



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2017 – 03:46 PM EST

PDB ID : 5E79  
Title : Macromolecular diffractive imaging using imperfect crystals  
Authors : Ayer, K.; Yefanov, O.; Oberthur, D.; Roy-Chowdhury, S.; Galli, L.; Mariani, V.; Basu, S.; Coe, J.; Conrad, C.E.; Fromme, R.; Schaffer, A.; Dorner, K.; James, D.; Kupitz, C.; Metz, M.; Nelson, G.; Xavier, P.L.; Beyerlein, K.R.; Schmidt, M.; Sarrou, I.; Spence, J.C.H.; Weierstall, U.; White, T.A.; Yang, J.-H.; Zhao, Y.; Liang, M.; Aquila, A.; Hunter, M.S.; Koglin, J.E.; Boutet, S.; Fromme, P.; Barty, A.; Chapman, H.N.  
Deposited on : 2015-10-12  
Resolution : 3.50 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
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

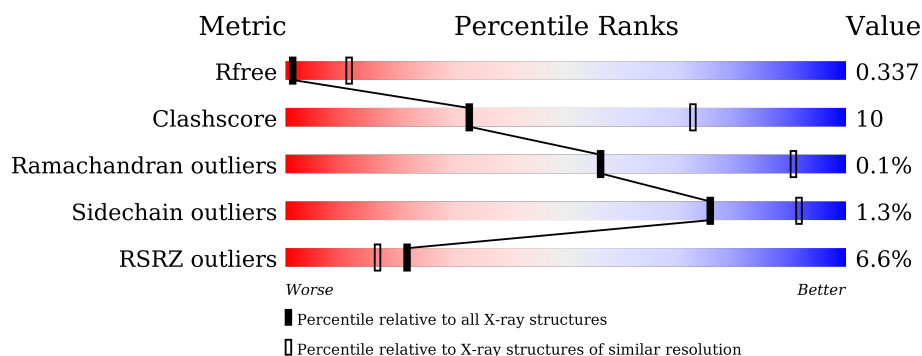
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	334	<div> <div>6%</div> <div>69%</div> <div>31%</div> </div>
1	a	334	<div> <div>7%</div> <div>100%</div> </div>
2	B	504	<div> <div>3%</div> <div>70%</div> <div>29%</div> </div>
2	b	504	<div> <div>9%</div> <div>99%</div> </div>
3	C	451	<div> <div>6%</div> <div>75%</div> <div>24%</div> </div>
3	c	451	<div> <div>9%</div> <div>99%</div> </div>

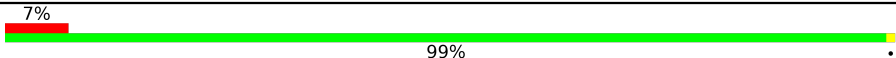
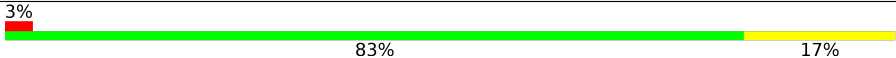

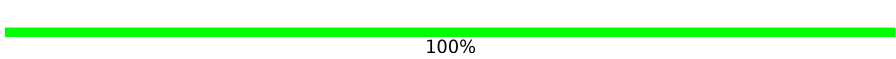
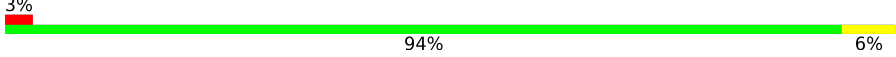
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Mol	Chain	Length	Quality of chain
4	D	342	<div> <div>5%</div> <div>68%</div> <div>32%</div> </div>
4	d	342	<div> <div>7%</div> <div>99%</div> <div>.</div> </div>
5	E	81	<div> <div>6%</div> <div>77%</div> <div>23%</div> </div>
5	e	81	<div> <div>10%</div> <div>99%</div> <div>.</div> </div>
6	F	34	<div> <div>3%</div> <div>50%</div> <div>50%</div> </div>
6	f	34	<div> <div>12%</div> <div>97%</div> <div>.</div> </div>
7	H	65	<div> <div>6%</div> <div>63%</div> <div>32%</div> <div>5%</div> </div>
7	h	65	<div> <div>12%</div> <div>95%</div> <div>5%</div> </div>
8	I	38	<div> <div>3%</div> <div>76%</div> <div>24%</div> </div>
8	i	38	<div> <div>5%</div> <div>100%</div> </div>
9	J	38	<div> <div>5%</div> <div>84%</div> <div>16%</div> </div>
9	j	38	<div> <div>5%</div> <div>100%</div> </div>
10	K	37	<div> <div>3%</div> <div>54%</div> <div>43%</div> <div>.</div> </div>
10	k	37	<div> <div>11%</div> <div>92%</div> <div>8%</div> </div>
11	L	37	<div> <div>5%</div> <div>59%</div> <div>41%</div> </div>
11	l	37	<div> <div>5%</div> <div>97%</div> <div>.</div> </div>
12	M	34	<div> <div>6%</div> <div>68%</div> <div>32%</div> </div>
12	m	34	<div> <div>6%</div> <div>97%</div> <div>.</div> </div>
13	O	243	<div> <div>6%</div> <div>80%</div> <div>20%</div> </div>
13	o	243	<div> <div>11%</div> <div>98%</div> <div>.</div> </div>
14	T	30	<div> <div>57%</div> <div>43%</div> </div>
14	t	30	<div> <div>100%</div> </div>
15	U	97	<div> <div>3%</div> <div>85%</div> <div>15%</div> </div>
15	u	97	<div> <div>6%</div> <div>99%</div> <div>.</div> </div>
16	V	137	<div> <div>7%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
16	v	137	
17	Y	29	
17	y	29	
18	X	39	
18	x	39	
19	Z	62	
19	z	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
22	CL	A	603	-	-	-	X
22	CL	A	604	-	-	-	X
23	BCT	A	605	-	-	-	X
23	BCT	a	605	-	-	-	X
24	CLA	A	606	X	-	-	X
24	CLA	A	607	X	-	-	X
24	CLA	A	609	X	-	-	X
24	CLA	B	602	X	-	-	X
24	CLA	B	603	X	-	-	X
24	CLA	B	604	X	-	-	X
24	CLA	B	605	X	-	-	X
24	CLA	B	606	X	-	-	X
24	CLA	B	607[A]	X	-	-	X
24	CLA	B	607[B]	X	-	-	X
24	CLA	B	608	X	-	-	X
24	CLA	B	609	X	-	-	X
24	CLA	B	610	X	-	-	X
24	CLA	B	611	X	-	-	X
24	CLA	B	612	X	-	-	X
24	CLA	B	613	X	-	-	X
24	CLA	B	614	X	-	-	X
24	CLA	B	615	X	-	-	X
24	CLA	B	616	X	-	-	X
24	CLA	B	617	X	-	-	X
24	CLA	C	501	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	502	X	-	-	X
24	CLA	C	503	X	-	-	X
24	CLA	C	504	X	-	-	X
24	CLA	C	505	X	-	-	X
24	CLA	C	506	X	-	-	X
24	CLA	C	507	X	-	-	X
24	CLA	C	508	X	-	-	X
24	CLA	C	509	X	-	-	X
24	CLA	C	510	X	-	-	X
24	CLA	C	511	X	-	-	X
24	CLA	C	512	X	-	-	X
24	CLA	C	513	X	-	-	X
24	CLA	D	402	X	-	-	X
24	CLA	D	403	X	-	-	X
24	CLA	D	404	X	-	-	X
24	CLA	a	606	X	-	-	X
24	CLA	a	607	X	-	-	X
24	CLA	a	609	X	-	-	X
24	CLA	a	615	X	-	-	X
24	CLA	b	603	X	-	-	X
24	CLA	b	604	X	-	-	X
24	CLA	b	605	X	-	-	X
24	CLA	b	606	X	-	-	X
24	CLA	b	607	X	-	-	X
24	CLA	b	608[A]	X	-	-	X
24	CLA	b	608[B]	X	-	-	X
24	CLA	b	609	X	-	-	X
24	CLA	b	610	X	-	-	X
24	CLA	b	611	X	-	-	X
24	CLA	b	612	X	-	-	X
24	CLA	b	613	X	-	-	X
24	CLA	b	614	X	-	-	X
24	CLA	b	615	X	-	-	X
24	CLA	b	616	X	-	-	X
24	CLA	b	617	X	-	-	X
24	CLA	b	618	X	-	-	X
24	CLA	c	501	X	-	-	X
24	CLA	c	502	X	-	-	X
24	CLA	c	503	X	-	-	X
24	CLA	c	504	X	-	-	X
24	CLA	c	505	X	-	-	X
24	CLA	c	506	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	c	507	X	-	-	X
24	CLA	c	508	X	-	-	X
24	CLA	c	509	X	-	-	X
24	CLA	c	510	X	-	-	X
24	CLA	c	511	X	-	-	X
24	CLA	c	512	X	-	-	X
24	CLA	c	513	X	-	-	X
24	CLA	d	402	X	-	-	X
24	CLA	d	403	X	-	-	-
25	PHO	A	608	-	-	-	X
25	PHO	D	401	-	-	-	X
25	PHO	a	608	-	-	-	X
25	PHO	d	401	-	-	-	X
26	BCR	A	610	-	-	-	X
26	BCR	B	618	-	-	X	X
26	BCR	B	619	-	-	X	X
26	BCR	B	620	-	-	X	X
26	BCR	C	514	-	-	X	X
26	BCR	F	101	-	-	X	X
26	BCR	H	101	-	-	X	X
26	BCR	I	101	-	-	-	X
26	BCR	K	101	-	-	X	X
26	BCR	K	102	-	-	-	X
26	BCR	T	101	-	-	X	X
26	BCR	a	610	-	-	-	X
26	BCR	b	619	-	-	-	X
26	BCR	b	620	-	-	-	X
26	BCR	b	621	-	-	-	X
26	BCR	c	514	-	X	-	X
26	BCR	c	515	-	-	-	X
26	BCR	c	521	-	-	-	X
26	BCR	f	101	-	-	-	X
26	BCR	h	101	-	X	-	X
26	BCR	k	101	-	-	-	X
26	BCR	t	101	-	-	-	X
27	PL9	A	611	-	-	-	X
27	PL9	D	405	-	-	-	X
27	PL9	a	611	-	-	-	X
27	PL9	d	404	-	-	-	X
28	SQD	A	612	-	-	-	X
28	SQD	A	614	-	-	-	X
28	SQD	B	622	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	SQD	L	102	-	-	-	X
28	SQD	X	101	-	-	-	X
28	SQD	a	612	-	-	-	X
28	SQD	a	614	-	-	-	X
28	SQD	b	601	-	-	-	X
28	SQD	l	101	-	-	-	X
28	SQD	x	101	-	-	-	X
29	LMG	A	613	-	-	-	X
29	LMG	B	621	-	-	-	X
29	LMG	C	518	-	-	-	X
29	LMG	C	519	-	-	-	X
29	LMG	D	408	-	-	-	X
29	LMG	Z	101	-	-	-	X
29	LMG	a	613	-	-	-	X
29	LMG	b	622	-	-	-	X
29	LMG	c	519	-	-	-	X
29	LMG	c	520	-	-	-	X
29	LMG	j	101	-	-	-	X
29	LMG	z	101	-	-	-	X
30	LHG	A	615	-	-	-	X
30	LHG	D	406	-	-	-	X
30	LHG	D	407	-	-	-	X
30	LHG	E	102	-	-	-	X
30	LHG	L	101	-	-	-	X
30	LHG	a	616	-	-	-	X
30	LHG	d	406	-	-	-	X
30	LHG	d	407	-	-	-	X
30	LHG	e	101	-	-	-	X
30	LHG	l	102	-	-	-	X
31	CA	o	301	-	-	-	X
32	DGD	C	515	-	-	-	X
32	DGD	C	516	-	-	-	X
32	DGD	C	517	-	-	-	X
32	DGD	E	101	-	-	-	X
32	DGD	H	102	-	-	-	X
32	DGD	c	516	-	-	-	X
32	DGD	c	517	-	-	-	X
32	DGD	c	518	-	-	-	X
32	DGD	d	405	-	-	-	X
32	DGD	h	102	-	-	-	X
33	HEM	E	103	-	-	-	X
33	HEM	V	201	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	HEM	e	102	-	-	-	X
33	HEM	v	201	-	-	-	X
34	MG	j	102	-	-	-	X



