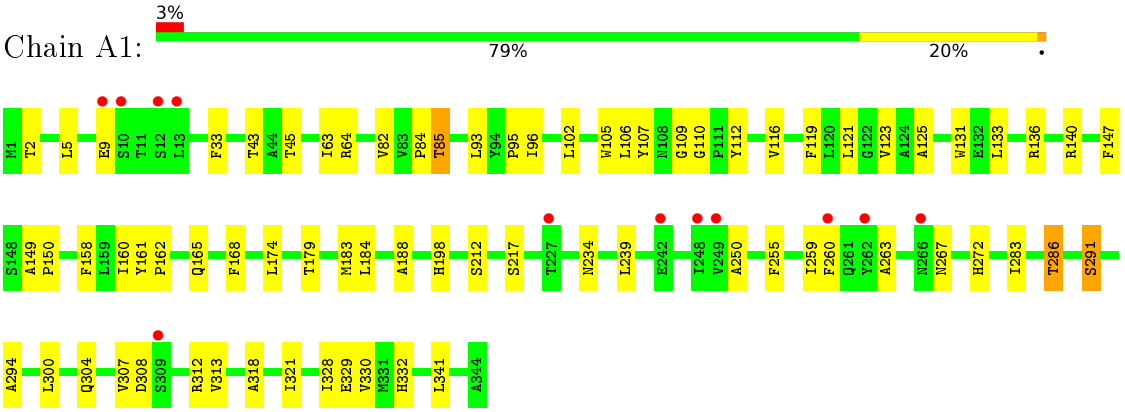
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	d2	1	Total O 1 1	0	0

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.

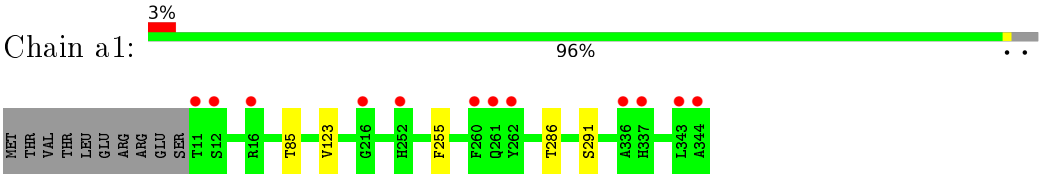
- Molecule 1: Photosystem II protein D1

Chain A1:



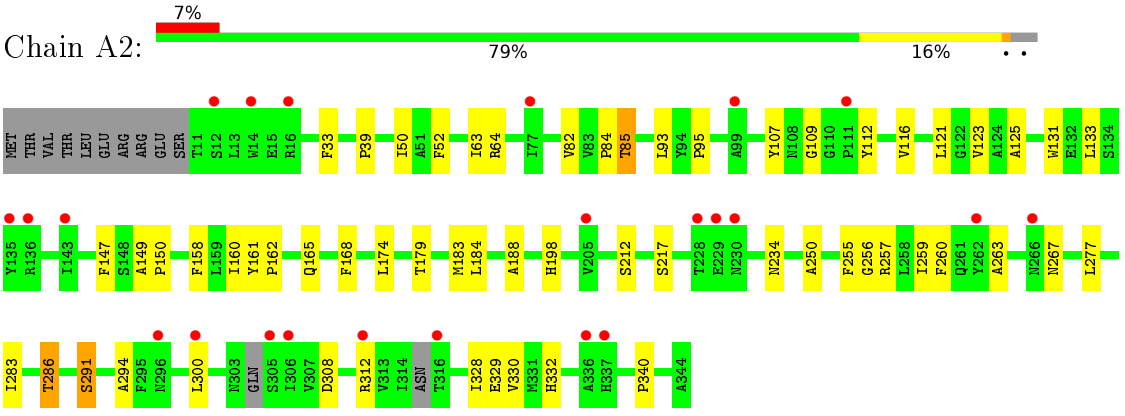
- Molecule 1: Photosystem II protein D1

Chain a1:



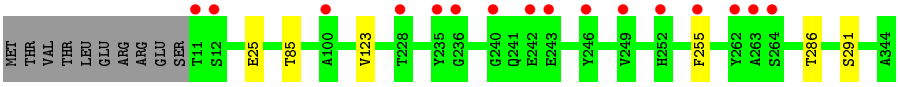
- Molecule 1: Photosystem II protein D1

Chain A2:



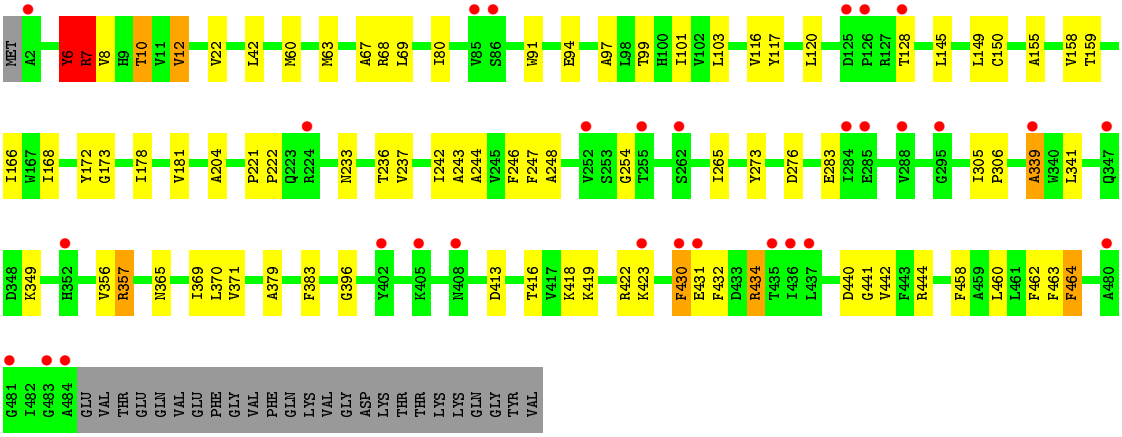
- Molecule 1: Photosystem II protein D1

Chain a2:



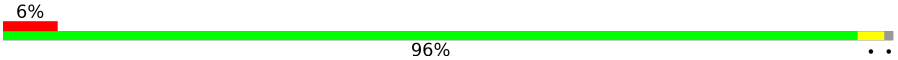
• Molecule 2: Photosystem II CP47 reaction center protein

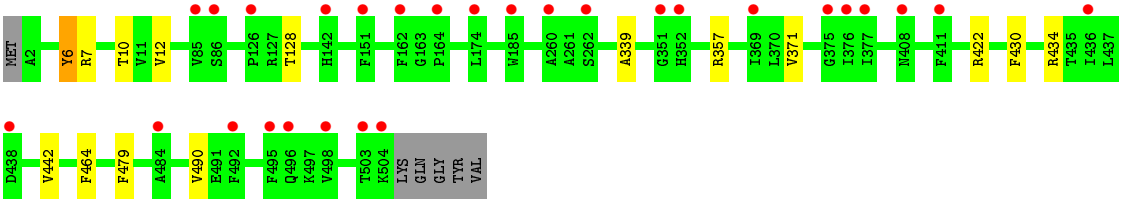
Chain B1:



• Molecule 2: Photosystem II CP47 reaction center protein

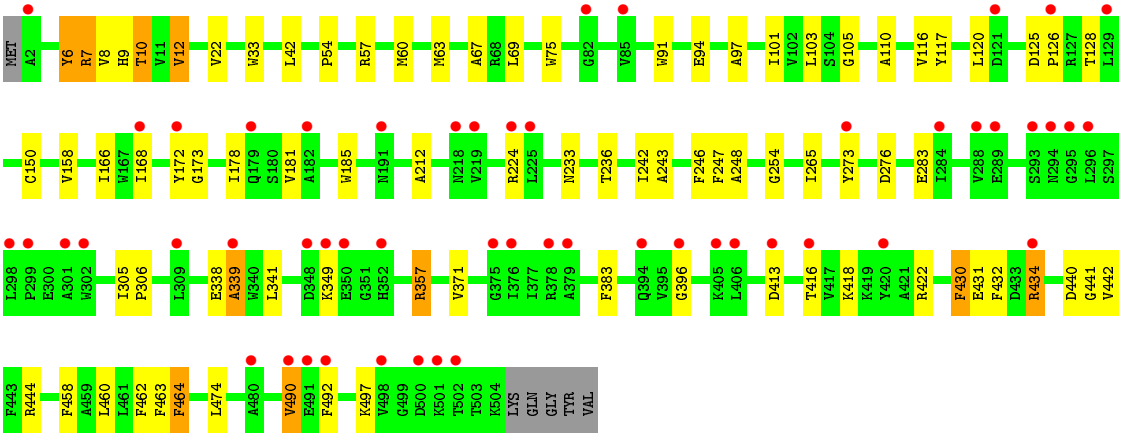
Chain b1:





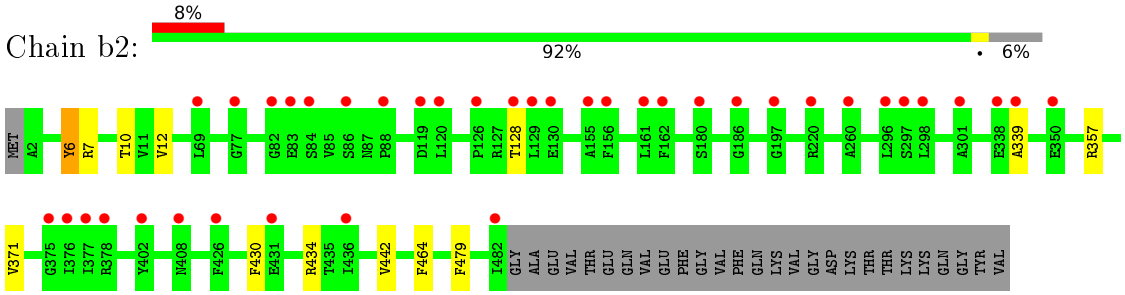
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B2:



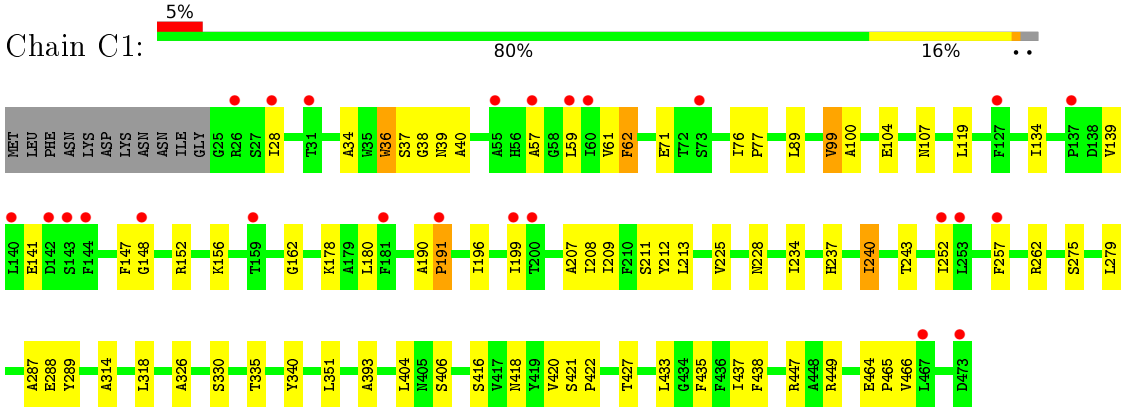
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b2:



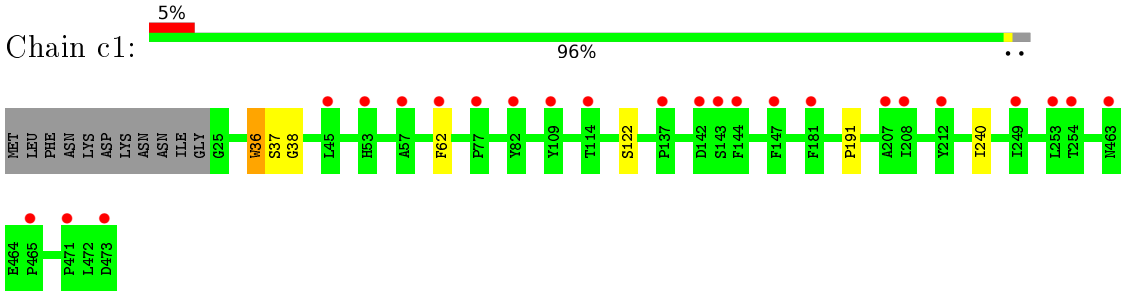
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C1:



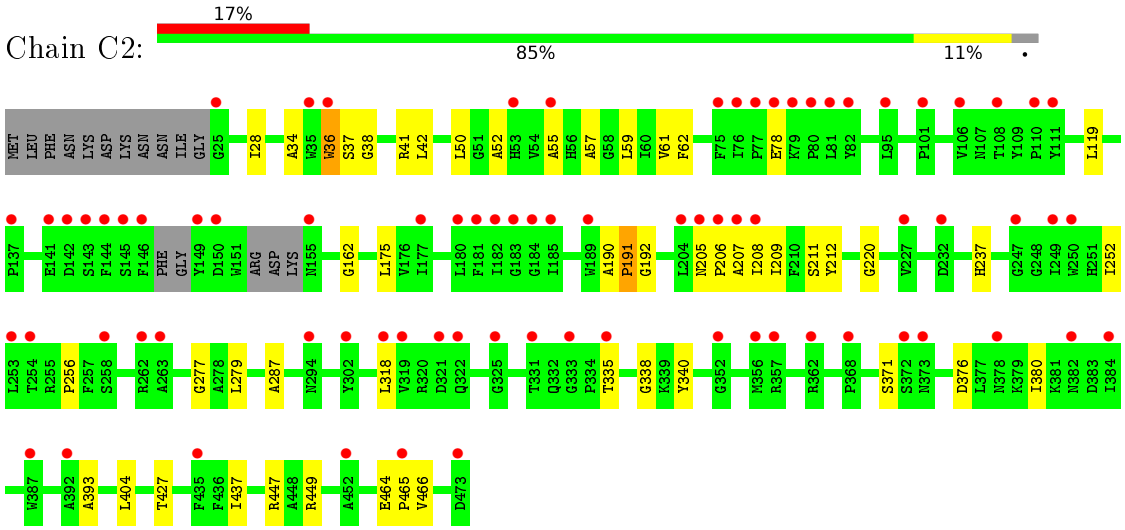
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c1:



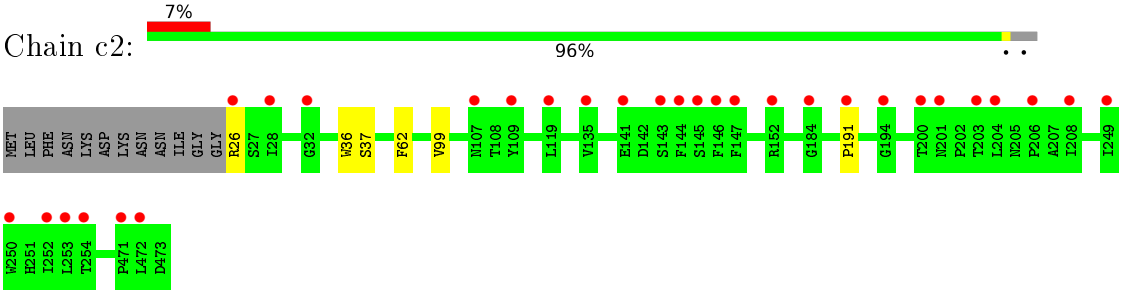
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C2:



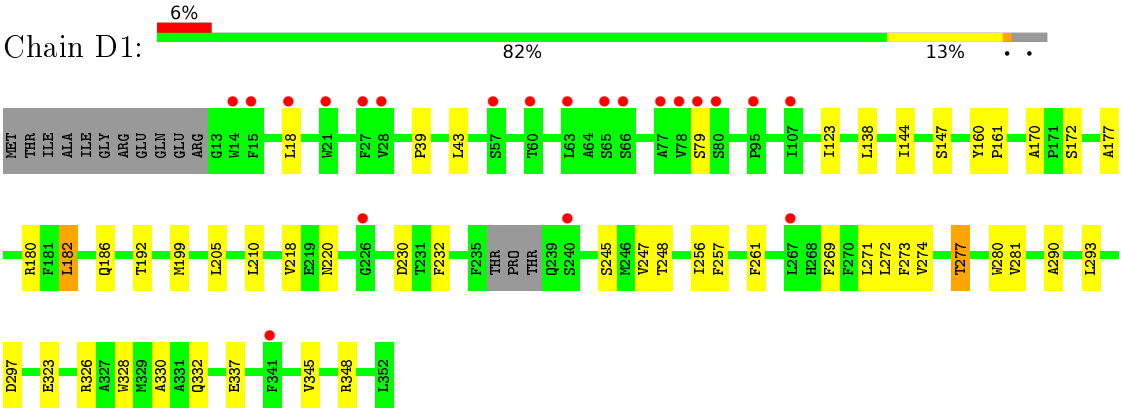
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c2:



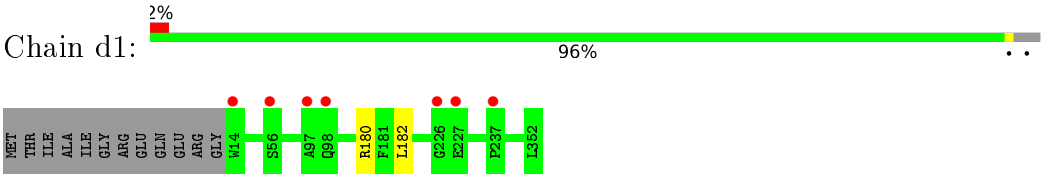
• Molecule 4: Photosystem II D2 protein

Chain D1:



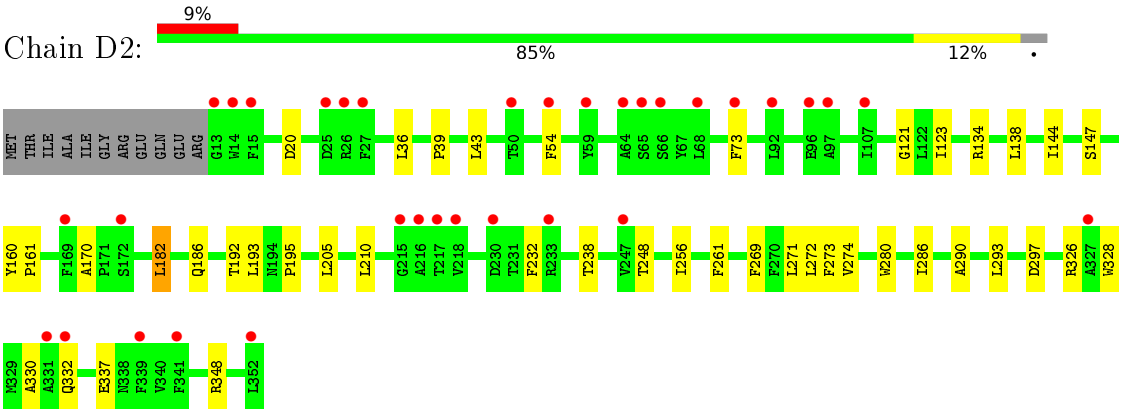
• Molecule 4: Photosystem II D2 protein

Chain d1:



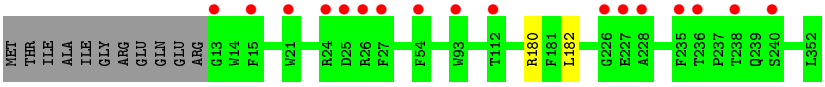
• Molecule 4: Photosystem II D2 protein

Chain D2:

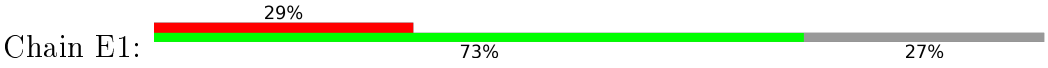


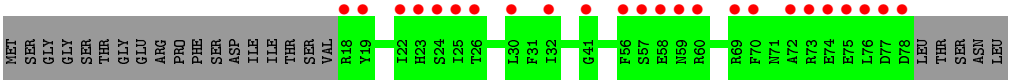
• Molecule 4: Photosystem II D2 protein

Chain d2:

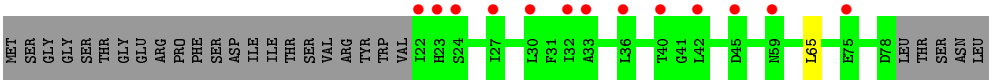


• Molecule 5: Cytochrome b559 subunit alpha

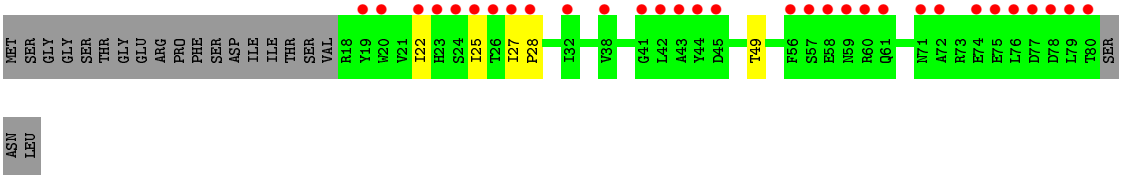




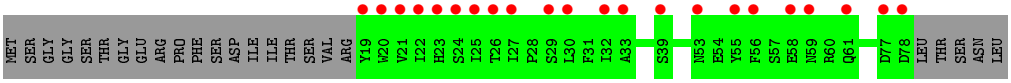
• Molecule 5: Cytochrome b559 subunit alpha



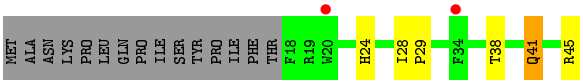
• Molecule 5: Cytochrome b559 subunit alpha



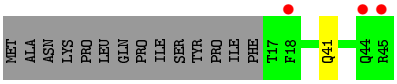
• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 6: Cytochrome b559 subunit beta

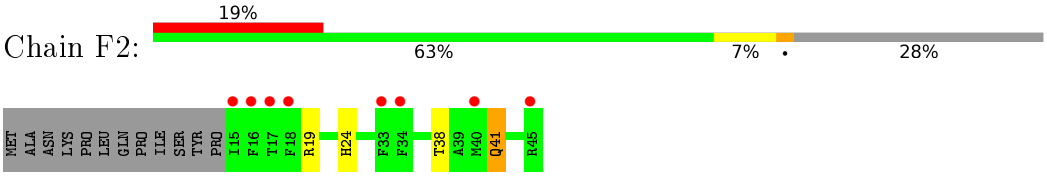


• Molecule 6: Cytochrome b559 subunit beta



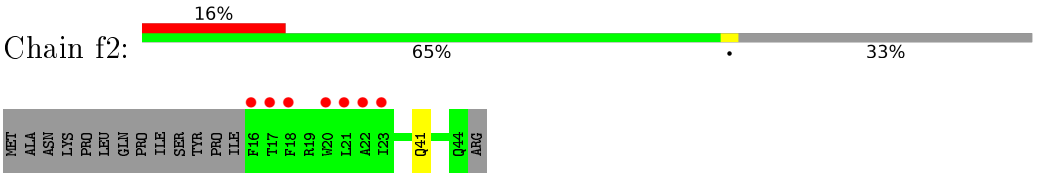
• Molecule 6: Cytochrome b559 subunit beta

Chain F2:



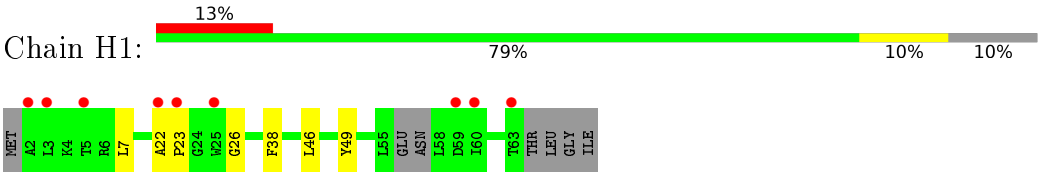
- Molecule 6: Cytochrome b559 subunit beta

Chain f2:



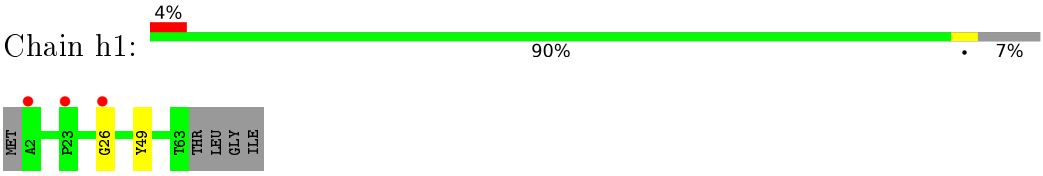
- Molecule 7: Photosystem II reaction center protein H

