



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 14, 2016 – 06:10 PM EST

PDB ID : 4FBY
Title : fs X-ray diffraction of Photosystem II
Authors : Kern, J.; Alonso-Mori, R.; Hellmich, J.; Tran, R.; Hattne, J.; Laksmono, H.; Gloeckner, C.; Echols, N.; Sierra, R.G.; Sellberg, J.; Lassalle-Kaiser, B.; Gildea, R.J.; Glatzel, P.; Grosse-Kunstleve, R.W.; Latimer, M.J.; McQueen, T.A.; Difiore, D.; Fry, A.R.; Messerschmidt, M.M.; Miahnahri, A.; Schafer, D.W.; Seibert, M.M.; Sokaras, D.; Weng, T.-C.; Zwart, P.H.; White, W.E.; Adams, P.D.; Bogan, M.J.; Boutet, S.; Williams, G.J.; Messinger, J.; Sauter, N.K.; Zouni, A.; Bergmann, U.; Yano, J.; Yachandra, V.K.
Deposited on : 2012-05-23
Resolution : 6.56 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

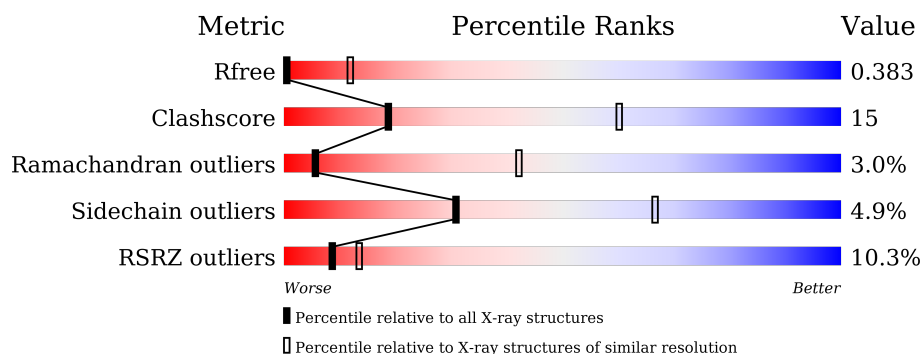
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.56 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	1012 (9.00-3.66)
Clashscore	102246	1060 (9.00-3.70)
Ramachandran outliers	100387	1033 (9.00-3.66)
Sidechain outliers	100360	1004 (9.00-3.66)
RSRZ outliers	91569	1011 (9.00-3.66)

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

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div>8%</div> <div>62%</div> <div>33%</div> <div>..</div> </div>
1	G	344	<div> <div>6%</div> <div>62%</div> <div>33%</div> <div>..</div> </div>
2	B	510	<div> <div>11%</div> <div>69%</div> <div>24%</div> <div>...</div> </div>
2	N	510	<div> <div>13%</div> <div>71%</div> <div>23%</div> <div>...</div> </div>
3	C	461	<div> <div>5%</div> <div>61%</div> <div>32%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
3	P	461	
4	D	352	
4	Q	352	
5	E	83	
5	R	83	
6	F	44	
6	S	44	
7	H	65	
7	W	65	
8	I	38	
8	a	38	
9	J	39	
9	b	39	
10	K	37	
10	c	37	
11	L	37	
11	d	37	
12	M	36	
12	e	36	
13	O	246	
13	f	246	
14	T	32	
14	g	32	
15	U	104	
15	h	104	

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Mol	Chain	Length	Quality of chain
16	V	137	
16	i	137	
17	m	46	
17	y	46	
18	X	40	
18	j	40	
19	Y	28	
19	k	28	
20	Z	62	
20	l	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
21	CLA	A	401	X	-	-	-
21	CLA	A	402	X	-	-	-
21	CLA	A	403	X	-	-	-
21	CLA	A	405	X	-	-	X
21	CLA	B	601	X	-	-	X
21	CLA	B	602	X	-	-	X
21	CLA	B	603	X	-	-	X
21	CLA	B	604	X	-	-	X
21	CLA	B	605	X	-	-	X
21	CLA	B	606	X	-	-	X
21	CLA	B	607	X	-	-	-
21	CLA	B	608	X	-	-	X
21	CLA	B	609	X	-	-	X
21	CLA	B	610	X	-	-	X
21	CLA	B	611	X	-	-	-
21	CLA	B	612	X	-	-	X
21	CLA	B	613	X	-	-	-
21	CLA	B	614	X	-	-	-
21	CLA	B	615	X	-	-	X
21	CLA	B	616	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	C	501	X	-	-	X
21	CLA	C	502	X	-	-	X
21	CLA	C	503	X	-	-	X
21	CLA	C	504	X	-	-	-
21	CLA	C	505	X	-	-	X
21	CLA	C	506	X	-	-	X
21	CLA	C	507	X	-	-	X
21	CLA	C	508	X	-	-	-
21	CLA	C	509	X	-	-	X
21	CLA	C	510	X	-	-	-
21	CLA	C	511	X	-	-	X
21	CLA	C	512	X	-	-	X
21	CLA	C	513	X	-	-	X
21	CLA	D	401	X	-	-	X
21	CLA	D	403	X	-	-	X
21	CLA	G	402	X	-	-	X
21	CLA	G	403	X	-	-	-
21	CLA	G	404	X	-	-	-
21	CLA	G	406	X	-	-	X
21	CLA	N	605	X	-	-	X
21	CLA	N	606	X	-	-	-
21	CLA	N	607	X	-	-	X
21	CLA	N	608	X	-	-	X
21	CLA	N	609	X	-	-	X
21	CLA	N	610	X	-	-	X
21	CLA	N	611	X	-	-	-
21	CLA	N	612	X	-	-	X
21	CLA	N	613	X	-	-	X
21	CLA	N	614	X	-	-	X
21	CLA	N	615	X	-	-	-
21	CLA	N	616	X	-	-	X
21	CLA	N	617	X	-	-	-
21	CLA	N	618	X	-	-	-
21	CLA	N	619	X	-	-	X
21	CLA	N	620	X	-	-	X
21	CLA	P	501	X	-	-	X
21	CLA	P	502	X	-	-	X
21	CLA	P	503	X	-	-	X
21	CLA	P	504	X	-	-	X
21	CLA	P	505	X	-	-	-
21	CLA	P	506	X	-	-	X
21	CLA	P	507	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	P	508	X	-	-	X
21	CLA	P	509	X	-	-	X
21	CLA	P	510	X	-	-	X
21	CLA	P	511	X	-	-	X
21	CLA	P	512	X	-	-	X
21	CLA	P	513	X	-	-	X
21	CLA	Q	402	X	-	-	X
21	CLA	Q	404	X	-	-	X
22	PHO	D	402	-	-	-	X
23	PL9	A	406	-	-	-	X
23	PL9	G	407	-	-	-	X
23	PL9	J	101	-	-	-	X
23	PL9	b	101	-	-	-	X
24	DGD	A	407	X	-	-	-
24	DGD	B	621	X	-	-	X
24	DGD	B	628	X	-	-	X
24	DGD	C	516	X	-	-	-
24	DGD	C	517	X	-	-	-
24	DGD	C	518	X	-	-	-
24	DGD	D	408	X	-	-	X
24	DGD	G	408	X	-	-	X
24	DGD	N	602	X	-	-	X
24	DGD	P	517	X	-	-	-
24	DGD	P	518	X	-	-	X
24	DGD	P	519	X	-	-	-
24	DGD	Q	409	X	-	-	X
24	DGD	W	102	X	-	-	-
25	LHG	A	411	-	-	-	X
25	LHG	G	412	-	-	-	X
26	SQD	A	414	-	-	-	X
26	SQD	B	624	-	-	-	X
26	SQD	B	627	-	-	-	X
26	SQD	F	101	-	-	-	X
26	SQD	N	601	-	-	-	X
26	SQD	Q	408	-	-	-	X
26	SQD	S	102	-	-	-	X
27	LMG	A	410	X	-	-	-
27	LMG	B	622	X	-	-	-
27	LMG	B	623	X	-	-	-
27	LMG	C	519	X	-	-	-
27	LMG	C	520	X	-	-	X
27	LMG	D	406	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	LMG	D	407	X	-	-	-
27	LMG	D	412	X	-	-	X
27	LMG	E	102	X	-	-	X
27	LMG	G	411	X	-	-	-
27	LMG	I	102	X	-	-	-
27	LMG	M	101	X	-	-	-
27	LMG	N	622	X	-	-	-
27	LMG	N	623	X	-	-	-
27	LMG	P	520	X	-	-	X
27	LMG	P	521	X	-	-	X
27	LMG	Q	401	X	-	-	X
27	LMG	Q	406	X	-	-	X
27	LMG	Q	407	X	-	-	-
27	LMG	R	102	X	-	-	X
27	LMG	a	102	X	-	-	-
27	LMG	e	102	X	-	-	-
28	OEC	A	412	-	-	-	X
28	OEC	G	413	-	-	-	X
30	BCR	B	620	-	-	-	X
30	BCR	C	514	-	-	-	X
30	BCR	C	515	-	-	-	X
30	BCR	D	405	-	-	-	X
30	BCR	H	101	-	-	-	X
30	BCR	I	101	-	-	-	X
30	BCR	J	102	-	-	-	X
30	BCR	K	101	-	-	-	X
30	BCR	P	514	-	-	-	X
30	BCR	P	515	-	-	-	X
30	BCR	P	516	-	-	-	X
30	BCR	S	101	-	-	-	X
30	BCR	T	103	-	-	-	X
30	BCR	W	101	-	-	-	X
30	BCR	Z	101	-	-	-	X
30	BCR	a	101	-	-	-	X
30	BCR	b	102	-	-	-	X
30	BCR	c	101	-	-	-	X
31	LMT	B	626	-	-	-	X
31	LMT	B	629	-	-	-	X
31	LMT	B	630	-	-	-	X
31	LMT	D	409	-	-	-	X
31	LMT	I	103	-	-	-	X
31	LMT	M	102	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	LMT	N	603	-	-	-	X
31	LMT	N	604	-	-	-	X
31	LMT	N	625	-	-	-	X
31	LMT	Q	410	-	-	-	X
31	LMT	a	103	-	-	-	X
31	LMT	e	101	-	-	-	X
32	BCT	Q	411	-	-	-	X
33	CL	D	411	-	-	-	X
33	CL	G	415	-	-	-	X
34	HEM	R	101	-	-	-	X
34	HEM	V	201	-	-	-	X
34	HEM	i	201	-	-	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50232 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			
4	Q	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			
9	b	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

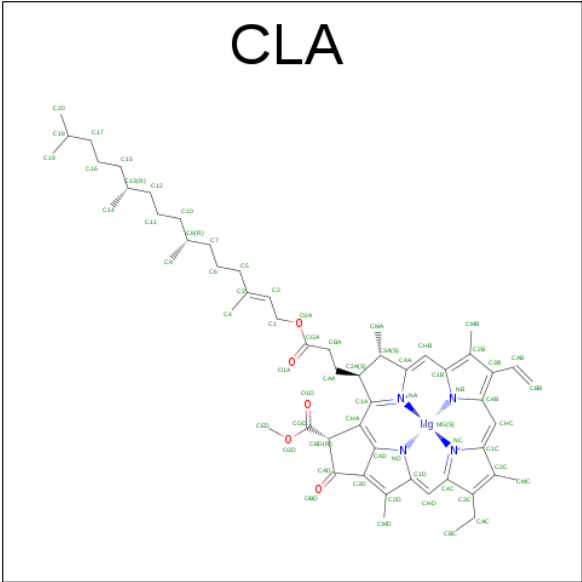
- Molecule 19 is a protein called Photosystem II reaction center protein Y.

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

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

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

- Molecule 21 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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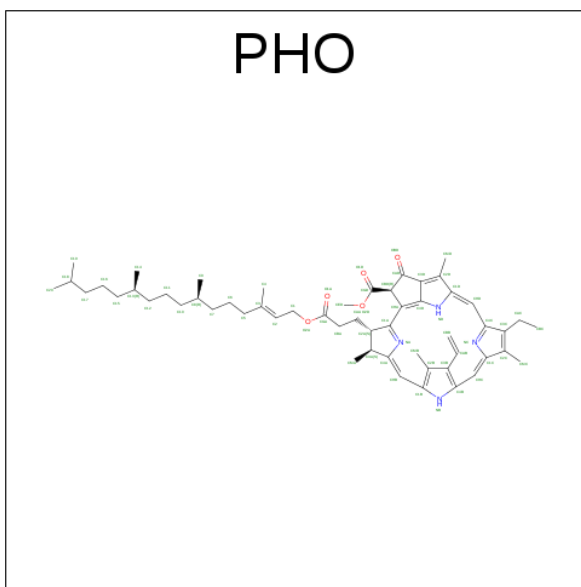
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	P	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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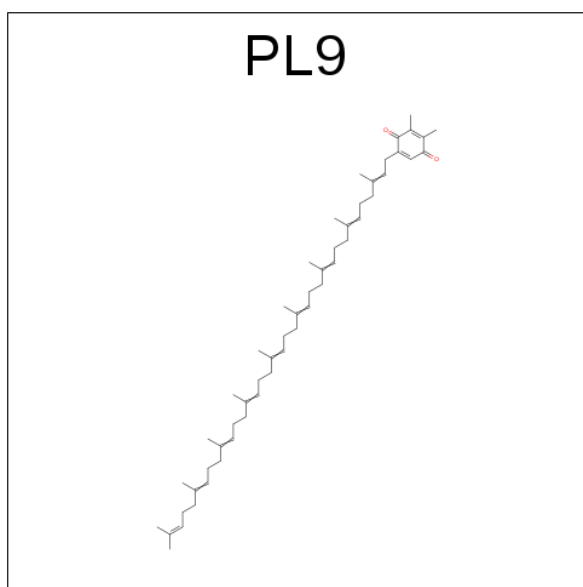
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	Q	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	Q	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 22 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	N	O	0	0
			64	55	4	5		
22	D	1	Total	C	N	O	0	0
			64	55	4	5		
22	G	1	Total	C	N	O	0	0
			64	55	4	5		
22	Q	1	Total	C	N	O	0	0
			64	55	4	5		

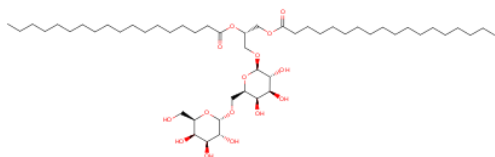
- Molecule 23 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: C₅₃H₈₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			45	43	2		
23	D	1	Total	C	O	0	0
			55	53	2		
23	J	1	Total	C	O	0	0
			35	33	2		
23	G	1	Total	C	O	0	0
			45	43	2		
23	Q	1	Total	C	O	0	0
			55	53	2		
23	b	1	Total	C	O	0	0
			35	33	2		

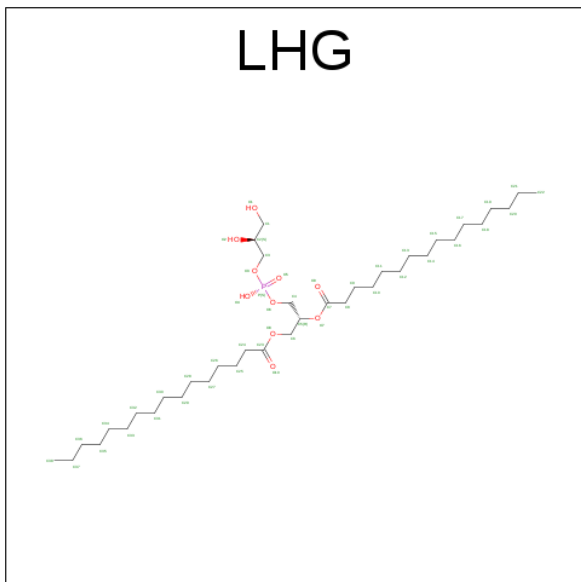
- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).