## 2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 50074 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	4	0
			2637	1730	432	460	15			
1	a	334	Total	C	N	O	S	3	4	0
			2637	1730	432	460	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	ALA	THR	conflict	UNP P0A444
a	286	ALA	THR	conflict	UNP P0A444

- 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	10	0
			4024	2641	668	702	13			
2	b	504	Total	C	N	O	S	0	10	0
			4024	2641	668	702	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	5	0
			3506	2296	584	613	13			
3	c	451	Total	C	N	O	S	0	5	0
			3506	2296	584	613	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	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	2	0
			668	436	107	125				
5	e	81	Total	C	N	O		0	2	0
			668	436	107	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	2	0
			525	351	86	86	2			
7	h	65	Total	C	N	O	S	0	2	0
			525	351	86	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	1	0
			320	215	49	54	2			
8	i	38	Total	C	N	O	S	0	1	0
			320	215	49	54	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	38	Total	C	N	O	S	0	0	0
			272	182	42	47	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			
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	5	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	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	1	0
			272	183	40	48	1			
12	m	34	Total	C	N	O	S	0	1	0
			272	183	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	4	0
			1883	1178	315	385	5			
13	o	243	Total	C	N	O	S	0	4	0
			1883	1178	315	385	5			

- 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	2	0
			270	189	37	41	3			
14	t	30	Total	C	N	O	S	0	2	0
			270	189	37	41	3			

- 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	1	0
			1072	680	180	208	4			
16	v	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

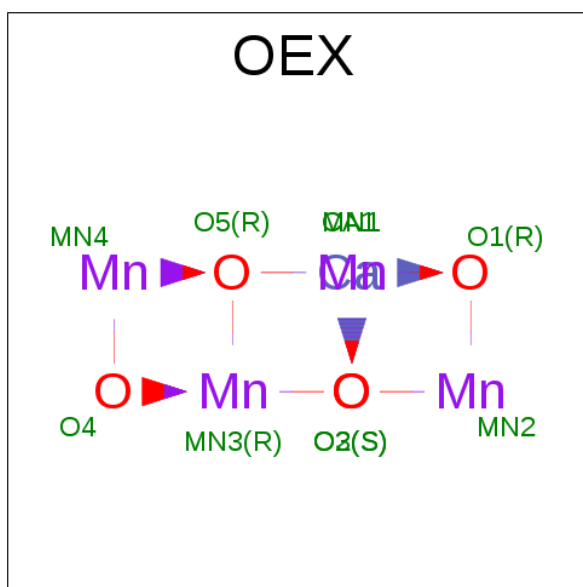
- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O	0	1	0
			292	196	46	50			
18	x	39	Total	C	N	O	0	1	0
			292	196	46	50			

- 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
			479	328	72	77	2			

- Molecule 20 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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

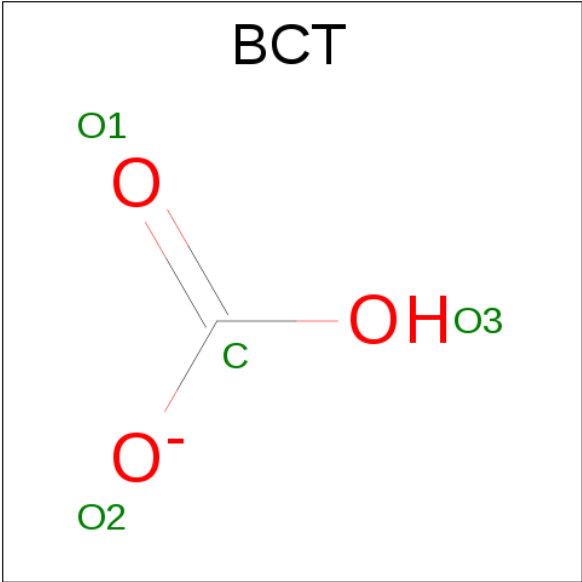
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

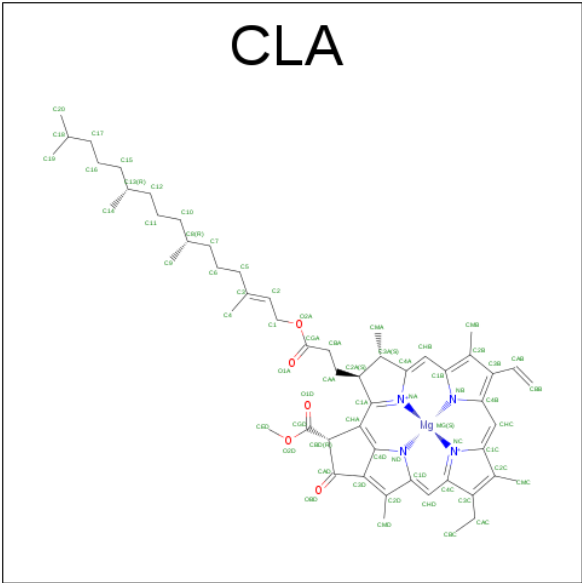
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	u	1	Total	Cl	0	0
			1	1		
22	a	2	Total	Cl	0	0
			2	2		
22	U	1	Total	Cl	0	0
			1	1		

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO<sub>3</sub>).



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

- Molecule 24 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
24	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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

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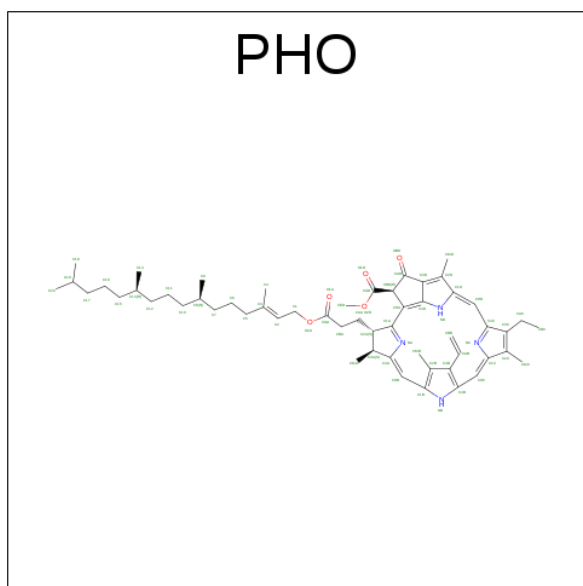
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	b	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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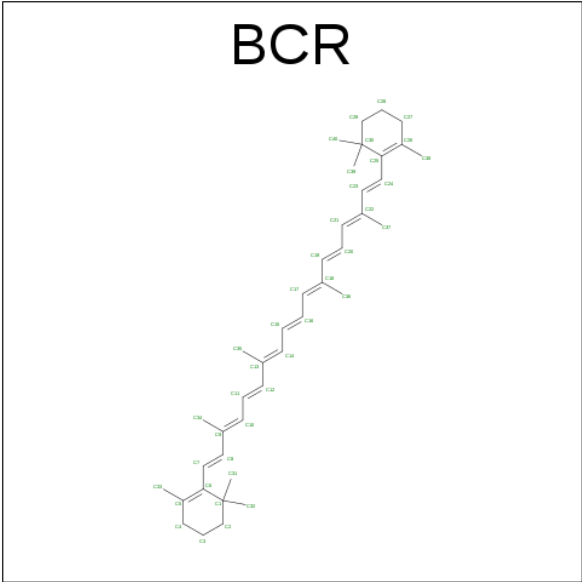
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



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

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



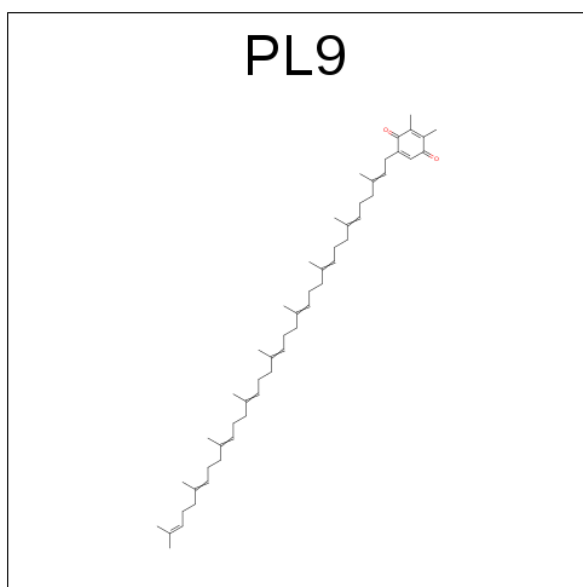
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	F	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	I	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	f	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0

- Molecule 27 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:  $C_{53}H_{80}O_2$ ).



