



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 19, 2016 – 09:03 PM EST

PDB ID : 5TIS  
Title : Room temperature XFEL structure of the native, doubly-illuminated photo-system II complex  
Authors : Young, I.D.; Ibrahim, M.; Chatterjee, R.; Gul, S.; Fuller, F.; Koroidov, S.; Brewster, A.S.; Tran, R.; Alonso-Mori, R.; Kroll, T.; Michels-Clark, T.; Laksmono, H.; Sierra, R.G.; Stan, C.A.; Hussein, R.; Zhang, M.; Douthit, L.; Kubin, M.; de Lichtenberg, C.; Pham, L.V.; Nilsson, H.; Cheah, M.H.; Shevela, D.; Saracini, C.; Bean, M.A.; Seuffert, I.; Sokaras, D.; Weng, T.-C.; Pastor, E.; Weninger, C.; Fransson, T.; Lassalle, L.; Braeuer, P.; Aller, P.; Docker, P.T.; Andi, B.; Orville, A.M.; Glowina, J.M.; Nelson, S.; Sikorski, M.; Zhu, D.; Hunter, M.S.; Aquila, A.; Koglin, J.E.; Robinson, J.; Liang, M.; Boutet, S.; Lyubimov, A.Y.; Uervirojnangkoorn, M.; Moriarty, N.W.; Liebschner, D.; Afonine, P.V.; Watermann, D.G.; Evans, G.; Wernet, P.; Dobbek, H.; Weis, W.I.; Brunger, A.T.; Zwart, P.H.; Adams, P.D.; Zouni, A.; Messinger, J.; Bergmann, U.; Sauter, N.K.; Kern, J.; Yachandra, V.K.; Yano, J.  
Deposited on : 2016-10-03  
Resolution : 2.25 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](mailto: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.

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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

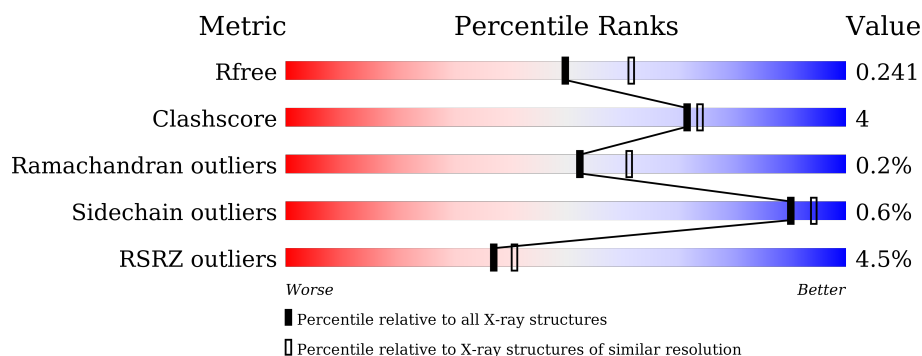
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

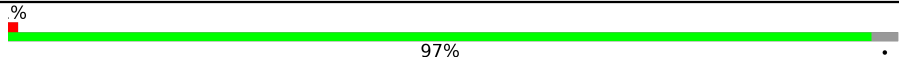

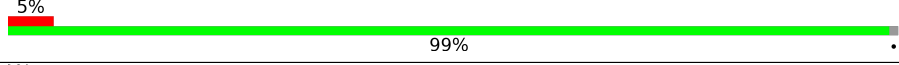

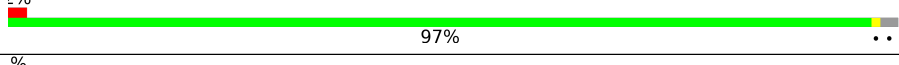
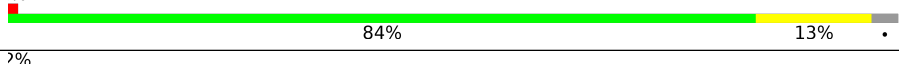
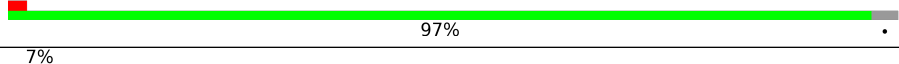

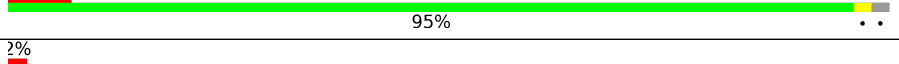


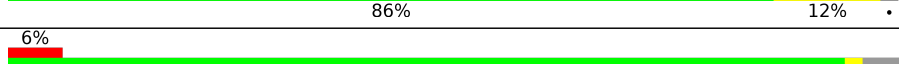
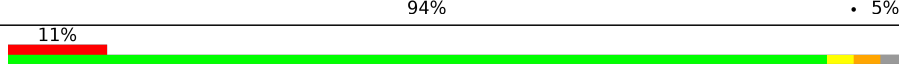
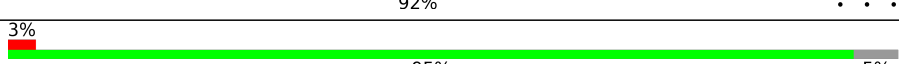
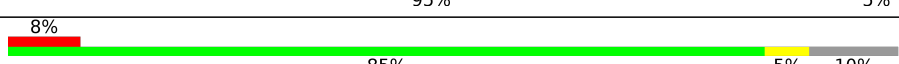
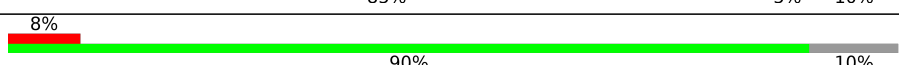
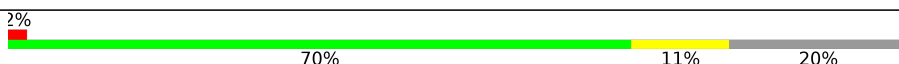
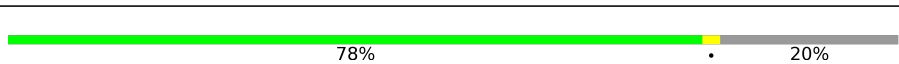
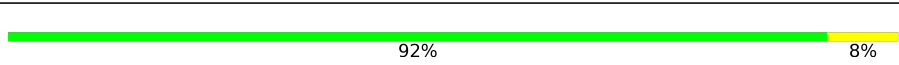
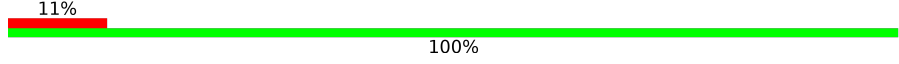

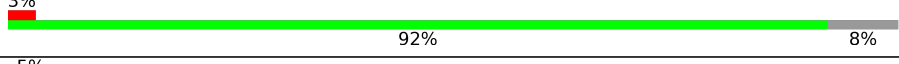
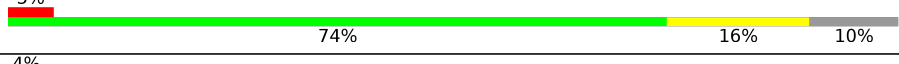
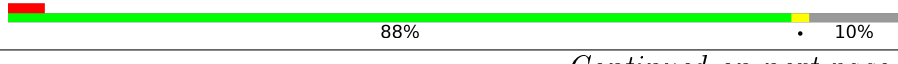

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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 style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; left: 0; top: -10px; width: 5px; height: 5px; background-color: red;"></div> <div style="position: absolute; left: 85%; top: -10px; width: 5px; height: 5px; background-color: yellow;"></div> <div style="position: absolute; left: 95%; top: -10px; width: 5px; height: 5px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>85%</span> <span>12%</span> <span>.</span> </div> </div>

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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

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Mol	Chain	Length	Quality of chain
1	a	344	
2	B	510	
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	

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Mol	Chain	Length	Quality of chain
14	T	32	
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

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
25	CLA	A	606	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	609	X	-	-	-
25	CLA	A	613	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	X
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	C	514	X	-	-	X
25	CLA	D	402	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	a	606	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	610	X	-	-	-
25	CLA	a	615	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606[A]	X	-	-	-
25	CLA	b	606[B]	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	b	616	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	401	X	-	-	-
25	CLA	d	402	X	-	-	-
28	PL9	A	611	-	-	-	X
28	PL9	a	612	-	-	-	X
29	SQD	B	625	-	-	-	X
29	SQD	D	409	-	-	-	X
30	LHG	A	618	-	-	-	X
30	LHG	a	617	-	-	-	X
30	LHG	d	406	-	-	-	X
31	UNL	A	615	-	-	-	X
31	UNL	A	617	-	-	-	X
31	UNL	B	627	-	-	-	X
31	UNL	C	522	-	-	-	X
31	UNL	D	410	-	-	-	X
31	UNL	M	101	-	-	-	X
31	UNL	M	102	-	-	-	X
31	UNL	a	619	-	-	-	X
31	UNL	c	525	-	-	-	X
31	UNL	d	409	-	-	-	X
31	UNL	j	801	-	-	-	X
31	UNL	m	103	-	-	-	X
31	UNL	t	102	-	-	-	X
32	LMG	B	621	-	-	-	X
32	LMG	B	626	-	-	-	X
32	LMG	C	521	-	-	-	X
32	LMG	b	620	-	-	-	X
32	LMG	c	520	-	-	-	X
32	LMG	d	408	-	-	-	X

## 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 51757 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	1	0
			2625	1719	431	460	15			
1	a	334	Total	C	N	O	S	0	0	0
			2622	1717	431	459	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	5	0
			4005	2629	667	696	13			
2	b	504	Total	C	N	O	S	0	2	0
			3982	2613	665	691	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	1	0
			3494	2287	585	609	13			
3	c	451	Total	C	N	O	S	0	1	0
			3494	2286	587	608	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	0	0
			2717	1800	444	461	12			
4	d	341	Total	C	N	O	S	0	0	0
			2716	1800	444	460	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	1	0
			670	437	109	124			
5	e	82	Total	C	N	O	0	1	0
			671	438	108	125			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	34	Total	C	N	O	S	0	0	0
			275	187	45	42	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
			510	341	82	85	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	37	Total	C	N	O	S	0	0	0
			304	206	47	50	1			
8	i	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			257	174	40	42	1			
9	j	36	Total	C	N	O	S	0	0	0
			257	174	40	42	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	k	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	l	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	33	Total	C	N	O	S	0	1	0
			269	178	39	51	1			
12	m	33	Total	C	N	O	S	0	0	0
			260	173	38	48	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	2	0
			1888	1179	320	385	4			
13	o	244	Total	C	N	O	S	0	2	0
			1888	1179	320	385	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	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	u	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
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	1	0
			1070	680	178	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0	0
			200	131	35	31	3			
17	y	30	Total	C	N	O	S	0	0	0
			224	147	38	36	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	S	0	0	0
			281	188	45	48				
18	x	38	Total	C	N	O	S	0	1	0
			285	192	46	47				

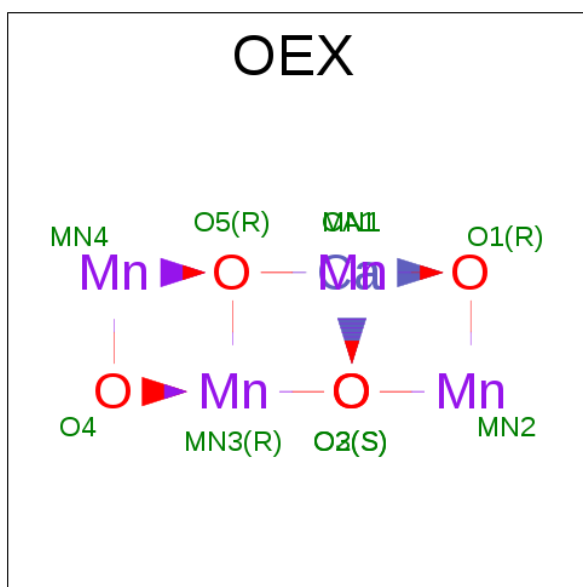
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			478	328	72	76	2			

- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	S	0	0	0
			273	186	47	40				
20	r	34	Total	C	N	O	S	0	0	0
			270	183	47	40				

- Molecule 21 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
21	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

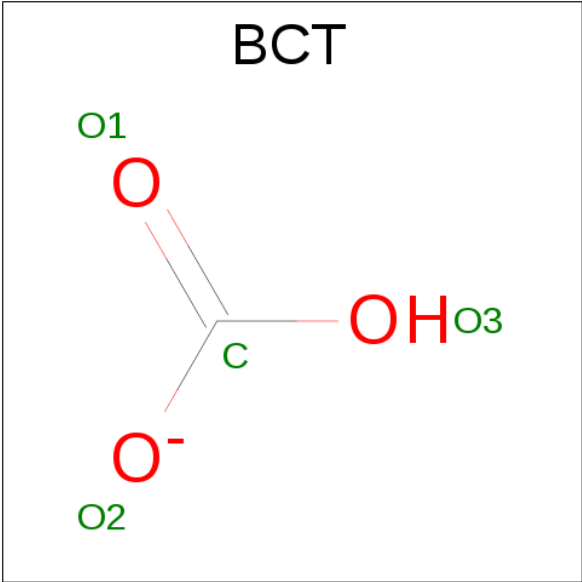
- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	1	Total	Fe	0	0
			1	1		
22	a	1	Total	Fe	0	0
			1	1		

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

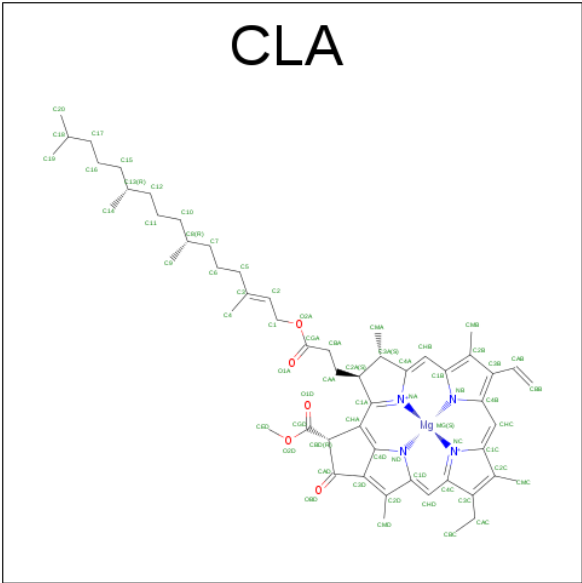
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	2	Total	Cl	0	0
			2	2		
23	a	2	Total	Cl	0	0
			2	2		

- Molecule 24 is BICARBONATE ION (three-letter code: BCT) (formula: CHO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	O		0	0
			4	1	3			
24	a	1	Total	C	O		0	0
			4	1	3			

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
25	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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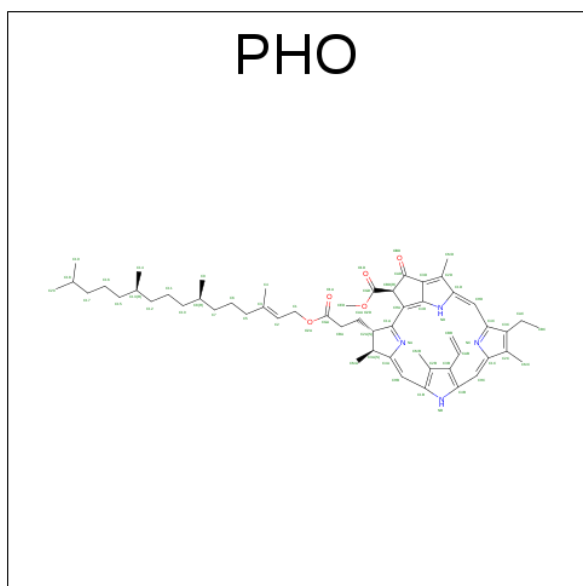
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total 129	C 110	Mg 1	N 8	O 10	0	1
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 64	C 54	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

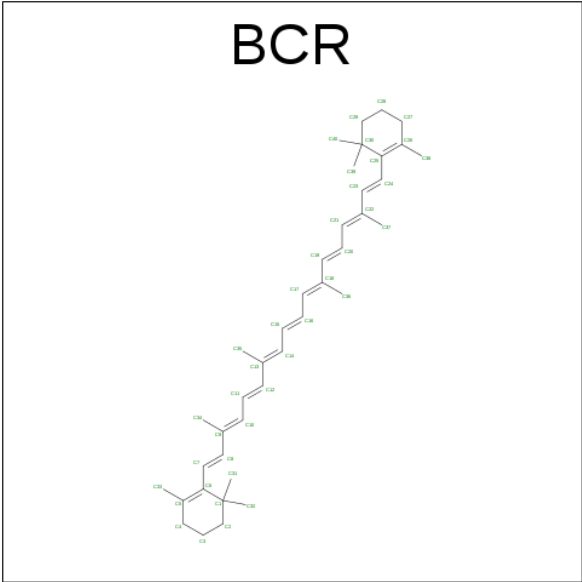
- Molecule 26 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	N	O	0	0
			64	55	4	5		
26	D	1	Total	C	N	O	0	0
			64	55	4	5		
26	a	1	Total	C	N	O	0	0
			64	55	4	5		
26	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).