DGD



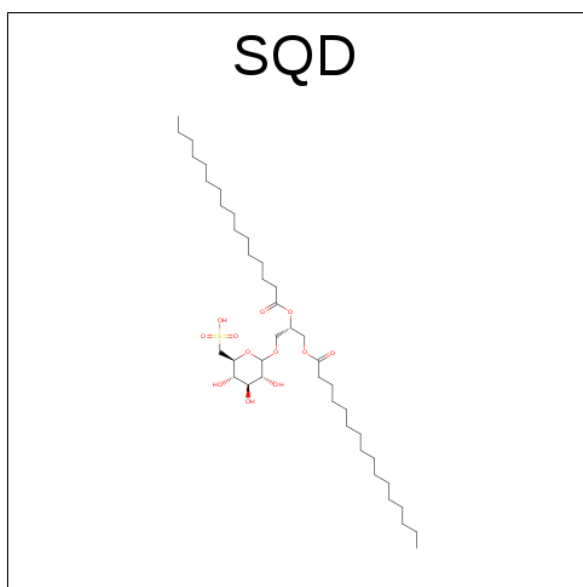
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	A	1	Total	C	O	0	0
			56	41	15		
24	B	1	Total	C	O	0	0
			58	43	15		
24	B	1	Total	C	O	0	0
			52	37	15		
24	C	1	Total	C	O	0	0
			53	38	15		
24	C	1	Total	C	O	0	0
			62	47	15		
24	C	1	Total	C	O	0	0
			66	51	15		
24	D	1	Total	C	O	0	0
			63	48	15		
24	G	1	Total	C	O	0	0
			56	41	15		
24	N	1	Total	C	O	0	0
			52	37	15		
24	P	1	Total	C	O	0	0
			53	38	15		
24	P	1	Total	C	O	0	0
			62	47	15		
24	P	1	Total	C	O	0	0
			66	51	15		
24	Q	1	Total	C	O	0	0
			63	48	15		
24	W	1	Total	C	O	0	0
			58	43	15		

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



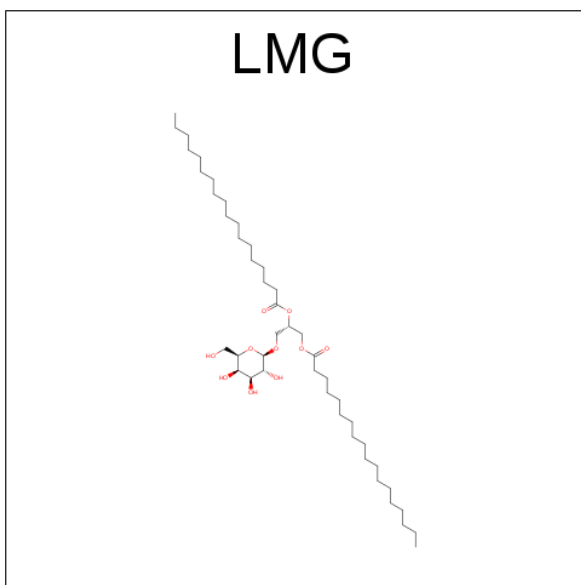
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	O	P	0	0
			39	28	10	1		
25	A	1	Total	C	O	P	0	0
			37	26	10	1		
25	G	1	Total	C	O	P	0	0
			39	28	10	1		
25	G	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 26 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
26	A	1	Total	C	O	S	0	0
			51	38	12	1		
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	B	1	Total	C	O	S	0	0
			43	30	12	1		
26	B	1	Total	C	O	S	0	0
			47	34	12	1		
26	F	1	Total	C	O	S	0	0
			45	32	12	1		
26	G	1	Total	C	O	S	0	0
			54	41	12	1		
26	G	1	Total	C	O	S	0	0
			51	38	12	1		
26	N	1	Total	C	O	S	0	0
			47	34	12	1		
26	Q	1	Total	C	O	S	0	0
			43	30	12	1		
26	S	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



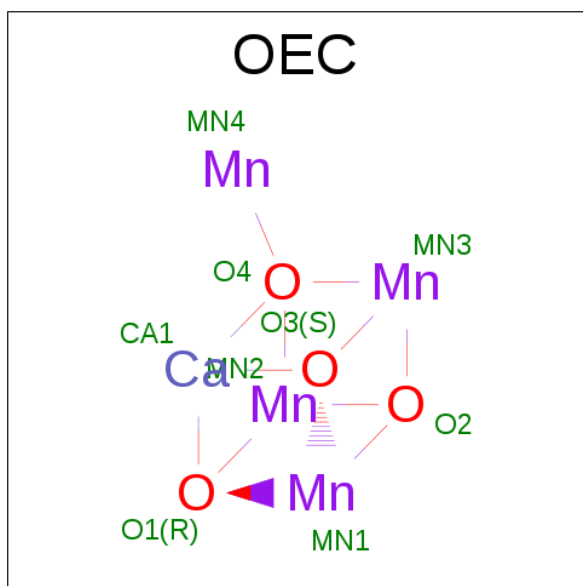
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			51	41	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	C	1	Total	C	O	0	0
			48	38	10		
27	C	1	Total	C	O	0	0
			45	35	10		
27	D	1	Total	C	O	0	0
			46	36	10		
27	D	1	Total	C	O	0	0
			48	38	10		
27	E	1	Total	C	O	0	0
			44	34	10		
27	D	1	Total	C	O	0	0
			42	32	10		
27	I	1	Total	C	O	0	0
			43	33	10		
27	M	1	Total	C	O	0	0
			42	32	10		
27	G	1	Total	C	O	0	0
			51	41	10		
27	N	1	Total	C	O	0	0
			49	39	10		
27	N	1	Total	C	O	0	0
			49	39	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	P	1	Total	C	O	0	0
			48	38	10		
27	P	1	Total	C	O	0	0
			45	35	10		
27	Q	1	Total	C	O	0	0
			42	32	10		
27	Q	1	Total	C	O	0	0
			48	38	10		
27	Q	1	Total	C	O	0	0
			46	36	10		
27	R	1	Total	C	O	0	0
			44	34	10		
27	a	1	Total	C	O	0	0
			43	33	10		
27	e	1	Total	C	O	0	0
			42	32	10		

- Molecule 28 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn_4O_4).

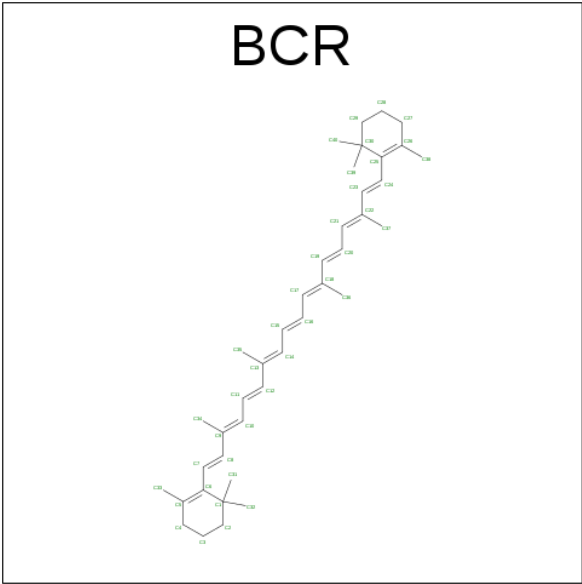


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	Ca	Mn	0	0
			5	1	4		
28	G	1	Total	Ca	Mn	0	0
			5	1	4		

- Molecule 29 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	G	1	Total Fe 1 1	0	0
29	A	1	Total Fe 1 1	0	0

- Molecule 30 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



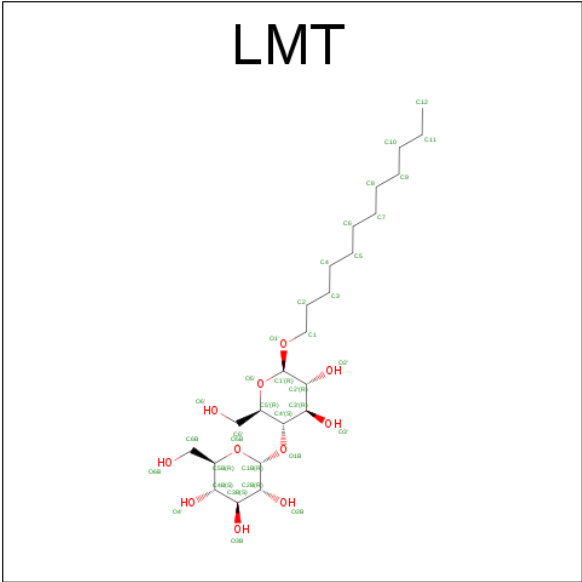
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	B	1	Total C 40 40	0	0
30	B	1	Total C 40 40	0	0
30	B	1	Total C 40 40	0	0
30	B	1	Total C 40 40	0	0
30	C	1	Total C 40 40	0	0
30	C	1	Total C 40 40	0	0
30	D	1	Total C 40 40	0	0
30	H	1	Total C 40 40	0	0
30	I	1	Total C 40 40	0	0
30	J	1	Total C 40 40	0	0

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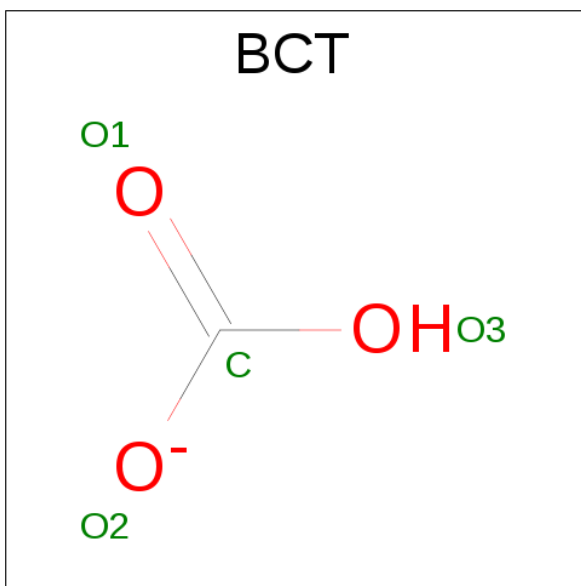
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	K	1	Total C 40 40	0	0
30	T	1	Total C 40 40	0	0
30	T	1	Total C 40 40	0	0
30	T	1	Total C 40 40	0	0
30	Z	1	Total C 40 40	0	0
30	N	1	Total C 40 40	0	0
30	P	1	Total C 40 40	0	0
30	P	1	Total C 40 40	0	0
30	P	1	Total C 40 40	0	0
30	S	1	Total C 40 40	0	0
30	W	1	Total C 40 40	0	0
30	b	1	Total C 40 40	0	0
30	a	1	Total C 40 40	0	0
30	c	1	Total C 40 40	0	0

- Molecule 31 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	D	1	Total	C	O	0	0
			31	20	11		
31	I	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	N	1	Total	C	O	0	0
			35	24	11		
31	N	1	Total	C	O	0	0
			35	24	11		
31	N	1	Total	C	O	0	0
			35	24	11		
31	N	1	Total	C	O	0	0
			35	24	11		
31	Q	1	Total	C	O	0	0
			31	20	11		
31	a	1	Total	C	O	0	0
			35	24	11		
31	e	1	Total	C	O	0	0
			35	24	11		

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	D	1	Total	C	O	0	0
			4	1	3		
32	Q	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	G	1	Total	Cl	0	0
			1	1		
33	D	1	Total	Cl	0	0
			1	1		

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
34	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
34	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
34	R	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
34	i	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

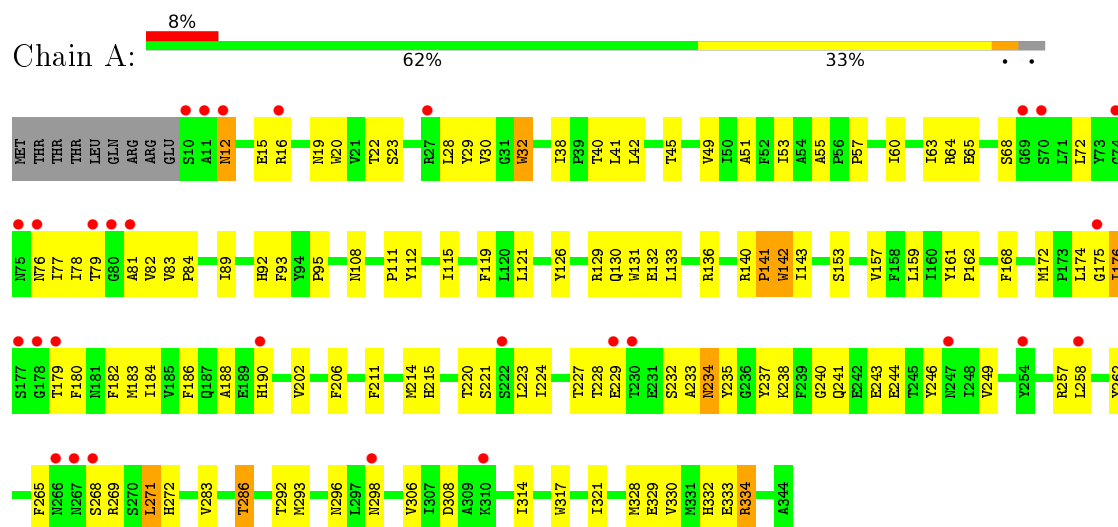
- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	O	1	Total	Ca	0	0
			1	1		
35	f	1	Total	Ca	0	0
			1	1		