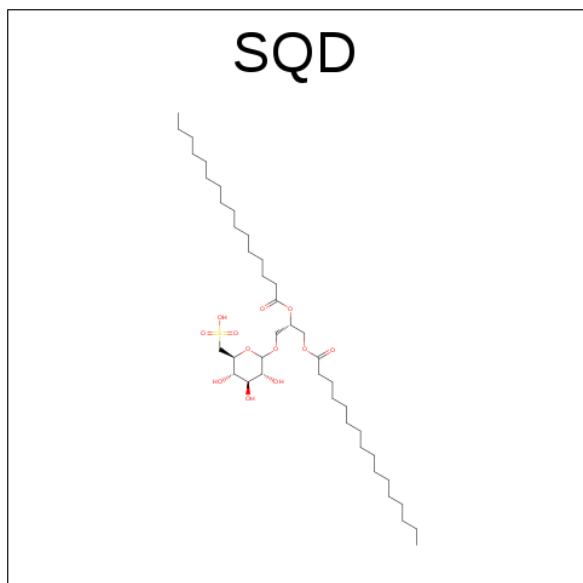
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 55 53 2	0	0
27	D	1	Total C O 55 53 2	0	0

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

- Molecule 28 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).



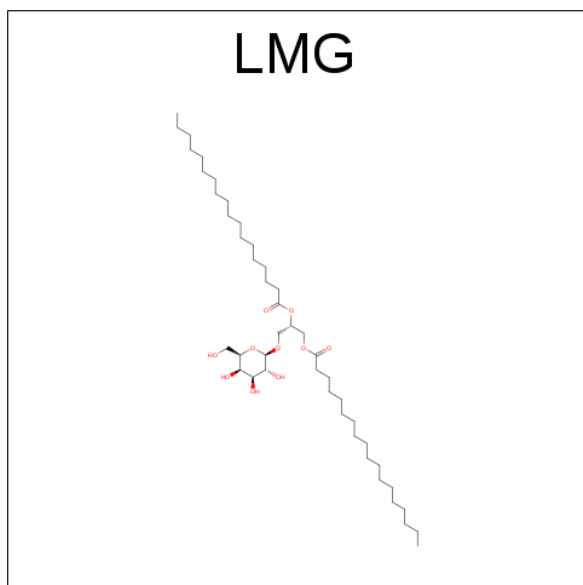
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	B	1	Total	C	O	S	0	0
			54	41	12	1		
28	L	1	Total	C	O	S	0	0
			54	41	12	1		
28	X	1	Total	C	O	S	0	0
			43	30	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	b	1	Total	C	O	S	0	0
			54	41	12	1		
28	l	1	Total	C	O	S	0	0
			54	41	12	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	x	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



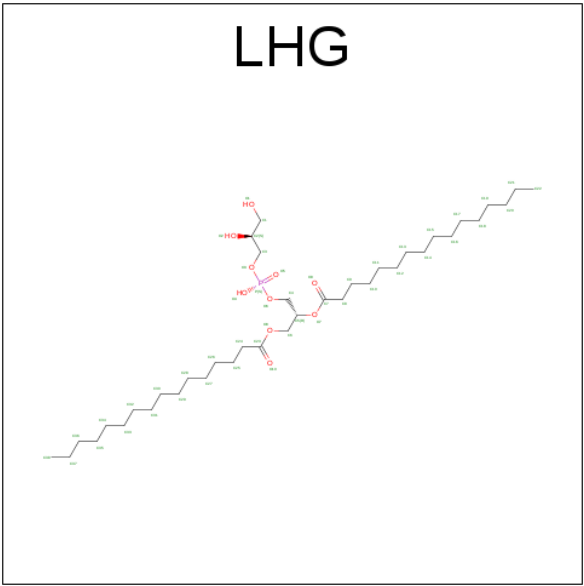
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O		0	0
			51	41	10			
29	B	1	Total	C	O		0	0
			51	41	10			
29	C	1	Total	C	O		0	0
			51	41	10			
29	C	1	Total	C	O		0	0
			51	41	10			
29	D	1	Total	C	O		0	0
			51	41	10			
29	Z	1	Total	C	O		0	0
			37	27	10			
29	a	1	Total	C	O		0	0
			51	41	10			
29	b	1	Total	C	O		0	0
			51	41	10			
29	c	1	Total	C	O		0	0
			51	41	10			
29	c	1	Total	C	O		0	0
			51	41	10			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	j	1	Total	C	O	0	0
			51	41	10		
29	z	1	Total	C	O	0	0
			37	27	10		

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	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	D	1	Total	C	O	P	0	0
			49	38	10	1		
30	E	1	Total	C	O	P	0	0
			42	31	10	1		
30	L	1	Total	C	O	P	0	0
			49	38	10	1		
30	a	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	d	1	Total	C	O	P	0	0
			49	38	10	1		
30	e	1	Total	C	O	P	0	0
			42	31	10	1		

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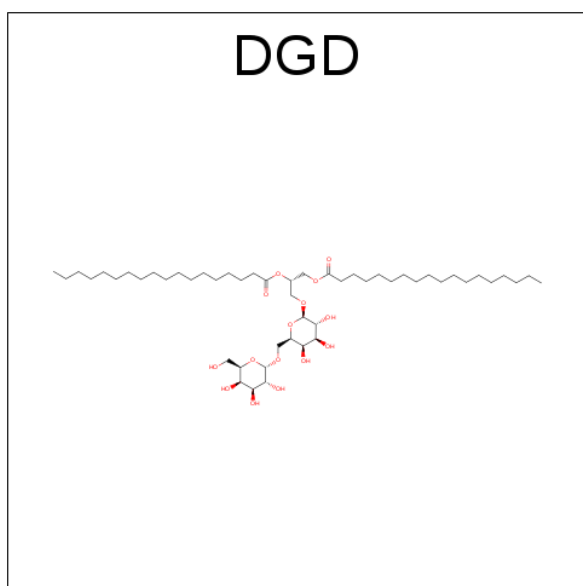
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 31 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	B	1	Total	Ca	0	0
			1	1		
31	F	1	Total	Ca	0	0
			1	1		
31	o	1	Total	Ca	0	0
			1	1		
31	O	1	Total	Ca	0	0
			1	1		
31	b	1	Total	Ca	0	0
			1	1		
31	f	1	Total	Ca	0	0
			1	1		

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	C	1	Total	C	O	0	0
			62	47	15		
32	C	1	Total	C	O	0	0
			62	47	15		

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

- # HEM
- 
- The diagram illustrates the chemical structure of Hemoglobin (HEM). It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The iron atom is also coordinated by a heme group (O2A) and a water molecule (O2D). The structure includes various side chains and heme groups, such as CAA, CBA, CAD, CBD, CMA, C3A, C2A, C3B, C4B, C1B, C2B, C3C, C4C, C1C, C2C, C3D, C4D, C1D, C2D, C3E, C4E, C1E, C2E, C3F, C4F, C1F, C2F, C3G, C4G, C1G, C2G, C3H, C4H, C1H, C2H, C3I, C4I, C1I, C2I, C3J, C4J, C1J, C2J, C3K, C4K, C1K, C2K, C3L, C4L, C1L, C2L, C3M, C4M, C1M, C2M, C3N, C4N, C1N, C2N, C3O, C4O, C1O, C2O, C3P, C4P, C1P, C2P, C3Q, C4Q, C1Q, C2Q, C3R, C4R, C1R, C2R, C3S, C4S, C1S, C2S, C3T, C4T, C1T, C2T, C3U, C4U, C1U, C2U, C3V, C4V, C1V, C2V, C3W, C4W, C1W, C2W, C3X, C4X, C1X, C2X, C3Y, C4Y, C1Y, C2Y, C3Z, C4Z, C1Z, C2Z, C3AA, C4AA, C1AA, C2AA, C3AB, C4AB, C1AB, C2AB, C3AC, C4AC, C1AC, C2AC, C3AD, C4AD, C1AD, C2AD, C3AE, C4AE, C1AE, C2AE, C3AF, C4AF, C1AF, C2AF, C3AG, C4AG, C1AG, C2AG, C3AH, C4AH, C1AH, C2AH, C3AI, C4AI, C1AI, C2AI, C3AJ, C4AJ, C1AJ, C2AJ, C3AK, C4AK, C1AK, C2AK, C3AL, C4AL, C1AL, C2AL, C3AM, C4AM, C1AM, C2AM, C3AN, C4AN, C1AN, C2AN, C3AO, C4AO, C1AO, C2AO, C3AP, C4AP, C1AP, C2AP, C3AQ, C4AQ, 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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
33	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
33	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0



*Continued from previous page...*

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

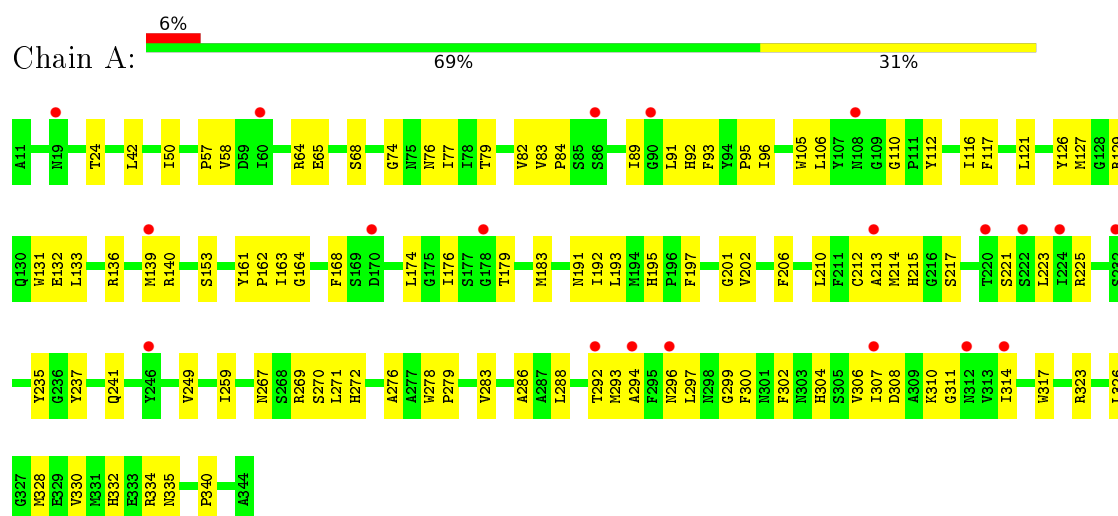
- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	J	1	Total	Mg	0	0
			1	1		
34	j	1	Total	Mg	0	0
			1	1		

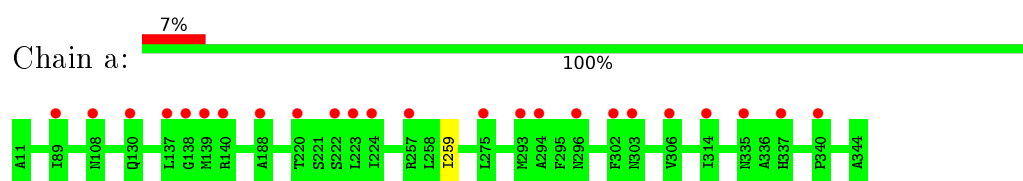
### 3 Residue-property plots

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.