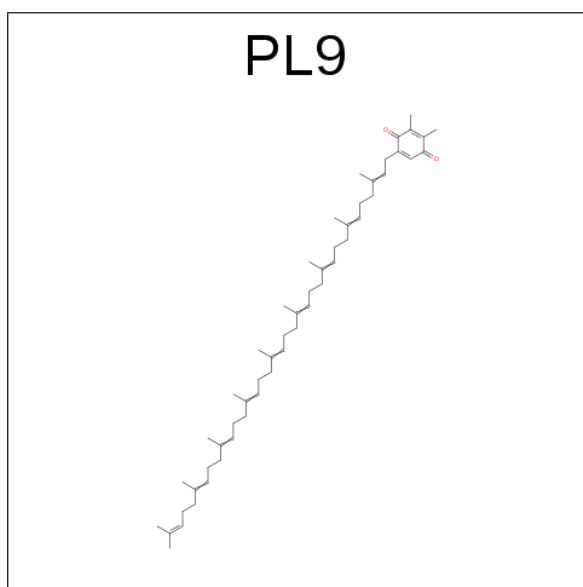
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	Y	1	Total C 40 40	0	0
27	a	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	d	1	Total C 40 40	0	0
27	h	1	Total C 40 40	0	0
27	t	1	Total C 40 40	0	0

- Molecule 28 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:  $C_{53}H_{80}O_2$ ).



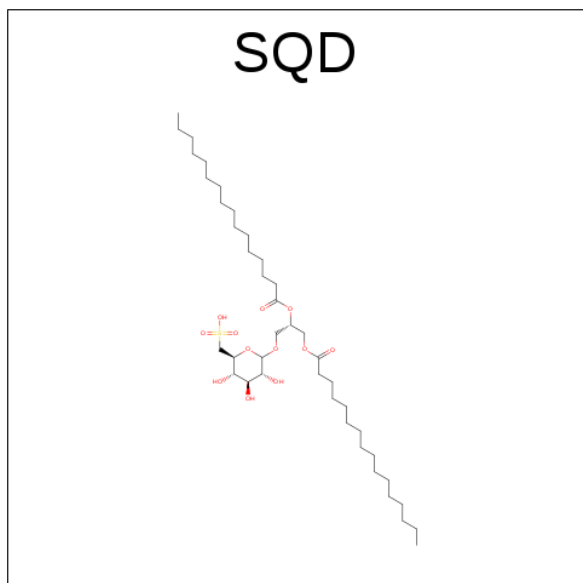
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 55 53 2	0	0
28	D	1	Total C O 55 53 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	a	1	Total	C	O	0	0
			55	53	2		
28	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



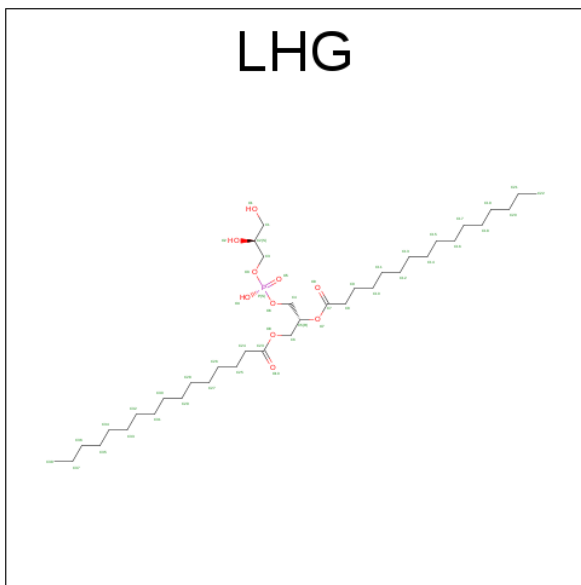
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	S	0	0
			52	39	12	1		
29	A	1	Total	C	O	S	0	0
			54	41	12	1		
29	B	1	Total	C	O	S	0	0
			54	41	12	1		
29	B	1	Total	C	O	S	0	0
			54	41	12	1		
29	D	1	Total	C	O	S	0	0
			43	30	12	1		
29	D	1	Total	C	O	S	0	0
			47	34	12	1		
29	L	1	Total	C	O	S	0	0
			49	36	12	1		
29	a	1	Total	C	O	S	0	0
			54	41	12	1		
29	b	1	Total	C	O		0	0
			40	35	5			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	f	1	Total	C	O	S	0	0
			41	28	12	1		

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).

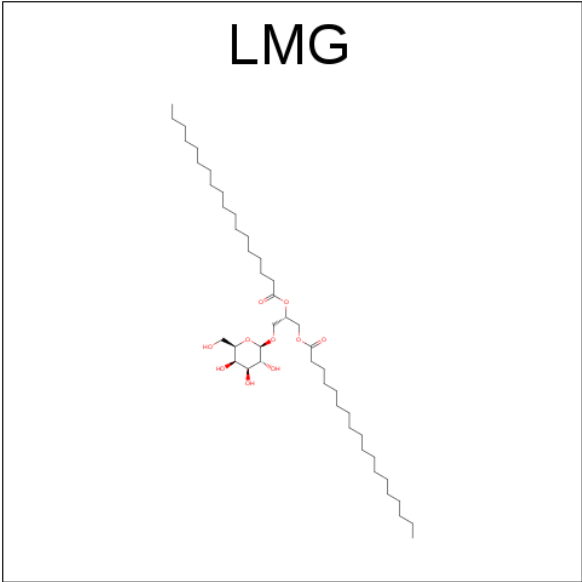


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	P	0	0
			47	36	10	1		
30	A	1	Total	C	O	P	0	0
			49	38	10	1		
30	B	1	Total	C	O	P	0	0
			49	38	10	1		
30	D	1	Total	C	O	P	0	0
			49	38	10	1		
30	L	1	Total	C	O	P	0	0
			49	38	10	1		
30	a	1	Total	C	O	P	0	0
			39	28	10	1		
30	a	1	Total	C	O	P	0	0
			42	31	10	1		
30	d	1	Total	C	O	P	0	0
			49	38	10	1		
30	d	1	Total	C	O	P	0	0
			49	38	10	1		
30	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 31 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

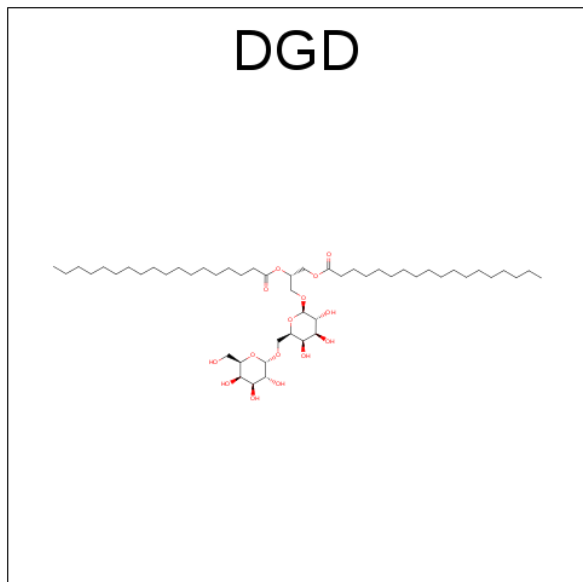
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	J	2	Total C O 23 21 2	0	0
31	i	1	Total C O 20 18 2	0	0
31	D	2	Total C 28 28	0	0
31	E	1	Total C O 12 10 2	0	0
31	H	1	Total C 7 7	0	0
31	B	2	Total C 26 26	0	0
31	I	2	Total C O 27 25 2	0	0
31	C	2	Total C O 33 31 2	0	0
31	a	2	Total C O 29 27 2	0	0
31	c	3	Total C O 40 34 6	0	0
31	x	1	Total C 16 16	0	0
31	A	2	Total C O 29 27 2	0	0
31	T	2	Total C 26 26	0	0
31	j	2	Total C O 27 25 2	0	0
31	d	1	Total C 17 17	0	0
31	t	1	Total C 18 18	0	0
31	m	2	Total C O 25 23 2	0	0
31	b	2	Total C 28 28	0	0
31	M	2	Total C O 32 30 2	0	0

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



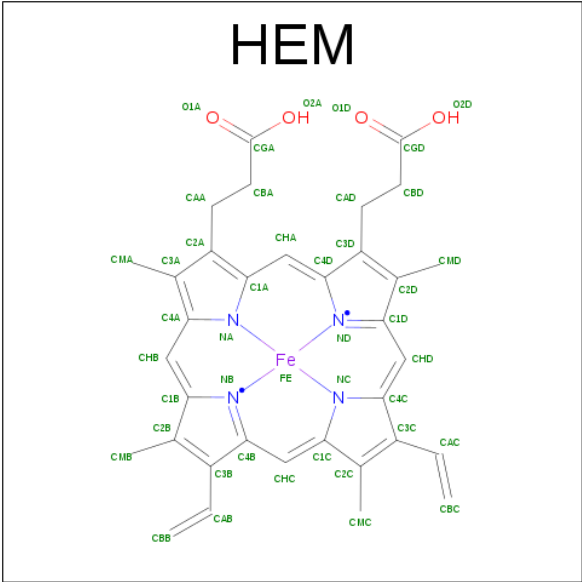
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B	1	Total	C	O	0	0
			51	41	10		
32	B	1	Total	C	O	0	0
			51	41	10		
32	B	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			48	38	10		
32	C	1	Total	C	O	0	0
			48	38	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	D	1	Total	C	O	0	0
			51	41	10		
32	a	1	Total	C	O	0	0
			51	41	10		
32	b	1	Total	C	O	0	0
			51	41	10		
32	c	1	Total	C	O	0	0
			37	27	10		
32	c	1	Total	C	O	0	0
			34	24	10		
32	d	1	Total	C	O	0	0
			51	41	10		
32	d	1	Total	C	O	0	0
			38	36	2		
32	m	1	Total	C	O	0	0
			51	41	10		

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			62	47	15		
33	C	1	Total	C	O	0	0
			62	47	15		
33	C	1	Total	C	O	0	0
			62	47	15		
33	H	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	h	1	Total	C	O	0	0
			62	47	15		

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



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

- Molecule 35 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	86	Total	O	0	0
			86	86		
35	B	109	Total	O	0	0
			109	109		
35	C	95	Total	O	0	0
			95	95		
35	D	82	Total	O	0	0
			82	82		
35	E	14	Total	O	0	0
			14	14		
35	F	3	Total	O	0	0
			3	3		
35	H	11	Total	O	0	0
			11	11		
35	I	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	J	5	Total 5	O 5	0	0
35	K	2	Total 2	O 2	0	0
35	L	3	Total 3	O 3	0	0
35	M	5	Total 5	O 5	0	0
35	O	72	Total 72	O 72	0	0
35	T	9	Total 9	O 9	0	0
35	U	22	Total 22	O 22	0	0
35	V	42	Total 42	O 42	0	0
35	X	5	Total 5	O 5	0	0
35	Z	3	Total 3	O 3	0	0
35	a	90	Total 90	O 90	0	0
35	b	129	Total 129	O 129	0	0
35	c	95	Total 95	O 95	0	0
35	d	87	Total 87	O 87	0	0
35	e	9	Total 9	O 9	0	0
35	f	2	Total 2	O 2	0	0
35	h	13	Total 13	O 13	0	0
35	i	6	Total 6	O 6	0	0
35	j	2	Total 2	O 2	0	0
35	k	4	Total 4	O 4	0	0
35	l	10	Total 10	O 10	0	0

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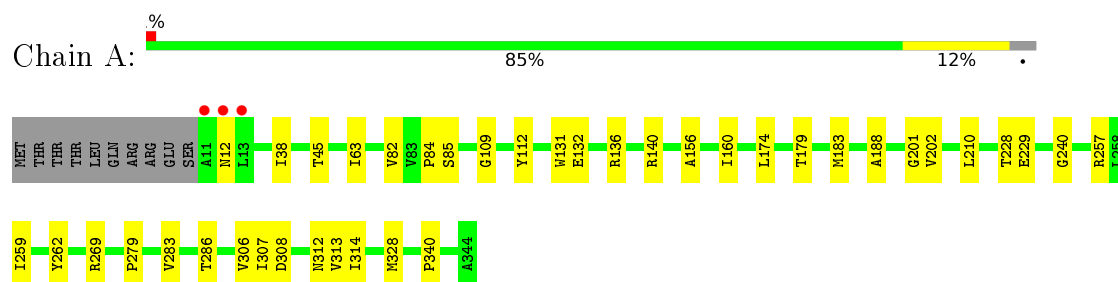
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	m	10	Total 10	O 10	0	0
35	o	69	Total 69	O 69	0	0
35	t	4	Total 4	O 4	0	0
35	u	34	Total 34	O 34	0	0
35	v	37	Total 37	O 37	0	0
35	y	1	Total 1	O 1	0	0
35	x	4	Total 4	O 4	0	0
35	z	1	Total 1	O 1	0	0
35	r	1	Total 1	O 1	0	0