Chain H1:



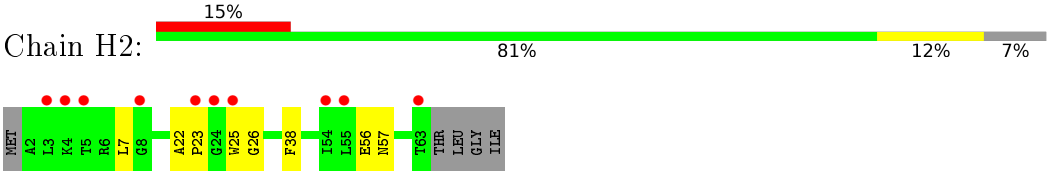
- Molecule 7: Photosystem II reaction center protein H

Chain h1:



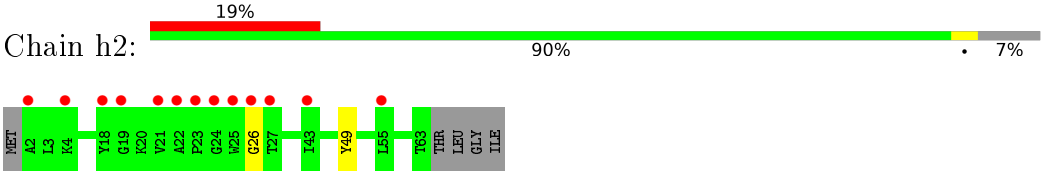
- Molecule 7: Photosystem II reaction center protein H

Chain H2:



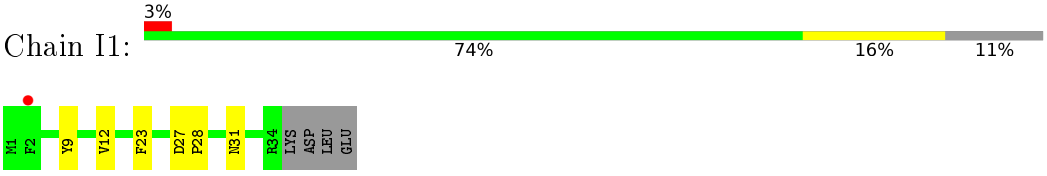
- Molecule 7: Photosystem II reaction center protein H

Chain h2:



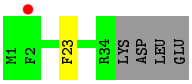
- Molecule 8: Photosystem II reaction center protein I

Chain I1:



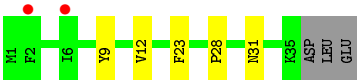
- Molecule 8: Photosystem II reaction center protein I

Chain i1:



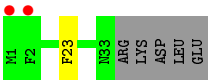
• Molecule 8: Photosystem II reaction center protein I

Chain I2:



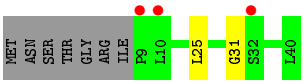
• Molecule 8: Photosystem II reaction center protein I

Chain i2:



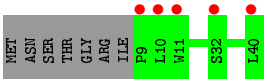
• Molecule 9: Photosystem II reaction center protein J

Chain J1:



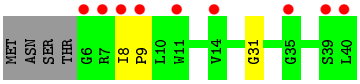
• Molecule 9: Photosystem II reaction center protein J

Chain j1:



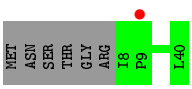
• Molecule 9: Photosystem II reaction center protein J

Chain J2:



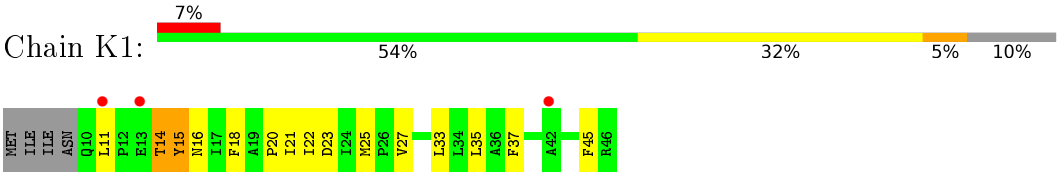
• Molecule 9: Photosystem II reaction center protein J

Chain j2:



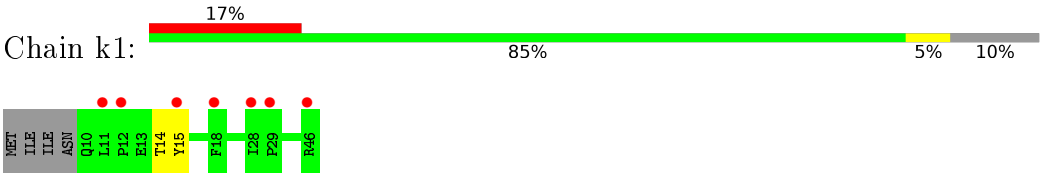
• Molecule 10: Photosystem II reaction center protein K

Chain K1:



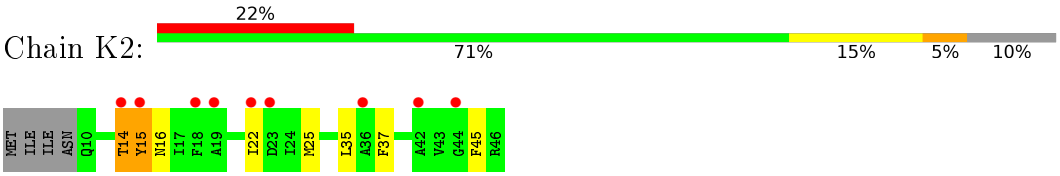
• Molecule 10: Photosystem II reaction center protein K

Chain k1:



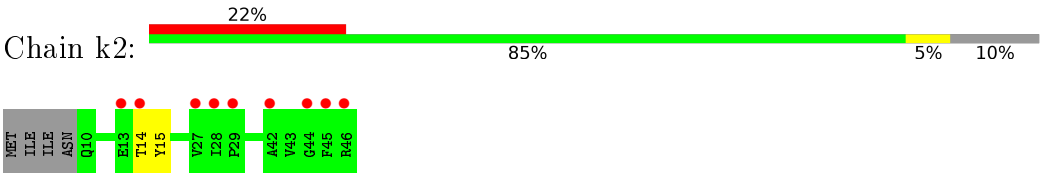
• Molecule 10: Photosystem II reaction center protein K

Chain K2:



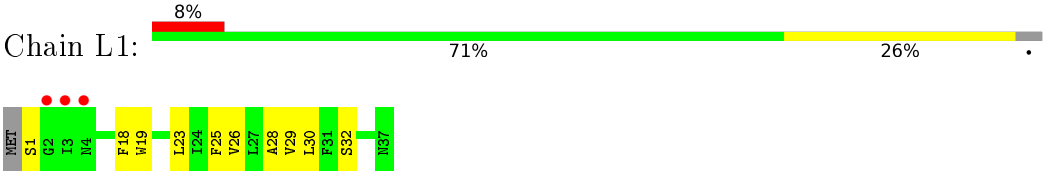
• Molecule 10: Photosystem II reaction center protein K

Chain k2:



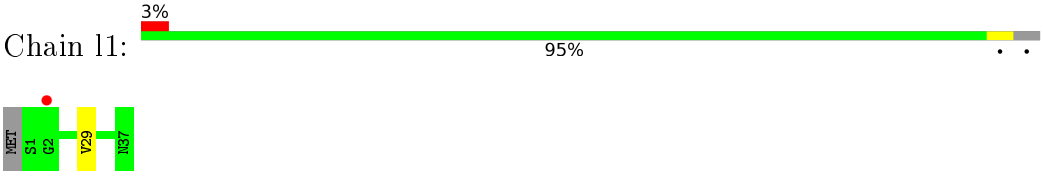
• Molecule 11: Photosystem II reaction center protein L

Chain L1:



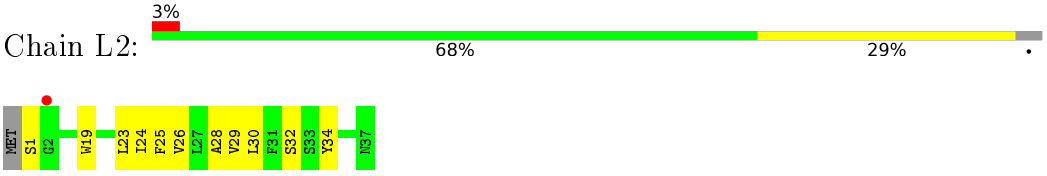
• Molecule 11: Photosystem II reaction center protein L

Chain l1:



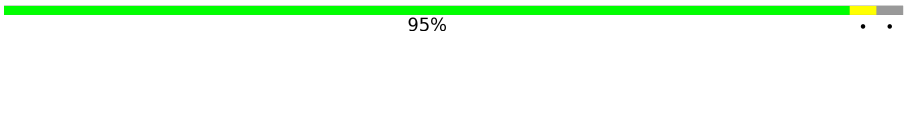
• Molecule 11: Photosystem II reaction center protein L

Chain L2:



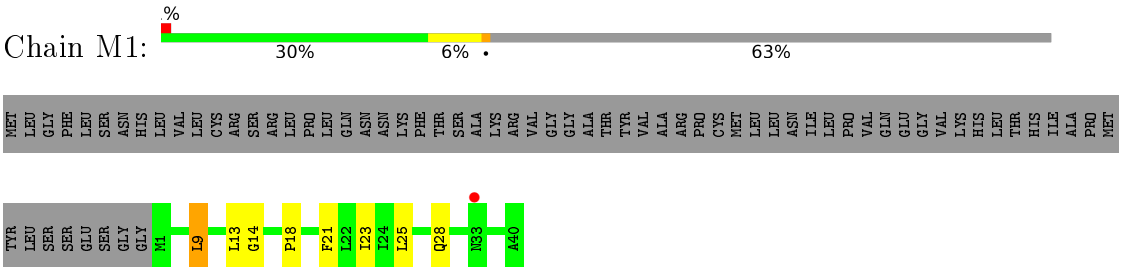
• Molecule 11: Photosystem II reaction center protein L

Chain l2:



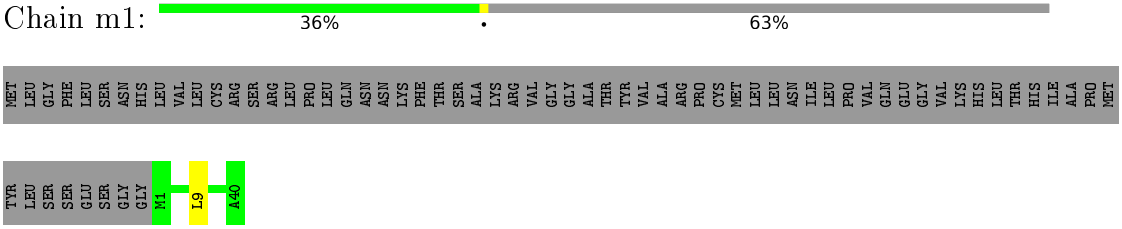
• Molecule 12: PHOTOSYSTEM II REACTION CENTER PROTEIN M

Chain M1:



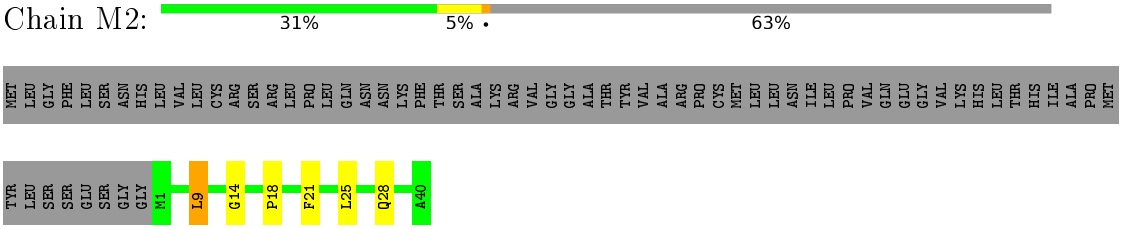
• Molecule 12: PHOTOSYSTEM II REACTION CENTER PROTEIN M

Chain m1:



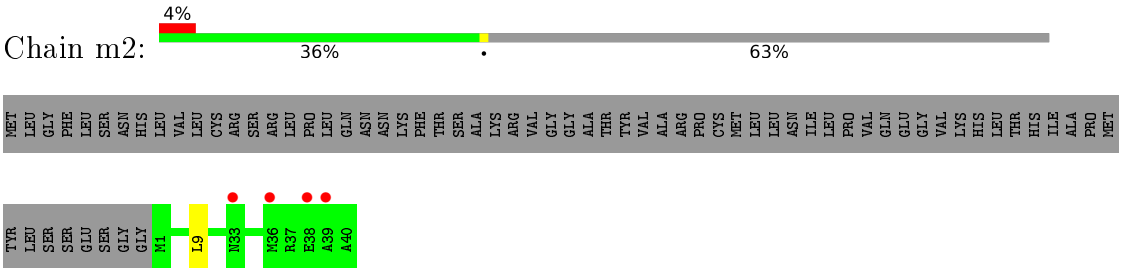
• Molecule 12: PHOTOSYSTEM II REACTION CENTER PROTEIN M

Chain M2:



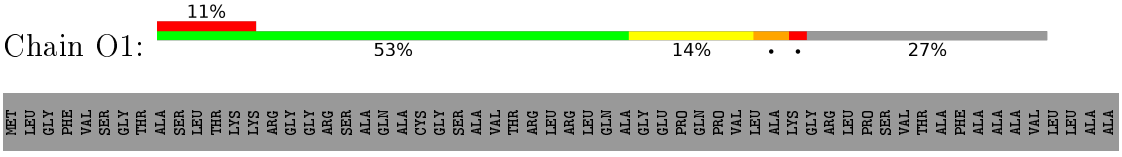
• Molecule 12: PHOTOSYSTEM II REACTION CENTER PROTEIN M

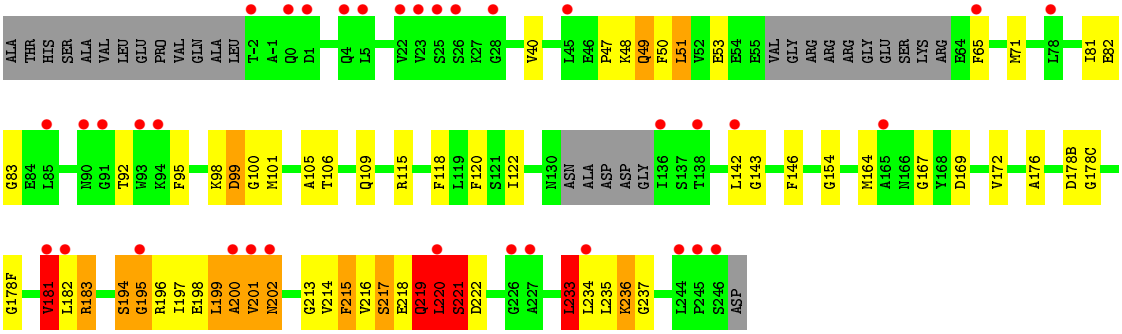
Chain m2:



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

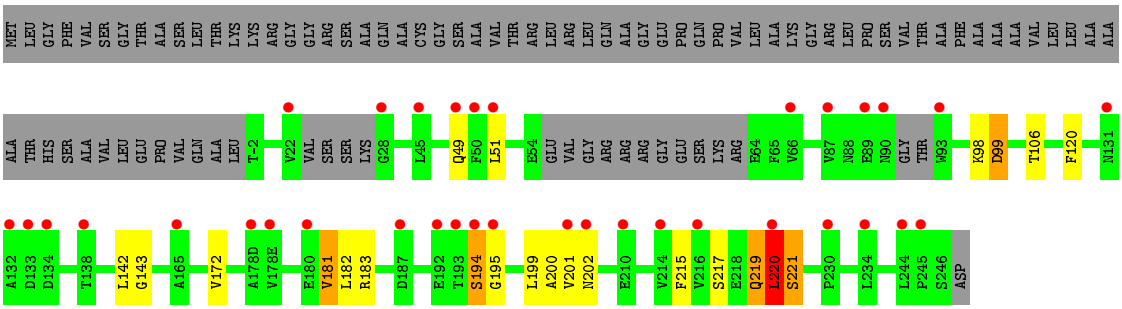
Chain O1:





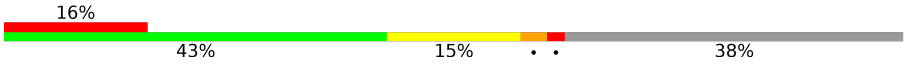
• Molecule 13: PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE, PSBO

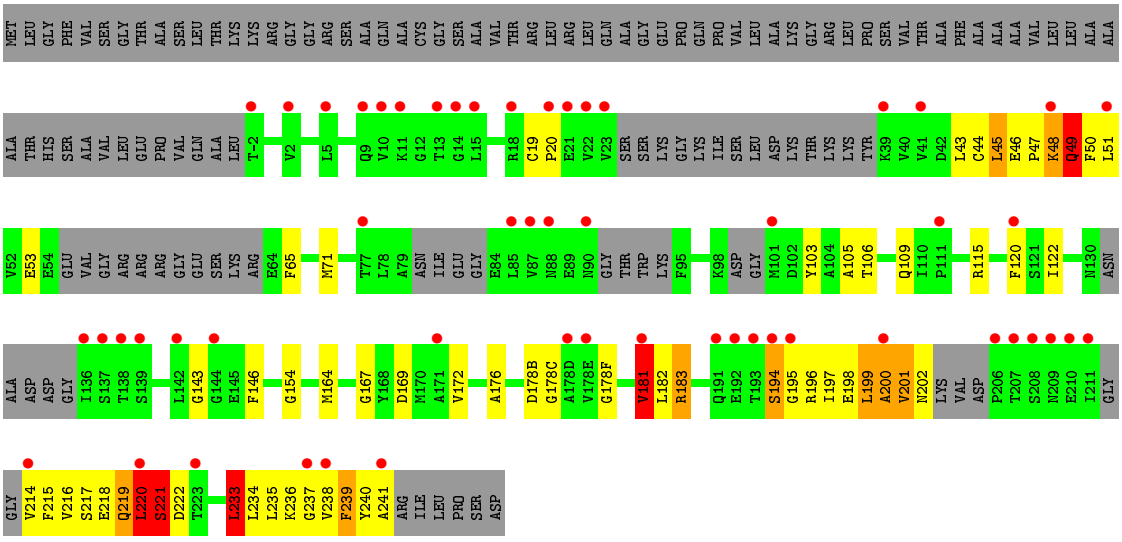
Chain o1:



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

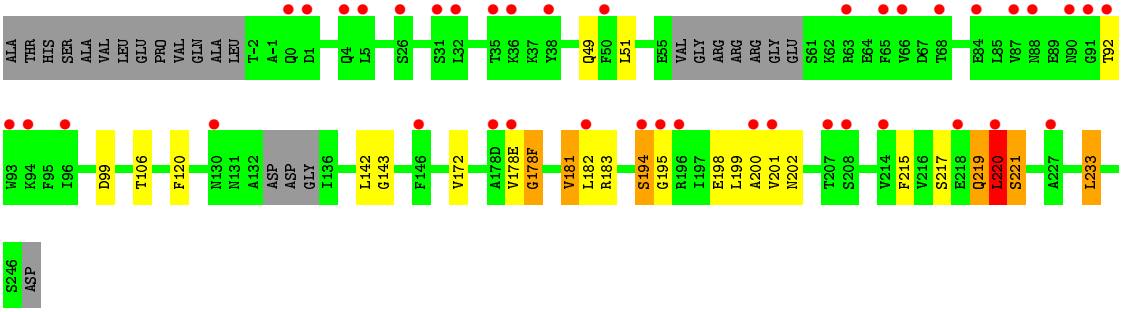
Chain O2:



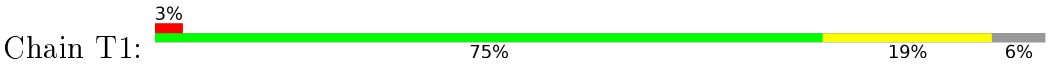


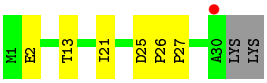
• Molecule 13: PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE, PSBO

Chain o2:

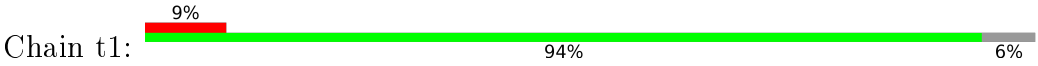


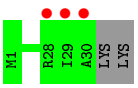
• Molecule 14: Photosystem II reaction center protein T



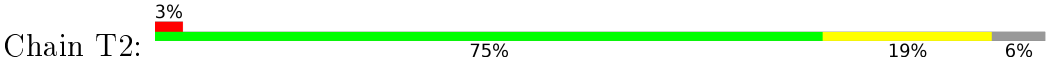


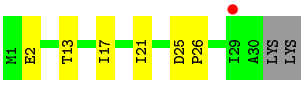
• Molecule 14: Photosystem II reaction center protein T



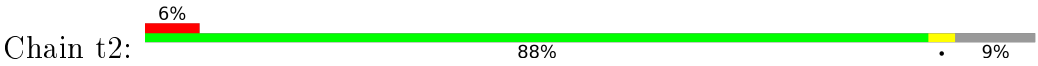


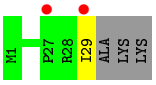
• Molecule 14: Photosystem II reaction center protein T



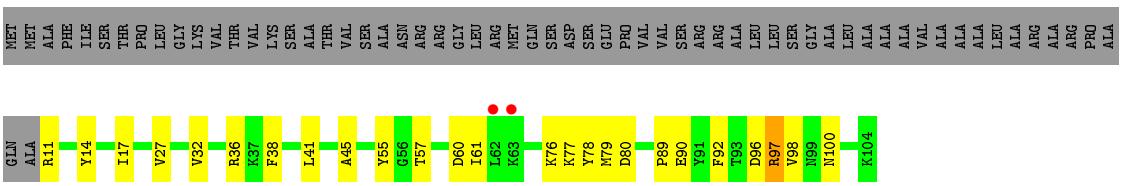


• Molecule 14: Photosystem II reaction center protein T



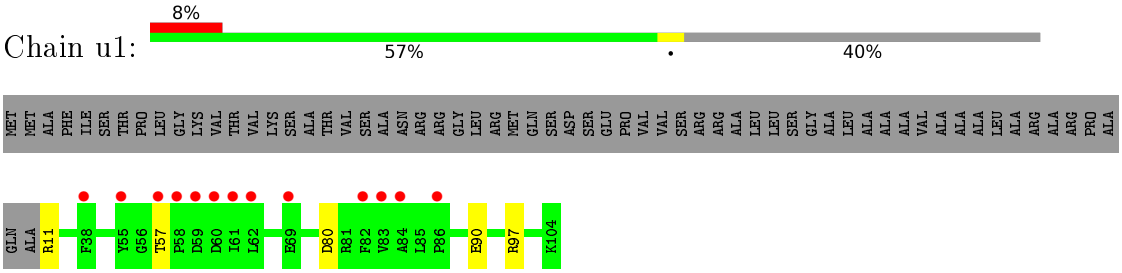


• Molecule 15: Photosystem II 12 kDa extrinsic protein, chloroplastic



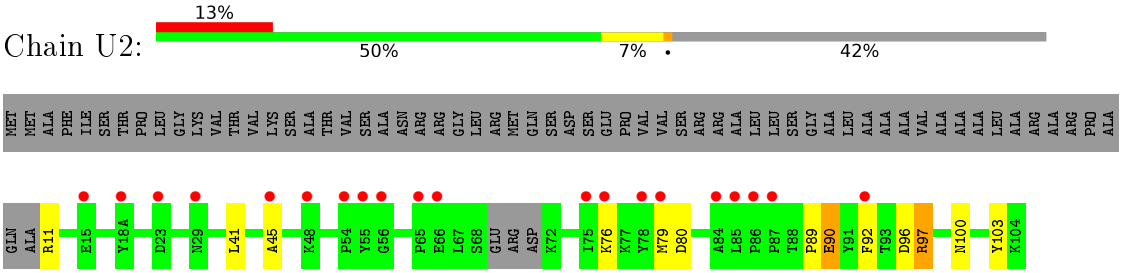
• Molecule 15: Photosystem II 12 kDa extrinsic protein, chloroplastic

Chain u1:



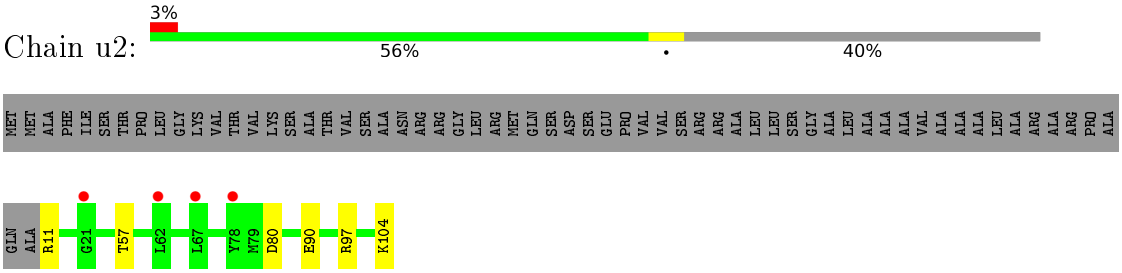
- Molecule 15: Photosystem II 12 kDa extrinsic protein, chloroplastic

Chain U2:



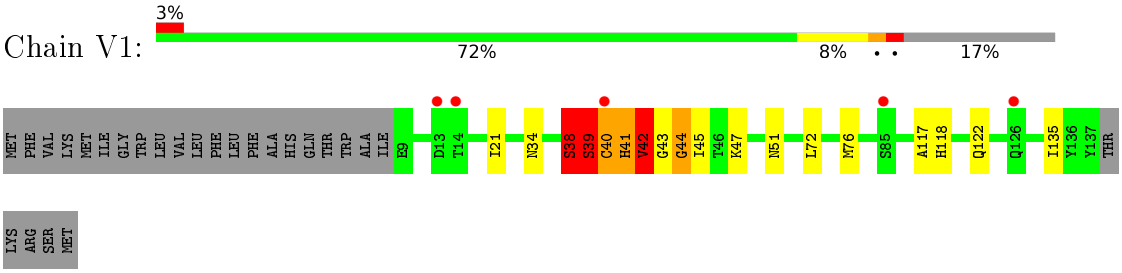
- Molecule 15: Photosystem II 12 kDa extrinsic protein, chloroplastic

Chain u2:



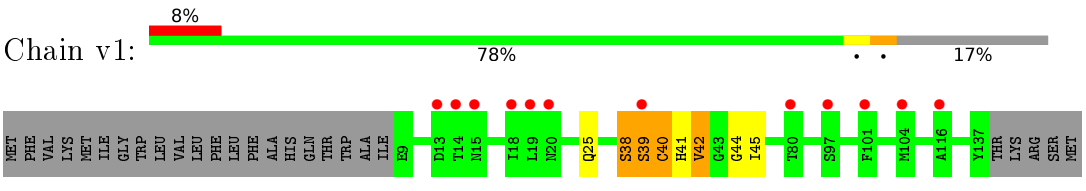
- Molecule 16: Cytochrome c-550

Chain V1:



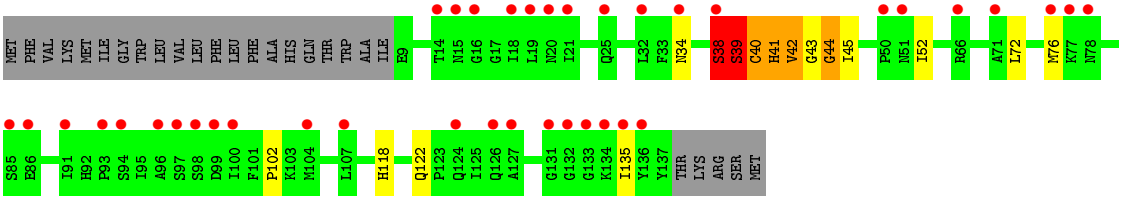
- Molecule 16: Cytochrome c-550

Chain v1:

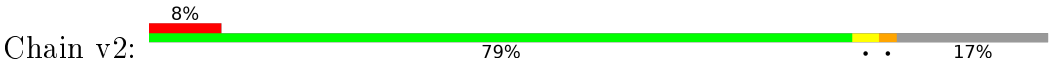


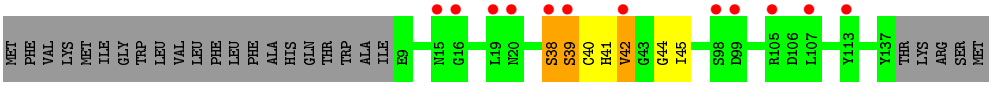
- Molecule 16: Cytochrome c-550

Chain V2:

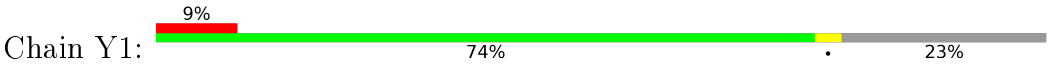


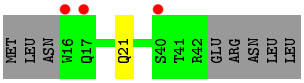
• Molecule 16: Cytochrome c-550



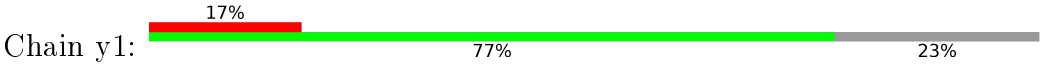


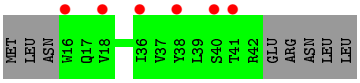
• Molecule 17: Photosystem II reaction center protein Ycf12



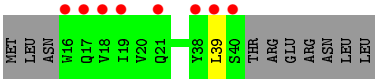


• Molecule 17: Photosystem II reaction center protein Ycf12

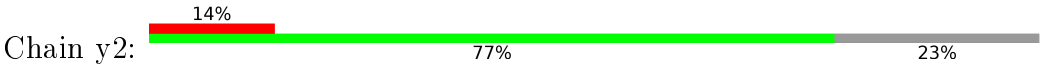


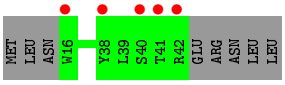


• Molecule 17: Photosystem II reaction center protein Ycf12

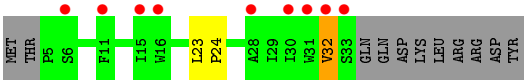


• Molecule 17: Photosystem II reaction center protein Ycf12



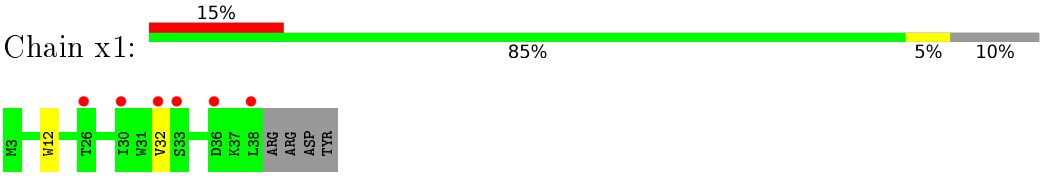


• Molecule 18: PHOTOSYSTEM II REACTION CENTER PROTEIN X



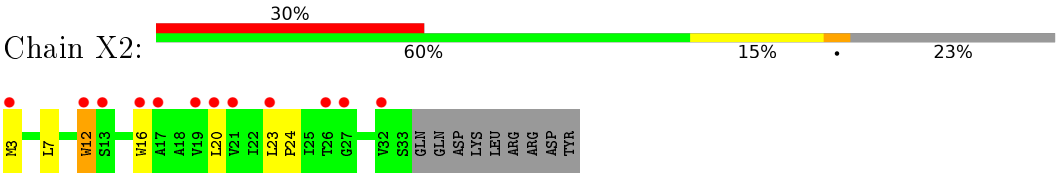
• Molecule 18: PHOTOSYSTEM II REACTION CENTER PROTEIN X

Chain x1:



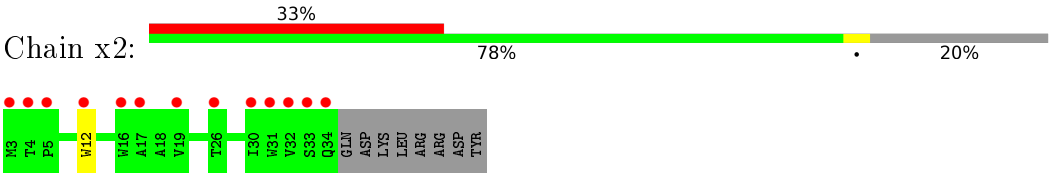
• Molecule 18: PHOTOSYSTEM II REACTION CENTER PROTEIN X