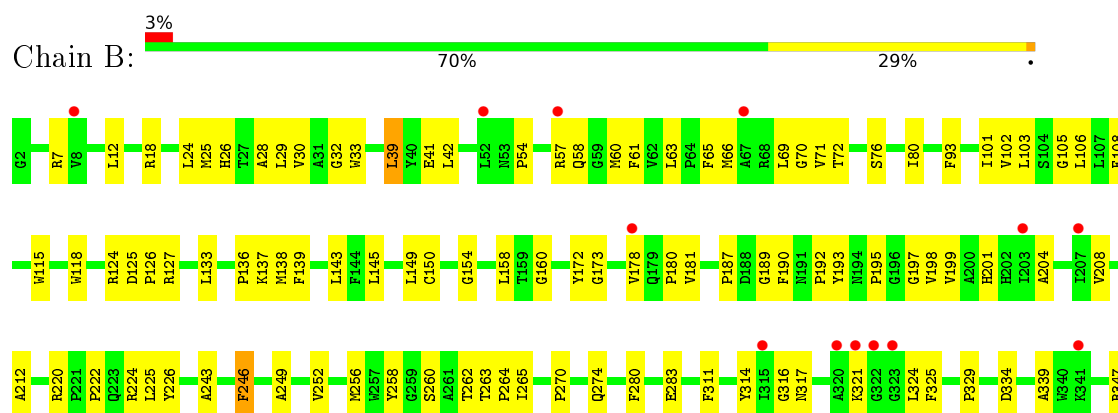
#### • Molecule 1: Photosystem II protein D1 1

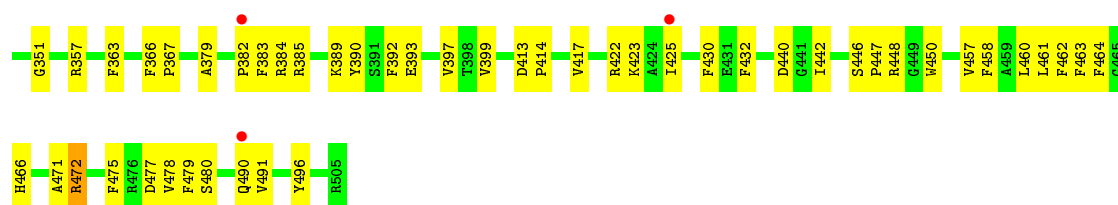


#### • Molecule 1: Photosystem II protein D1 1

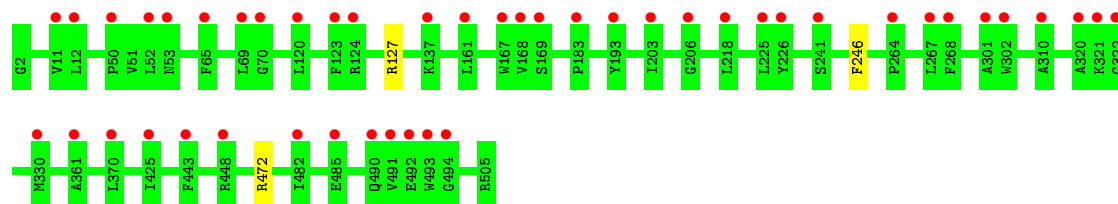


#### • Molecule 2: Photosystem II CP47 reaction center protein

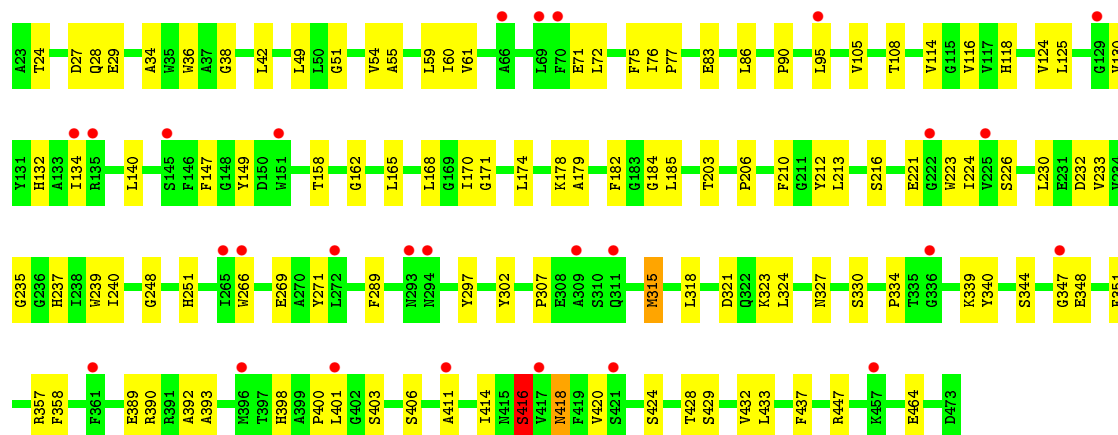
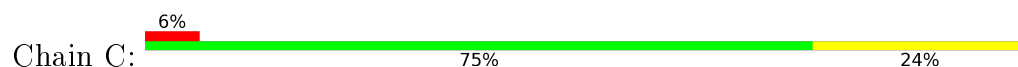




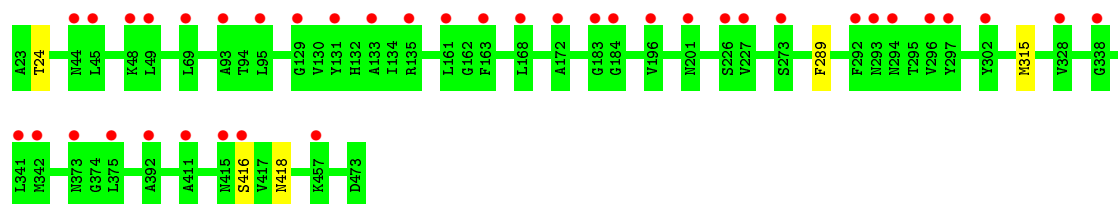
• Molecule 2: Photosystem II CP47 reaction center protein



• Molecule 3: Photosystem II CP43 reaction center protein

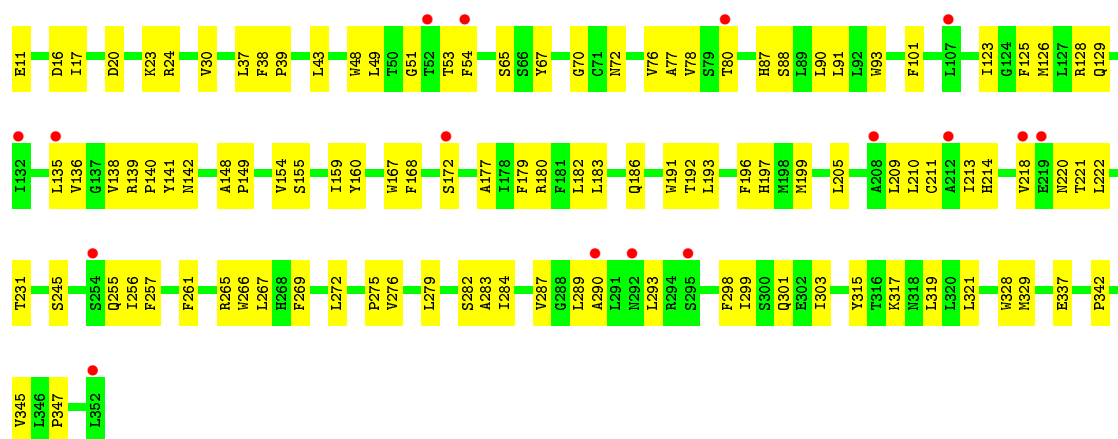


• Molecule 3: Photosystem II CP43 reaction center protein

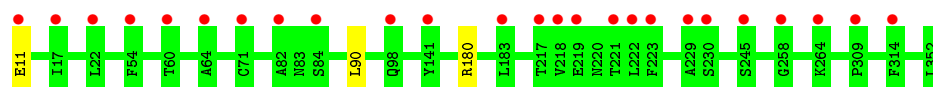


• Molecule 4: Photosystem II D2 protein

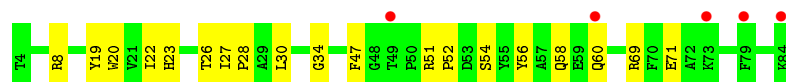
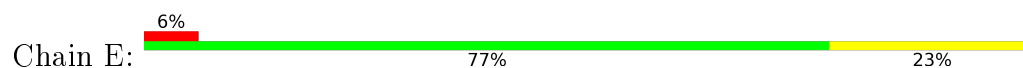




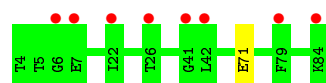
• Molecule 4: Photosystem II D2 protein



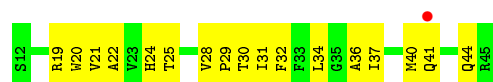
• Molecule 5: Cytochrome b559 subunit alpha