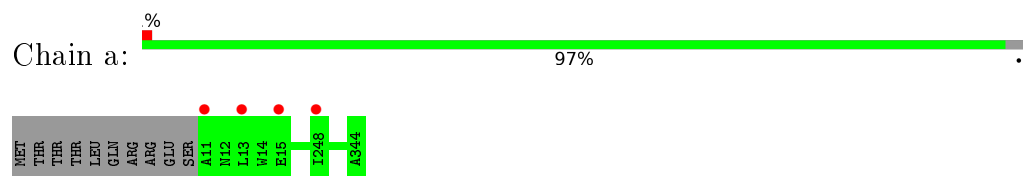
### 3 Residue-property plots [i](#)

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

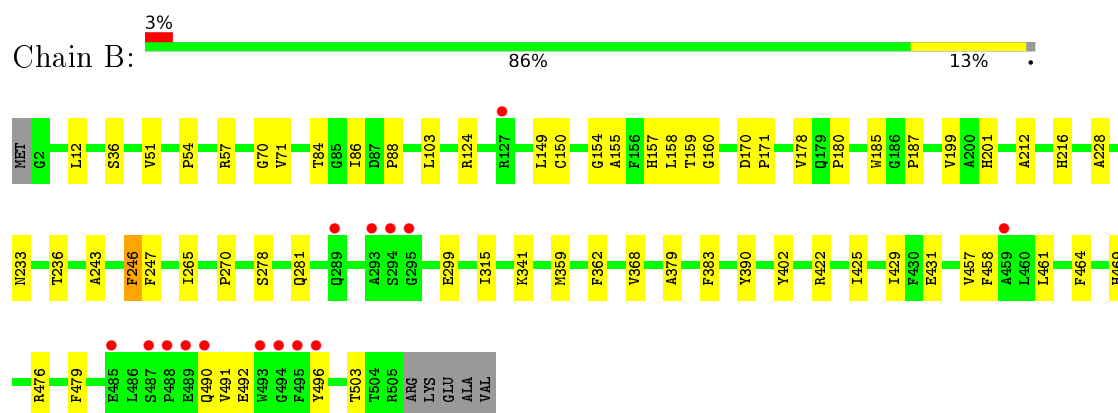
- Molecule 1: Photosystem II protein D1 1



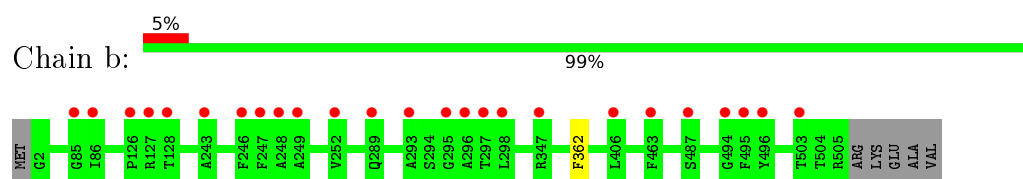
- Molecule 1: Photosystem II protein D1 1



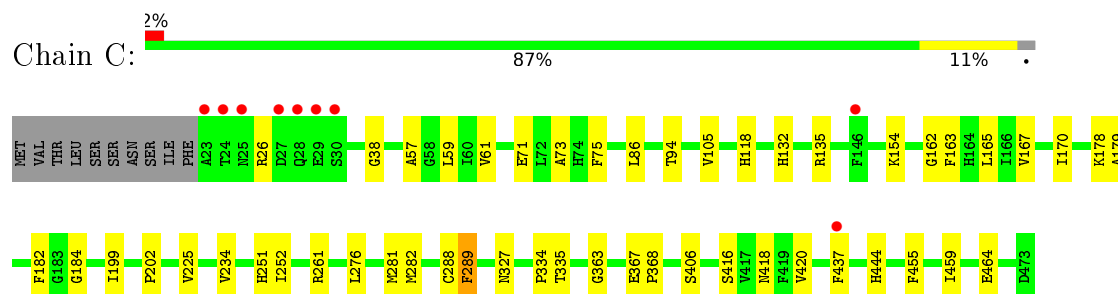
- Molecule 2: Photosystem II CP47 reaction center protein



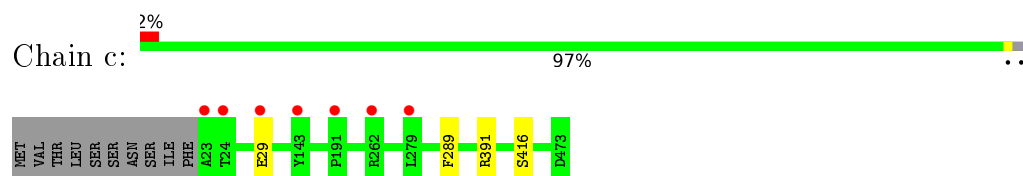
- Molecule 2: Photosystem II CP47 reaction center protein



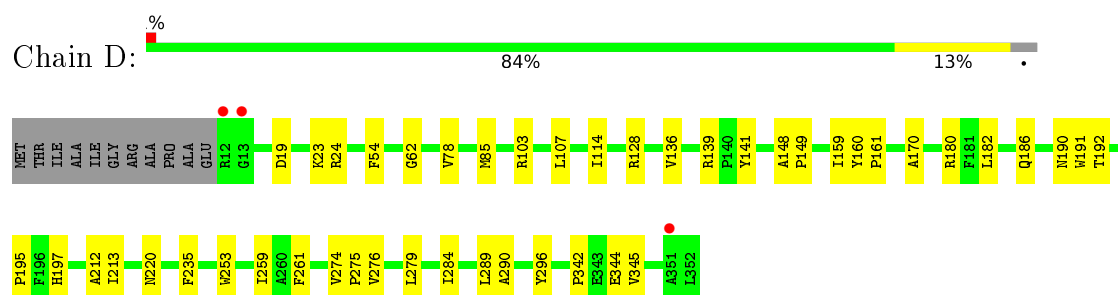
- Molecule 3: Photosystem II CP43 reaction center protein



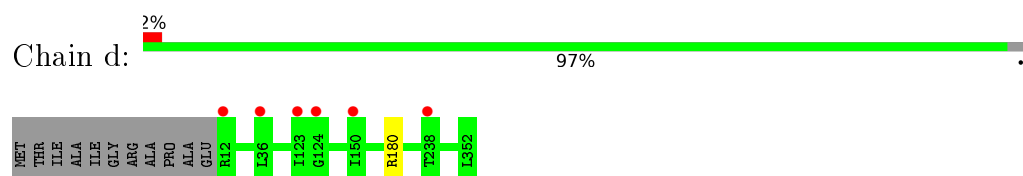
- Molecule 3: Photosystem II CP43 reaction center protein



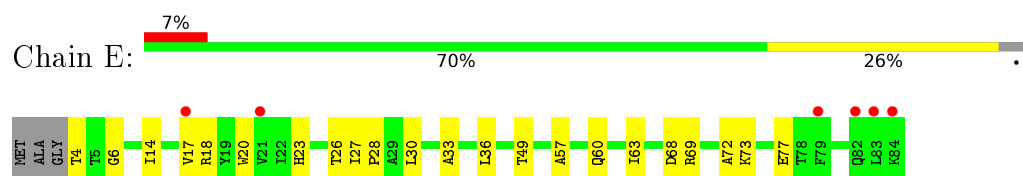
- Molecule 4: Photosystem II D2 protein



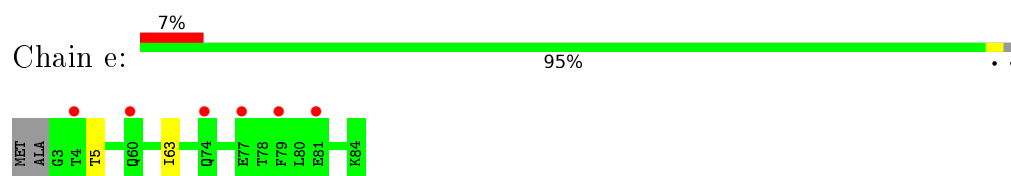
- Molecule 4: Photosystem II D2 protein



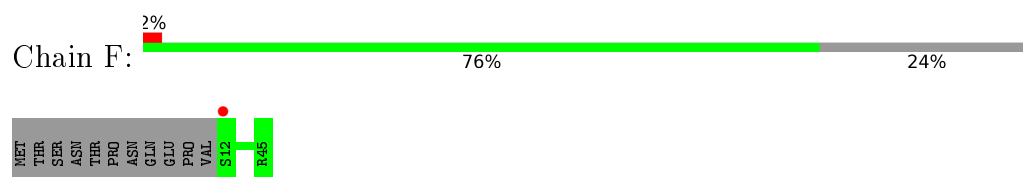
- Molecule 5: Cytochrome b559 subunit alpha



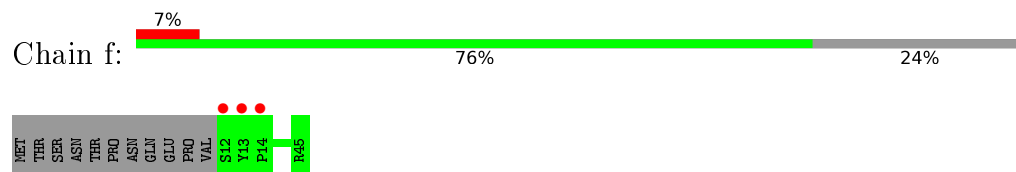
- Molecule 5: Cytochrome b559 subunit alpha



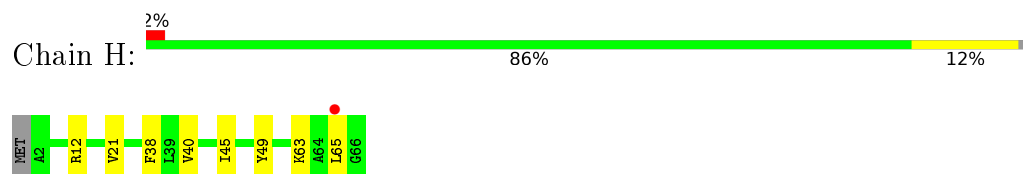
- Molecule 6: Cytochrome b559 subunit beta



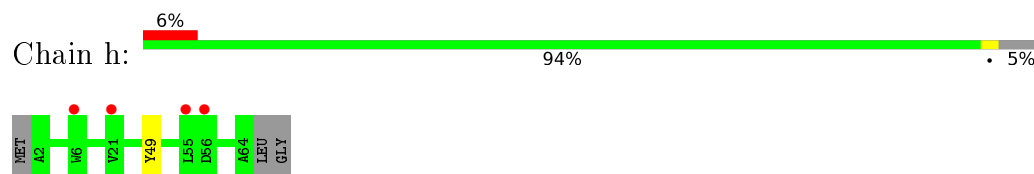
- Molecule 6: Cytochrome b559 subunit beta



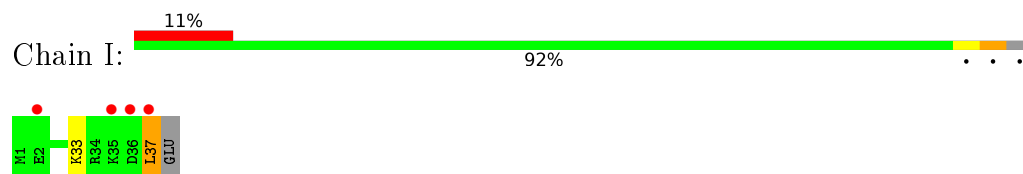
- Molecule 7: Photosystem II reaction center protein H



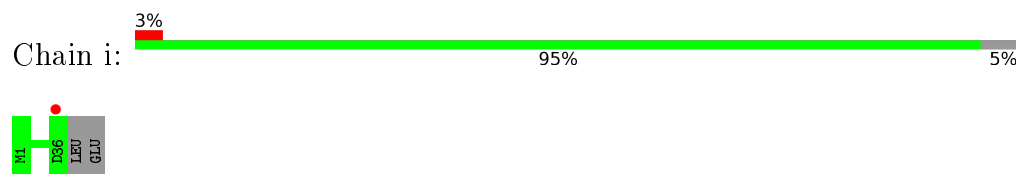
- Molecule 7: Photosystem II reaction center protein H



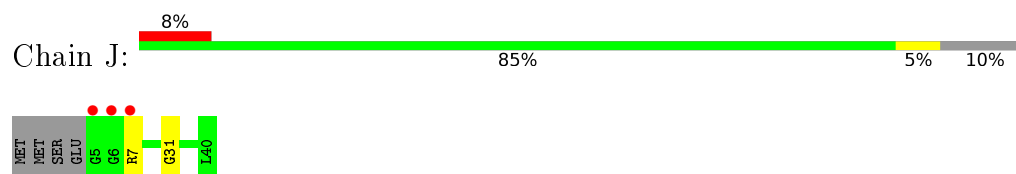
- Molecule 8: Photosystem II reaction center protein I



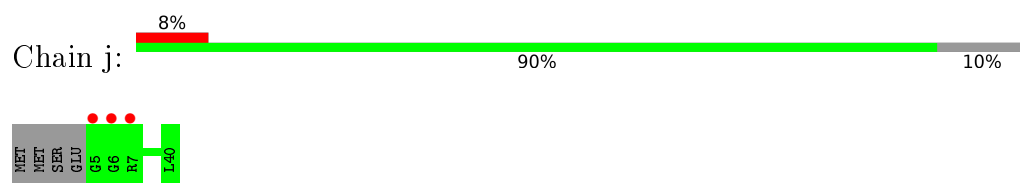
- Molecule 8: Photosystem II reaction center protein I



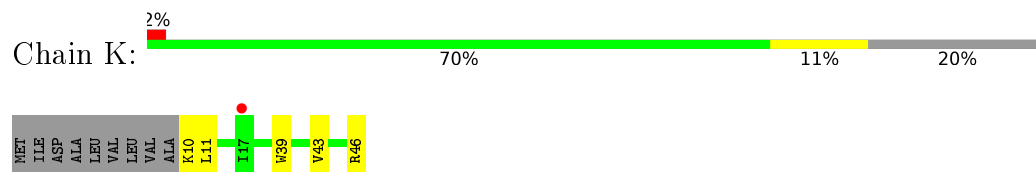
- Molecule 9: Photosystem II reaction center protein J



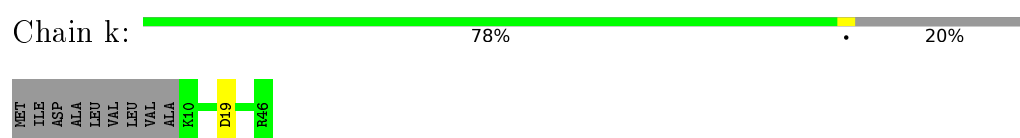
- Molecule 9: Photosystem II reaction center protein J



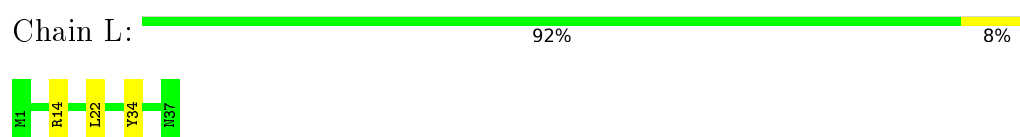
- Molecule 10: Photosystem II reaction center protein K