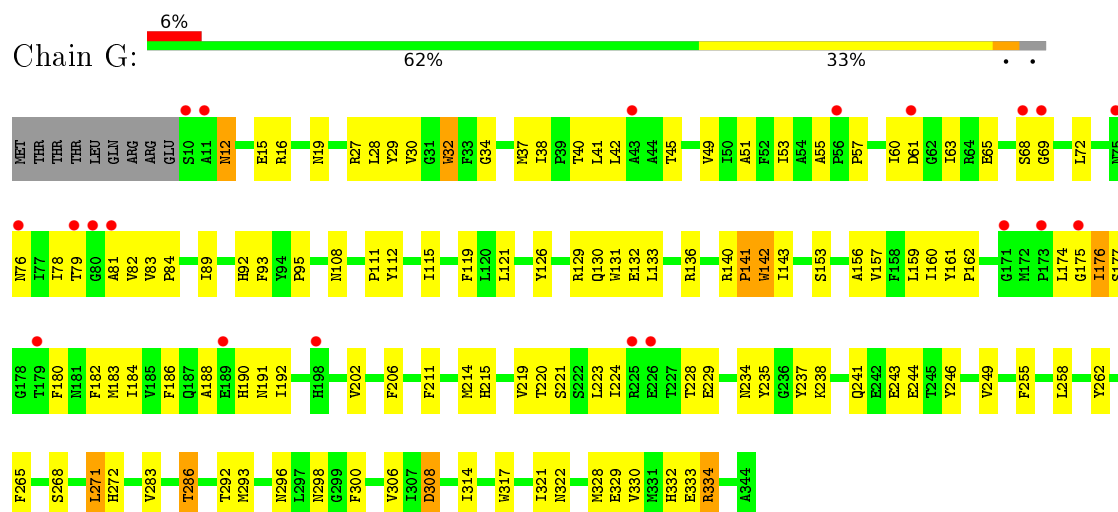
3 Residue-property plots

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

• Molecule 1: Photosystem Q(B) protein 1

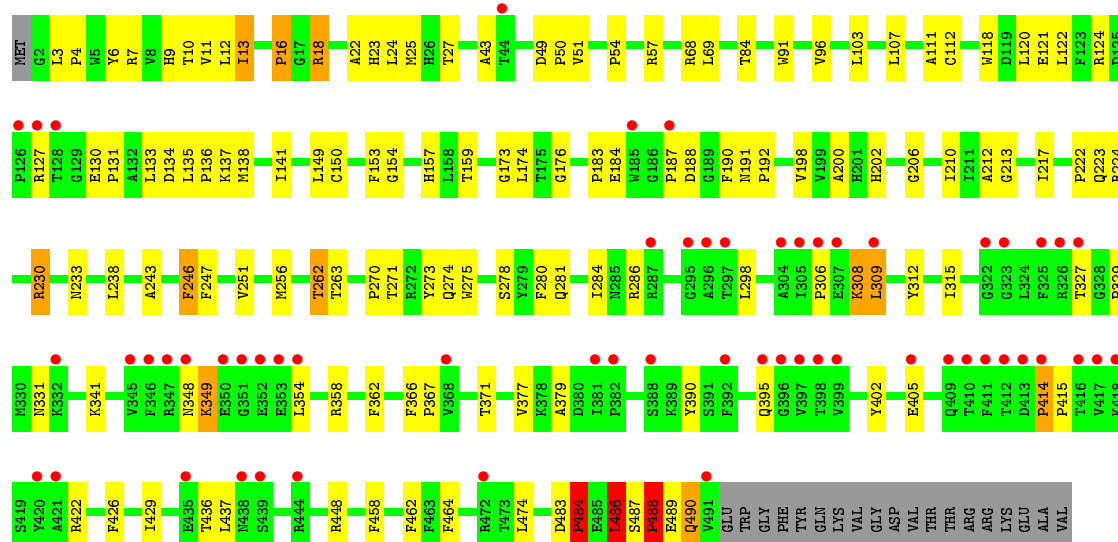


• Molecule 1: Photosystem Q(B) protein 1

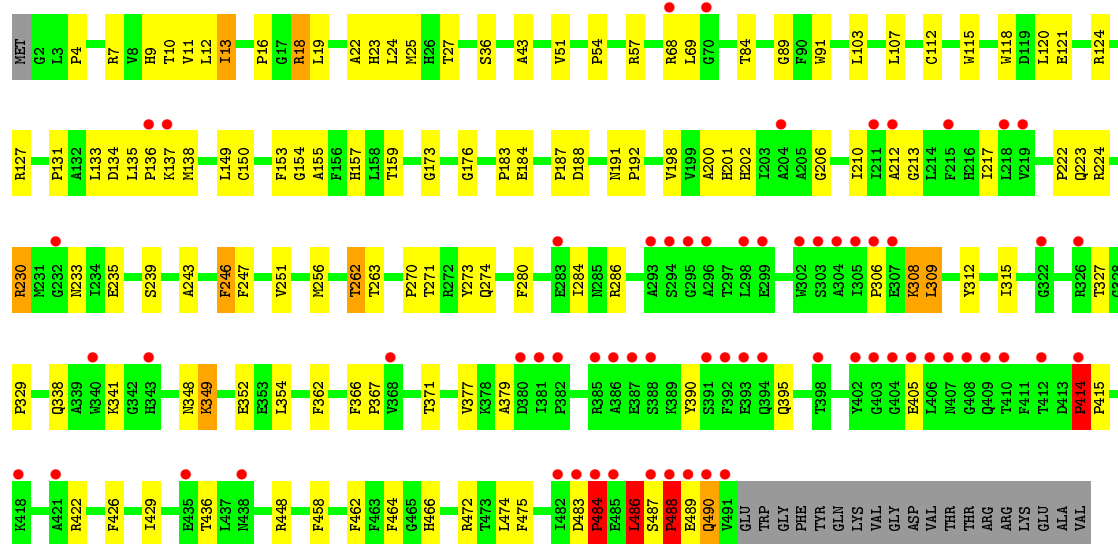


• Molecule 2: Photosystem II core light harvesting protein

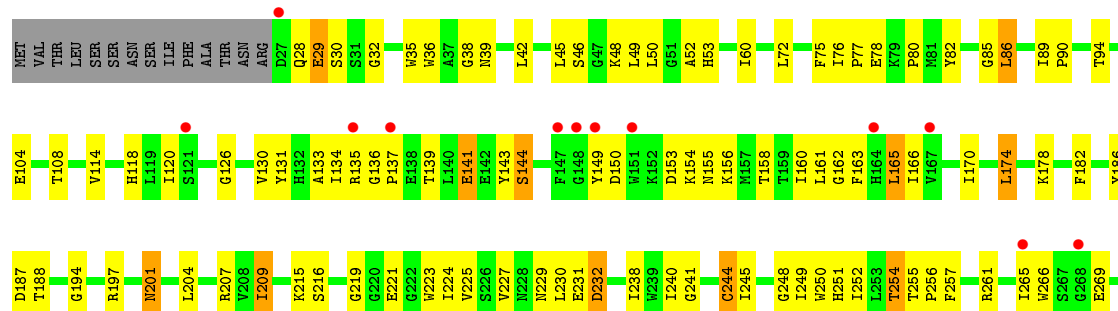


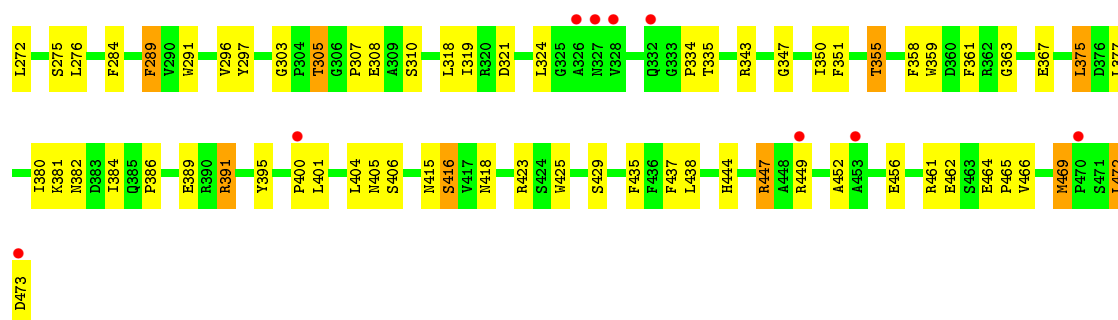


• Molecule 2: Photosystem II core light harvesting protein

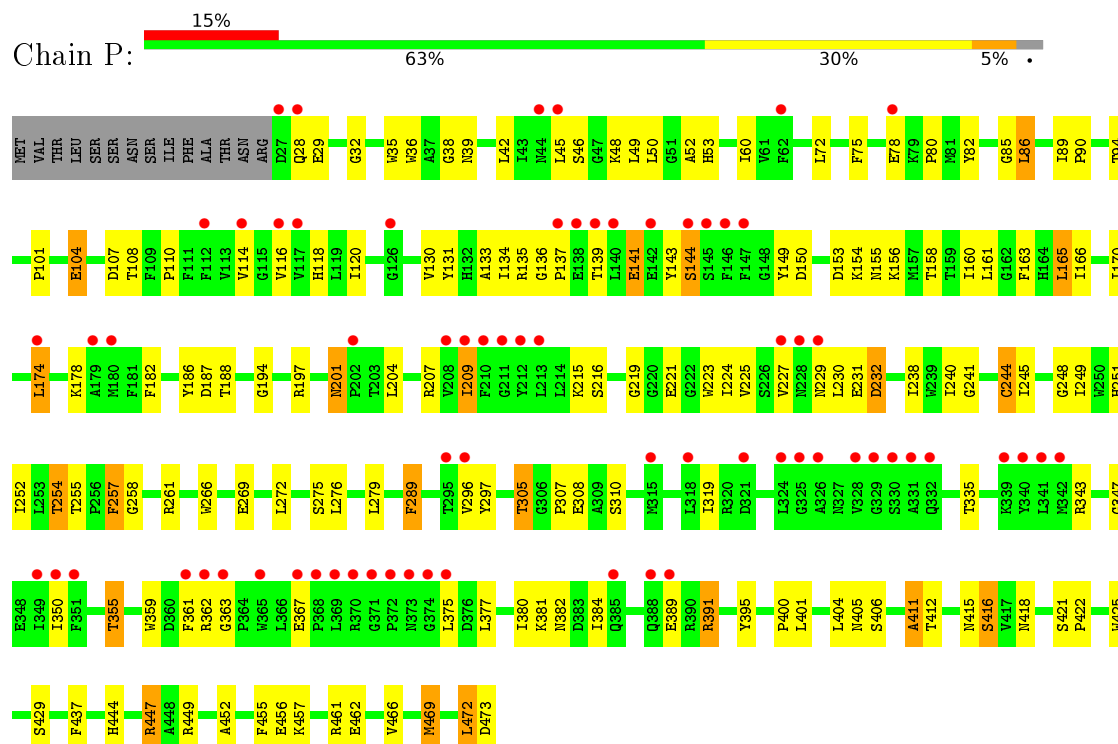


• Molecule 3: Photosystem II CP43 protein

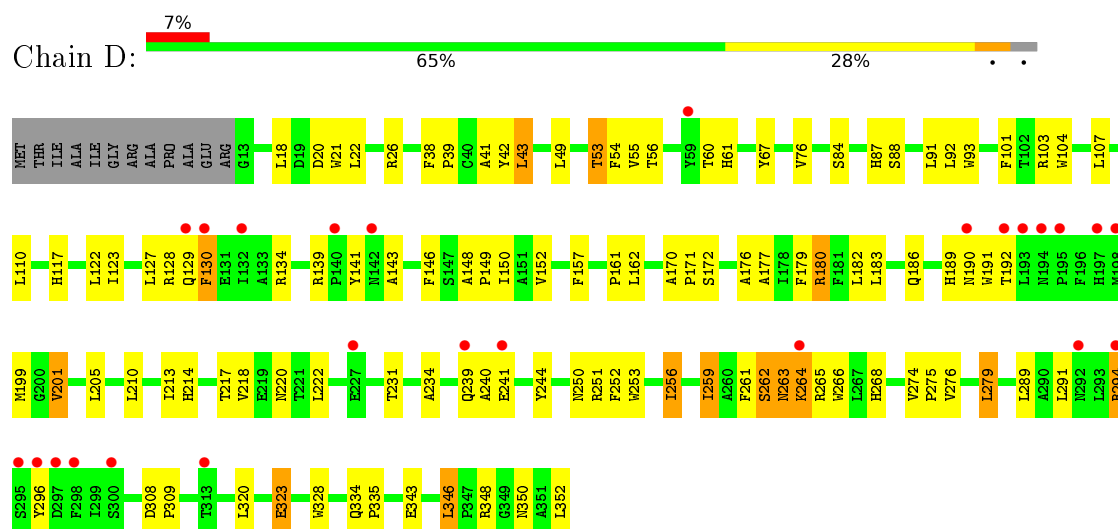




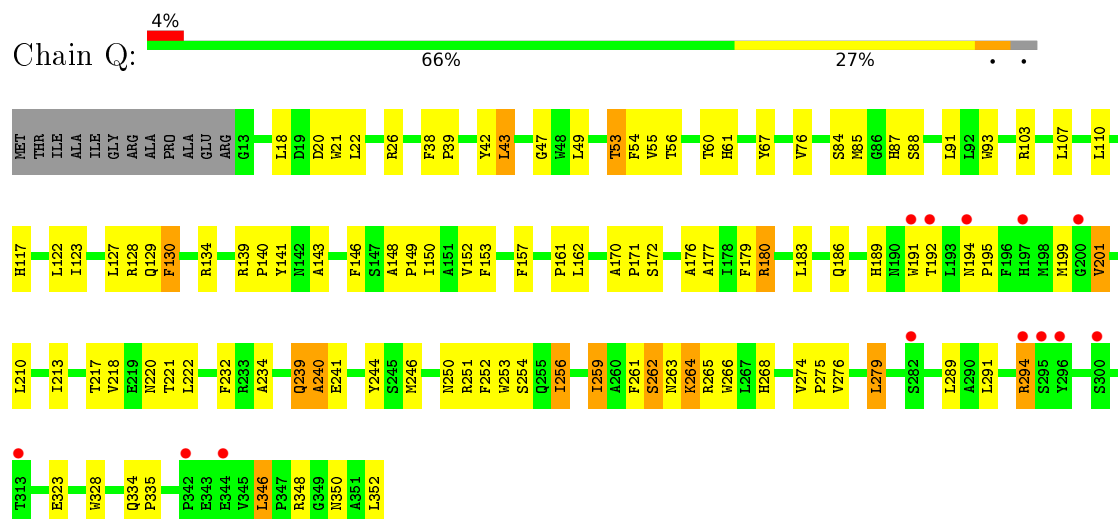
• Molecule 3: Photosystem II CP43 protein



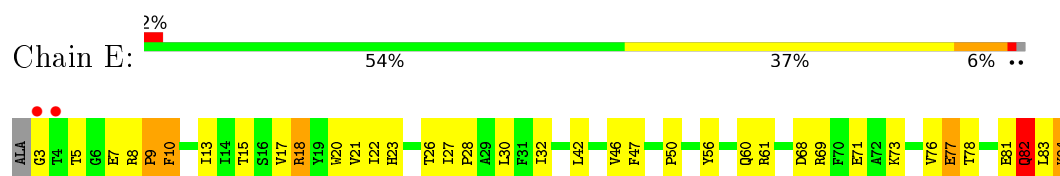
• Molecule 4: Photosystem II D2 protein



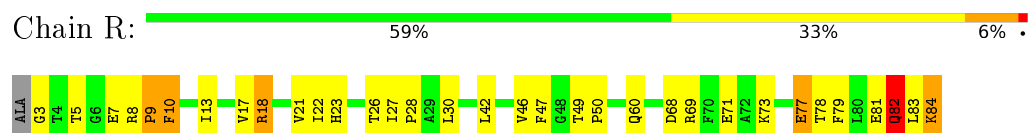
- Molecule 4: Photosystem II D2 protein



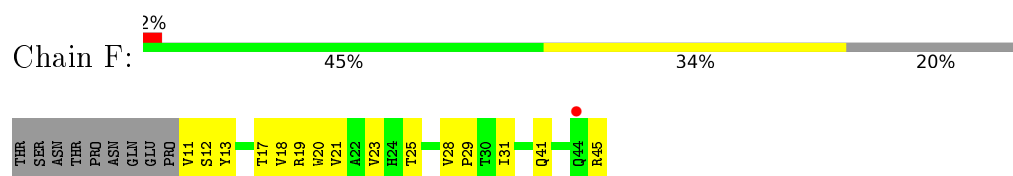
- Molecule 5: Cytochrome b559 subunit alpha



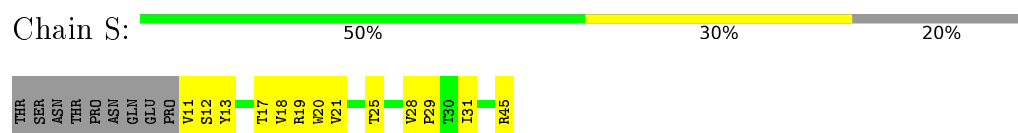
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta

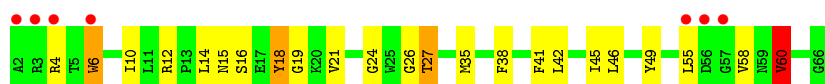


- Molecule 6: Cytochrome b559 subunit beta

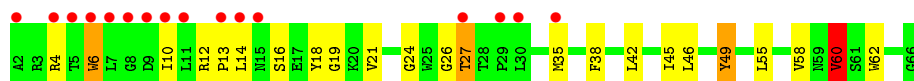


- Molecule 7: Photosystem II reaction center protein H

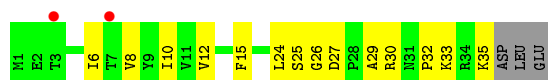




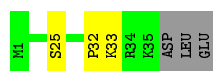
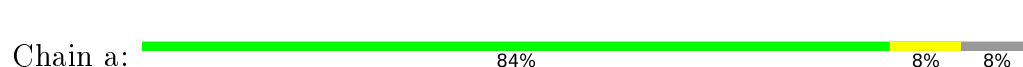
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