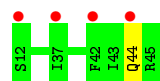
• Molecule 5: Cytochrome b559 subunit alpha



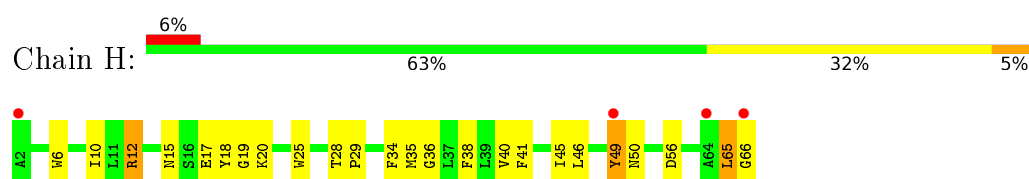
• Molecule 6: Cytochrome b559 subunit beta



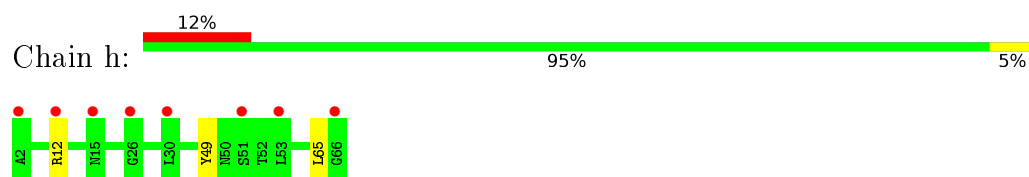
• Molecule 6: Cytochrome b559 subunit beta



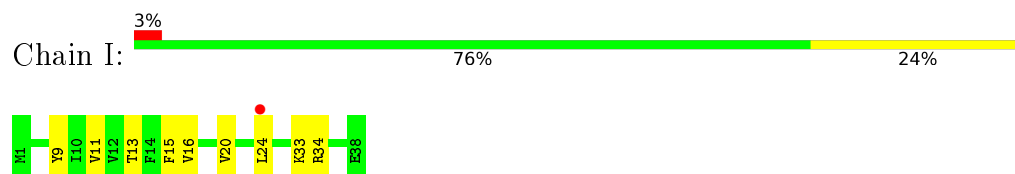
• Molecule 7: Photosystem II reaction center protein H



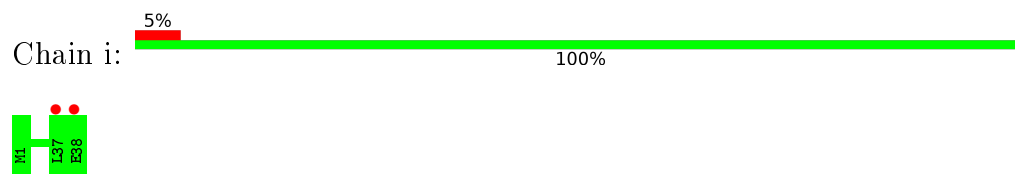
- Molecule 7: Photosystem II reaction center protein H



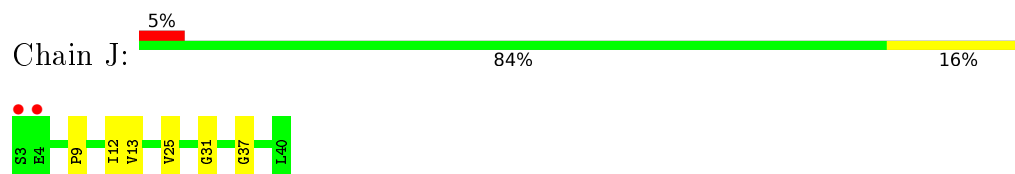
- Molecule 8: Photosystem II reaction center protein I



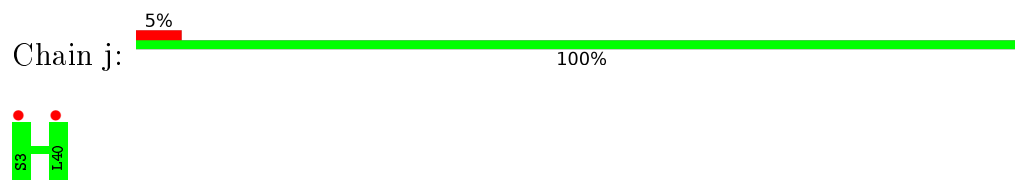
- Molecule 8: Photosystem II reaction center protein I



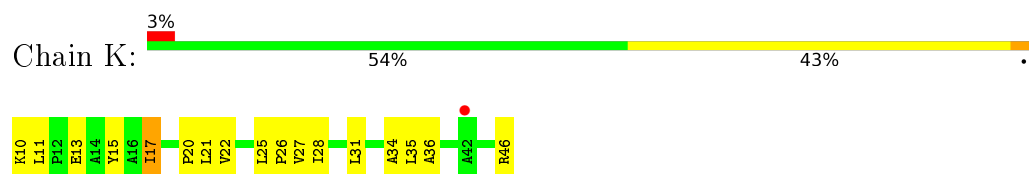
- Molecule 9: Photosystem II reaction center protein J



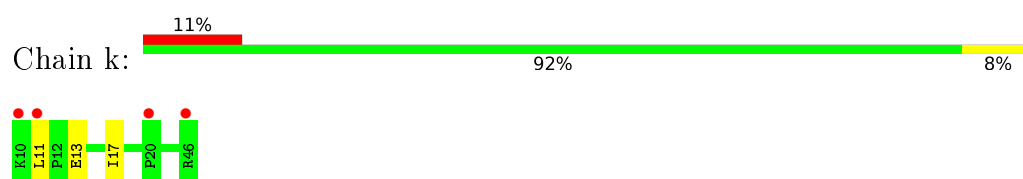
- Molecule 9: Photosystem II reaction center protein J



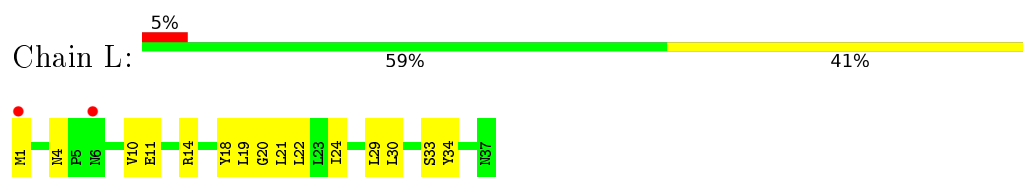
- Molecule 10: Photosystem II reaction center protein K



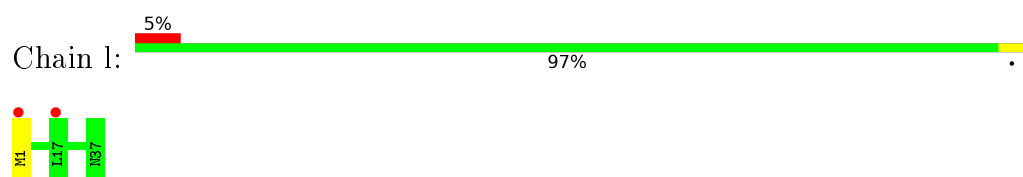
- Molecule 10: Photosystem II reaction center protein K



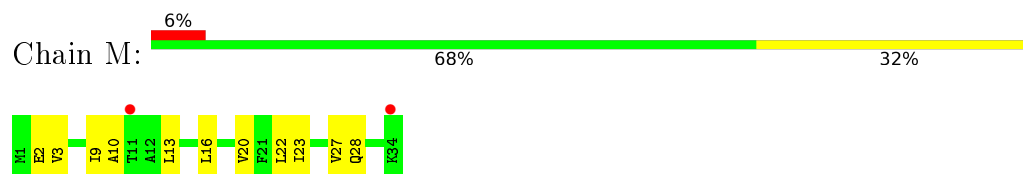
- Molecule 11: Photosystem II reaction center protein L



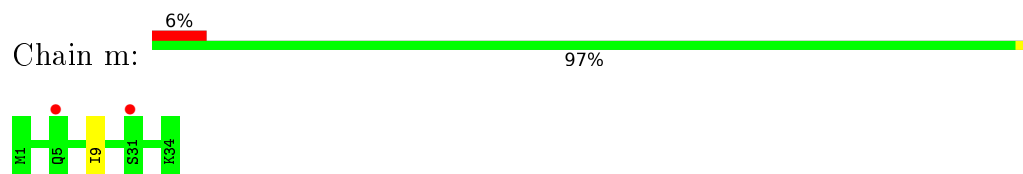
- Molecule 11: Photosystem II reaction center protein L



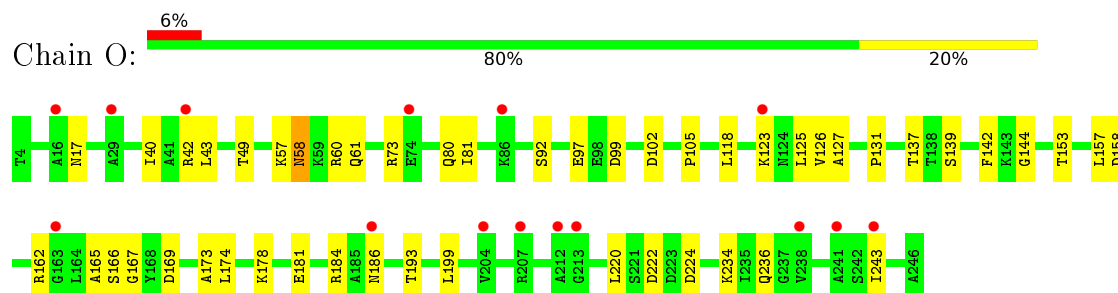
- Molecule 12: Photosystem II reaction center protein M



- Molecule 12: Photosystem II reaction center protein M

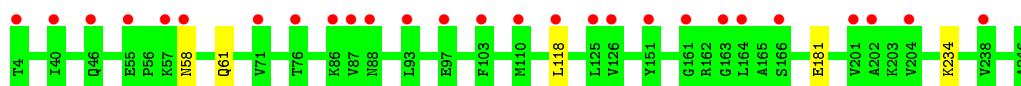


- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide





- Molecule 14: Photosystem II reaction center protein T

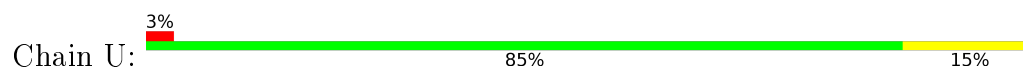


- Molecule 14: Photosystem II reaction center protein T

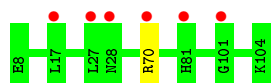


There are no outlier residues recorded for this chain.