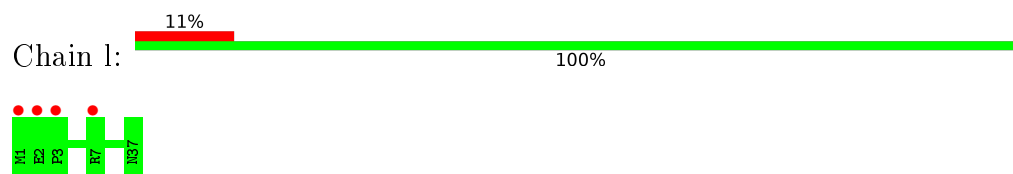
- Molecule 10: Photosystem II reaction center protein K



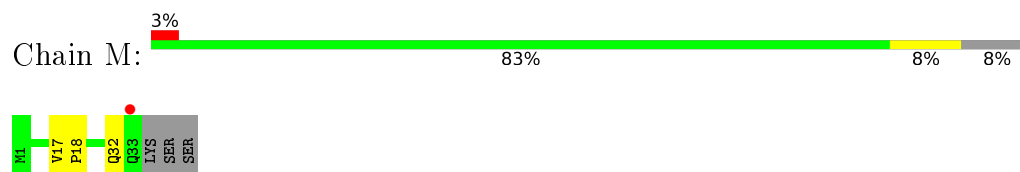
- Molecule 11: Photosystem II reaction center protein L



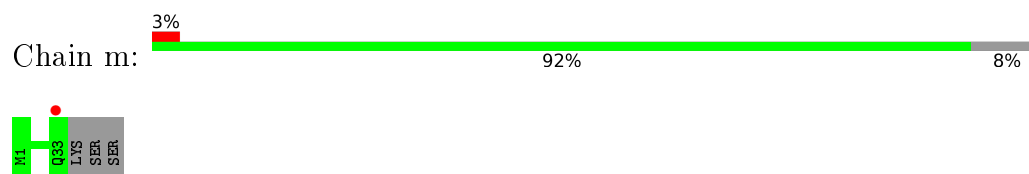
- Molecule 11: Photosystem II reaction center protein L



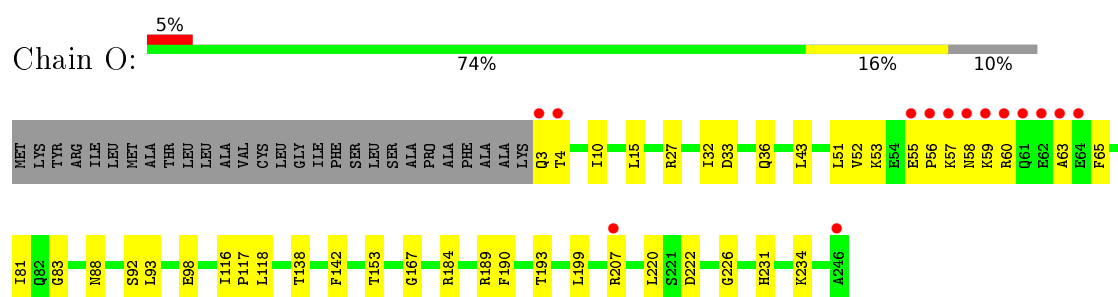
- Molecule 12: Photosystem II reaction center protein M



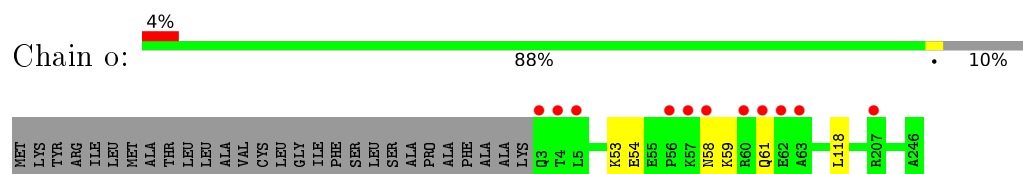
- Molecule 12: Photosystem II reaction center protein M



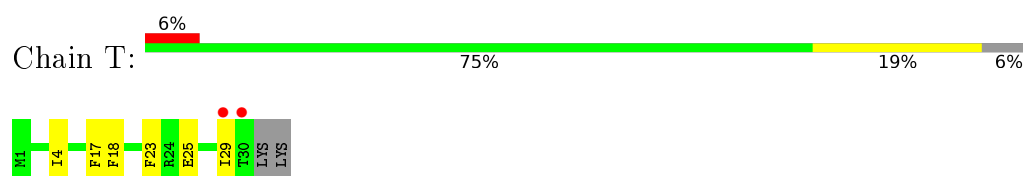
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



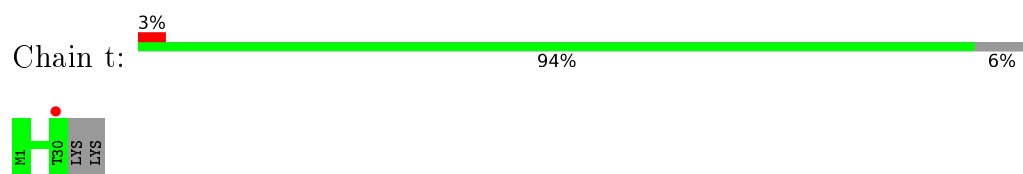
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



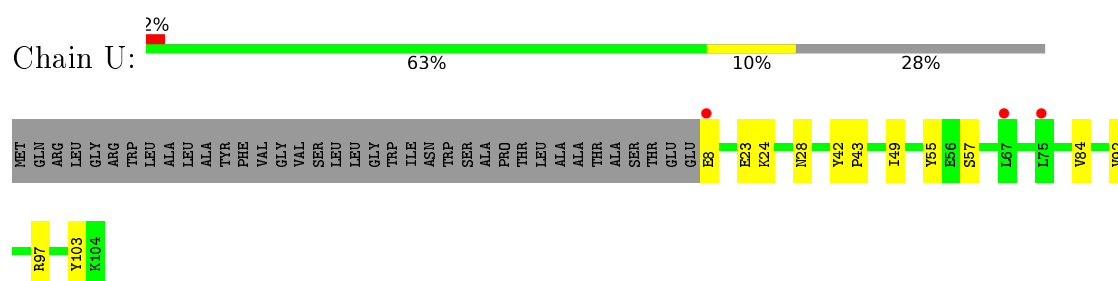
- Molecule 14: Photosystem II reaction center protein T



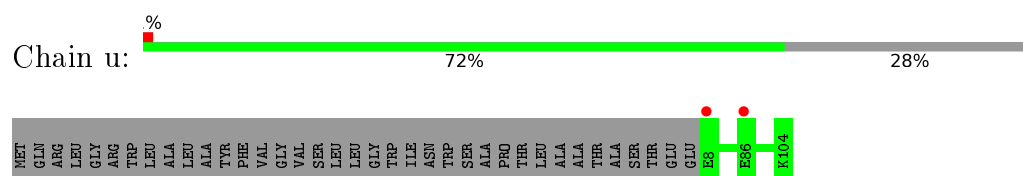
- Molecule 14: Photosystem II reaction center protein T



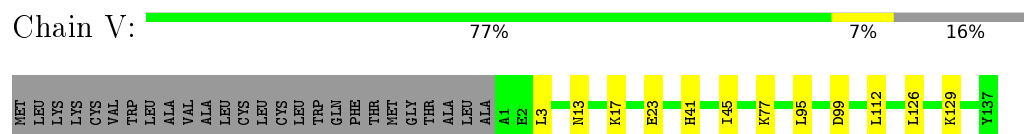
- Molecule 15: Photosystem II 12 kDa extrinsic protein



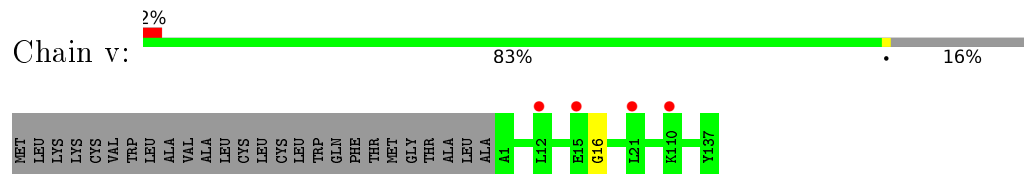
- Molecule 15: Photosystem II 12 kDa extrinsic protein



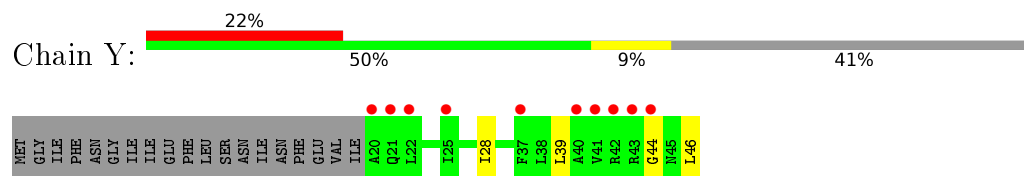
- Molecule 16: Cytochrome c-550



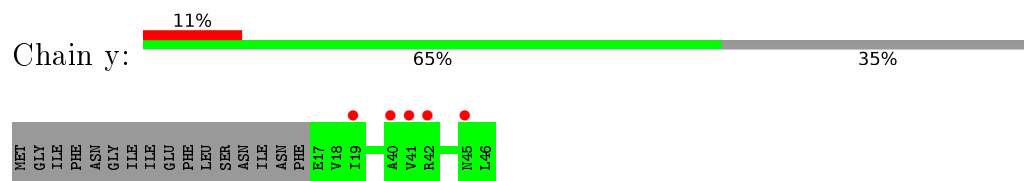
- Molecule 16: Cytochrome c-550



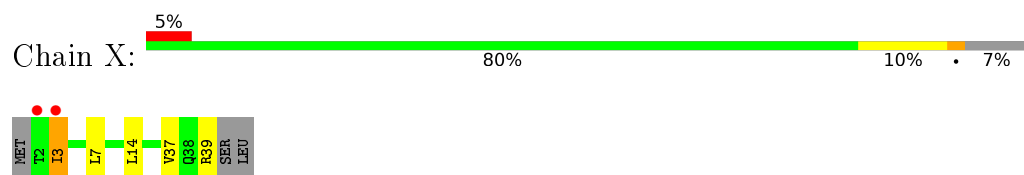
- Molecule 17: Photosystem II reaction center protein Ycf12



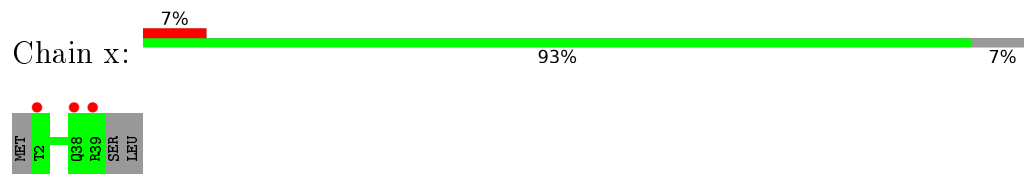
- Molecule 17: Photosystem II reaction center protein Ycf12



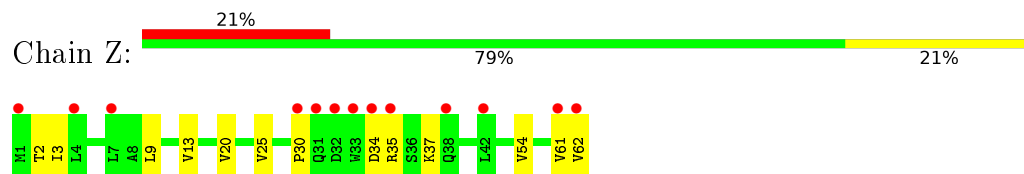
- Molecule 18: Photosystem II reaction center X protein



- Molecule 18: Photosystem II reaction center X protein

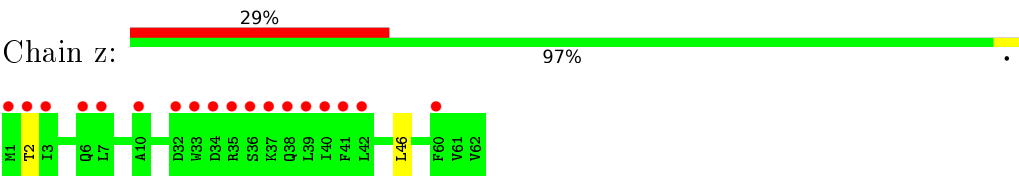


- Molecule 19: Photosystem II reaction center protein Z

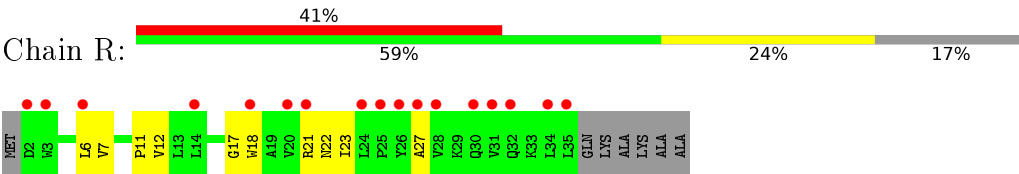


- Molecule 19: Photosystem II reaction center protein Z

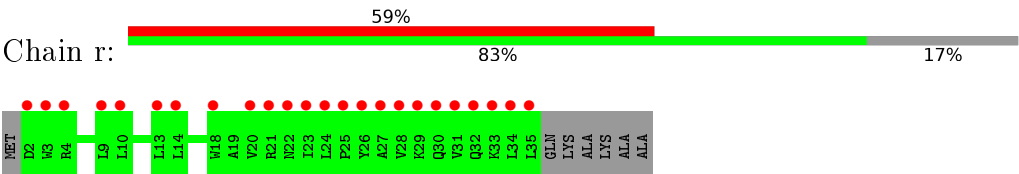




● Molecule 20: Photosystem II protein Y



● Molecule 20: Photosystem II protein Y



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.87Å 223.14Å 310.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.28 – 2.25 44.28 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.28-2.25) 90.6 (44.28-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_2481)	Depositor
R, $R_{free}$	0.193 , 0.231 0.202 , 0.241	Depositor DCC
$R_{free}$ test set	3426 reflections (0.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.5	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 62.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	51757	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, OEX, PHO, DGD, CL, CLA, PL9, FE2, SQD, BCT, HEM, FME, UNL, 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	0.25	0/2713	0.40	0/3700
1	a	0.25	0/2707	0.40	0/3692
2	B	0.25	0/4155	0.40	0/5661
2	b	0.25	0/4125	0.40	0/5621
3	C	0.25	0/3607	0.40	0/4911
3	c	0.25	0/3610	0.40	0/4914
4	D	0.26	0/2812	0.41	0/3832
4	d	0.25	0/2811	0.41	0/3830
5	E	0.23	0/689	0.37	0/940
5	e	0.30	1/693 (0.1%)	0.38	0/945
6	F	0.24	0/284	0.36	0/387
6	f	0.24	0/284	0.35	0/387
7	H	0.25	0/523	0.41	0/713
7	h	0.24	0/511	0.39	0/697
8	I	0.25	0/301	0.43	0/407
8	i	0.26	0/293	0.38	0/396
9	J	0.25	0/263	0.40	0/356
9	j	0.25	0/263	0.39	0/356
10	K	0.26	0/303	0.39	0/416
10	k	0.26	0/303	0.37	0/416
11	L	0.24	0/311	0.37	0/422
11	l	0.24	0/311	0.37	0/422
12	M	0.24	0/262	0.34	0/358
12	m	0.24	0/253	0.35	0/346
13	O	0.24	0/1925	0.46	0/2610
13	o	0.25	0/1925	0.47	0/2609
14	T	0.27	0/257	0.34	0/349
14	t	0.27	0/257	0.36	0/349
15	U	0.24	0/785	0.42	0/1064
15	u	0.24	0/785	0.42	0/1064
16	V	0.23	0/1085	0.41	0/1473
16	v	0.23	0/1094	0.40	0/1484