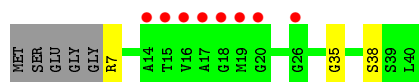
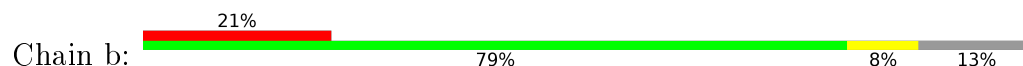
- Molecule 8: Photosystem II reaction center protein I



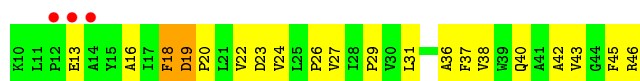
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J

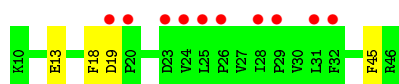


- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K

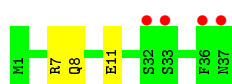




- Molecule 11: Photosystem II reaction center protein L



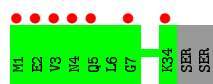
- Molecule 11: Photosystem II reaction center protein L



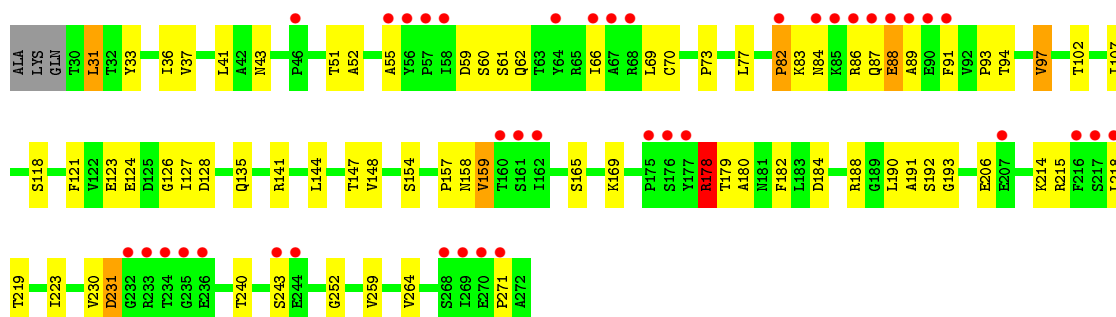
- Molecule 12: Photosystem II reaction center protein M



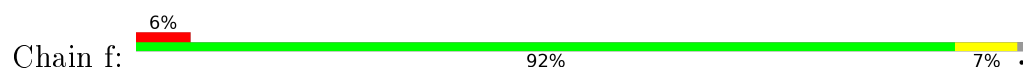
- Molecule 12: Photosystem II reaction center protein M

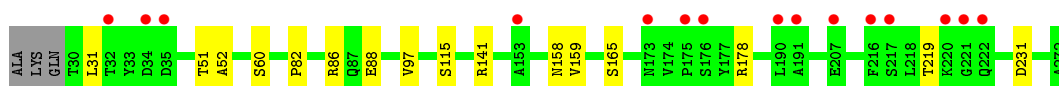


- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide





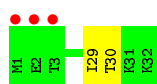
- Molecule 14: Photosystem II reaction center protein T

Chain T: 63% 34% .



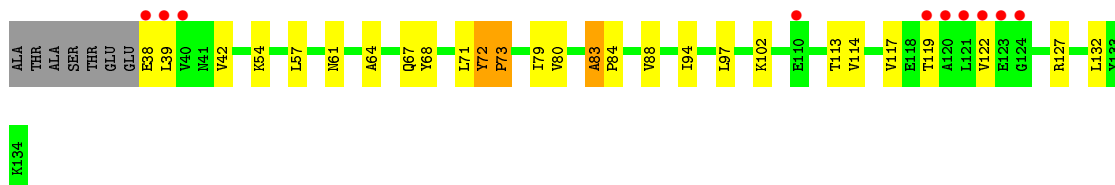
- Molecule 14: Photosystem II reaction center protein T

Chain g: 9% 94% 6%



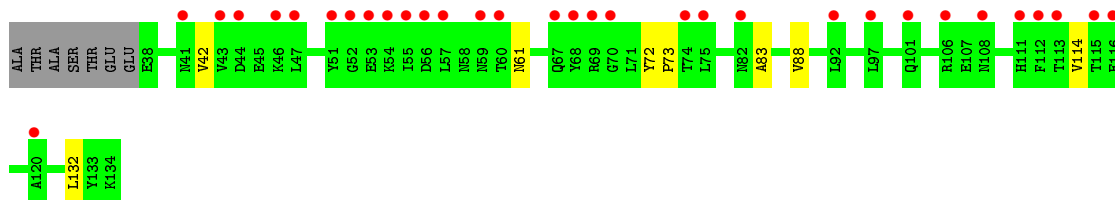
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 10% 67% 23% . 7%



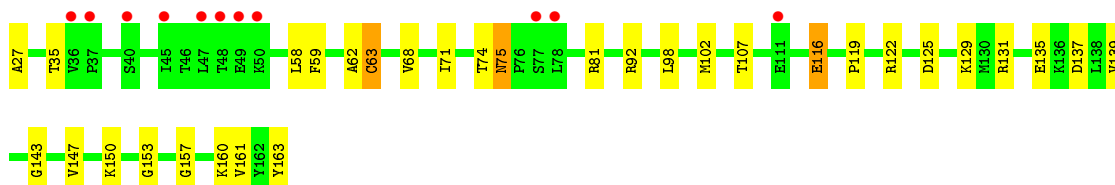
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain h: 31% 86% 8% 7%

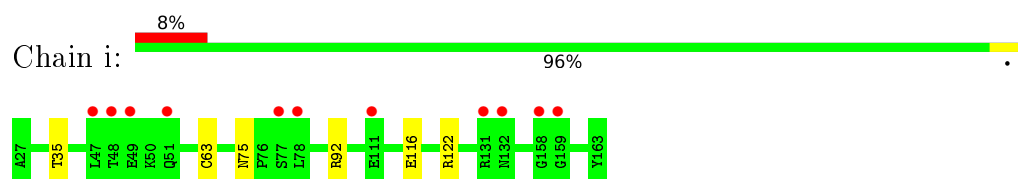


- Molecule 16: Cytochrome c-550

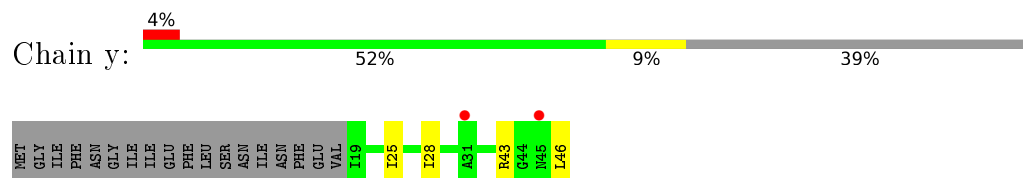
Chain V: 8% 77% 21% .



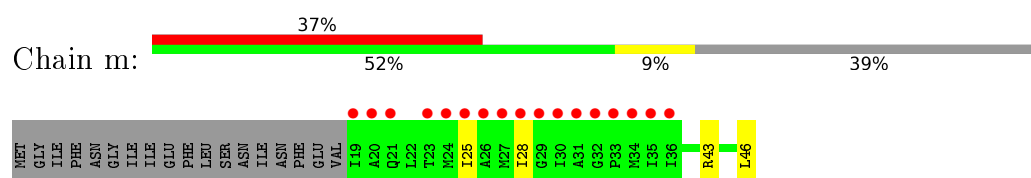
- Molecule 16: Cytochrome c-550



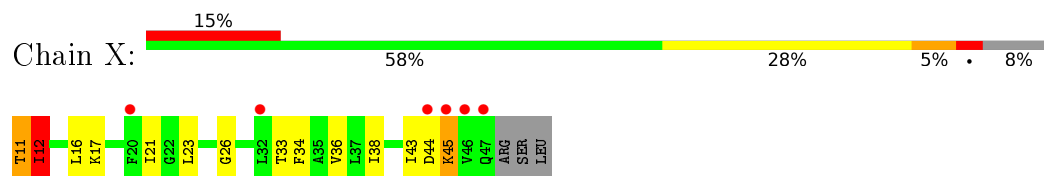
- Molecule 17: Photosystem II reaction center protein ycf12



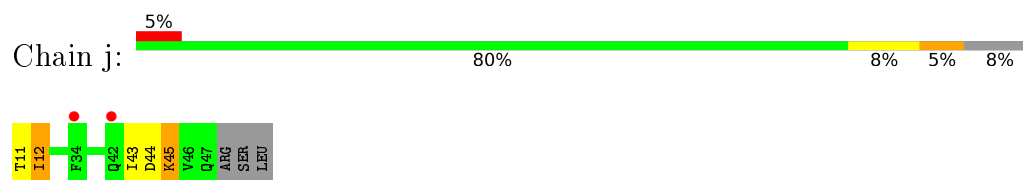
- Molecule 17: Photosystem II reaction center protein ycf12



- Molecule 18: Photosystem II reaction center protein X



- Molecule 18: Photosystem II reaction center protein X



- Molecule 19: Photosystem II reaction center protein Y



There are no outlier residues recorded for this chain.

- Molecule 19: Photosystem II reaction center protein Y



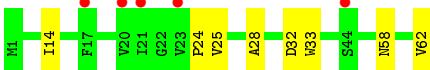
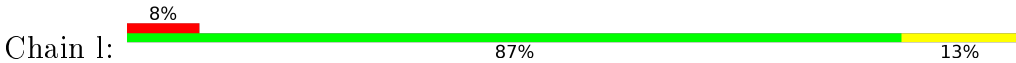
There are no outlier residues recorded for this chain.

- Molecule 20: Photosystem II reaction center protein Z





● Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	130.78 Å 227.76 Å 308.63 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.89 – 6.56 85.88 – 6.56	Depositor EDS
% Data completeness (in resolution range)	97.8 (85.89-6.56) 97.8 (85.88-6.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.06 (at 6.72 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3)	Depositor
R, R_{free}	0.366 , 0.385 0.361 , 0.383	Depositor DCC
R_{free} test set	895 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	10.8	Xtriage
Anisotropy	6.750	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 88.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.64	EDS
Total number of atoms	50232	wwPDB-VP
Average B, all atoms (Å ²)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, PHO, DGD, CL, CA, LMT, CLA, PL9, BCT, FE2, OEC, HEM, SQD, BCR, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/2713	0.55	0/3700
1	G	0.26	0/2713	0.54	0/3700
2	B	0.26	0/3986	0.55	2/5433 (0.0%)
2	N	0.27	0/3986	0.56	2/5433 (0.0%)
3	C	0.25	0/3556	0.56	0/4842
3	P	0.25	0/3556	0.56	0/4842
4	D	0.26	0/2801	0.55	0/3818
4	Q	0.26	0/2801	0.54	0/3818
5	E	0.27	0/685	0.58	0/933
5	R	0.27	0/685	0.58	0/933
6	F	0.25	0/291	0.49	0/397
6	S	0.23	0/291	0.48	0/397
7	H	0.27	0/520	0.61	0/709
7	W	0.28	0/520	0.61	0/709
8	I	0.26	0/293	0.53	0/395
8	a	0.27	0/293	0.53	0/395
9	J	0.24	0/255	0.56	0/346
9	b	0.24	0/255	0.57	0/346
10	K	0.30	0/303	0.59	0/416
10	c	0.30	0/303	0.59	0/416
11	L	0.25	0/311	0.52	0/422
11	d	0.26	0/311	0.52	0/422
12	M	0.28	0/270	0.58	0/367
12	e	0.29	0/270	0.57	0/367
13	O	0.26	0/1876	0.60	1/2548 (0.0%)
13	f	0.26	0/1876	0.61	0/2548
14	T	0.27	0/284	0.53	0/381
14	g	0.27	0/284	0.53	0/381
15	U	0.27	0/785	0.61	0/1064
15	h	0.27	0/785	0.62	0/1064
16	V	0.24	0/1081	0.54	0/1468
16	i	0.24	0/1081	0.53	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	m	0.27	0/202	0.68	0/272
17	y	0.30	0/202	0.69	0/272
18	X	0.32	0/273	0.59	0/370
18	j	0.32	0/273	0.59	0/370
20	Z	0.28	0/490	0.62	0/669
20	l	0.28	0/490	0.62	0/669
All	All	0.26	0/41950	0.56	5/57100 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	486	LEU	CA-CB-CG	7.03	131.46	115.30
2	N	486	LEU	CA-CB-CG	6.79	130.91	115.30
2	N	484	PRO	N-CA-C	5.16	125.51	112.10
2	B	484	PRO	N-CA-C	5.05	125.24	112.10
13	O	178	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	23	HIS	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2628	0	2524	98	0
1	G	2628	0	2524	97	0
2	B	3850	0	3718	107	0
2	N	3850	0	3718	105	0
3	C	3444	0	3365	127	0
3	P	3444	0	3365	111	0
4	D	2706	0	2608	98	0
4	Q	2706	0	2608	97	0
5	E	666	0	651	39	0
5	R	666	0	651	33	0
6	F	282	0	291	13	0
6	S	282	0	291	12	0
7	H	507	0	521	24	0
7	W	507	0	521	21	0
8	I	286	0	308	7	0
8	a	286	0	308	0	0
9	J	249	0	262	19	0
9	b	249	0	262	0	0
10	K	293	0	305	16	0
10	c	293	0	305	0	0
11	L	304	0	316	12	0
11	d	304	0	316	0	0
12	M	267	0	289	7	0
12	e	267	0	289	0	0
13	O	1845	0	1801	45	0
13	f	1845	0	1801	0	1
14	T	275	0	288	13	0
14	g	275	0	288	0	0
15	U	774	0	773	15	0
15	h	774	0	773	0	0
16	V	1060	0	1068	21	0
16	i	1060	0	1068	0	0
17	m	201	0	226	0	0
17	y	201	0	226	0	0
18	X	270	0	299	10	0
18	j	270	0	299	0	0
19	Y	140	0	32	0	0
19	k	140	0	32	0	0
20	Z	479	0	516	18	1
20	l	479	0	516	0	0
21	A	260	0	288	32	0
21	B	1040	0	1152	75	0
21	C	845	0	936	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	D	130	0	144	13	0
21	G	260	0	288	27	0
21	N	1040	0	1152	74	0
21	P	845	0	936	51	0
21	Q	130	0	144	14	0
22	A	64	0	74	7	0
22	D	64	0	74	4	0
22	G	64	0	74	7	0
22	Q	64	0	74	6	0
23	A	45	0	61	5	0
23	D	55	0	80	7	0
23	G	45	0	61	6	0
23	J	35	0	45	0	0
23	Q	55	0	80	6	0
23	b	35	0	45	0	0
24	A	56	0	70	1	0
24	B	110	0	136	5	0
24	C	181	0	245	16	0
24	D	63	0	87	0	0
24	G	56	0	70	2	0
24	N	52	0	62	4	0
24	P	181	0	245	12	0
24	Q	63	0	87	1	0
24	W	58	0	74	3	0
25	A	76	0	95	4	0
25	G	76	0	95	4	0
26	A	105	0	147	11	0
26	B	90	0	111	10	0
26	F	45	0	54	2	0
26	G	105	0	147	12	0
26	N	47	0	61	7	0
26	Q	43	0	50	3	0
26	S	45	0	54	0	0
27	A	51	0	72	2	0
27	B	98	0	136	2	0
27	C	93	0	126	4	0
27	D	136	0	182	15	0
27	E	44	0	58	3	0
27	G	51	0	72	0	0
27	I	43	0	56	4	0
27	M	42	0	54	3	0
27	N	98	0	136	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	P	93	0	126	4	0
27	Q	136	0	182	10	0
27	R	44	0	58	2	0
27	a	43	0	56	0	0
27	e	42	0	54	0	0
28	A	5	0	0	0	0
28	G	5	0	0	0	0
29	A	1	0	0	0	0
29	G	1	0	0	0	0
30	B	160	0	224	15	0
30	C	80	0	112	18	0
30	D	40	0	56	3	0
30	H	40	0	56	3	0
30	I	40	0	56	5	0
30	J	40	0	56	4	0
30	K	40	0	56	11	0
30	N	40	0	56	4	0
30	P	120	0	168	17	0
30	S	40	0	56	4	0
30	T	120	0	168	15	0
30	W	40	0	56	4	0
30	Z	40	0	56	3	0
30	a	40	0	56	0	0
30	b	40	0	56	0	0
30	c	40	0	56	0	0
31	B	140	0	184	7	0
31	D	31	0	35	1	0
31	I	35	0	46	2	0
31	M	35	0	46	1	0
31	N	140	0	184	9	0
31	Q	31	0	35	0	0
31	a	35	0	46	0	0
31	e	35	0	46	0	0
32	D	4	0	1	0	0
32	Q	4	0	1	0	0
33	D	1	0	0	0	0
33	G	1	0	0	0	0
34	E	43	0	30	7	0
34	R	43	0	30	6	0
34	V	43	0	30	4	0
34	i	43	0	30	0	0
35	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	f	1	0	0	0	0
All	All	50232	0	51376	1336	1

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 15.