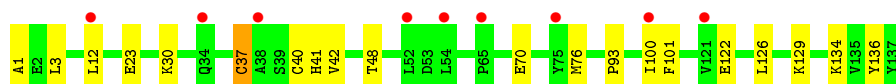
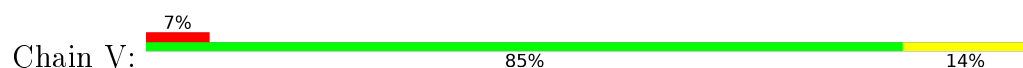
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein



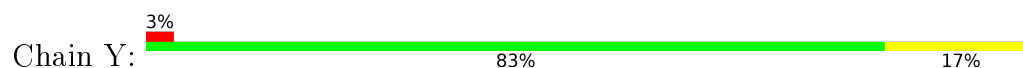
- Molecule 16: Cytochrome c-550



- Molecule 16: Cytochrome c-550



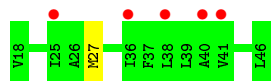
- Molecule 17: Photosystem II reaction center protein Ycf12



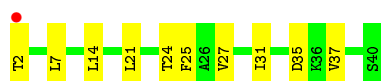
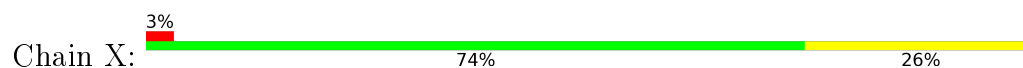




- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein

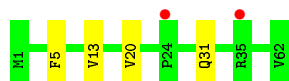
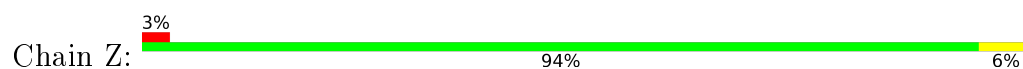


- Molecule 18: Photosystem II reaction center X protein

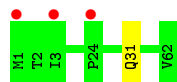


There are no outlier residues recorded for this chain.

- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	250.80 Å   250.80 Å   250.80 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	29.98 – 3.50 250.80 – 3.28	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.98-3.50) 100.0 (250.80-3.28)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.324 , 0.331 0.332 , 0.337	Depositor DCC
$R_{free}$ test set	37670 reflections (4.89%)	DCC
Wilson B-factor (Å <sup>2</sup> )	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 1.5	EDS
L-test for twinning <sup>1</sup>	$\langle  L  \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	50074	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: (*Not available*)

<sup>1</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, MG, OEX, PHO, DGD, CL, CA, CLA, PL9, FE2, BCT, 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	0.56	0/2734	0.68	0/3727
1	a	0.49	0/2734	0.64	0/3727
2	B	0.51	0/4194	0.65	1/5713 (0.0%)
2	b	0.48	0/4194	0.63	1/5713 (0.0%)
3	C	0.51	0/3634	0.64	0/4947
3	c	0.47	0/3634	0.60	0/4947
4	D	0.53	0/2821	0.65	0/3844
4	d	0.48	0/2821	0.60	0/3844
5	E	0.46	0/693	0.63	0/944
5	e	0.43	0/693	0.58	0/944
6	F	0.51	0/284	0.61	0/387
6	f	0.41	0/284	0.56	0/387
7	H	0.47	0/544	0.64	0/739
7	h	0.46	0/544	0.66	0/739
8	I	0.52	0/327	0.68	0/439
8	i	0.46	0/327	0.60	0/439
9	J	0.46	0/278	0.59	0/376
9	j	0.43	0/278	0.53	0/376
10	K	0.48	0/303	0.70	0/416
10	k	0.55	0/303	0.79	0/416
11	L	0.55	0/319	0.70	0/433
11	l	0.48	0/319	0.62	0/433
12	M	0.52	0/278	0.74	0/378
12	m	0.49	0/278	0.69	0/378
13	O	0.46	0/1926	0.65	0/2611
13	o	0.41	0/1926	0.61	0/2611
14	T	0.60	0/282	0.68	0/382
14	t	0.49	0/282	0.60	0/382
15	U	0.48	0/785	0.64	0/1064
15	u	0.46	0/785	0.63	0/1064
16	V	0.52	1/1096 (0.1%)	0.66	0/1487
16	v	0.42	0/1096	0.62	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	Y	0.44	0/216	0.61	0/289
17	y	0.44	0/216	0.59	0/289
18	X	0.43	0/298	0.53	0/403
18	x	0.44	0/298	0.54	0/403
19	Z	0.44	0/490	0.58	0/669
19	z	0.46	0/490	0.56	0/669
All	All	0.49	1/43004 (0.0%)	0.63	2/58496 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	37	CYS	CB-SG	-5.25	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	127	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	B	39	LEU	CA-CB-CG	-5.25	103.23	115.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2637	0	2551	104	0
1	a	2637	0	2551	0	0
2	B	4024	0	3901	160	0
2	b	4024	0	3901	0	0
3	C	3506	0	3439	96	0
3	c	3506	0	3439	0	0
4	D	2726	0	2627	107	0
4	d	2726	0	2627	0	0
5	E	668	0	658	17	0
5	e	668	0	658	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	275	0	282	17	0
6	f	275	0	282	0	0
7	H	525	0	558	26	0
7	h	525	0	558	0	0
8	I	320	0	339	7	0
8	i	320	0	339	0	0
9	J	272	0	279	5	0
9	j	272	0	279	0	0
10	K	293	0	305	19	0
10	k	293	0	305	0	0
11	L	309	0	327	19	0
11	l	309	0	327	0	0
12	M	272	0	300	12	0
12	m	272	0	300	0	0
13	O	1883	0	1865	35	0
13	o	1883	0	1865	0	0
14	T	270	0	278	18	0
14	t	270	0	278	0	0
15	U	774	0	773	12	0
15	u	774	0	773	0	0
16	V	1072	0	1088	17	0
16	v	1072	0	1088	0	0
17	Y	215	0	246	8	0
17	y	215	0	246	0	0
18	X	292	0	328	13	0
18	x	292	0	328	0	0
19	Z	479	0	516	3	0
19	z	479	0	516	0	0
20	A	10	0	0	1	0
20	a	10	0	0	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	1	0
22	U	1	0	0	0	0
22	a	2	0	0	0	0
22	u	1	0	0	0	0
23	A	4	0	1	0	0
23	a	4	0	1	0	0
24	A	195	0	216	29	0
24	B	1105	0	1224	115	0
24	C	845	0	936	74	0
24	D	195	0	216	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	260	0	288	0	0
24	b	1105	0	1224	0	0
24	c	845	0	936	0	0
24	d	130	0	144	0	0
25	A	64	0	74	4	0
25	D	64	0	74	12	0
25	a	64	0	74	0	0
25	d	64	0	74	0	0
26	A	40	0	55	19	0
26	B	120	0	165	82	0
26	C	40	0	55	21	0
26	F	40	0	55	28	0
26	H	40	0	55	25	0
26	I	40	0	55	18	0
26	K	80	0	110	36	0
26	T	40	0	55	29	0
26	a	40	0	55	0	0
26	b	120	0	166	0	0
26	c	120	0	165	0	0
26	f	40	0	55	0	0
26	h	40	0	55	0	0
26	k	40	0	55	0	0
26	t	40	0	55	0	0
27	A	55	0	80	17	0
27	D	55	0	80	14	0
27	a	55	0	80	0	0
27	d	55	0	80	0	0
28	A	108	0	156	4	0
28	B	54	0	30	6	0
28	L	54	0	26	6	0
28	X	43	0	53	4	0
28	a	108	0	156	0	0
28	b	54	0	30	0	0
28	l	54	0	29	0	0
28	x	43	0	53	0	0
29	A	51	0	72	3	0
29	B	51	0	72	2	0
29	C	102	0	144	6	0
29	D	51	0	72	7	0
29	Z	37	0	44	1	0
29	a	51	0	72	0	0
29	b	51	0	72	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	c	102	0	144	0	0
29	j	51	0	72	0	0
29	z	37	0	44	0	0
30	A	49	0	74	10	0
30	D	98	0	148	10	0
30	E	42	0	57	0	0
30	L	49	0	74	6	0
30	a	49	0	74	0	0
30	d	98	0	148	0	0
30	e	42	0	57	0	0
30	l	49	0	74	0	0
31	B	1	0	0	0	0
31	F	1	0	0	0	0
31	O	1	0	0	0	0
31	b	1	0	0	0	0
31	f	1	0	0	0	0
31	o	1	0	0	0	0
32	C	186	0	246	10	0
32	E	62	0	82	1	0
32	H	62	0	82	11	0
32	c	186	0	246	0	0
32	d	62	0	82	0	0
32	h	62	0	82	0	0
33	E	43	0	30	6	0
33	V	43	0	30	10	0
33	e	43	0	30	0	0
33	v	43	0	30	0	0
34	J	1	0	0	0	0
34	j	1	0	0	0	0
All	All	50074	0	51320	924	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 10.