Chain X2:



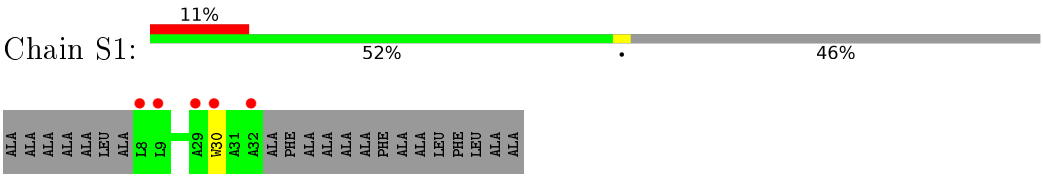
• Molecule 18: PHOTOSYSTEM II REACTION CENTER PROTEIN X

Chain x2:



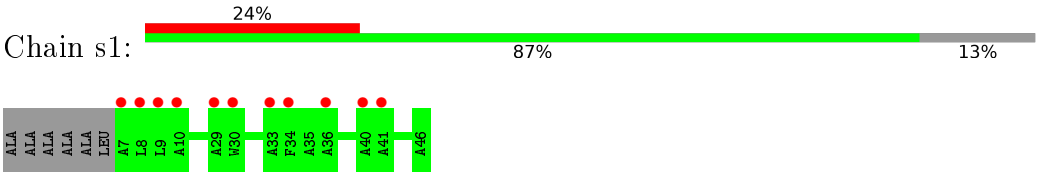
• Molecule 19: PEPTIDE CHAIN UNASSIGNED

Chain S1:



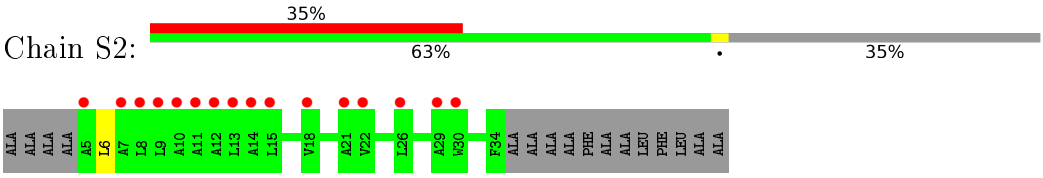
• Molecule 19: PEPTIDE CHAIN UNASSIGNED

Chain s1:



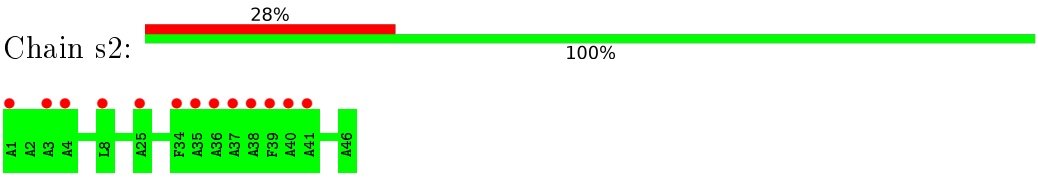
• Molecule 19: PEPTIDE CHAIN UNASSIGNED

Chain S2:



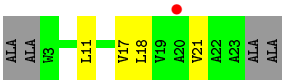
• Molecule 19: PEPTIDE CHAIN UNASSIGNED

Chain s2:



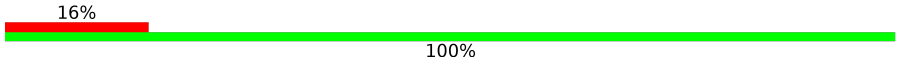
• Molecule 20: PEPTIDE CHAIN UNASSIGNED

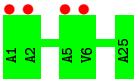
Chain W1:



• Molecule 20: PEPTIDE CHAIN UNASSIGNED

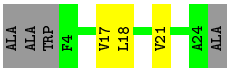
Chain w1:





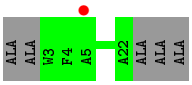
• Molecule 20: PEPTIDE CHAIN UNASSIGNED

Chain W2:



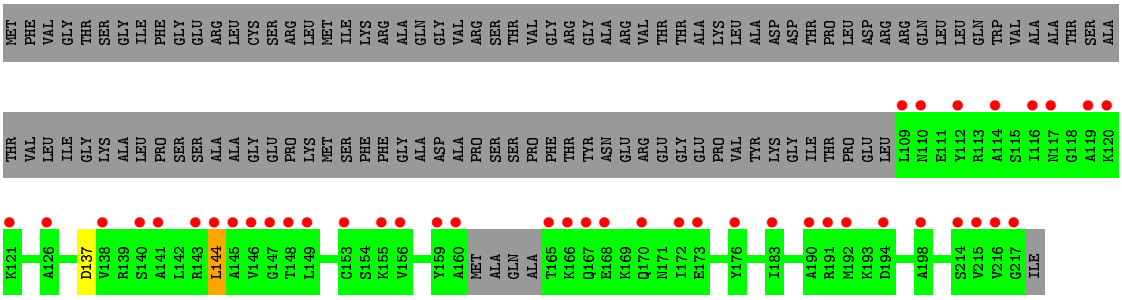
• Molecule 20: PEPTIDE CHAIN UNASSIGNED

Chain w2:



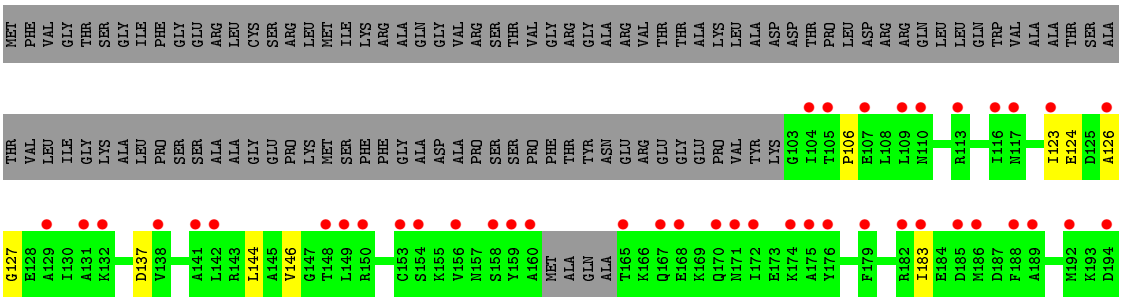
• Molecule 21: Extrinsic protein in photosystem II

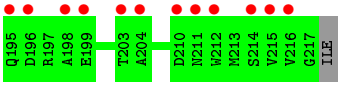
Chain q1:



• Molecule 21: Extrinsic protein in photosystem II

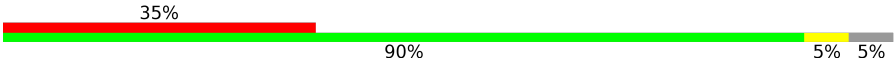
Chain Q2:

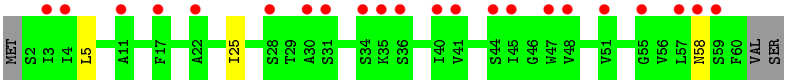




• Molecule 22: Photosystem II reaction center protein Z

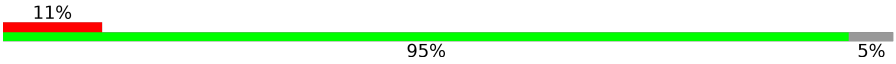
Chain Z2:

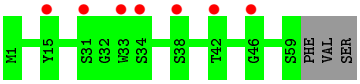




• Molecule 22: Photosystem II reaction center protein Z

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

The worst 5 of 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

The worst 5 of 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	O1	194	SER	Peptide
13	O1	220	LEU	Peptide
16	V1	38	SER	Peptide
16	V1	41	HIS	Peptide
16	V1	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

The worst 5 of 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

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

5 of 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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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

5 of 162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	o1	220	LEU
2	B2	6	TYR
13	o2	183	ARG
15	u1	57	THR
18	x1	12	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
2	b1	489	GLN
3	c1	418	ASN
13	o2	109	GLN
3	c1	56	HIS
13	o1	109	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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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%)
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

The worst 5 of 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

The worst 5 of 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

5 of 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

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

The worst 5 of 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

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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.