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	Y	0.24	0/201	0.39	0/268
17	y	0.24	0/225	0.37	0/301
18	X	0.24	0/284	0.37	0/384
18	x	0.24	0/291	0.38	0/392
19	Z	0.24	0/490	0.35	0/669
19	z	0.24	0/489	0.36	0/669
20	R	0.22	0/279	0.40	0/383
20	r	0.22	0/276	0.36	0/379
All	All	0.25	1/43035 (0.0%)	0.40	0/58572

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	63	ILE	C-N	5.06	1.43	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 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	A	2625	0	2524	32	0
1	a	2622	0	2519	0	0
2	B	4005	0	3865	54	0
2	b	3982	0	3842	0	0
3	C	3494	0	3417	45	0
3	c	3494	0	3420	0	0
4	D	2717	0	2621	38	0
4	d	2716	0	2621	0	0
5	E	670	0	655	17	0
5	e	671	0	657	0	0
6	F	275	0	282	0	0
6	f	275	0	282	0	0
7	H	510	0	532	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	h	498	0	518	0	0
8	I	304	0	322	3	0
8	i	296	0	311	0	0
9	J	257	0	268	2	0
9	j	257	0	268	0	0
10	K	293	0	305	5	0
10	k	293	0	305	0	0
11	L	304	0	316	6	0
11	l	304	0	316	0	0
12	M	269	0	280	1	0
12	m	260	0	275	0	0
13	O	1888	0	1865	24	0
13	o	1888	0	1865	0	0
14	T	258	0	261	7	0
14	t	258	0	261	0	0
15	U	774	0	773	9	0
15	u	774	0	773	0	0
16	V	1064	0	1073	7	0
16	v	1070	0	1086	0	0
17	Y	200	0	226	5	0
17	y	224	0	252	0	0
18	X	281	0	312	4	0
18	x	285	0	320	0	0
19	Z	479	0	516	9	0
19	z	478	0	516	0	0
20	R	273	0	305	6	0
20	r	270	0	296	0	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	2	0	0	0	0
23	a	2	0	0	0	0
24	A	4	0	1	0	0
24	a	4	0	1	0	0
25	A	249	0	264	17	0
25	B	1040	0	1152	65	0
25	C	845	0	936	57	0
25	D	130	0	144	9	0
25	a	260	0	288	0	0
25	b	1086	0	1187	0	0
25	c	839	0	919	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	d	130	0	144	0	0
26	A	64	0	74	4	0
26	D	64	0	74	0	0
26	a	128	0	148	0	0
27	A	40	0	56	2	0
27	B	120	0	168	12	0
27	C	80	0	112	8	0
27	D	40	0	56	4	0
27	H	40	0	56	4	0
27	K	40	0	56	2	0
27	T	40	0	56	5	0
27	Y	40	0	56	4	0
27	a	40	0	56	0	0
27	b	120	0	168	0	0
27	c	160	0	224	0	0
27	d	40	0	56	0	0
27	h	40	0	56	0	0
27	t	40	0	56	0	0
28	A	55	0	80	3	0
28	D	55	0	80	0	0
28	a	55	0	80	0	0
28	d	55	0	80	0	0
29	A	106	0	148	2	0
29	B	108	0	156	6	0
29	D	90	0	111	3	0
29	L	49	0	65	3	0
29	a	54	0	78	0	0
29	b	40	0	67	0	0
29	f	41	0	49	0	0
30	A	96	0	141	3	0
30	B	49	0	74	4	0
30	D	49	0	74	4	0
30	L	49	0	74	1	0
30	a	81	0	108	0	0
30	d	98	0	148	0	0
30	l	49	0	74	0	0
31	A	29	0	0	0	0
31	B	26	0	0	0	0
31	C	33	0	0	0	0
31	D	28	0	0	0	0
31	E	12	0	0	0	0
31	H	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	I	27	0	0	0	0
31	J	23	0	0	0	0
31	M	32	0	0	0	0
31	T	26	0	0	0	0
31	a	29	0	0	0	0
31	b	28	0	0	0	0
31	c	40	0	0	0	0
31	d	17	0	0	0	0
31	i	20	0	0	0	0
31	j	27	0	0	0	0
31	m	25	0	0	0	0
31	t	18	0	0	0	0
31	x	16	0	0	0	0
32	B	153	0	216	3	0
32	C	147	0	204	2	0
32	D	51	0	72	2	0
32	a	51	0	72	0	0
32	b	51	0	72	0	0
32	c	71	0	82	0	0
32	d	89	0	142	0	0
32	m	51	0	72	0	0
33	C	186	0	246	7	0
33	H	62	0	82	2	0
33	c	186	0	246	0	0
33	h	62	0	82	0	0
34	E	43	0	30	5	0
34	V	43	0	30	2	0
34	e	43	0	30	0	0
34	v	43	0	30	0	0
35	A	86	0	0	1	0
35	B	109	0	0	2	0
35	C	95	0	0	1	0
35	D	82	0	0	1	0
35	E	14	0	0	0	0
35	F	3	0	0	0	0
35	H	11	0	0	0	0
35	I	3	0	0	1	0
35	J	5	0	0	1	0
35	K	2	0	0	0	0
35	L	3	0	0	0	0
35	M	5	0	0	0	0
35	O	72	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	T	9	0	0	0	0
35	U	22	0	0	3	0
35	V	42	0	0	0	0
35	X	5	0	0	0	0
35	Z	3	0	0	0	0
35	a	90	0	0	0	0
35	b	129	0	0	0	0
35	c	95	0	0	0	0
35	d	87	0	0	0	0
35	e	9	0	0	0	0
35	f	2	0	0	0	0
35	h	13	0	0	0	0
35	i	6	0	0	0	0
35	j	2	0	0	0	0
35	k	4	0	0	0	0
35	l	10	0	0	0	0
35	m	10	0	0	0	0
35	o	69	0	0	0	0
35	r	1	0	0	0	0
35	t	4	0	0	0	0
35	u	34	0	0	0	0
35	v	37	0	0	0	0
35	x	4	0	0	0	0
35	y	1	0	0	0	0
35	z	1	0	0	0	0
All	All	51757	0	51380	383	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 4.

The worst 5 of 383 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:B:157:HIS:HE1	25:B:606:CLA:NA	1.78	0.81
2:B:359:MET:SD	35:B:703:HOH:O	32.98	0.75
3:C:165:LEU:HD21	25:C:507:CLA:HAB	1.67	0.74
5:E:17:VAL:H	9:J:7:ARG:HH21	2.15	0.74
15:U:55:TYR:OH	35:U:201:HOH:O	20.33	0.73

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	327 (98%)	5 (2%)	1 (0%)	46	52
1	a	332/344 (96%)	327 (98%)	5 (2%)	0	100	100
2	B	507/510 (99%)	498 (98%)	9 (2%)	0	100	100
2	b	504/510 (99%)	491 (97%)	13 (3%)	0	100	100
3	C	450/461 (98%)	439 (98%)	10 (2%)	1 (0%)	52	61
3	c	450/461 (98%)	440 (98%)	9 (2%)	1 (0%)	52	61
4	D	339/352 (96%)	329 (97%)	10 (3%)	0	100	100
4	d	339/352 (96%)	328 (97%)	11 (3%)	0	100	100
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	15	10
5	e	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	35/38 (92%)	32 (91%)	3 (9%)	0	100	100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	30 (94%)	1 (3%)	1 (3%)	5	2
12	m	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
13	O	244/272 (90%)	235 (96%)	8 (3%)	1 (0%)	39	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	244/272 (90%)	229 (94%)	11 (4%)	4 (2%)	12	7
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
15	u	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	V	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
16	v	136/163 (83%)	130 (96%)	5 (4%)	1 (1%)	26	26
17	Y	25/46 (54%)	25 (100%)	0	0	100	100
17	y	28/46 (61%)	27 (96%)	1 (4%)	0	100	100
18	X	36/41 (88%)	34 (94%)	1 (3%)	1 (3%)	6	3
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	11	6
20	R	32/41 (78%)	32 (100%)	0	0	100	100
20	r	32/41 (78%)	31 (97%)	1 (3%)	0	100	100
All	All	5258/5700 (92%)	5108 (97%)	137 (3%)	13 (0%)	52	61

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	o	53	LYS
13	o	58	ASN
3	C	416	SER
3	c	416	SER
13	o	59	LYS

### 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%)	270 (100%)	1 (0%)	93	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	270/280 (96%)	270 (100%)	0	100	100
2	B	407/407 (100%)	403 (99%)	4 (1%)	82	89
2	b	403/407 (99%)	402 (100%)	1 (0%)	95	98
3	C	353/362 (98%)	352 (100%)	1 (0%)	94	97
3	c	353/362 (98%)	349 (99%)	4 (1%)	80	88
4	D	276/283 (98%)	275 (100%)	1 (0%)	93	96
4	d	276/283 (98%)	275 (100%)	1 (0%)	93	96
5	E	73/73 (100%)	72 (99%)	1 (1%)	74	84
5	e	73/73 (100%)	72 (99%)	1 (1%)	74	84
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	54/55 (98%)	52 (96%)	2 (4%)	41	50
7	h	53/55 (96%)	52 (98%)	1 (2%)	65	75
8	I	33/34 (97%)	32 (97%)	1 (3%)	48	59
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	30/37 (81%)	29 (97%)	1 (3%)	45	56
10	k	30/37 (81%)	29 (97%)	1 (3%)	45	56
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	29/32 (91%)	29 (100%)	0	100	100
13	O	209/228 (92%)	207 (99%)	2 (1%)	82	89
13	o	209/228 (92%)	207 (99%)	2 (1%)	82	89
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	84/112 (75%)	84 (100%)	0	100	100
15	u	84/112 (75%)	84 (100%)	0	100	100
16	V	117/138 (85%)	117 (100%)	0	100	100
16	v	118/138 (86%)	118 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Y	20/37 (54%)	20 (100%)	0	100	100
17	y	23/37 (62%)	23 (100%)	0	100	100
18	X	31/34 (91%)	31 (100%)	0	100	100
18	x	31/34 (91%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	65	75
19	z	52/52 (100%)	51 (98%)	1 (2%)	65	75
20	R	29/33 (88%)	28 (97%)	1 (3%)	44	54
20	r	28/33 (85%)	28 (100%)	0	100	100
All	All	4359/4654 (94%)	4331 (99%)	28 (1%)	90	94

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	O	118	LEU
20	R	6	LEU
13	o	61	GLN
13	O	207	ARG
19	Z	35	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
19	Z	31	GLN
1	a	312	ASN
3	c	418	ASN
15	U	63	ASN
16	V	86	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
8	FME	I	1	8	8,9,10	0.87	0	5,9,11	0.82	0
12	FME	M	1	12	8,9,10	0.86	0	5,9,11	0.95	0
14	FME	T	1	14	8,9,10	0.84	0	5,9,11	0.84	0
8	FME	i	1	8	8,9,10	0.88	0	5,9,11	0.90	0
12	FME	m	1	12	8,9,10	0.87	0	5,9,11	0.82	0
14	FME	t	1	14	8,9,10	0.89	0	5,9,11	0.98	0