The worst 5 of 1336 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)
2:N:121:GLU:HG2	7:W:4:ARG:HG2	1.49	0.94
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.50	0.93
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.52	0.92
4:Q:26:ARG:HD3	6:S:18:VAL:HG11	1.54	0.88
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.54	0.88

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:60:PHE:O	13:f:115:SER:OG[3_755]	2.16	0.04

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	A	333/344 (97%)	297 (89%)	31 (9%)	5 (2%)	13	57
1	G	333/344 (97%)	297 (89%)	31 (9%)	5 (2%)	13	57
2	B	488/510 (96%)	422 (86%)	54 (11%)	12 (2%)	7	46
2	N	488/510 (96%)	422 (86%)	54 (11%)	12 (2%)	7	46
3	C	445/461 (96%)	375 (84%)	55 (12%)	15 (3%)	5	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	445/461 (96%)	376 (84%)	53 (12%)	16 (4%)	4	38
4	D	338/352 (96%)	292 (86%)	40 (12%)	6 (2%)	11	53
4	Q	338/352 (96%)	291 (86%)	41 (12%)	6 (2%)	11	53
5	E	80/83 (96%)	72 (90%)	5 (6%)	3 (4%)	4	37
5	R	80/83 (96%)	72 (90%)	5 (6%)	3 (4%)	4	37
6	F	33/44 (75%)	24 (73%)	9 (27%)	0	100	100
6	S	33/44 (75%)	24 (73%)	9 (27%)	0	100	100
7	H	63/65 (97%)	48 (76%)	10 (16%)	5 (8%)	1	19
7	W	63/65 (97%)	48 (76%)	10 (16%)	5 (8%)	1	19
8	I	33/38 (87%)	24 (73%)	7 (21%)	2 (6%)	2	26
8	a	33/38 (87%)	25 (76%)	6 (18%)	2 (6%)	2	26
9	J	32/39 (82%)	26 (81%)	4 (12%)	2 (6%)	2	25
9	b	32/39 (82%)	26 (81%)	4 (12%)	2 (6%)	2	25
10	K	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	2	27
10	c	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	2	27
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	d	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	M	32/36 (89%)	23 (72%)	9 (28%)	0	100	100
12	e	32/36 (89%)	23 (72%)	9 (28%)	0	100	100
13	O	241/246 (98%)	203 (84%)	27 (11%)	11 (5%)	3	32
13	f	241/246 (98%)	203 (84%)	29 (12%)	9 (4%)	4	37
14	T	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	5	40
14	g	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	5	40
15	U	95/104 (91%)	81 (85%)	10 (10%)	4 (4%)	3	34
15	h	95/104 (91%)	81 (85%)	10 (10%)	4 (4%)	3	34
16	V	135/137 (98%)	113 (84%)	21 (16%)	1 (1%)	26	71
16	i	135/137 (98%)	113 (84%)	21 (16%)	1 (1%)	26	71
17	m	26/46 (56%)	15 (58%)	9 (35%)	2 (8%)	1	20
17	y	26/46 (56%)	15 (58%)	9 (35%)	2 (8%)	1	20
18	X	35/40 (88%)	27 (77%)	4 (11%)	4 (11%)	0	10
18	j	35/40 (88%)	27 (77%)	4 (11%)	4 (11%)	0	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	Z	60/62 (97%)	49 (82%)	8 (13%)	3 (5%)	3	31
20	l	60/62 (97%)	49 (82%)	8 (13%)	3 (5%)	3	31
All	All	5138/5426 (95%)	4357 (85%)	626 (12%)	155 (3%)	5	42

5 of 155 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	142	TRP
2	B	176	GLY
2	B	230	ARG
2	B	484	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/280 (97%)	260 (96%)	11 (4%)	37	71
1	G	271/280 (97%)	260 (96%)	11 (4%)	37	71
2	B	390/407 (96%)	377 (97%)	13 (3%)	45	76
2	N	390/407 (96%)	376 (96%)	14 (4%)	42	74
3	C	347/362 (96%)	327 (94%)	20 (6%)	25	61
3	P	347/362 (96%)	327 (94%)	20 (6%)	25	61
4	D	275/283 (97%)	259 (94%)	16 (6%)	25	61
4	Q	275/283 (97%)	258 (94%)	17 (6%)	23	59
5	E	72/72 (100%)	66 (92%)	6 (8%)	14	49
5	R	72/72 (100%)	66 (92%)	6 (8%)	14	49
6	F	29/38 (76%)	29 (100%)	0	100	100
6	S	29/38 (76%)	29 (100%)	0	100	100
7	H	53/54 (98%)	50 (94%)	3 (6%)	25	62
7	W	53/54 (98%)	50 (94%)	3 (6%)	25	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	32/35 (91%)	31 (97%)	1 (3%)	47	77
8	a	32/35 (91%)	31 (97%)	1 (3%)	47	77
9	J	24/27 (89%)	23 (96%)	1 (4%)	36	70
9	b	24/27 (89%)	23 (96%)	1 (4%)	36	70
10	K	30/30 (100%)	28 (93%)	2 (7%)	20	57
10	c	30/30 (100%)	28 (93%)	2 (7%)	20	57
11	L	35/35 (100%)	32 (91%)	3 (9%)	13	47
11	d	35/35 (100%)	32 (91%)	3 (9%)	13	47
12	M	31/33 (94%)	31 (100%)	0	100	100
12	e	31/33 (94%)	31 (100%)	0	100	100
13	O	202/208 (97%)	196 (97%)	6 (3%)	48	77
13	f	202/208 (97%)	196 (97%)	6 (3%)	48	77
14	T	29/29 (100%)	28 (97%)	1 (3%)	44	75
14	g	29/29 (100%)	28 (97%)	1 (3%)	44	75
15	U	84/89 (94%)	80 (95%)	4 (5%)	31	67
15	h	84/89 (94%)	80 (95%)	4 (5%)	31	67
16	V	116/117 (99%)	111 (96%)	5 (4%)	35	70
16	i	116/117 (99%)	111 (96%)	5 (4%)	35	70
17	m	20/37 (54%)	18 (90%)	2 (10%)	9	38
17	y	20/37 (54%)	18 (90%)	2 (10%)	9	38
18	X	30/33 (91%)	27 (90%)	3 (10%)	9	38
18	j	30/33 (91%)	27 (90%)	3 (10%)	9	38
20	Z	52/52 (100%)	47 (90%)	5 (10%)	10	40
20	l	52/52 (100%)	47 (90%)	5 (10%)	10	40
All	All	4244/4442 (96%)	4038 (95%)	206 (5%)	31	66