The worst 5 of 924 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)
26:T:101:BCR:C37	26:T:101:BCR:C22	1.74	1.65
26:B:619:BCR:C19	26:B:619:BCR:C20	1.76	1.64
26:B:620:BCR:C22	26:B:620:BCR:C37	1.76	1.64
26:C:514:BCR:C19	26:C:514:BCR:C20	1.73	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:619:BCR:C37	26:B:619:BCR:C22	1.74	1.62

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/334 (101%)	332 (99%)	3 (1%)	1 (0%)	46	84
1	a	336/334 (101%)	331 (98%)	4 (1%)	1 (0%)	46	84
2	B	512/504 (102%)	506 (99%)	6 (1%)	0	100	100
2	b	512/504 (102%)	505 (99%)	7 (1%)	0	100	100
3	C	454/451 (101%)	444 (98%)	8 (2%)	2 (0%)	39	81
3	c	454/451 (101%)	444 (98%)	8 (2%)	2 (0%)	39	81
4	D	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
5	e	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	32/34 (94%)	32 (100%)	0	0	100	100
7	H	65/65 (100%)	60 (92%)	5 (8%)	0	100	100
7	h	65/65 (100%)	60 (92%)	5 (8%)	0	100	100
8	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
9	J	36/38 (95%)	36 (100%)	0	0	100	100
9	j	36/38 (95%)	36 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	k	35/37 (95%)	30 (86%)	4 (11%)	1 (3%)	6	42
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/34 (97%)	33 (100%)	0	0	100	100
12	m	33/34 (97%)	33 (100%)	0	0	100	100
13	O	245/243 (101%)	237 (97%)	7 (3%)	1 (0%)	39	81
13	o	245/243 (101%)	237 (97%)	7 (3%)	1 (0%)	39	81
14	T	29/30 (97%)	28 (97%)	1 (3%)	0	100	100
14	t	29/30 (97%)	28 (97%)	1 (3%)	0	100	100
15	U	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
15	u	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
17	Y	27/29 (93%)	27 (100%)	0	0	100	100
17	y	27/29 (93%)	27 (100%)	0	0	100	100
18	X	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
18	x	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	5252/5264 (100%)	5139 (98%)	104 (2%)	9 (0%)	56	88

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	58	ASN
13	o	58	ASN
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER

### 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	273/269 (102%)	273 (100%)	0	100	100
1	a	273/269 (102%)	273 (100%)	0	100	100
2	B	412/402 (102%)	408 (99%)	4 (1%)	82	93
2	b	412/402 (102%)	410 (100%)	2 (0%)	92	97
3	C	357/352 (101%)	351 (98%)	6 (2%)	68	89
3	c	357/352 (101%)	353 (99%)	4 (1%)	80	92
4	D	277/277 (100%)	274 (99%)	3 (1%)	80	92
4	d	277/277 (100%)	274 (99%)	3 (1%)	80	92
5	E	74/72 (103%)	73 (99%)	1 (1%)	74	91
5	e	74/72 (103%)	73 (99%)	1 (1%)	74	91
6	F	28/28 (100%)	27 (96%)	1 (4%)	42	77
6	f	28/28 (100%)	27 (96%)	1 (4%)	42	77
7	H	56/54 (104%)	52 (93%)	4 (7%)	18	58
7	h	56/54 (104%)	52 (93%)	4 (7%)	18	58
8	I	36/35 (103%)	36 (100%)	0	100	100
8	i	36/35 (103%)	36 (100%)	0	100	100
9	J	26/26 (100%)	26 (100%)	0	100	100
9	j	26/26 (100%)	26 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	20	61
10	k	30/30 (100%)	28 (93%)	2 (7%)	20	61
11	L	36/35 (103%)	35 (97%)	1 (3%)	51	82
11	l	36/35 (103%)	35 (97%)	1 (3%)	51	82
12	M	32/31 (103%)	31 (97%)	1 (3%)	47	81
12	m	32/31 (103%)	31 (97%)	1 (3%)	47	81
13	O	210/206 (102%)	206 (98%)	4 (2%)	65	87
13	o	210/206 (102%)	206 (98%)	4 (2%)	65	87
14	T	29/27 (107%)	29 (100%)	0	100	100
14	t	29/27 (107%)	29 (100%)	0	100	100
15	U	84/84 (100%)	83 (99%)	1 (1%)	78	92
15	u	84/84 (100%)	83 (99%)	1 (1%)	78	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	V	118/117 (101%)	117 (99%)	1 (1%)	86	95
16	v	118/117 (101%)	117 (99%)	1 (1%)	86	95
17	Y	22/22 (100%)	21 (96%)	1 (4%)	34	73
17	y	22/22 (100%)	21 (96%)	1 (4%)	34	73
18	X	33/32 (103%)	33 (100%)	0	100	100
18	x	33/32 (103%)	33 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	65	87
19	z	52/52 (100%)	51 (98%)	1 (2%)	65	87
All	All	4370/4302 (102%)	4312 (99%)	58 (1%)	76	91