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
8	FME	I	1	8	-	0/6/9/11	0/0/0/0
12	FME	M	1	12	-	0/6/9/11	0/0/0/0
14	FME	T	1	14	-	0/6/9/11	0/0/0/0
8	FME	i	1	8	-	0/6/9/11	0/0/0/0
12	FME	m	1	12	-	0/6/9/11	0/0/0/0
14	FME	t	1	14	-	0/6/9/11	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 190 ligands modelled in this entry, 33 are unknown and 6 are monoatomic - leaving 151 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	OEX	A	601	1,3,35	0,15,15	0.00	-	0,32,32	0.00	-
24	BCT	A	605	22	0,3,3	0.00	-	0,3,3	0.00	-
25	CLA	A	606	-	57,73,73	1.13	4 (7%)	61,113,113	1.09	3 (4%)
25	CLA	A	607	35	57,73,73	1.14	5 (8%)	61,113,113	1.10	5 (8%)
26	PHO	A	608	-	67,69,69	1.24	9 (13%)	86,99,99	1.08	8 (9%)
25	CLA	A	609	-	46,62,73	1.26	5 (10%)	47,99,113	1.25	7 (14%)
27	BCR	A	610	-	41,41,41	1.10	2 (4%)	56,56,56	1.20	5 (8%)
28	PL9	A	611	-	54,55,55	0.84	2 (3%)	68,69,69	1.44	13 (19%)
29	SQD	A	612	-	51,52,54	0.96	5 (9%)	60,63,65	1.85	9 (15%)
25	CLA	A	613	35	57,73,73	1.13	4 (7%)	61,113,113	1.08	5 (8%)
30	LHG	A	614	-	46,46,48	0.62	1 (2%)	47,52,54	1.25	5 (10%)
29	SQD	A	616	-	53,54,54	0.95	5 (9%)	62,65,65	1.79	9 (14%)
30	LHG	A	618	-	48,48,48	0.63	1 (2%)	49,54,54	1.25	6 (12%)
25	CLA	B	601	35	57,73,73	1.14	5 (8%)	61,113,113	1.10	5 (8%)
25	CLA	B	602	-	57,73,73	1.12	4 (7%)	61,113,113	1.13	4 (6%)
25	CLA	B	603	-	57,73,73	1.13	4 (7%)	61,113,113	1.10	6 (9%)
25	CLA	B	604	-	57,73,73	1.15	4 (7%)	61,113,113	1.14	6 (9%)
25	CLA	B	605	-	57,73,73	1.12	4 (7%)	61,113,113	1.10	6 (9%)
25	CLA	B	606	-	57,73,73	1.15	5 (8%)	61,113,113	1.11	5 (8%)
25	CLA	B	607	35	57,73,73	1.11	4 (7%)	61,113,113	1.10	6 (9%)
25	CLA	B	608	-	57,73,73	1.13	4 (7%)	61,113,113	1.08	5 (8%)
25	CLA	B	609	-	57,73,73	1.14	4 (7%)	61,113,113	1.10	7 (11%)
25	CLA	B	610	35	57,73,73	1.13	4 (7%)	61,113,113	1.12	7 (11%)
25	CLA	B	611	-	57,73,73	1.14	4 (7%)	61,113,113	1.15	7 (11%)
25	CLA	B	612	-	57,73,73	1.12	4 (7%)	61,113,113	1.18	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	B	613	-	57,73,73	1.11	4 (7%)	61,113,113	1.20	6 (9%)
25	CLA	B	614	-	57,73,73	1.12	4 (7%)	61,113,113	1.12	7 (11%)
25	CLA	B	615	-	57,73,73	1.15	4 (7%)	61,113,113	1.11	7 (11%)
25	CLA	B	616	-	57,73,73	1.13	6 (10%)	61,113,113	1.17	6 (9%)
27	BCR	B	617	-	41,41,41	1.07	2 (4%)	56,56,56	1.18	4 (7%)
27	BCR	B	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	5 (8%)
27	BCR	B	619	-	41,41,41	1.07	2 (4%)	56,56,56	1.21	4 (7%)
32	LMG	B	620	-	51,51,55	0.71	0	59,59,63	1.34	6 (10%)
32	LMG	B	621	-	51,51,55	0.71	0	59,59,63	1.32	7 (11%)
30	LHG	B	623	-	48,48,48	0.61	0	49,54,54	1.27	6 (12%)
29	SQD	B	624	-	53,54,54	0.95	5 (9%)	62,65,65	1.90	10 (16%)
29	SQD	B	625	-	53,54,54	0.95	5 (9%)	62,65,65	1.78	9 (14%)
32	LMG	B	626	-	51,51,55	0.71	1 (1%)	59,59,63	1.29	4 (6%)
32	LMG	C	501	-	48,48,55	0.72	0	56,56,63	1.29	5 (8%)
25	CLA	C	502	-	57,73,73	1.14	5 (8%)	61,113,113	1.12	6 (9%)
25	CLA	C	503	-	57,73,73	1.13	4 (7%)	61,113,113	1.10	6 (9%)
25	CLA	C	504	-	57,73,73	1.14	4 (7%)	61,113,113	1.11	6 (9%)
25	CLA	C	505	35	57,73,73	1.14	5 (8%)	61,113,113	1.12	5 (8%)
25	CLA	C	506	-	57,73,73	1.12	4 (7%)	61,113,113	1.14	6 (9%)
25	CLA	C	507	-	57,73,73	1.14	5 (8%)	61,113,113	1.14	7 (11%)
25	CLA	C	508	35	57,73,73	1.12	4 (7%)	61,113,113	1.15	6 (9%)
25	CLA	C	509	-	57,73,73	1.13	5 (8%)	61,113,113	1.15	6 (9%)
25	CLA	C	510	-	57,73,73	1.12	4 (7%)	61,113,113	1.16	5 (8%)
25	CLA	C	511	-	57,73,73	1.13	4 (7%)	61,113,113	1.11	5 (8%)
25	CLA	C	512	3	57,73,73	1.14	5 (8%)	61,113,113	1.09	6 (9%)
25	CLA	C	513	-	57,73,73	1.14	4 (7%)	61,113,113	1.14	6 (9%)
25	CLA	C	514	-	57,73,73	1.13	5 (8%)	61,113,113	1.12	6 (9%)
27	BCR	C	515	-	41,41,41	1.10	2 (4%)	56,56,56	1.20	4 (7%)
27	BCR	C	516	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	6 (10%)
33	DGD	C	517	-	63,63,67	0.81	0	77,77,81	1.35	8 (10%)
33	DGD	C	518	-	63,63,67	0.86	1 (1%)	77,77,81	1.41	9 (11%)
33	DGD	C	519	-	63,63,67	0.85	1 (1%)	77,77,81	1.39	11 (14%)
32	LMG	C	520	-	48,48,55	0.74	0	56,56,63	1.33	7 (12%)
32	LMG	C	521	-	51,51,55	0.77	1 (1%)	59,59,63	1.34	6 (10%)
26	PHO	D	401	-	67,69,69	1.24	7 (10%)	86,99,99	1.07	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	D	402	-	57,73,73	1.14	5 (8%)	61,113,113	1.07	5 (8%)
25	CLA	D	403	-	57,73,73	1.11	5 (8%)	61,113,113	1.19	7 (11%)
27	BCR	D	404	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	4 (7%)
28	PL9	D	405	-	54,55,55	0.82	1 (1%)	68,69,69	1.45	12 (17%)
30	LHG	D	406	-	48,48,48	0.60	0	49,54,54	1.25	6 (12%)
32	LMG	D	407	-	51,51,55	0.71	0	59,59,63	1.31	6 (10%)
29	SQD	D	408	-	42,43,54	1.06	5 (11%)	51,54,65	2.03	9 (17%)
29	SQD	D	409	-	46,47,54	1.02	5 (10%)	55,58,65	1.95	10 (18%)
34	HEM	E	101	5,6	24,50,50	2.03	5 (20%)	16,82,82	1.43	3 (18%)
27	BCR	H	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.21	4 (7%)
33	DGD	H	102	-	63,63,67	0.87	1 (1%)	77,77,81	1.36	7 (9%)
27	BCR	K	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	5 (8%)
29	SQD	L	101	-	48,49,54	0.99	4 (8%)	57,60,65	1.92	10 (17%)
30	LHG	L	102	-	48,48,48	0.61	1 (2%)	49,54,54	1.24	6 (12%)
27	BCR	T	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	6 (10%)
34	HEM	V	201	16	24,50,50	1.94	4 (16%)	16,82,82	1.42	2 (12%)
27	BCR	Y	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.17	3 (5%)
21	OEX	a	601	1,3,35	0,15,15	0.00	-	0,32,32	0.00	-
24	BCT	a	605	22	0,3,3	0.00	-	0,3,3	0.00	-
25	CLA	a	606	-	57,73,73	1.14	5 (8%)	61,113,113	1.11	5 (8%)
25	CLA	a	607	35	57,73,73	1.14	5 (8%)	61,113,113	1.09	4 (6%)
26	PHO	a	608	-	67,69,69	1.23	7 (10%)	86,99,99	1.07	8 (9%)
26	PHO	a	609	-	67,69,69	1.24	7 (10%)	86,99,99	1.07	7 (8%)
25	CLA	a	610	-	57,73,73	1.12	4 (7%)	61,113,113	1.13	6 (9%)
27	BCR	a	611	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	5 (8%)
28	PL9	a	612	-	54,55,55	0.83	2 (3%)	68,69,69	1.44	12 (17%)
29	SQD	a	613	-	53,54,54	0.94	5 (9%)	62,65,65	1.79	8 (12%)
32	LMG	a	614	-	51,51,55	0.72	0	59,59,63	1.34	7 (11%)
25	CLA	a	615	35	57,73,73	1.14	4 (7%)	61,113,113	1.07	4 (6%)
30	LHG	a	616	-	38,38,48	0.68	1 (2%)	39,44,54	1.17	3 (7%)
30	LHG	a	617	-	41,41,48	0.66	0	42,47,54	1.33	6 (14%)
25	CLA	b	601	35	57,73,73	1.15	5 (8%)	61,113,113	1.10	5 (8%)
25	CLA	b	602	-	57,73,73	1.13	4 (7%)	61,113,113	1.15	5 (8%)
25	CLA	b	603	-	57,73,73	1.12	4 (7%)	61,113,113	1.13	6 (9%)
25	CLA	b	604	-	57,73,73	1.13	4 (7%)	61,113,113	1.16	6 (9%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	b	605	-	57,73,73	1.14	5 (8%)	61,113,113	1.10	5 (8%)
25	CLA	b	606[A]	-	57,73,73	1.14	4 (7%)	61,113,113	1.10	6 (9%)
25	CLA	b	606[B]	-	57,73,73	1.14	4 (7%)	61,113,113	1.09	6 (9%)
25	CLA	b	607	35	57,73,73	1.12	4 (7%)	61,113,113	1.10	5 (8%)
25	CLA	b	608	-	57,73,73	1.13	5 (8%)	61,113,113	1.12	6 (9%)
25	CLA	b	609	-	57,73,73	1.14	4 (7%)	61,113,113	1.11	6 (9%)
25	CLA	b	610	35	57,73,73	1.14	4 (7%)	61,113,113	1.10	6 (9%)
25	CLA	b	611	-	57,73,73	1.12	4 (7%)	61,113,113	1.14	5 (8%)
25	CLA	b	612	-	57,73,73	1.13	4 (7%)	61,113,113	1.16	6 (9%)
25	CLA	b	613	-	57,73,73	1.12	4 (7%)	61,113,113	1.17	7 (11%)
25	CLA	b	614	-	57,73,73	1.13	4 (7%)	61,113,113	1.13	5 (8%)
25	CLA	b	615	-	57,73,73	1.16	4 (7%)	61,113,113	1.09	5 (8%)
25	CLA	b	616	-	39,55,73	1.36	6 (15%)	42,91,113	1.31	5 (11%)
27	BCR	b	617	-	41,41,41	1.11	2 (4%)	56,56,56	1.23	5 (8%)
27	BCR	b	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.24	5 (8%)
27	BCR	b	619	-	41,41,41	1.08	2 (4%)	56,56,56	1.19	3 (5%)
32	LMG	b	620	-	51,51,55	0.71	0	59,59,63	1.35	7 (11%)
29	SQD	b	621	-	39,39,54	0.86	2 (5%)	41,41,65	1.15	2 (4%)
25	CLA	c	501	-	57,73,73	1.13	4 (7%)	61,113,113	1.14	5 (8%)
25	CLA	c	502	-	57,73,73	1.14	5 (8%)	61,113,113	1.11	6 (9%)
25	CLA	c	503	-	57,73,73	1.14	4 (7%)	61,113,113	1.12	5 (8%)
25	CLA	c	504	35	52,68,73	1.19	4 (7%)	55,107,113	1.15	6 (10%)
25	CLA	c	505	-	57,73,73	1.12	4 (7%)	61,113,113	1.13	5 (8%)
25	CLA	c	506	-	57,73,73	1.14	4 (7%)	61,113,113	1.09	6 (9%)
25	CLA	c	507	35	57,73,73	1.14	4 (7%)	61,113,113	1.15	7 (11%)
25	CLA	c	508	-	56,72,73	1.14	5 (8%)	59,111,113	1.17	6 (10%)
25	CLA	c	509	-	57,73,73	1.13	4 (7%)	61,113,113	1.15	7 (11%)
25	CLA	c	510	-	57,73,73	1.14	5 (8%)	61,113,113	1.14	5 (8%)
25	CLA	c	511	3	57,73,73	1.13	4 (7%)	61,113,113	1.10	6 (9%)
25	CLA	c	512	-	57,73,73	1.15	5 (8%)	61,113,113	1.13	6 (9%)
25	CLA	c	513	-	57,73,73	1.13	5 (8%)	61,113,113	1.12	5 (8%)
27	BCR	c	514	-	41,41,41	1.10	2 (4%)	56,56,56	1.23	5 (8%)
27	BCR	c	515	-	41,41,41	1.11	2 (4%)	56,56,56	1.19	4 (7%)
33	DGD	c	516	-	63,63,67	0.82	1 (1%)	77,77,81	1.42	9 (11%)
33	DGD	c	517	-	63,63,67	0.88	1 (1%)	77,77,81	1.38	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	DGD	c	518	-	63,63,67	0.83	0	77,77,81	1.37	9 (11%)
32	LMG	c	519	-	37,37,55	0.84	0	45,45,63	1.35	7 (15%)
32	LMG	c	520	-	34,34,55	0.85	0	42,42,63	1.24	4 (9%)
27	BCR	c	521	-	41,41,41	1.12	3 (7%)	56,56,56	1.17	3 (5%)
27	BCR	c	522	-	41,41,41	1.11	2 (4%)	56,56,56	1.20	4 (7%)
25	CLA	d	401	-	57,73,73	1.14	4 (7%)	61,113,113	1.07	7 (11%)
25	CLA	d	402	-	57,73,73	1.14	5 (8%)	61,113,113	1.08	5 (8%)
27	BCR	d	403	-	41,41,41	1.11	2 (4%)	56,56,56	1.19	5 (8%)
28	PL9	d	404	-	54,55,55	0.86	3 (5%)	68,69,69	1.42	15 (22%)
30	LHG	d	405	-	48,48,48	0.60	0	49,54,54	1.28	6 (12%)
30	LHG	d	406	-	48,48,48	0.60	0	49,54,54	1.24	6 (12%)
32	LMG	d	407	-	51,51,55	0.72	0	59,59,63	1.34	7 (11%)
32	LMG	d	408	-	33,36,55	0.13	0	32,35,63	1.38	3 (9%)
34	HEM	e	101	5,6	24,50,50	2.12	4 (16%)	16,82,82	1.43	2 (12%)
29	SQD	f	101	-	40,41,54	1.08	5 (12%)	49,52,65	1.90	9 (18%)
27	BCR	h	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	6 (10%)
33	DGD	h	102	-	63,63,67	0.86	0	77,77,81	1.36	9 (11%)
30	LHG	l	101	-	48,48,48	0.61	0	49,54,54	1.24	6 (12%)
32	LMG	m	102	-	51,51,55	0.71	0	59,59,63	1.37	7 (11%)
27	BCR	t	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.24	6 (10%)
34	HEM	v	201	16	24,50,50	1.93	5 (20%)	16,82,82	1.37	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	OEX	A	601	1,3,35	-	0/0/68/68	0/0/6/6
24	BCT	A	605	22	-	0/0/0/0	0/0/0/0
25	CLA	A	606	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	A	607	35	3/3/20/25	0/37/135/135	0/0/9/9
26	PHO	A	608	-	-	0/53/103/103	0/1/6/6
25	CLA	A	609	-	3/3/17/25	0/24/122/135	0/0/9/9
27	BCR	A	610	-	-	0/29/63/63	0/2/2/2
28	PL9	A	611	-	-	0/53/73/73	0/1/1/1
29	SQD	A	612	-	-	0/47/67/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	613	35	3/3/20/25	0/37/135/135	0/0/9/9
30	LHG	A	614	-	-	0/51/51/53	0/0/0/0
29	SQD	A	616	-	-	0/49/69/69	0/1/1/1
30	LHG	A	618	-	-	0/53/53/53	0/0/0/0
25	CLA	B	601	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	602	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	607	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	609	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	610	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	B	617	-	-	0/29/63/63	0/2/2/2
27	BCR	B	618	-	-	0/29/63/63	0/2/2/2
27	BCR	B	619	-	-	0/29/63/63	0/2/2/2
32	LMG	B	620	-	-	0/46/66/70	0/1/1/1
32	LMG	B	621	-	-	0/46/66/70	0/1/1/1
30	LHG	B	623	-	-	0/53/53/53	0/0/0/0
29	SQD	B	624	-	-	0/49/69/69	0/1/1/1
29	SQD	B	625	-	-	0/49/69/69	0/1/1/1
32	LMG	B	626	-	-	0/46/66/70	0/1/1/1
32	LMG	C	501	-	-	0/43/63/70	0/1/1/1
25	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	505	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	508	35	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	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	511	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	512	3	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	513	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	514	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	C	515	-	-	0/29/63/63	0/2/2/2
27	BCR	C	516	-	-	0/29/63/63	0/2/2/2
33	DGD	C	517	-	-	0/51/91/95	0/2/2/2
33	DGD	C	518	-	-	0/51/91/95	0/2/2/2
33	DGD	C	519	-	-	0/51/91/95	0/2/2/2
32	LMG	C	520	-	-	0/43/63/70	0/1/1/1
32	LMG	C	521	-	-	1/46/66/70	0/1/1/1
26	PHO	D	401	-	-	0/53/103/103	0/1/6/6
25	CLA	D	402	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	D	403	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	D	404	-	-	0/29/63/63	0/2/2/2
28	PL9	D	405	-	-	0/53/73/73	0/1/1/1
30	LHG	D	406	-	-	0/53/53/53	0/0/0/0
32	LMG	D	407	-	-	0/46/66/70	0/1/1/1
29	SQD	D	408	-	-	0/38/58/69	0/1/1/1
29	SQD	D	409	-	-	0/42/62/69	0/1/1/1
34	HEM	E	101	5,6	-	0/6/54/54	0/0/8/8
27	BCR	H	101	-	-	0/29/63/63	0/2/2/2
33	DGD	H	102	-	-	0/51/91/95	0/2/2/2
27	BCR	K	101	-	-	0/29/63/63	0/2/2/2
29	SQD	L	101	-	-	0/44/64/69	0/1/1/1
30	LHG	L	102	-	-	0/53/53/53	0/0/0/0
27	BCR	T	101	-	-	0/29/63/63	0/2/2/2
34	HEM	V	201	16	-	0/6/54/54	0/0/8/8
27	BCR	Y	101	-	-	0/29/63/63	0/2/2/2
21	OEX	a	601	1,3,35	-	0/0/68/68	0/0/6/6
24	BCT	a	605	22	-	0/0/0/0	0/0/0/0
25	CLA	a	606	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	a	607	35	3/3/20/25	0/37/135/135	0/0/9/9
26	PHO	a	608	-	-	0/53/103/103	0/1/6/6
26	PHO	a	609	-	-	0/53/103/103	0/1/6/6
25	CLA	a	610	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	a	611	-	-	0/29/63/63	0/2/2/2
28	PL9	a	612	-	-	0/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	a	613	-	-	0/49/69/69	0/1/1/1
32	LMG	a	614	-	-	0/46/66/70	0/1/1/1
25	CLA	a	615	35	3/3/20/25	0/37/135/135	0/0/9/9
30	LHG	a	616	-	-	0/43/43/53	0/0/0/0
30	LHG	a	617	-	-	0/46/46/53	0/0/0/0
25	CLA	b	601	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	602	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	603	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	604	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	606[A]	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	606[B]	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	607	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	609	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	610	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	612	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	616	-	3/3/16/25	0/16/114/135	0/0/9/9
27	BCR	b	617	-	-	0/29/63/63	0/2/2/2
27	BCR	b	618	-	-	0/29/63/63	0/2/2/2
27	BCR	b	619	-	-	0/29/63/63	0/2/2/2
32	LMG	b	620	-	-	0/46/66/70	0/1/1/1
29	SQD	b	621	-	-	0/41/41/69	0/0/0/1
25	CLA	c	501	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	502	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	504	35	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	c	505	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	506	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	507	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	508	-	3/3/19/25	0/36/134/135	0/0/9/9
25	CLA	c	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	c	510	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	511	3	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	512	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	513	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	c	514	-	-	0/29/63/63	0/2/2/2
27	BCR	c	515	-	-	0/29/63/63	0/2/2/2
33	DGD	c	516	-	-	0/51/91/95	0/2/2/2
33	DGD	c	517	-	-	0/51/91/95	0/2/2/2
33	DGD	c	518	-	-	0/51/91/95	0/2/2/2
32	LMG	c	519	-	-	0/31/51/70	0/1/1/1
32	LMG	c	520	-	-	0/29/49/70	0/1/1/1
27	BCR	c	521	-	-	0/29/63/63	0/2/2/2
27	BCR	c	522	-	-	0/29/63/63	0/2/2/2
25	CLA	d	401	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	d	402	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	d	403	-	-	0/29/63/63	0/2/2/2
28	PL9	d	404	-	-	0/53/73/73	0/1/1/1
30	LHG	d	405	-	-	0/53/53/53	0/0/0/0
30	LHG	d	406	-	-	0/53/53/53	0/0/0/0
32	LMG	d	407	-	-	0/46/66/70	0/1/1/1
32	LMG	d	408	-	-	0/30/32/70	0/0/0/1
34	HEM	e	101	5,6	-	0/6/54/54	0/0/8/8
29	SQD	f	101	-	-	0/36/56/69	0/1/1/1
27	BCR	h	101	-	-	0/29/63/63	0/2/2/2
33	DGD	h	102	-	-	0/51/91/95	0/2/2/2
30	LHG	l	101	-	-	0/53/53/53	0/0/0/0
32	LMG	m	102	-	-	0/46/66/70	0/1/1/1
27	BCR	t	101	-	-	0/29/63/63	0/2/2/2
34	HEM	v	201	16	-	0/6/54/54	0/0/8/8