5 of 206 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	y	46	LEU
2	N	84	THR
15	h	132	LEU
18	X	12	ILE
1	G	157	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	234	ASN
1	G	241	GLN
4	Q	250	ASN
11	L	8	GLN
4	Q	129	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 182 ligands modelled in this entry, 6 are monoatomic - leaving 176 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	$\# Z > 2$
21	CLA	A	401	-	57,73,73	1.39	12 (21%)	61,113,113	1.67	10 (16%)
21	CLA	A	402	-	57,73,73	1.39	13 (22%)	61,113,113	1.72	9 (14%)
21	CLA	A	403	-	57,73,73	1.39	10 (17%)	61,113,113	1.71	8 (13%)
22	PHO	A	404	-	67,69,69	2.10	17 (25%)	86,99,99	1.98	24 (27%)
21	CLA	A	405	-	57,73,73	1.38	12 (21%)	61,113,113	1.69	10 (16%)
23	PL9	A	406	-	44,45,55	1.19	7 (15%)	56,57,69	1.73	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	DGD	A	407	-	57,57,67	0.96	3 (5%)	71,71,81	1.46	8 (11%)
25	LHG	A	408	-	38,38,48	1.04	2 (5%)	39,44,54	0.97	2 (5%)
26	SQD	A	409	-	50,51,54	1.72	4 (8%)	59,62,65	1.62	9 (15%)
27	LMG	A	410	-	51,51,55	0.93	2 (3%)	59,59,63	1.28	5 (8%)
25	LHG	A	411	-	36,36,48	1.05	2 (5%)	37,42,54	1.11	2 (5%)
28	OEC	A	412	1,3	0,0,13	0.00	-	0,0,27	0.00	-
26	SQD	A	414	-	53,54,54	1.71	4 (7%)	62,65,65	1.24	4 (6%)
21	CLA	B	601	-	57,73,73	1.38	12 (21%)	61,113,113	1.73	10 (16%)
21	CLA	B	602	-	57,73,73	1.39	10 (17%)	61,113,113	1.66	9 (14%)
21	CLA	B	603	-	57,73,73	1.40	11 (19%)	61,113,113	1.70	10 (16%)
21	CLA	B	604	-	57,73,73	1.39	11 (19%)	61,113,113	1.67	10 (16%)
21	CLA	B	605	-	57,73,73	1.38	11 (19%)	61,113,113	1.68	13 (21%)
21	CLA	B	606	-	57,73,73	1.38	11 (19%)	61,113,113	1.73	10 (16%)
21	CLA	B	607	-	57,73,73	1.40	9 (15%)	61,113,113	1.70	10 (16%)
21	CLA	B	608	-	57,73,73	1.39	10 (17%)	61,113,113	1.61	8 (13%)
21	CLA	B	609	-	57,73,73	1.39	12 (21%)	61,113,113	1.60	10 (16%)
21	CLA	B	610	-	57,73,73	1.39	12 (21%)	61,113,113	1.69	9 (14%)
21	CLA	B	611	-	57,73,73	1.39	11 (19%)	61,113,113	1.69	12 (19%)
21	CLA	B	612	-	57,73,73	1.39	12 (21%)	61,113,113	1.70	9 (14%)
21	CLA	B	613	-	57,73,73	1.38	11 (19%)	61,113,113	1.63	9 (14%)
21	CLA	B	614	-	57,73,73	1.39	9 (15%)	61,113,113	1.63	9 (14%)
21	CLA	B	615	-	57,73,73	1.38	10 (17%)	61,113,113	1.71	9 (14%)
21	CLA	B	616	-	57,73,73	1.37	12 (21%)	61,113,113	1.73	9 (14%)
30	BCR	B	617	-	41,41,41	0.70	0	56,56,56	1.60	11 (19%)
30	BCR	B	618	-	41,41,41	0.69	0	56,56,56	1.91	14 (25%)
30	BCR	B	619	-	41,41,41	0.73	0	56,56,56	1.53	11 (19%)
30	BCR	B	620	-	41,41,41	0.70	0	56,56,56	1.63	10 (17%)
24	DGD	B	621	-	59,59,67	0.92	3 (5%)	73,73,81	1.41	9 (12%)
27	LMG	B	622	-	49,49,55	0.91	2 (4%)	57,57,63	1.30	9 (15%)
27	LMG	B	623	-	49,49,55	0.92	2 (4%)	57,57,63	1.30	8 (14%)
26	SQD	B	624	-	42,43,54	1.91	4 (9%)	51,54,65	1.70	9 (17%)
31	LMT	B	625	-	36,36,36	0.40	0	47,47,47	0.72	1 (2%)
31	LMT	B	626	-	36,36,36	0.43	0	47,47,47	0.67	1 (2%)
26	SQD	B	627	-	46,47,54	1.86	4 (8%)	55,58,65	1.88	9 (16%)
24	DGD	B	628	-	53,53,67	0.99	3 (5%)	67,67,81	1.56	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMT	B	629	-	36,36,36	0.44	0	47,47,47	0.80	2 (4%)
31	LMT	B	630	-	36,36,36	0.38	0	47,47,47	0.62	0
21	CLA	C	501	-	57,73,73	1.39	10 (17%)	61,113,113	1.64	8 (13%)
21	CLA	C	502	-	57,73,73	1.37	12 (21%)	61,113,113	1.68	10 (16%)
21	CLA	C	503	-	57,73,73	1.37	10 (17%)	61,113,113	1.66	10 (16%)
21	CLA	C	504	-	57,73,73	1.40	11 (19%)	61,113,113	1.65	10 (16%)
21	CLA	C	505	-	57,73,73	1.38	12 (21%)	61,113,113	1.67	10 (16%)
21	CLA	C	506	-	57,73,73	1.40	12 (21%)	61,113,113	1.68	11 (18%)
21	CLA	C	507	-	57,73,73	1.37	11 (19%)	61,113,113	1.67	9 (14%)
21	CLA	C	508	-	57,73,73	1.38	12 (21%)	61,113,113	1.72	11 (18%)
21	CLA	C	509	-	57,73,73	1.40	11 (19%)	61,113,113	1.64	9 (14%)
21	CLA	C	510	-	57,73,73	1.39	11 (19%)	61,113,113	1.68	9 (14%)
21	CLA	C	511	3	57,73,73	1.38	11 (19%)	61,113,113	1.71	9 (14%)
21	CLA	C	512	-	57,73,73	1.38	9 (15%)	61,113,113	1.78	10 (16%)
21	CLA	C	513	-	57,73,73	1.39	10 (17%)	61,113,113	1.67	8 (13%)
30	BCR	C	514	-	41,41,41	0.71	0	56,56,56	2.33	17 (30%)
30	BCR	C	515	-	41,41,41	0.74	0	56,56,56	1.71	11 (19%)
24	DGD	C	516	-	54,54,67	0.95	3 (5%)	68,68,81	1.55	11 (16%)
24	DGD	C	517	-	63,63,67	0.89	3 (4%)	77,77,81	1.51	14 (18%)
24	DGD	C	518	-	67,67,67	0.90	4 (5%)	81,81,81	1.34	9 (11%)
27	LMG	C	519	-	48,48,55	0.94	2 (4%)	56,56,63	1.33	6 (10%)
27	LMG	C	520	-	45,45,55	1.01	2 (4%)	53,53,63	1.31	7 (13%)
21	CLA	D	401	-	57,73,73	1.39	9 (15%)	61,113,113	1.61	9 (14%)
22	PHO	D	402	-	67,69,69	2.12	16 (23%)	86,99,99	1.88	23 (26%)
21	CLA	D	403	-	57,73,73	1.38	12 (21%)	61,113,113	1.74	10 (16%)
23	PL9	D	404	-	54,55,55	1.19	8 (14%)	68,69,69	1.69	19 (27%)
30	BCR	D	405	-	41,41,41	0.70	0	56,56,56	1.73	10 (17%)
27	LMG	D	406	-	46,46,55	0.96	2 (4%)	54,54,63	1.35	7 (12%)
27	LMG	D	407	-	48,48,55	0.92	2 (4%)	56,56,63	1.29	5 (8%)
24	DGD	D	408	-	64,64,67	0.89	2 (3%)	78,78,81	1.35	10 (12%)
31	LMT	D	409	-	32,32,36	0.46	0	43,43,47	0.65	1 (2%)
32	BCT	D	410	29	0,3,3	0.00	-	0,3,3	0.00	-
27	LMG	D	412	-	42,42,55	1.01	2 (4%)	50,50,63	1.28	5 (10%)
34	HEM	E	101	5,6	24,50,50	2.31	5 (20%)	16,82,82	2.06	4 (25%)
27	LMG	E	102	-	44,44,55	0.99	2 (4%)	52,52,63	1.12	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SQD	F	101	-	44,45,54	1.82	4 (9%)	53,56,65	1.38	8 (15%)
26	SQD	G	401	-	53,54,54	1.69	4 (7%)	62,65,65	1.21	4 (6%)
21	CLA	G	402	-	57,73,73	1.39	12 (21%)	61,113,113	1.69	10 (16%)
21	CLA	G	403	-	57,73,73	1.38	11 (19%)	61,113,113	1.70	9 (14%)
21	CLA	G	404	-	57,73,73	1.37	10 (17%)	61,113,113	1.74	9 (14%)
22	PHO	G	405	-	67,69,69	2.09	16 (23%)	86,99,99	2.00	25 (29%)
21	CLA	G	406	-	57,73,73	1.36	9 (15%)	61,113,113	1.69	10 (16%)
23	PL9	G	407	-	44,45,55	1.19	7 (15%)	56,57,69	1.72	16 (28%)
24	DGD	G	408	-	57,57,67	0.95	3 (5%)	71,71,81	1.46	9 (12%)
25	LHG	G	409	-	38,38,48	1.04	2 (5%)	39,44,54	0.97	3 (7%)
26	SQD	G	410	-	50,51,54	1.72	4 (8%)	59,62,65	1.68	8 (13%)
27	LMG	G	411	-	51,51,55	0.93	2 (3%)	59,59,63	1.25	5 (8%)
25	LHG	G	412	-	36,36,48	1.06	2 (5%)	37,42,54	1.08	2 (5%)
28	OEC	G	413	1	0,0,13	0.00	-	0,0,27	0.00	-
30	BCR	H	101	-	41,41,41	0.74	0	56,56,56	1.47	11 (19%)
30	BCR	I	101	-	41,41,41	0.68	0	56,56,56	1.57	10 (17%)
27	LMG	I	102	-	43,43,55	0.98	2 (4%)	51,51,63	1.37	5 (9%)
31	LMT	I	103	-	36,36,36	0.46	0	47,47,47	0.74	2 (4%)
23	PL9	J	101	-	34,35,55	1.15	5 (14%)	44,45,69	1.49	10 (22%)
30	BCR	J	102	-	41,41,41	0.78	0	56,56,56	3.15	20 (35%)
30	BCR	K	101	-	41,41,41	0.77	0	56,56,56	1.63	13 (23%)
27	LMG	M	101	-	42,42,55	1.00	2 (4%)	50,50,63	1.32	5 (10%)
31	LMT	M	102	-	36,36,36	0.40	0	47,47,47	0.69	1 (2%)
26	SQD	N	601	-	46,47,54	1.86	4 (8%)	55,58,65	1.95	10 (18%)
24	DGD	N	602	-	53,53,67	0.99	3 (5%)	67,67,81	1.56	9 (13%)
31	LMT	N	603	-	36,36,36	0.44	0	47,47,47	0.82	2 (4%)
31	LMT	N	604	-	36,36,36	0.41	0	47,47,47	0.62	0
21	CLA	N	605	-	57,73,73	1.37	11 (19%)	61,113,113	1.73	10 (16%)
21	CLA	N	606	-	57,73,73	1.40	14 (24%)	61,113,113	1.69	10 (16%)
21	CLA	N	607	-	57,73,73	1.40	11 (19%)	61,113,113	1.68	11 (18%)
21	CLA	N	608	-	57,73,73	1.39	11 (19%)	61,113,113	1.68	10 (16%)
21	CLA	N	609	-	57,73,73	1.38	11 (19%)	61,113,113	1.70	13 (21%)
21	CLA	N	610	-	57,73,73	1.39	11 (19%)	61,113,113	1.73	10 (16%)
21	CLA	N	611	-	57,73,73	1.41	10 (17%)	61,113,113	1.69	10 (16%)
21	CLA	N	612	-	57,73,73	1.40	10 (17%)	61,113,113	1.61	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	N	613	-	57,73,73	1.37	11 (19%)	61,113,113	1.60	11 (18%)
21	CLA	N	614	-	57,73,73	1.39	11 (19%)	61,113,113	1.69	9 (14%)
21	CLA	N	615	-	57,73,73	1.39	12 (21%)	61,113,113	1.70	12 (19%)
21	CLA	N	616	-	57,73,73	1.40	12 (21%)	61,113,113	1.79	9 (14%)
21	CLA	N	617	-	57,73,73	1.41	12 (21%)	61,113,113	1.62	10 (16%)
21	CLA	N	618	-	57,73,73	1.39	10 (17%)	61,113,113	1.64	9 (14%)
21	CLA	N	619	-	57,73,73	1.36	11 (19%)	61,113,113	1.71	10 (16%)
21	CLA	N	620	-	57,73,73	1.38	12 (21%)	61,113,113	1.73	9 (14%)
30	BCR	N	621	-	41,41,41	0.73	0	56,56,56	1.55	14 (25%)
27	LMG	N	622	-	49,49,55	0.91	2 (4%)	57,57,63	1.37	8 (14%)
27	LMG	N	623	-	49,49,55	0.92	2 (4%)	57,57,63	1.29	8 (14%)
31	LMT	N	624	-	36,36,36	0.40	0	47,47,47	0.69	1 (2%)
31	LMT	N	625	-	36,36,36	0.41	0	47,47,47	0.67	1 (2%)
21	CLA	P	501	-	57,73,73	1.39	10 (17%)	61,113,113	1.65	8 (13%)
21	CLA	P	502	-	57,73,73	1.39	12 (21%)	61,113,113	1.68	11 (18%)
21	CLA	P	503	-	57,73,73	1.37	11 (19%)	61,113,113	1.66	10 (16%)
21	CLA	P	504	-	57,73,73	1.40	9 (15%)	61,113,113	1.62	10 (16%)
21	CLA	P	505	-	57,73,73	1.37	11 (19%)	61,113,113	1.66	9 (14%)
21	CLA	P	506	-	57,73,73	1.40	13 (22%)	61,113,113	1.66	11 (18%)
21	CLA	P	507	-	57,73,73	1.37	10 (17%)	61,113,113	1.66	8 (13%)
21	CLA	P	508	-	57,73,73	1.38	10 (17%)	61,113,113	1.75	10 (16%)
21	CLA	P	509	-	57,73,73	1.39	12 (21%)	61,113,113	1.64	9 (14%)
21	CLA	P	510	-	57,73,73	1.38	11 (19%)	61,113,113	1.70	9 (14%)
21	CLA	P	511	3	57,73,73	1.38	11 (19%)	61,113,113	1.69	9 (14%)
21	CLA	P	512	-	57,73,73	1.38	10 (17%)	61,113,113	1.76	8 (13%)
21	CLA	P	513	-	57,73,73	1.40	11 (19%)	61,113,113	1.66	8 (13%)
30	BCR	P	514	-	41,41,41	0.69	0	56,56,56	2.36	18 (32%)
30	BCR	P	515	-	41,41,41	0.67	0	56,56,56	1.56	10 (17%)
30	BCR	P	516	-	41,41,41	0.74	0	56,56,56	1.71	11 (19%)
24	DGD	P	517	-	54,54,67	0.96	3 (5%)	68,68,81	1.59	11 (16%)
24	DGD	P	518	-	63,63,67	0.89	3 (4%)	77,77,81	1.51	13 (16%)
24	DGD	P	519	-	67,67,67	0.87	3 (4%)	81,81,81	1.28	7 (8%)
27	LMG	P	520	-	48,48,55	0.93	2 (4%)	56,56,63	1.33	7 (12%)
27	LMG	P	521	-	45,45,55	1.00	2 (4%)	53,53,63	1.27	5 (9%)
27	LMG	Q	401	-	42,42,55	1.01	2 (4%)	50,50,63	1.26	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	Q	402	-	57,73,73	1.39	9 (15%)	61,113,113	1.60	9 (14%)
22	PHO	Q	403	-	67,69,69	2.11	16 (23%)	86,99,99	1.86	23 (26%)
21	CLA	Q	404	-	57,73,73	1.39	10 (17%)	61,113,113	1.74	10 (16%)
23	PL9	Q	405	-	54,55,55	1.20	8 (14%)	68,69,69	1.68	18 (26%)
27	LMG	Q	406	-	46,46,55	0.96	2 (4%)	54,54,63	1.32	4 (7%)
27	LMG	Q	407	-	48,48,55	0.93	2 (4%)	56,56,63	1.31	5 (8%)
26	SQD	Q	408	-	42,43,54	1.92	5 (11%)	51,54,65	1.72	8 (15%)
24	DGD	Q	409	-	64,64,67	0.89	2 (3%)	78,78,81	1.35	9 (11%)
31	LMT	Q	410	-	32,32,36	0.46	0	43,43,47	0.65	1 (2%)
32	BCT	Q	411	29	0,3,3	0.00	-	0,3,3	0.00	-
34	HEM	R	101	5,6	24,50,50	2.31	5 (20%)	16,82,82	2.25	3 (18%)
27	LMG	R	102	-	44,44,55	0.97	2 (4%)	52,52,63	1.13	5 (9%)
30	BCR	S	101	-	41,41,41	0.71	0	56,56,56	1.75	10 (17%)
26	SQD	S	102	-	44,45,54	1.83	5 (11%)	53,56,65	1.37	8 (15%)
30	BCR	T	101	-	41,41,41	0.70	0	56,56,56	1.58	10 (17%)
30	BCR	T	102	-	41,41,41	0.68	0	56,56,56	1.89	14 (25%)
30	BCR	T	103	-	41,41,41	0.68	0	56,56,56	1.65	12 (21%)
34	HEM	V	201	16	24,50,50	2.34	6 (25%)	16,82,82	1.99	2 (12%)
30	BCR	W	101	-	41,41,41	0.74	0	56,56,56	1.47	10 (17%)
24	DGD	W	102	-	59,59,67	0.93	3 (5%)	73,73,81	1.42	9 (12%)
30	BCR	Z	101	-	41,41,41	0.66	0	56,56,56	1.61	12 (21%)
30	BCR	a	101	-	41,41,41	0.68	0	56,56,56	1.59	10 (17%)
27	LMG	a	102	-	43,43,55	0.98	2 (4%)	51,51,63	1.39	6 (11%)
31	LMT	a	103	-	36,36,36	0.45	0	47,47,47	0.74	2 (4%)
23	PL9	b	101	-	34,35,55	1.15	5 (14%)	44,45,69	1.48	10 (22%)
30	BCR	b	102	-	41,41,41	0.77	0	56,56,56	3.18	20 (35%)
30	BCR	c	101	-	41,41,41	0.76	0	56,56,56	1.57	9 (16%)
31	LMT	e	101	-	36,36,36	0.40	0	47,47,47	0.67	1 (2%)
27	LMG	e	102	-	42,42,55	1.01	2 (4%)	50,50,63	1.34	5 (10%)
34	HEM	i	201	16	24,50,50	2.34	6 (25%)	16,82,82	2.01	3 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	401	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	402	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	403	-	3/3/20/25	0/37/135/135	0/0/9/9
22	PHO	A	404	-	-	0/53/103/103	0/1/6/6
21	CLA	A	405	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PL9	A	406	-	-	0/41/61/73	0/1/1/1
24	DGD	A	407	-	3/3/13/13	0/45/85/95	0/2/2/2
25	LHG	A	408	-	-	0/43/43/53	0/0/0/0
26	SQD	A	409	-	-	0/46/66/69	0/1/1/1
27	LMG	A	410	-	2/2/8/8	0/46/66/70	0/1/1/1
25	LHG	A	411	-	-	0/41/41/53	0/0/0/0
28	OEC	A	412	1,3	-	0/0/0/54	0/0/0/5
26	SQD	A	414	-	-	0/49/69/69	0/1/1/1
21	CLA	B	601	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	602	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	607	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	609	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	610	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
30	BCR	B	617	-	-	0/29/63/63	0/2/2/2
30	BCR	B	618	-	-	0/29/63/63	0/2/2/2
30	BCR	B	619	-	-	0/29/63/63	0/2/2/2
30	BCR	B	620	-	-	0/29/63/63	0/2/2/2
24	DGD	B	621	-	3/3/13/13	0/47/87/95	0/2/2/2
27	LMG	B	622	-	2/2/8/8	0/44/64/70	0/1/1/1
27	LMG	B	623	-	2/2/8/8	0/44/64/70	0/1/1/1
26	SQD	B	624	-	-	1/38/58/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	B	625	-	-	0/21/61/61	0/2/2/2
31	LMT	B	626	-	-	0/21/61/61	0/2/2/2
26	SQD	B	627	-	-	0/42/62/69	0/1/1/1
24	DGD	B	628	-	3/3/13/13	0/41/81/95	0/2/2/2
31	LMT	B	629	-	-	0/21/61/61	0/2/2/2
31	LMT	B	630	-	-	0/21/61/61	0/2/2/2
21	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	C	505	-	3/3/20/25	1/37/135/135	0/0/9/9
21	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	C	508	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	C	509	-	3/3/20/25	1/37/135/135	0/0/9/9
21	CLA	C	510	-	3/3/20/25	1/37/135/135	0/0/9/9
21	CLA	C	511	3	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	C	512	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	C	513	-	3/3/20/25	1/37/135/135	0/0/9/9
30	BCR	C	514	-	-	0/29/63/63	0/2/2/2
30	BCR	C	515	-	-	0/29/63/63	0/2/2/2
24	DGD	C	516	-	3/3/13/13	0/42/82/95	0/2/2/2
24	DGD	C	517	-	3/3/13/13	0/51/91/95	0/2/2/2
24	DGD	C	518	-	3/3/13/13	0/55/95/95	0/2/2/2
27	LMG	C	519	-	2/2/8/8	0/43/63/70	0/1/1/1
27	LMG	C	520	-	2/2/8/8	0/40/60/70	0/1/1/1
21	CLA	D	401	-	3/3/20/25	0/37/135/135	0/0/9/9
22	PHO	D	402	-	-	0/53/103/103	0/1/6/6
21	CLA	D	403	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PL9	D	404	-	-	0/53/73/73	0/1/1/1
30	BCR	D	405	-	-	0/29/63/63	0/2/2/2
27	LMG	D	406	-	2/2/8/8	0/41/61/70	0/1/1/1
27	LMG	D	407	-	2/2/8/8	1/43/63/70	0/1/1/1
24	DGD	D	408	-	3/3/13/13	0/52/92/95	0/2/2/2
31	LMT	D	409	-	-	0/17/57/61	0/2/2/2
32	BCT	D	410	29	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	D	412	-	2/2/8/8	0/37/57/70	0/1/1/1
34	HEM	E	101	5,6	-	0/6/54/54	0/0/8/8
27	LMG	E	102	-	2/2/8/8	0/39/59/70	0/1/1/1
26	SQD	F	101	-	-	0/40/60/69	0/1/1/1
26	SQD	G	401	-	-	0/49/69/69	0/1/1/1
21	CLA	G	402	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	G	403	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	G	404	-	3/3/20/25	0/37/135/135	0/0/9/9
22	PHO	G	405	-	-	0/53/103/103	0/1/6/6
21	CLA	G	406	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PL9	G	407	-	-	0/41/61/73	0/1/1/1
24	DGD	G	408	-	3/3/13/13	0/45/85/95	0/2/2/2
25	LHG	G	409	-	-	0/43/43/53	0/0/0/0
26	SQD	G	410	-	-	0/46/66/69	0/1/1/1
27	LMG	G	411	-	2/2/8/8	0/46/66/70	0/1/1/1
25	LHG	G	412	-	-	0/41/41/53	0/0/0/0
28	OEC	G	413	1	-	0/0/0/54	0/0/0/5
30	BCR	H	101	-	-	0/29/63/63	0/2/2/2
30	BCR	I	101	-	-	0/29/63/63	0/2/2/2
27	LMG	I	102	-	2/2/8/8	0/38/58/70	0/1/1/1
31	LMT	I	103	-	-	0/21/61/61	0/2/2/2
23	PL9	J	101	-	-	0/29/49/73	0/1/1/1
30	BCR	J	102	-	-	0/29/63/63	0/2/2/2
30	BCR	K	101	-	-	0/29/63/63	0/2/2/2
27	LMG	M	101	-	2/2/8/8	0/37/57/70	0/1/1/1
31	LMT	M	102	-	-	0/21/61/61	0/2/2/2
26	SQD	N	601	-	-	0/42/62/69	0/1/1/1
24	DGD	N	602	-	3/3/13/13	0/41/81/95	0/2/2/2
31	LMT	N	603	-	-	0/21/61/61	0/2/2/2
31	LMT	N	604	-	-	0/21/61/61	0/2/2/2
21	CLA	N	605	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	606	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	607	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	608	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	609	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	610	-	3/3/20/25	1/37/135/135	0/0/9/9
21	CLA	N	611	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	612	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	N	613	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	614	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	615	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	616	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	617	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	618	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	619	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	620	-	3/3/20/25	0/37/135/135	0/0/9/9
30	BCR	N	621	-	-	0/29/63/63	0/2/2/2
27	LMG	N	622	-	2/2/8/8	0/44/64/70	0/1/1/1
27	LMG	N	623	-	2/2/8/8	0/44/64/70	0/1/1/1
31	LMT	N	624	-	-	0/21/61/61	0/2/2/2
31	LMT	N	625	-	-	0/21/61/61	0/2/2/2
21	CLA	P	501	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	P	502	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	P	503	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	P	504	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	P	505	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	P	506	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	P	507	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	P	508	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	P	509	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	P	510	-	3/3/20/25	1/37/135/135	0/0/9/9
21	CLA	P	511	3	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	P	512	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	P	513	-	3/3/20/25	1/37/135/135	0/0/9/9
30	BCR	P	514	-	-	0/29/63/63	0/2/2/2
30	BCR	P	515	-	-	0/29/63/63	0/2/2/2
30	BCR	P	516	-	-	0/29/63/63	0/2/2/2
24	DGD	P	517	-	3/3/13/13	0/42/82/95	0/2/2/2
24	DGD	P	518	-	3/3/13/13	0/51/91/95	0/2/2/2
24	DGD	P	519	-	3/3/13/13	0/55/95/95	0/2/2/2
27	LMG	P	520	-	2/2/8/8	0/43/63/70	0/1/1/1
27	LMG	P	521	-	2/2/8/8	0/40/60/70	0/1/1/1
27	LMG	Q	401	-	2/2/8/8	0/37/57/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	Q	402	-	3/3/20/25	0/37/135/135	0/0/9/9
22	PHO	Q	403	-	-	0/53/103/103	0/1/6/6
21	CLA	Q	404	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PL9	Q	405	-	-	0/53/73/73	0/1/1/1
27	LMG	Q	406	-	2/2/8/8	0/41/61/70	0/1/1/1
27	LMG	Q	407	-	2/2/8/8	1/43/63/70	0/1/1/1
26	SQD	Q	408	-	-	1/38/58/69	0/1/1/1
24	DGD	Q	409	-	3/3/13/13	0/52/92/95	0/2/2/2
31	LMT	Q	410	-	-	0/17/57/61	0/2/2/2
32	BCT	Q	411	29	-	0/0/0/0	0/0/0/0
34	HEM	R	101	5,6	-	0/6/54/54	0/0/8/8
27	LMG	R	102	-	2/2/8/8	0/39/59/70	0/1/1/1
30	BCR	S	101	-	-	0/29/63/63	0/2/2/2
26	SQD	S	102	-	-	0/40/60/69	0/1/1/1
30	BCR	T	101	-	-	0/29/63/63	0/2/2/2
30	BCR	T	102	-	-	0/29/63/63	0/2/2/2
30	BCR	T	103	-	-	0/29/63/63	0/2/2/2
34	HEM	V	201	16	-	0/6/54/54	0/0/8/8
30	BCR	W	101	-	-	0/29/63/63	0/2/2/2
24	DGD	W	102	-	3/3/13/13	0/47/87/95	0/2/2/2
30	BCR	Z	101	-	-	0/29/63/63	0/2/2/2
30	BCR	a	101	-	-	0/29/63/63	0/2/2/2
27	LMG	a	102	-	2/2/8/8	0/38/58/70	0/1/1/1
31	LMT	a	103	-	-	0/21/61/61	0/2/2/2
23	PL9	b	101	-	-	0/29/49/73	0/1/1/1
30	BCR	b	102	-	-	0/29/63/63	0/2/2/2
30	BCR	c	101	-	-	0/29/63/63	0/2/2/2
31	LMT	e	101	-	-	0/21/61/61	0/2/2/2
27	LMG	e	102	-	2/2/8/8	0/37/57/70	0/1/1/1
34	HEM	i	201	16	-	0/6/54/54	0/0/8/8

The worst 5 of 1028 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	N	601	SQD	C6-S	-9.60	1.66	1.77
26	B	627	SQD	C6-S	-9.59	1.66	1.77
26	A	414	SQD	C6-S	-9.53	1.66	1.77
26	Q	408	SQD	C6-S	-9.31	1.66	1.77
26	G	401	SQD	C6-S	-9.30	1.66	1.77

The worst 5 of 1539 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	102	BCR	C32-C1-C6	-14.32	88.45	110.33
30	J	102	BCR	C32-C1-C6	-14.25	88.56	110.33
30	b	102	BCR	C32-C1-C31	-8.07	82.38	108.36
30	J	102	BCR	C32-C1-C31	-8.06	82.42	108.36
34	R	101	HEM	CBD-CAD-C3D	-7.02	100.15	112.47

5 of 296 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	B	628	DGD	C2D
24	B	628	DGD	C5D
24	B	628	DGD	C5E
21	B	615	CLA	NC
21	B	615	CLA	ND

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	C	505	CLA	C1-C2-C3-C4
21	N	610	CLA	C1-C2-C3-C4
21	C	509	CLA	C1-C2-C3-C4
21	P	510	CLA	C1-C2-C3-C4
21	C	510	CLA	C1-C2-C3-C4

There are no ring outliers.

154 monomers are involved in 576 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	401	CLA	13	0
21	A	402	CLA	11	0
21	A	403	CLA	8	0
22	A	404	PHO	7	0
21	A	405	CLA	3	0
23	A	406	PL9	5	0
24	A	407	DGD	1	0
25	A	408	LHG	2	0
26	A	409	SQD	4	0
27	A	410	LMG	2	0
25	A	411	LHG	2	0
26	A	414	SQD	7	0
21	B	601	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	602	CLA	4	0
21	B	603	CLA	8	0
21	B	604	CLA	5	0
21	B	605	CLA	7	0
21	B	606	CLA	9	0
21	B	607	CLA	6	0
21	B	608	CLA	10	0
21	B	609	CLA	6	0
21	B	610	CLA	4	0
21	B	611	CLA	2	0
21	B	612	CLA	7	0
21	B	613	CLA	5	0
21	B	614	CLA	6	0
21	B	615	CLA	3	0
21	B	616	CLA	7	0
30	B	617	BCR	8	0
30	B	618	BCR	4	0
30	B	619	BCR	2	0
30	B	620	BCR	2	0
24	B	621	DGD	2	0
27	B	622	LMG	1	0
27	B	623	LMG	1	0
26	B	624	SQD	5	0
31	B	625	LMT	1	0
31	B	626	LMT	1	0
26	B	627	SQD	5	0
24	B	628	DGD	3	0
31	B	629	LMT	2	0
31	B	630	LMT	3	0
21	C	501	CLA	8	0
21	C	503	CLA	6	0
21	C	504	CLA	6	0
21	C	505	CLA	6	0
21	C	506	CLA	3	0
21	C	507	CLA	5	0
21	C	508	CLA	6	0
21	C	509	CLA	8	0
21	C	510	CLA	7	0
21	C	511	CLA	9	0
21	C	512	CLA	3	0
21	C	513	CLA	3	0
30	C	514	BCR	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	C	515	BCR	6	0
24	C	516	DGD	2	0
24	C	517	DGD	7	0
24	C	518	DGD	7	0
27	C	520	LMG	4	0
21	D	401	CLA	8	0
22	D	402	PHO	4	0
21	D	403	CLA	5	0
23	D	404	PL9	7	0
30	D	405	BCR	3	0
27	D	406	LMG	4	0
27	D	407	LMG	9	0
31	D	409	LMT	1	0
27	D	412	LMG	2	0
34	E	101	HEM	7	0
27	E	102	LMG	3	0
26	F	101	SQD	2	0
26	G	401	SQD	6	0
21	G	402	CLA	13	0
21	G	403	CLA	9	0
21	G	404	CLA	6	0
22	G	405	PHO	7	0
21	G	406	CLA	3	0
23	G	407	PL9	6	0
24	G	408	DGD	2	0
25	G	409	LHG	1	0
26	G	410	SQD	6	0
25	G	412	LHG	3	0
30	H	101	BCR	3	0
30	I	101	BCR	5	0
27	I	102	LMG	4	0
31	I	103	LMT	2	0
30	J	102	BCR	4	0
30	K	101	BCR	11	0
27	M	101	LMG	3	0
31	M	102	LMT	1	0
26	N	601	SQD	7	0
24	N	602	DGD	4	0
31	N	603	LMT	3	0
31	N	604	LMT	4	0
21	N	605	CLA	2	0
21	N	606	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	N	607	CLA	9	0
21	N	608	CLA	6	0
21	N	609	CLA	8	0
21	N	610	CLA	6	0
21	N	611	CLA	5	0
21	N	612	CLA	8	0
21	N	613	CLA	4	0
21	N	614	CLA	4	0
21	N	615	CLA	2	0
21	N	616	CLA	9	0
21	N	617	CLA	4	0
21	N	618	CLA	9	0
21	N	619	CLA	4	0
21	N	620	CLA	5	0
30	N	621	BCR	4	0
27	N	622	LMG	2	0
31	N	624	LMT	1	0
31	N	625	LMT	1	0
21	P	501	CLA	5	0
21	P	502	CLA	2	0
21	P	503	CLA	7	0
21	P	504	CLA	5	0
21	P	505	CLA	5	0
21	P	506	CLA	2	0
21	P	507	CLA	5	0
21	P	508	CLA	5	0
21	P	509	CLA	7	0
21	P	510	CLA	7	0
21	P	511	CLA	7	0
21	P	512	CLA	4	0
21	P	513	CLA	3	0
30	P	514	BCR	8	0
30	P	515	BCR	4	0
30	P	516	BCR	5	0
24	P	517	DGD	2	0
24	P	518	DGD	4	0
24	P	519	DGD	6	0
27	P	521	LMG	4	0
27	Q	401	LMG	2	0
21	Q	402	CLA	11	0
22	Q	403	PHO	6	0
21	Q	404	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	Q	405	PL9	6	0
27	Q	406	LMG	2	0
27	Q	407	LMG	6	0
26	Q	408	SQD	3	0
24	Q	409	DGD	1	0
34	R	101	HEM	6	0
27	R	102	LMG	2	0
30	S	101	BCR	4	0
30	T	101	BCR	3	0
30	T	102	BCR	9	0
30	T	103	BCR	3	0
34	V	201	HEM	4	0
30	W	101	BCR	4	0
24	W	102	DGD	3	0
30	Z	101	BCR	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/344 (97%)	0.46	29 (8%) 13 17	131, 152, 182, 204	0
1	G	335/344 (97%)	0.29	20 (5%) 25 26	128, 156, 184, 213	0
2	B	490/510 (96%)	0.57	58 (11%) 6 11	128, 158, 178, 195	0
2	N	490/510 (96%)	0.62	65 (13%) 4 10	129, 160, 180, 207	0
3	C	447/461 (96%)	0.30	21 (4%) 35 35	129, 164, 183, 211	0
3	P	447/461 (96%)	0.66	69 (15%) 3 8	139, 165, 183, 197	0
4	D	340/352 (96%)	0.33	25 (7%) 17 21	125, 152, 176, 198	0
4	Q	340/352 (96%)	0.18	13 (3%) 44 42	130, 155, 175, 184	0
5	E	82/83 (98%)	0.17	2 (2%) 62 58	148, 171, 188, 198	0
5	R	82/83 (98%)	-0.15	0 100 100	148, 171, 188, 195	0
6	F	35/44 (79%)	-0.19	1 (2%) 55 50	140, 168, 185, 199	0
6	S	35/44 (79%)	0.37	0 100 100	148, 165, 187, 188	0
7	H	65/65 (100%)	0.77	7 (10%) 8 12	154, 172, 189, 195	0
7	W	65/65 (100%)	0.85	16 (24%) 1 5	154, 173, 188, 196	0
8	I	35/38 (92%)	0.19	2 (5%) 27 28	147, 163, 174, 178	0
8	a	35/38 (92%)	0.03	0 100 100	148, 164, 179, 190	0
9	J	34/39 (87%)	0.04	0 100 100	155, 165, 183, 189	0
9	b	34/39 (87%)	1.21	8 (23%) 1 5	156, 176, 190, 190	0
10	K	37/37 (100%)	0.21	3 (8%) 15 18	158, 170, 181, 185	0
10	c	37/37 (100%)	1.36	10 (27%) 1 5	152, 171, 187, 195	0
11	L	37/37 (100%)	0.27	4 (10%) 8 12	137, 155, 186, 190	0
11	d	37/37 (100%)	0.26	4 (10%) 8 12	143, 158, 194, 201	0
12	M	34/36 (94%)	0.37	5 (14%) 3 9	147, 163, 179, 195	0
12	e	34/36 (94%)	0.43	7 (20%) 1 6	147, 159, 176, 192	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/246 (98%)	0.83	39 (16%) 3 8	132, 162, 190, 201	0
13	f	243/246 (98%)	0.54	15 (6%) 24 25	127, 164, 191, 211	0
14	T	32/32 (100%)	0.21	0 100 100	144, 157, 187, 198	0
14	g	32/32 (100%)	0.28	3 (9%) 11 15	145, 158, 179, 198	0
15	U	97/104 (93%)	0.88	10 (10%) 9 13	136, 154, 173, 177	0
15	h	97/104 (93%)	1.73	32 (32%) 0 4	140, 154, 165, 174	0
16	V	137/137 (100%)	0.45	11 (8%) 15 19	135, 156, 170, 180	0
16	i	137/137 (100%)	0.54	11 (8%) 15 19	131, 158, 176, 185	0
17	m	28/46 (60%)	2.13	17 (60%) 0 3	167, 183, 198, 205	0
17	y	28/46 (60%)	0.45	2 (7%) 19 21	164, 182, 197, 201	0
18	X	37/40 (92%)	1.19	6 (16%) 3 8	158, 173, 188, 190	0
18	j	37/40 (92%)	0.76	2 (5%) 29 30	161, 175, 191, 202	0
19	Y	0/28	-	-	-	-
19	k	0/28	-	-	-	-
20	Z	62/62 (100%)	1.55	17 (27%) 1 5	159, 178, 198, 208	0
20	l	62/62 (100%)	0.97	5 (8%) 15 18	164, 178, 199, 208	0
All	All	5214/5482 (95%)	0.53	539 (10%) 9 13	125, 161, 185, 213	0