The worst 5 of 469 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	e	101	HEM	C3B-C2B	-5.17	1.33	1.40
34	e	101	HEM	C3C-C2C	-5.05	1.33	1.40
34	E	101	HEM	C3C-C2C	-5.04	1.34	1.40
34	E	101	HEM	C3B-C2B	-4.09	1.35	1.40
34	v	201	HEM	C3B-C2B	-4.01	1.35	1.40

The worst 5 of 893 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	516	DGD	O3G-C3G-C2G	-4.62	100.00	110.99
33	C	518	DGD	O3G-C3G-C2G	-4.56	100.15	110.99
29	D	408	SQD	O9-S-O7	-4.54	101.13	113.96
29	B	625	SQD	O9-S-O7	-4.54	101.15	113.96
29	L	101	SQD	O9-S-O7	-4.53	101.16	113.96

5 of 213 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	C	508	CLA	NC
25	C	508	CLA	ND
25	C	508	CLA	NA
25	b	613	CLA	NC
25	b	613	CLA	ND

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	C	521	LMG	C7-O1-C1-O6

There are no ring outliers.

70 monomers are involved in 216 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	606	CLA	7	0
25	A	607	CLA	9	0
26	A	608	PHO	4	0
25	A	609	CLA	1	0
27	A	610	BCR	2	0
28	A	611	PL9	3	0
25	A	613	CLA	1	0
29	A	616	SQD	2	0
30	A	618	LHG	3	0
25	B	601	CLA	7	0
25	B	602	CLA	5	0
25	B	603	CLA	4	0
25	B	604	CLA	6	0
25	B	605	CLA	6	0
25	B	606	CLA	3	0
25	B	607	CLA	2	0
25	B	608	CLA	4	0
25	B	609	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	610	CLA	4	0
25	B	611	CLA	4	0
25	B	612	CLA	2	0
25	B	613	CLA	3	0
25	B	614	CLA	8	0
25	B	615	CLA	8	0
25	B	616	CLA	1	0
27	B	617	BCR	4	0
27	B	618	BCR	4	0
27	B	619	BCR	4	0
32	B	620	LMG	1	0
32	B	621	LMG	1	0
30	B	623	LHG	4	0
29	B	624	SQD	4	0
29	B	625	SQD	2	0
32	B	626	LMG	1	0
32	C	501	LMG	1	0
25	C	502	CLA	4	0
25	C	503	CLA	3	0
25	C	504	CLA	6	0
25	C	505	CLA	6	0
25	C	506	CLA	5	0
25	C	507	CLA	4	0
25	C	508	CLA	7	0
25	C	509	CLA	8	0
25	C	510	CLA	5	0
25	C	511	CLA	7	0
25	C	512	CLA	4	0
25	C	513	CLA	5	0
25	C	514	CLA	3	0
27	C	515	BCR	6	0
27	C	516	BCR	2	0
33	C	517	DGD	3	0
33	C	518	DGD	3	0
33	C	519	DGD	1	0
32	C	521	LMG	1	0
25	D	402	CLA	6	0
25	D	403	CLA	3	0
27	D	404	BCR	4	0
30	D	406	LHG	4	0
32	D	407	LMG	2	0
29	D	408	SQD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	D	409	SQD	1	0
34	E	101	HEM	5	0
27	H	101	BCR	4	0
33	H	102	DGD	2	0
27	K	101	BCR	2	0
29	L	101	SQD	3	0
30	L	102	LHG	1	0
27	T	101	BCR	5	0
34	V	201	HEM	2	0
27	Y	101	BCR	4	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	334/344 (97%)	-0.36	3 (0%) 85 87	28, 34, 52, 81	0
1	a	334/344 (97%)	-0.21	4 (1%) 81 83	28, 36, 63, 83	0
2	B	504/510 (98%)	-0.31	15 (2%) 54 58	28, 38, 65, 97	0
2	b	504/510 (98%)	-0.10	25 (4%) 32 36	29, 41, 76, 102	0
3	C	451/461 (97%)	-0.20	9 (1%) 68 72	30, 41, 61, 101	0
3	c	451/461 (97%)	-0.15	7 (1%) 74 77	31, 44, 65, 97	0
4	D	341/352 (96%)	-0.35	3 (0%) 85 87	28, 35, 52, 92	0
4	d	341/352 (96%)	-0.18	6 (1%) 71 75	28, 39, 61, 98	0
5	E	81/84 (96%)	0.12	6 (7%) 17 18	37, 55, 75, 97	0
5	e	82/84 (97%)	0.54	6 (7%) 18 19	42, 61, 83, 99	0
6	F	34/45 (75%)	-0.45	1 (2%) 55 60	41, 48, 70, 82	0
6	f	34/45 (75%)	-0.08	3 (8%) 12 14	44, 55, 83, 91	0
7	H	65/66 (98%)	-0.32	1 (1%) 76 79	36, 44, 61, 93	0
7	h	63/66 (95%)	0.14	4 (6%) 23 25	42, 51, 66, 70	0
8	I	36/38 (94%)	0.38	4 (11%) 7 7	36, 44, 78, 90	0
8	i	35/38 (92%)	-0.23	1 (2%) 55 60	36, 45, 72, 94	0
9	J	36/40 (90%)	-0.18	3 (8%) 14 15	39, 54, 81, 88	0
9	j	36/40 (90%)	0.14	3 (8%) 14 15	41, 57, 87, 96	0
10	K	37/46 (80%)	-0.02	1 (2%) 58 62	47, 56, 76, 83	0
10	k	37/46 (80%)	-0.22	0 100 100	52, 58, 74, 89	0
11	L	37/37 (100%)	-0.15	0 100 100	31, 34, 67, 72	0
11	l	37/37 (100%)	-0.18	4 (10%) 8 7	30, 37, 80, 104	0
12	M	32/36 (88%)	-0.37	1 (3%) 52 57	34, 39, 69, 93	0
12	m	32/36 (88%)	-0.46	1 (3%) 52 57	34, 40, 60, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	244/272 (89%)	-0.13	14 (5%) 27 30	28, 46, 84, 131	0
13	o	244/272 (89%)	-0.06	11 (4%) 37 41	30, 46, 85, 133	0
14	T	29/32 (90%)	0.30	2 (6%) 20 22	33, 37, 58, 84	0
14	t	29/32 (90%)	-0.13	1 (3%) 49 53	32, 37, 71, 88	0
15	U	97/134 (72%)	0.11	3 (3%) 52 57	36, 47, 74, 103	0
15	u	97/134 (72%)	-0.24	2 (2%) 67 71	34, 44, 62, 102	0
16	V	137/163 (84%)	-0.43	0 100 100	35, 44, 60, 85	0
16	v	137/163 (84%)	0.08	4 (2%) 55 60	37, 50, 71, 92	0
17	Y	27/46 (58%)	1.63	10 (37%) 0 0	57, 75, 102, 112	0
17	y	30/46 (65%)	0.42	5 (16%) 2 2	59, 74, 88, 97	0
18	X	38/41 (92%)	0.00	2 (5%) 30 33	43, 51, 76, 83	0
18	x	38/41 (92%)	0.51	3 (7%) 15 17	48, 60, 81, 100	0
19	Z	62/62 (100%)	1.15	13 (20%) 1 1	57, 72, 113, 123	0
19	z	62/62 (100%)	1.48	18 (29%) 1 0	59, 74, 111, 124	0
20	R	34/41 (82%)	1.79	17 (50%) 0 0	64, 76, 94, 102	0
20	r	34/41 (82%)	3.50	24 (70%) 0 0	75, 91, 109, 110	0
All	All	5313/5700 (93%)	-0.08	240 (4%) 37 41	28, 42, 78, 133	0

The worst 5 of 240 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Z	30	PRO	11.3
8	I	37	LEU	10.6
13	o	61	GLN	9.5
2	b	127	ARG	8.6
20	r	35	LEU	8.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
8	FME	I	1	10/11	0.96	0.17	-	45,49,54,55	0
8	FME	i	1	10/11	0.93	0.18	-	45,53,58,58	0
14	FME	T	1	10/11	0.95	0.10	-	32,40,59,74	0
12	FME	m	1	10/11	0.96	0.14	-	39,51,70,77	0
14	FME	t	1	10/11	0.96	0.10	-	31,38,58,64	0
12	FME	M	1	10/11	0.94	0.15	-	41,53,62,63	0