The worst 5 of 539 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	295	SER	7.7
12	M	2	GLU	6.5
16	i	132	ASN	6.5
15	U	123	GLU	6.2
9	b	15	THR	6.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
33	CL	G	415	1/1	0.86	0.89	5.23	122,122,122,122	0
27	LMG	C	520	45/55	0.29	1.14	4.78	164,178,186,187	0
31	LMT	D	409	31/35	0.56	1.06	4.73	162,187,202,208	0
30	BCR	T	103	40/40	0.49	0.88	4.69	155,168,181,184	0
33	CL	D	411	1/1	0.71	0.87	4.63	121,121,121,121	0
30	BCR	B	620	40/40	0.61	0.76	4.46	161,168,186,196	0
31	LMT	Q	410	31/35	0.38	0.73	4.20	165,182,193,197	0
30	BCR	P	514	40/40	0.71	1.52	4.09	139,152,173,175	0
21	CLA	B	603	65/65	0.82	1.03	4.00	147,166,178,179	0
31	LMT	a	103	35/35	0.47	0.87	3.70	169,180,206,216	0
24	DGD	B	628	52/66	0.73	0.47	3.64	148,173,194,200	0
30	BCR	Z	101	40/40	0.85	1.17	3.64	163,178,192,197	0
24	DGD	D	408	63/66	0.58	0.78	3.44	167,181,198,212	0
21	CLA	P	503	65/65	0.78	1.06	3.37	144,174,187,195	0
21	CLA	P	501	65/65	0.81	0.97	3.25	149,170,185,188	0
30	BCR	D	405	40/40	0.65	0.69	3.22	145,161,176,179	0
30	BCR	P	515	40/40	0.84	1.38	3.08	165,176,185,189	0
27	LMG	P	521	45/55	0.43	1.10	3.08	149,175,191,198	0
30	BCR	C	514	40/40	0.74	0.84	3.04	153,160,171,173	0
21	CLA	B	610	65/65	0.82	0.57	2.95	146,163,174,176	0
21	CLA	B	605	65/65	0.75	0.75	2.89	156,167,176,179	0
31	LMT	N	604	35/35	0.59	0.51	2.83	145,180,209,212	0
31	LMT	B	630	35/35	0.64	0.54	2.82	157,169,199,220	0
21	CLA	D	403	65/65	0.83	0.89	2.70	153,160,181,189	0
32	BCT	Q	411	4/4	0.89	0.41	2.64	164,166,168,173	0
30	BCR	H	101	40/40	0.62	0.96	2.62	165,178,188,190	0
21	CLA	C	512	65/65	0.76	1.22	2.60	173,183,196,199	0
21	CLA	P	512	65/65	0.81	1.29	2.56	172,184,194,199	0
21	CLA	P	509	65/65	0.74	0.84	2.48	152,174,181,184	0
31	LMT	N	625	35/35	0.59	0.86	2.47	165,184,206,216	0
21	CLA	B	601	65/65	0.49	1.00	2.44	167,188,199,203	0
21	CLA	B	609	65/65	0.82	0.79	2.43	162,177,185,186	0
31	LMT	I	103	35/35	0.31	1.02	2.41	153,189,201,206	0
30	BCR	K	101	40/40	0.76	0.80	2.33	154,167,176,181	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	BCR	C	515	40/40	0.79	0.66	2.20	139,164,177,180	0
21	CLA	B	608	65/65	0.79	0.72	2.15	147,165,180,186	0
21	CLA	C	513	65/65	0.66	1.15	2.13	173,193,206,213	0
21	CLA	B	615	65/65	0.79	0.67	2.09	162,178,191,194	0
21	CLA	B	602	65/65	0.84	0.72	2.09	152,172,182,185	0
21	CLA	P	502	65/65	0.64	0.87	2.01	146,161,175,182	0
21	CLA	B	612	65/65	0.80	0.55	1.94	152,163,174,176	0
21	CLA	P	507	65/65	0.75	0.66	1.92	162,172,191,194	0
21	CLA	B	604	65/65	0.68	0.69	1.89	148,158,172,182	0
21	CLA	N	612	65/65	0.84	0.49	1.84	151,164,181,190	0
21	CLA	C	507	65/65	0.67	0.81	1.81	159,172,185,187	0
21	CLA	N	610	65/65	0.70	0.77	1.80	152,178,191,194	0
21	CLA	G	406	65/65	0.70	0.61	1.74	145,159,181,186	0
21	CLA	P	511	65/65	0.72	1.03	1.69	156,174,184,187	0
27	LMG	D	406	46/55	0.88	0.36	1.63	140,153,176,181	0
30	BCR	J	102	40/40	0.50	0.48	1.62	167,182,207,208	0
21	CLA	A	405	65/65	0.75	0.51	1.58	144,155,176,187	0
21	CLA	C	503	65/65	0.74	0.54	1.58	155,171,181,183	0
21	CLA	N	609	65/65	0.68	0.68	1.54	148,165,174,178	0
27	LMG	Q	401	42/55	0.60	0.65	1.54	131,168,174,183	0
21	CLA	Q	404	65/65	0.81	0.60	1.51	152,162,187,194	0
21	CLA	C	502	65/65	0.68	0.51	1.51	142,157,179,185	0
21	CLA	P	513	65/65	0.67	1.01	1.51	168,182,207,216	0
24	DGD	P	518	62/66	0.82	0.44	1.47	144,168,195,200	0
24	DGD	Q	409	63/66	0.67	0.54	1.46	157,183,208,238	0
31	LMT	N	603	35/35	0.54	0.61	1.45	153,179,189,190	0
21	CLA	N	616	65/65	0.78	0.56	1.44	156,167,181,184	0
21	CLA	N	607	65/65	0.69	0.71	1.44	133,163,170,175	0
30	BCR	a	101	40/40	0.40	0.56	1.40	139,159,176,181	0
24	DGD	B	621	58/66	0.74	0.49	1.36	142,158,168,171	0
21	CLA	C	501	65/65	0.75	0.55	1.35	160,174,184,185	0
21	CLA	C	509	65/65	0.70	0.80	1.26	145,170,180,183	0
26	SQD	N	601	47/54	0.70	0.44	1.24	141,176,198,202	0
24	DGD	N	602	52/66	0.74	0.46	1.23	154,176,204,206	0
30	BCR	P	516	40/40	0.68	0.85	1.23	164,173,180,187	0
30	BCR	I	101	40/40	0.47	0.54	1.23	143,155,171,183	0
27	LMG	R	102	44/55	0.67	0.42	1.17	161,177,189,192	0
31	LMT	B	629	35/35	0.57	0.75	1.17	153,166,181,185	0
21	CLA	N	605	65/65	0.46	0.79	1.14	170,189,202,205	0
23	PL9	J	101	35/55	0.46	0.50	1.13	177,190,200,204	0
26	SQD	F	101	45/54	0.77	0.60	1.09	157,176,196,198	0
30	BCR	W	101	40/40	0.78	0.79	1.09	164,176,182,186	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
27	LMG	C	519	48/55	0.69	0.39	1.06	132,169,183,188	0
30	BCR	S	101	40/40	0.83	0.63	1.02	145,159,176,178	0
26	SQD	A	414	54/54	0.63	0.57	0.99	139,173,190,200	0
26	SQD	S	102	45/54	0.81	0.58	0.98	160,188,201,203	0
23	PL9	G	407	45/55	0.72	0.44	0.97	148,160,183,188	0
21	CLA	N	619	65/65	0.75	0.86	0.95	158,180,190,193	0
26	SQD	Q	408	43/54	0.64	0.59	0.95	143,180,193,194	0
21	CLA	N	608	65/65	0.63	0.59	0.94	146,158,176,191	0
30	BCR	c	101	40/40	0.40	1.10	0.93	151,171,188,190	0
21	CLA	N	620	65/65	0.65	0.79	0.92	156,175,192,194	0
21	CLA	N	614	65/65	0.80	0.75	0.89	150,162,173,178	0
21	CLA	B	606	65/65	0.82	0.54	0.85	156,173,194,204	0
22	PHO	D	402	64/64	0.72	0.49	0.84	135,155,161,168	0
34	HEM	E	101	43/43	0.86	0.36	0.80	166,179,188,190	0
21	CLA	C	506	65/65	0.78	0.44	0.79	159,175,202,211	0
34	HEM	R	101	43/43	0.90	0.50	0.78	164,184,192,199	0
26	SQD	B	627	47/54	0.68	0.42	0.76	143,179,209,227	0
25	LHG	G	412	37/49	0.59	0.52	0.69	147,176,193,204	0
24	DGD	W	102	58/66	0.84	0.34	0.68	145,157,168,172	0
21	CLA	A	403	65/65	0.68	0.40	0.68	142,161,183,185	0
27	LMG	E	102	44/55	0.77	0.44	0.64	168,188,198,203	0
34	HEM	i	201	43/43	0.83	0.48	0.63	131,158,169,172	0
27	LMG	D	412	42/55	0.53	0.43	0.62	147,178,195,199	0
21	CLA	N	613	65/65	0.76	0.78	0.62	160,170,177,182	0
26	SQD	G	401	54/54	0.80	0.38	0.59	158,176,209,210	0
21	CLA	C	505	65/65	0.68	0.50	0.59	147,172,186,188	0
21	CLA	B	613	65/65	0.87	0.31	0.58	148,160,171,175	0
21	CLA	P	508	65/65	0.89	0.43	0.56	157,168,182,193	0
21	CLA	P	506	65/65	0.83	0.43	0.55	159,176,194,202	0
31	LMT	B	626	35/35	0.69	0.41	0.52	163,194,202,213	0
26	SQD	B	624	43/54	0.68	0.45	0.47	150,181,199,206	0
24	DGD	A	407	56/66	0.75	0.35	0.46	147,171,188,195	0
34	HEM	V	201	43/43	0.81	0.43	0.46	139,151,166,173	0
23	PL9	A	406	45/55	0.88	0.51	0.45	152,174,185,188	0
21	CLA	P	510	65/65	0.81	0.69	0.45	145,161,170,178	0
21	CLA	P	505	65/65	0.82	0.37	0.44	134,164,180,183	0
25	LHG	A	408	39/49	0.83	0.35	0.44	146,167,179,179	0
22	PHO	Q	403	64/64	0.80	0.37	0.42	144,155,164,168	0
21	CLA	B	616	65/65	0.79	0.46	0.41	155,166,199,214	0
25	LHG	G	409	39/49	0.88	0.39	0.38	156,168,188,191	0
27	LMG	M	101	42/55	0.84	0.32	0.37	166,174,184,188	0
21	CLA	N	618	65/65	0.85	0.31	0.37	153,171,180,185	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	CLA	N	617	65/65	0.89	0.28	0.35	149,168,182,188	0
21	CLA	P	504	65/65	0.83	0.46	0.33	155,169,181,186	0
21	CLA	D	401	65/65	0.68	0.42	0.33	137,149,176,181	0
21	CLA	N	606	65/65	0.86	0.37	0.27	152,172,178,182	0
21	CLA	C	511	65/65	0.79	0.46	0.25	155,172,181,184	0
27	LMG	Q	406	46/55	0.84	0.41	0.23	135,162,171,180	0
21	CLA	C	508	65/65	0.90	0.34	0.19	154,170,194,203	0
21	CLA	Q	402	65/65	0.77	0.50	0.12	136,144,158,169	0
24	DGD	G	408	56/66	0.74	0.43	0.10	163,179,188,193	0
27	LMG	e	102	42/55	0.85	0.30	0.09	155,166,183,191	0
21	CLA	G	402	65/65	0.84	0.43	0.05	136,148,155,166	0
24	DGD	C	516	53/66	0.83	0.34	0.05	141,158,168,170	0
28	OEC	A	412	5/9	0.96	0.47	-0.01	122,122,126,129	0
28	OEC	G	413	5/9	0.91	0.47	-0.05	91,102,115,124	0
27	LMG	D	407	48/55	0.82	0.32	-0.05	145,159,169,175	0
30	BCR	B	617	40/40	0.74	0.28	-0.07	151,158,176,180	0
30	BCR	B	618	40/40	0.71	0.30	-0.08	149,162,168,169	0
24	DGD	C	518	66/66	0.71	0.35	-0.08	139,157,179,185	0
27	LMG	B	622	49/55	0.78	0.36	-0.12	148,163,174,176	0
27	LMG	A	410	51/55	0.87	0.30	-0.13	138,157,168,171	0
21	CLA	C	504	65/65	0.85	0.29	-0.16	153,172,198,204	0
30	BCR	B	619	40/40	0.79	0.25	-0.17	140,156,169,178	0
31	LMT	e	101	35/35	0.65	0.52	-0.18	164,176,191,195	0
26	SQD	G	410	51/54	0.77	0.39	-0.21	161,172,184,190	0
27	LMG	P	520	48/55	0.79	0.58	-0.21	147,168,177,184	0
24	DGD	C	517	62/66	0.78	0.35	-0.22	145,169,193,200	0
21	CLA	B	614	65/65	0.83	0.29	-0.22	157,172,181,184	0
21	CLA	C	510	65/65	0.89	0.27	-0.22	149,161,171,178	0
22	PHO	A	404	64/64	0.73	0.32	-0.25	129,151,167,177	0
26	SQD	A	409	51/54	0.80	0.35	-0.26	156,178,191,194	0
21	CLA	B	611	65/65	0.89	0.32	-0.26	149,160,167,169	0
21	CLA	N	615	65/65	0.88	0.30	-0.26	152,158,168,173	0
24	DGD	P	517	53/66	0.85	0.33	-0.31	141,160,173,176	0
30	BCR	b	102	40/40	0.63	0.55	-0.32	158,178,202,203	0
27	LMG	B	623	49/55	0.74	0.36	-0.34	128,147,164,167	0
31	LMT	M	102	35/35	0.69	0.59	-0.37	134,165,196,205	0
30	BCR	T	102	40/40	0.80	0.29	-0.40	143,167,176,178	0
22	PHO	G	405	64/64	0.75	0.37	-0.40	131,149,159,162	0
24	DGD	P	519	66/66	0.83	0.32	-0.43	142,157,177,186	0
32	BCT	D	410	4/4	0.86	0.36	-0.44	166,167,167,169	0
21	CLA	G	404	65/65	0.74	0.36	-0.46	141,159,179,181	0
21	CLA	A	401	65/65	0.85	0.27	-0.52	138,146,156,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	BCR	T	101	40/40	0.75	0.29	-0.52	144,167,181,184	0
21	CLA	B	607	65/65	0.79	0.30	-0.62	135,152,161,165	0
27	LMG	N	622	49/55	0.88	0.28	-0.66	145,154,172,174	0
25	LHG	A	411	37/49	0.69	0.40	-0.69	156,178,214,232	0
21	CLA	N	611	65/65	0.88	0.29	-0.71	145,156,164,166	0
30	BCR	N	621	40/40	0.79	0.21	-0.72	132,154,165,172	0
27	LMG	Q	407	48/55	0.81	0.25	-0.72	142,156,168,176	0
27	LMG	N	623	49/55	0.83	0.27	-0.77	139,152,164,171	0
21	CLA	G	403	65/65	0.79	0.33	-0.81	123,139,149,162	0
23	PL9	D	404	55/55	0.86	0.23	-0.84	129,150,158,160	0
21	CLA	A	402	65/65	0.81	0.26	-0.90	139,147,158,164	0
27	LMG	G	411	51/55	0.85	0.24	-1.00	152,164,177,178	0
23	PL9	Q	405	55/55	0.80	0.22	-1.18	137,146,166,170	0
23	PL9	b	101	35/55	0.28	0.47	-1.59	168,188,199,208	0
29	FE2	A	413	1/1	0.88	0.17	-1.73	166,166,166,166	0
29	FE2	G	414	1/1	0.92	0.17	-1.78	149,149,149,149	0
31	LMT	N	624	35/35	0.43	0.92	-	166,201,210,213	0
27	LMG	a	102	43/55	0.72	0.64	-	160,179,196,200	0
27	LMG	I	102	43/55	0.60	0.79	-	152,184,203,207	0
35	CA	O	301	1/1	0.05	0.78	-	138,138,138,138	0
35	CA	f	301	1/1	0.30	0.81	-	210,210,210,210	0
31	LMT	B	625	35/35	0.49	0.88	-	163,196,218,227	0

6.5 Other polymers

There are no such residues in this entry.