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
32	LMG	B	626	51/55	0.61	0.31	6.97	55,76,89,91	0
31	UNL	c	525	12/-	0.79	0.25	6.66	50,62,73,73	0
31	UNL	a	619	12/-	0.78	0.26	5.78	60,65,71,76	0
32	LMG	C	521	51/55	0.82	0.27	5.74	45,65,116,118	0
31	UNL	A	617	20/-	0.65	0.23	5.63	58,66,76,77	0
32	LMG	c	520	34/55	0.87	0.26	4.35	58,66,78,88	0
32	LMG	b	620	51/55	0.83	0.27	4.12	55,72,98,110	0
31	UNL	D	410	18/-	0.66	0.20	4.04	41,53,74,74	0
28	PL9	A	611	55/55	0.80	0.27	3.75	42,60,82,88	55
32	LMG	d	408	38/55	0.69	0.27	3.74	58,68,101,106	0
28	PL9	a	612	55/55	0.77	0.28	3.69	51,67,89,96	0
31	UNL	B	627	15/-	0.86	0.18	3.51	48,55,65,68	0
31	UNL	j	801	15/-	0.88	0.18	3.46	50,60,77,77	0
29	SQD	B	625	54/54	0.74	0.26	3.46	52,72,92,105	0
30	LHG	A	618	49/49	0.80	0.27	3.44	56,90,112,115	0
31	UNL	C	522	17/-	0.82	0.21	3.14	42,56,67,75	0
29	SQD	D	409	47/54	0.74	0.21	3.13	41,59,109,125	0
32	LMG	B	621	51/55	0.88	0.23	3.05	54,71,102,110	0
31	UNL	M	102	17/-	0.81	0.21	2.93	52,61,73,74	0
30	LHG	a	617	42/49	0.83	0.30	2.66	67,88,102,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
25	CLA	C	514	65/65	0.91	0.23	2.55	49,60,136,139	0
31	UNL	m	103	16/-	0.85	0.16	2.55	39,51,73,76	0
31	UNL	M	101	15/-	0.88	0.15	2.37	42,52,63,75	0
31	UNL	d	409	17/-	0.87	0.28	2.35	51,58,67,70	0
31	UNL	t	102	18/-	0.87	0.17	2.31	43,56,65,66	0
30	LHG	d	406	49/49	0.95	0.17	2.28	31,44,55,64	0
31	UNL	A	615	9/-	0.91	0.17	2.20	41,52,68,70	0
25	CLA	B	616	65/65	0.94	0.15	2.00	29,39,96,102	0
32	LMG	C	501	48/55	0.79	0.20	1.99	46,61,76,89	0
25	CLA	D	403	65/65	0.91	0.19	1.96	31,37,89,99	0
29	SQD	b	621	40/54	0.75	0.20	1.91	48,58,68,70	0
32	LMG	D	407	51/55	0.94	0.14	1.90	32,52,72,82	0
29	SQD	B	624	54/54	0.81	0.20	1.88	43,62,96,106	0
31	UNL	c	524	20/-	0.81	0.18	1.83	45,67,82,83	0
32	LMG	c	519	37/55	0.88	0.15	1.75	48,67,76,77	0
31	UNL	T	102	14/-	0.90	0.16	1.73	36,53,63,67	0
31	UNL	x	101	16/-	0.79	0.22	1.73	41,51,65,68	0
31	UNL	J	102	12/-	0.63	0.39	1.63	61,79,84,86	0
25	CLA	A	607	65/65	0.94	0.16	1.56	25,35,123,129	0
29	SQD	A	616	54/54	0.80	0.21	1.54	50,70,96,103	0
27	BCR	d	403	40/40	0.88	0.15	1.49	41,54,79,82	0
25	CLA	c	506	65/65	0.91	0.15	1.48	33,48,82,95	0
31	UNL	T	103	12/-	0.86	0.14	1.45	42,54,59,61	0
32	LMG	a	614	51/55	0.84	0.19	1.45	41,60,74,80	0
32	LMG	B	620	51/55	0.84	0.18	1.35	32,57,73,77	0
25	CLA	B	601	65/65	0.91	0.15	1.32	39,54,81,87	0
30	LHG	D	406	49/49	0.94	0.18	1.31	32,40,56,74	0
33	DGD	c	516	62/66	0.95	0.17	1.29	28,44,67,72	0
25	CLA	B	606	65/65	0.92	0.13	1.22	28,37,63,74	0
25	CLA	a	610	65/65	0.91	0.15	1.21	24,32,77,81	0
25	CLA	b	601	65/65	0.87	0.21	1.20	40,61,83,94	0
27	BCR	B	618	40/40	0.94	0.16	1.18	30,44,55,60	0
27	BCR	D	404	40/40	0.90	0.16	1.15	31,44,82,86	0
24	BCT	a	605	4/4	0.95	0.14	1.13	37,45,46,53	2
30	LHG	B	623	49/49	0.94	0.17	1.10	36,47,63,70	0
33	DGD	C	518	62/66	0.93	0.15	1.09	40,50,89,97	0
25	CLA	b	605	65/65	0.95	0.14	1.08	25,37,46,52	0
27	BCR	B	617	40/40	0.94	0.13	1.08	29,45,53,57	0
31	UNL	b	623	11/-	0.84	0.18	1.08	59,66,68,71	0
27	BCR	T	101	40/40	0.91	0.17	1.06	35,46,57,68	0
30	LHG	L	102	49/49	0.95	0.15	0.99	35,42,50,58	0
31	UNL	H	103	7/-	0.89	0.15	0.97	48,53,60,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
25	CLA	B	613	65/65	0.95	0.20	0.97	26,33,63,76	0
33	DGD	c	517	62/66	0.93	0.13	0.96	39,52,81,86	0
29	SQD	D	408	43/54	0.91	0.22	0.96	54,76,105,108	0
25	CLA	b	606[B]	65/65	0.93	0.15	0.91	37,43,52,58	64
25	CLA	b	606[A]	65/65	0.93	0.15	0.90	37,43,52,55	64
25	CLA	C	510	65/65	0.94	0.17	0.88	32,42,66,70	0
25	CLA	C	508	65/65	0.89	0.18	0.88	30,42,59,78	0
25	CLA	B	607	65/65	0.94	0.16	0.87	27,36,63,71	0
33	DGD	h	102	62/66	0.88	0.21	0.87	38,51,60,64	0
31	UNL	a	618	17/-	0.80	0.16	0.86	46,57,71,72	0
32	LMG	d	407	51/55	0.94	0.15	0.86	38,58,88,93	0
25	CLA	B	603	65/65	0.96	0.15	0.85	25,36,56,63	0
25	CLA	d	402	65/65	0.89	0.17	0.84	36,43,83,90	0
25	CLA	C	502	65/65	0.94	0.17	0.84	31,37,50,59	0
28	PL9	d	404	55/55	0.94	0.14	0.82	27,39,50,54	0
25	CLA	B	605	65/65	0.96	0.14	0.80	26,33,48,53	0
27	BCR	C	516	40/40	0.93	0.14	0.80	34,44,55,57	0
33	DGD	C	517	62/66	0.95	0.16	0.80	29,42,72,81	0
26	PHO	D	401	64/64	0.96	0.14	0.77	23,33,38,44	0
25	CLA	C	505	65/65	0.95	0.17	0.76	34,42,80,85	0
32	LMG	m	102	51/55	0.89	0.16	0.75	43,56,69,77	0
25	CLA	B	614	65/65	0.94	0.13	0.73	25,37,75,81	0
27	BCR	t	101	40/40	0.94	0.15	0.73	33,43,53,62	0
25	CLA	C	504	65/65	0.91	0.17	0.73	36,44,50,59	0
27	BCR	b	618	40/40	0.91	0.17	0.71	33,44,56,59	0
25	CLA	C	503	65/65	0.93	0.18	0.71	28,39,53,65	0
27	BCR	b	617	40/40	0.91	0.14	0.67	33,44,52,52	0
29	SQD	L	101	49/54	0.84	0.18	0.61	41,66,96,109	0
30	LHG	A	614	47/49	0.95	0.13	0.61	33,44,73,76	0
26	PHO	a	608	64/64	0.94	0.14	0.61	28,34,42,49	0
25	CLA	B	612	65/65	0.95	0.15	0.59	25,33,42,45	0
25	CLA	b	602	65/65	0.92	0.17	0.59	33,41,59,66	0
25	CLA	b	610	65/65	0.94	0.15	0.58	31,40,51,66	0
25	CLA	C	513	65/65	0.89	0.17	0.56	41,54,81,86	0
25	CLA	c	502	65/65	0.93	0.18	0.55	31,41,55,63	0
25	CLA	c	501	65/65	0.94	0.15	0.54	29,38,53,56	0
27	BCR	c	515	40/40	0.94	0.13	0.54	30,46,51,63	0
28	PL9	D	405	55/55	0.95	0.14	0.54	25,35,47,49	0
25	CLA	c	509	65/65	0.93	0.15	0.52	37,45,61,64	0
25	CLA	a	615	65/65	0.95	0.13	0.51	24,34,52,62	0
30	LHG	d	405	49/49	0.93	0.15	0.50	43,53,68,72	0
25	CLA	b	608	65/65	0.95	0.22	0.50	32,41,56,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	DGD	H	102	62/66	0.91	0.17	0.50	39,47,63,65	0
25	CLA	B	611	65/65	0.94	0.15	0.49	25,34,48,52	0
25	CLA	b	609	65/65	0.91	0.14	0.49	35,46,60,66	0
30	LHG	l	101	49/49	0.94	0.12	0.48	37,49,62,76	0
33	DGD	C	519	62/66	0.94	0.12	0.48	33,50,79,84	0
25	CLA	c	512	65/65	0.89	0.15	0.47	45,57,89,94	0
29	SQD	A	612	52/54	0.92	0.16	0.46	48,63,85,91	0
25	CLA	A	609	54/65	0.96	0.12	0.44	25,32,72,78	0
30	LHG	a	616	39/49	0.94	0.13	0.42	39,48,66,71	0
29	SQD	a	613	54/54	0.89	0.14	0.40	40,62,72,76	0
25	CLA	b	603	65/65	0.96	0.16	0.38	29,38,57,62	0
25	CLA	b	613	65/65	0.95	0.18	0.38	29,38,74,89	0
25	CLA	B	610	65/65	0.95	0.13	0.37	26,37,47,55	0
26	PHO	a	609	64/64	0.94	0.17	0.34	34,40,49,52	0
25	CLA	c	513	65/65	0.90	0.18	0.33	48,63,86,90	0
25	CLA	C	511	65/65	0.95	0.18	0.32	30,43,58,70	0
25	CLA	B	608	65/65	0.95	0.18	0.32	30,38,57,60	0
25	CLA	a	607	65/65	0.95	0.13	0.31	28,43,84,90	0
25	CLA	A	606	65/65	0.93	0.12	0.27	23,32,50,59	0
25	CLA	b	612	65/65	0.95	0.14	0.26	26,38,49,56	0
25	CLA	B	609	65/65	0.91	0.12	0.26	28,39,58,69	0
27	BCR	h	101	40/40	0.83	0.17	0.26	40,48,64,68	0
27	BCR	K	101	40/40	0.93	0.14	0.24	37,52,63,66	0
25	CLA	b	607	65/65	0.95	0.12	0.24	29,37,62,68	0
27	BCR	c	522	40/40	0.91	0.14	0.24	42,54,63,69	0
33	DGD	c	518	62/66	0.94	0.12	0.23	34,48,73,77	0
26	PHO	A	608	64/64	0.95	0.15	0.22	29,37,43,46	0
34	HEM	v	201	43/43	0.97	0.11	0.22	31,40,47,54	0
25	CLA	B	615	65/65	0.95	0.11	0.14	28,40,58,66	0
25	CLA	C	506	65/65	0.94	0.12	0.14	27,40,65,70	0
25	CLA	A	613	65/65	0.95	0.13	0.13	25,33,44,53	0
25	CLA	B	604	65/65	0.93	0.16	0.12	27,33,72,81	0
25	CLA	c	503	65/65	0.93	0.15	0.12	36,45,50,57	0
25	CLA	b	604	65/65	0.94	0.18	0.11	25,35,69,82	0
25	CLA	b	614	65/65	0.94	0.13	0.11	31,39,75,79	0
27	BCR	C	515	40/40	0.92	0.13	0.10	44,53,65,67	0
25	CLA	B	602	65/65	0.95	0.12	0.10	26,36,57,66	0
25	CLA	c	507	65/65	0.92	0.14	0.09	36,46,62,72	0
25	CLA	a	606	65/65	0.94	0.12	0.09	26,33,42,58	0
27	BCR	H	101	40/40	0.87	0.15	0.07	36,50,64,65	0
27	BCR	c	521	40/40	0.91	0.12	0.07	49,59,72,73	0
29	SQD	f	101	41/54	0.89	0.20	0.06	59,84,105,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
27	BCR	Y	101	40/40	0.91	0.12	0.05	43,51,62,68	0
27	BCR	a	611	40/40	0.94	0.11	0.04	26,37,49,54	0
32	LMG	C	520	48/55	0.82	0.19	0.00	47,69,88,95	0
25	CLA	c	505	65/65	0.95	0.12	-0.08	32,41,69,76	0
27	BCR	B	619	40/40	0.92	0.10	-0.08	34,45,56,58	0
25	CLA	C	509	65/65	0.94	0.12	-0.10	31,41,86,89	0
25	CLA	c	510	65/65	0.92	0.16	-0.11	36,46,61,72	0
25	CLA	d	401	65/65	0.95	0.12	-0.15	25,34,55,69	0
21	OEX	A	601	10/10	0.99	0.11	-0.20	32,34,40,41	1
25	CLA	C	507	65/65	0.93	0.12	-0.22	34,46,77,89	0
25	CLA	C	512	65/65	0.93	0.13	-0.27	39,52,67,71	0
34	HEM	e	101	43/43	0.95	0.13	-0.30	47,58,73,80	0
34	HEM	V	201	43/43	0.97	0.09	-0.31	29,36,44,46	0
25	CLA	D	402	65/65	0.95	0.12	-0.32	21,31,54,78	0
25	CLA	c	508	64/65	0.95	0.11	-0.32	36,45,82,87	0
27	BCR	c	514	40/40	0.92	0.13	-0.40	49,58,62,64	0
25	CLA	b	615	65/65	0.93	0.11	-0.41	33,44,62,69	0
25	CLA	b	611	65/65	0.94	0.12	-0.42	29,36,55,66	0
23	CL	A	604	1/1	0.99	0.13	-0.52	33,33,33,33	0
34	HEM	E	101	43/43	0.96	0.11	-0.56	43,49,57,65	0
25	CLA	c	504	60/65	0.95	0.12	-0.59	34,47,69,77	0
25	CLA	c	511	65/65	0.94	0.12	-0.60	40,54,66,73	0
24	BCT	A	605	4/4	0.98	0.07	-0.66	42,43,44,53	0
27	BCR	A	610	40/40	0.95	0.09	-0.69	31,37,41,41	0
27	BCR	b	619	40/40	0.93	0.10	-0.70	32,48,60,61	0
25	CLA	b	616	47/65	0.94	0.09	-0.70	31,42,53,57	0
21	OEX	a	601	10/10	0.99	0.10	-1.56	28,32,35,42	0
23	CL	a	603	1/1	0.98	0.07	-2.21	33,33,33,33	0
22	FE2	A	602	1/1	0.99	0.04	-2.55	36,36,36,36	0
23	CL	A	603	1/1	0.99	0.06	-3.19	32,32,32,32	0
22	FE2	a	602	1/1	0.99	0.05	-3.22	43,43,43,43	0
23	CL	a	604	1/1	0.99	0.08	-5.01	35,35,35,35	0
31	UNL	B	622	11/-	0.89	0.14	-	41,47,60,61	0
31	UNL	C	523	16/-	0.68	0.22	-	55,71,94,101	0
31	UNL	c	523	8/-	0.81	0.15	-	49,59,77,84	0
31	UNL	I	101	7/-	0.80	0.19	-	53,57,64,65	0
31	UNL	b	622	17/-	0.81	0.19	-	47,53,63,65	0
31	UNL	J	101	11/-	0.78	0.23	-	48,61,68,68	0
31	UNL	i	101	20/-	0.87	0.23	-	51,59,77,79	0
31	UNL	E	102	12/-	0.51	0.25	-	63,85,93,95	0
31	UNL	I	102	20/-	0.74	0.21	-	46,64,81,84	0
31	UNL	j	802	12/-	0.66	0.21	-	62,72,86,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	UNL	m	101	9/-	0.85	0.18	-	51,53,61,62	0
31	UNL	D	411	10/-	0.86	0.20	-	49,55,72,79	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.