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	O	234	LYS
2	b	472	ARG
13	o	234	LYS
15	U	70	ARG
17	Y	27	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	216	HIS
2	B	409	GLN
4	d	197	HIS
15	u	78	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 168 ligands modelled in this entry, 16 are monoatomic - leaving 152 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	$\# Z  > 2$
20	OEX	A	601	1,3	0,15,15	0.00	-	0,32,32	0.00	-
23	BCT	A	605	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	A	606	-	57,73,73	2.60	22 (38%)	61,113,113	1.89	14 (22%)
24	CLA	A	607	-	57,73,73	2.52	21 (36%)	61,113,113	2.11	14 (22%)
25	PHO	A	608	-	67,69,69	1.22	9 (13%)	86,99,99	1.07	5 (5%)
24	CLA	A	609	-	57,73,73	2.59	22 (38%)	61,113,113	1.95	14 (22%)
26	BCR	A	610	-	41,41,41	9.24	30 (73%)	56,56,56	5.60	27 (48%)
27	PL9	A	611	-	54,55,55	3.94	16 (29%)	68,69,69	4.39	34 (50%)
28	SQD	A	612	-	53,54,54	1.49	3 (5%)	62,65,65	1.78	12 (19%)
29	LMG	A	613	-	51,51,55	1.31	5 (9%)	59,59,63	0.96	4 (6%)
28	SQD	A	614	-	53,54,54	1.50	3 (5%)	62,65,65	1.42	6 (9%)
30	LHG	A	615	-	48,48,48	1.09	3 (6%)	49,54,54	1.32	6 (12%)
24	CLA	B	602	-	57,73,73	2.49	22 (38%)	61,113,113	1.84	12 (19%)
24	CLA	B	603	-	57,73,73	2.52	23 (40%)	61,113,113	2.01	11 (18%)
24	CLA	B	604	-	57,73,73	2.48	24 (42%)	61,113,113	2.00	15 (24%)
24	CLA	B	605	-	57,73,73	2.51	21 (36%)	61,113,113	2.19	14 (22%)
24	CLA	B	606	-	57,73,73	2.52	21 (36%)	61,113,113	1.99	11 (18%)
24	CLA	B	607[A]	-	57,73,73	2.52	22 (38%)	61,113,113	2.07	13 (21%)
24	CLA	B	607[B]	-	57,73,73	2.54	22 (38%)	61,113,113	2.07	12 (19%)
24	CLA	B	608	-	57,73,73	2.56	23 (40%)	61,113,113	2.01	14 (22%)
24	CLA	B	609	-	57,73,73	2.48	22 (38%)	61,113,113	2.15	17 (27%)
24	CLA	B	610	-	57,73,73	2.55	23 (40%)	61,113,113	1.95	12 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	B	611	-	57,73,73	2.50	23 (40%)	61,113,113	1.84	13 (21%)
24	CLA	B	612	-	57,73,73	2.51	22 (38%)	61,113,113	2.00	11 (18%)
24	CLA	B	613	-	57,73,73	2.58	24 (42%)	61,113,113	2.08	15 (24%)
24	CLA	B	614	-	57,73,73	2.55	21 (36%)	61,113,113	1.98	10 (16%)
24	CLA	B	615	-	57,73,73	2.52	22 (38%)	61,113,113	1.90	10 (16%)
24	CLA	B	616	-	57,73,73	2.47	19 (33%)	61,113,113	1.94	15 (24%)
24	CLA	B	617	-	57,73,73	2.50	21 (36%)	61,113,113	1.87	13 (21%)
26	BCR	B	618	-	41,41,41	9.01	29 (70%)	56,56,56	6.05	30 (53%)
26	BCR	B	619	-	41,41,41	9.02	29 (70%)	56,56,56	5.63	29 (51%)
26	BCR	B	620	-	41,41,41	9.20	30 (73%)	56,56,56	5.86	32 (57%)
29	LMG	B	621	-	51,51,55	1.27	4 (7%)	59,59,63	1.01	5 (8%)
28	SQD	B	622	-	53,54,54	1.47	4 (7%)	62,65,65	1.73	9 (14%)
24	CLA	C	501	-	57,73,73	2.54	23 (40%)	61,113,113	2.06	13 (21%)
24	CLA	C	502	-	57,73,73	2.48	22 (38%)	61,113,113	1.93	13 (21%)
24	CLA	C	503	-	57,73,73	2.56	22 (38%)	61,113,113	1.72	11 (18%)
24	CLA	C	504	-	57,73,73	2.54	22 (38%)	61,113,113	2.04	14 (22%)
24	CLA	C	505	-	57,73,73	2.45	21 (36%)	61,113,113	1.95	11 (18%)
24	CLA	C	506	-	57,73,73	2.49	19 (33%)	61,113,113	1.94	10 (16%)
24	CLA	C	507	-	57,73,73	2.44	21 (36%)	61,113,113	2.22	13 (21%)
24	CLA	C	508	-	57,73,73	2.61	23 (40%)	61,113,113	1.92	10 (16%)
24	CLA	C	509	-	57,73,73	2.49	22 (38%)	61,113,113	1.91	13 (21%)
24	CLA	C	510	-	57,73,73	2.57	23 (40%)	61,113,113	1.79	12 (19%)
24	CLA	C	511	3	57,73,73	2.53	22 (38%)	61,113,113	2.02	16 (26%)
24	CLA	C	512	-	57,73,73	2.50	20 (35%)	61,113,113	1.94	14 (22%)
24	CLA	C	513	-	57,73,73	2.42	20 (35%)	61,113,113	1.96	16 (26%)
26	BCR	C	514	-	41,41,41	9.06	29 (70%)	56,56,56	5.96	33 (58%)
32	DGD	C	515	-	63,63,67	1.66	15 (23%)	77,77,81	1.04	5 (6%)
32	DGD	C	516	-	63,63,67	1.63	14 (22%)	77,77,81	1.21	9 (11%)
32	DGD	C	517	-	63,63,67	1.62	14 (22%)	77,77,81	1.15	6 (7%)
29	LMG	C	518	-	51,51,55	1.39	6 (11%)	59,59,63	1.29	8 (13%)
29	LMG	C	519	-	51,51,55	1.31	5 (9%)	59,59,63	1.03	3 (5%)
25	PHO	D	401	-	67,69,69	1.27	10 (14%)	86,99,99	1.11	6 (6%)
24	CLA	D	402	-	57,73,73	2.61	23 (40%)	61,113,113	1.95	16 (26%)
24	CLA	D	403	-	57,73,73	2.65	21 (36%)	61,113,113	1.91	16 (26%)
24	CLA	D	404	-	57,73,73	2.55	22 (38%)	61,113,113	2.01	14 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	PL9	D	405	-	54,55,55	3.98	17 (31%)	68,69,69	4.22	36 (52%)
30	LHG	D	406	-	48,48,48	1.12	3 (6%)	49,54,54	0.98	4 (8%)
30	LHG	D	407	-	48,48,48	1.09	3 (6%)	49,54,54	0.91	3 (6%)
29	LMG	D	408	-	51,51,55	1.31	5 (9%)	59,59,63	1.10	8 (13%)
32	DGD	E	101	-	63,63,67	1.70	15 (23%)	77,77,81	1.24	10 (12%)
30	LHG	E	102	-	41,41,48	1.20	3 (7%)	42,47,54	1.01	2 (4%)
33	HEM	E	103	5,6	24,50,50	2.36	6 (25%)	16,82,82	1.69	1 (6%)
26	BCR	F	101	-	41,41,41	9.10	26 (63%)	56,56,56	6.17	27 (48%)
26	BCR	H	101	-	41,41,41	9.11	30 (73%)	56,56,56	5.80	30 (53%)
32	DGD	H	102	-	63,63,67	1.65	14 (22%)	77,77,81	1.05	6 (7%)
26	BCR	I	101	-	41,41,41	9.12	28 (68%)	56,56,56	6.05	30 (53%)
26	BCR	K	101	-	41,41,41	9.19	31 (75%)	56,56,56	5.50	29 (51%)
26	BCR	K	102	-	41,41,41	9.21	30 (73%)	56,56,56	5.68	25 (44%)
30	LHG	L	101	-	48,48,48	1.09	2 (4%)	49,54,54	0.89	2 (4%)
28	SQD	L	102	-	53,54,54	1.43	4 (7%)	62,65,65	1.62	7 (11%)
26	BCR	T	101	-	41,41,41	9.12	29 (70%)	56,56,56	6.20	33 (58%)
33	HEM	V	201	16	24,50,50	2.32	6 (25%)	16,82,82	1.64	1 (6%)
28	SQD	X	101	-	42,43,54	1.70	3 (7%)	51,54,65	1.78	8 (15%)
29	LMG	Z	101	-	37,37,55	1.41	4 (10%)	45,45,63	1.42	5 (11%)
20	OEX	a	601	1,3	0,15,15	0.00	-	0,32,32	0.00	-
23	BCT	a	605	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	a	606	-	57,73,73	2.59	22 (38%)	61,113,113	1.94	14 (22%)
24	CLA	a	607	-	57,73,73	2.53	21 (36%)	61,113,113	1.88	13 (21%)
25	PHO	a	608	-	67,69,69	1.20	6 (8%)	86,99,99	1.06	6 (6%)
24	CLA	a	609	-	57,73,73	2.52	22 (38%)	61,113,113	1.93	14 (22%)
26	BCR	a	610	-	41,41,41	9.05	30 (73%)	56,56,56	5.69	24 (42%)
27	PL9	a	611	-	54,55,55	3.95	17 (31%)	68,69,69	4.38	37 (54%)
28	SQD	a	612	-	53,54,54	1.49	3 (5%)	62,65,65	1.79	12 (19%)
29	LMG	a	613	-	51,51,55	1.31	5 (9%)	59,59,63	1.02	5 (8%)
28	SQD	a	614	-	53,54,54	1.50	3 (5%)	62,65,65	1.42	6 (9%)
24	CLA	a	615	-	57,73,73	2.60	22 (38%)	61,113,113	2.08	16 (26%)
30	LHG	a	616	-	48,48,48	1.08	2 (4%)	49,54,54	1.20	3 (6%)
28	SQD	b	601	-	53,54,54	1.49	4 (7%)	62,65,65	1.73	9 (14%)
24	CLA	b	603	-	57,73,73	2.52	19 (33%)	61,113,113	1.94	14 (22%)
24	CLA	b	604	-	57,73,73	2.58	21 (36%)	61,113,113	2.08	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	b	605	-	57,73,73	2.58	22 (38%)	61,113,113	2.09	15 (24%)
24	CLA	b	606	-	57,73,73	2.55	20 (35%)	61,113,113	2.00	13 (21%)
24	CLA	b	607	-	57,73,73	2.55	22 (38%)	61,113,113	1.95	12 (19%)
24	CLA	b	608[A]	-	57,73,73	2.50	23 (40%)	61,113,113	2.07	13 (21%)
24	CLA	b	608[B]	-	57,73,73	2.52	23 (40%)	61,113,113	2.07	13 (21%)
24	CLA	b	609	-	57,73,73	2.58	22 (38%)	61,113,113	1.94	13 (21%)
24	CLA	b	610	-	57,73,73	2.50	22 (38%)	61,113,113	1.94	12 (19%)
24	CLA	b	611	-	57,73,73	2.50	21 (36%)	61,113,113	1.97	11 (18%)
24	CLA	b	612	-	57,73,73	2.49	23 (40%)	61,113,113	2.00	15 (24%)
24	CLA	b	613	-	57,73,73	2.55	22 (38%)	61,113,113	2.07	11 (18%)
24	CLA	b	614	-	57,73,73	2.58	23 (40%)	61,113,113	2.15	14 (22%)
24	CLA	b	615	-	57,73,73	2.49	22 (38%)	61,113,113	1.89	10 (16%)
24	CLA	b	616	-	57,73,73	2.51	21 (36%)	61,113,113	1.89	10 (16%)
24	CLA	b	617	-	57,73,73	2.54	22 (38%)	61,113,113	1.96	12 (19%)
24	CLA	b	618	-	57,73,73	2.53	20 (35%)	61,113,113	2.01	15 (24%)
26	BCR	b	619	-	41,41,41	9.31	29 (70%)	56,56,56	5.89	28 (50%)
26	BCR	b	620	-	41,41,41	8.95	29 (70%)	56,56,56	5.77	29 (51%)
26	BCR	b	621	-	41,41,41	9.20	31 (75%)	56,56,56	6.46	32 (57%)
29	LMG	b	622	-	51,51,55	1.30	4 (7%)	59,59,63	1.05	5 (8%)
24	CLA	c	501	-	57,73,73	2.46	19 (33%)	61,113,113	1.96	15 (24%)
24	CLA	c	502	-	57,73,73	2.52	23 (40%)	61,113,113	1.93	10 (16%)
24	CLA	c	503	-	57,73,73	2.54	22 (38%)	61,113,113	1.77	11 (18%)
24	CLA	c	504	-	57,73,73	2.59	23 (40%)	61,113,113	1.98	14 (22%)
24	CLA	c	505	-	57,73,73	2.48	21 (36%)	61,113,113	1.90	9 (14%)
24	CLA	c	506	-	57,73,73	2.52	20 (35%)	61,113,113	1.95	11 (18%)
24	CLA	c	507	-	57,73,73	2.44	20 (35%)	61,113,113	2.16	13 (21%)
24	CLA	c	508	-	57,73,73	2.51	21 (36%)	61,113,113	2.00	11 (18%)
24	CLA	c	509	-	57,73,73	2.52	23 (40%)	61,113,113	2.02	12 (19%)
24	CLA	c	510	-	57,73,73	2.49	21 (36%)	61,113,113	1.91	12 (19%)
24	CLA	c	511	3	57,73,73	2.54	21 (36%)	61,113,113	1.88	11 (18%)
24	CLA	c	512	-	57,73,73	2.53	24 (42%)	61,113,113	1.90	13 (21%)
24	CLA	c	513	-	57,73,73	2.47	23 (40%)	61,113,113	1.88	11 (18%)
26	BCR	c	514	-	41,41,41	9.06	30 (73%)	56,56,56	5.96	34 (60%)
26	BCR	c	515	-	41,41,41	9.22	31 (75%)	56,56,56	5.69	27 (48%)
32	DGD	c	516	-	63,63,67	1.66	15 (23%)	77,77,81	1.10	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	DGD	c	517	-	63,63,67	1.58	15 (23%)	77,77,81	1.14	7 (9%)
32	DGD	c	518	-	63,63,67	1.64	14 (22%)	77,77,81	1.29	8 (10%)
29	LMG	c	519	-	51,51,55	1.36	5 (9%)	59,59,63	1.06	5 (8%)
29	LMG	c	520	-	51,51,55	1.35	5 (9%)	59,59,63	1.13	4 (6%)
26	BCR	c	521	-	41,41,41	9.48	29 (70%)	56,56,56	5.66	25 (44%)
25	PHO	d	401	-	67,69,69	1.27	7 (10%)	86,99,99	1.07	6 (6%)
24	CLA	d	402	-	57,73,73	2.57	22 (38%)	61,113,113	1.92	13 (21%)
24	CLA	d	403	-	57,73,73	2.54	21 (36%)	61,113,113	1.91	13 (21%)
27	PL9	d	404	-	54,55,55	3.95	16 (29%)	68,69,69	4.27	35 (51%)
32	DGD	d	405	-	63,63,67	1.67	15 (23%)	77,77,81	1.16	8 (10%)
30	LHG	d	406	-	48,48,48	1.09	3 (6%)	49,54,54	1.04	3 (6%)
30	LHG	d	407	-	48,48,48	1.13	3 (6%)	49,54,54	1.10	3 (6%)
30	LHG	e	101	-	41,41,48	1.21	3 (7%)	42,47,54	1.08	2 (4%)
33	HEM	e	102	5,6	24,50,50	2.24	6 (25%)	16,82,82	1.78	2 (12%)
26	BCR	f	101	-	41,41,41	9.06	29 (70%)	56,56,56	5.72	25 (44%)
26	BCR	h	101	-	41,41,41	9.24	30 (73%)	56,56,56	5.73	33 (58%)
32	DGD	h	102	-	63,63,67	1.64	15 (23%)	77,77,81	1.24	8 (10%)
29	LMG	j	101	34	51,51,55	1.29	5 (9%)	59,59,63	0.87	2 (3%)
26	BCR	k	101	-	41,41,41	9.28	31 (75%)	56,56,56	5.71	27 (48%)
28	SQD	l	101	-	53,54,54	1.44	3 (5%)	62,65,65	1.62	7 (11%)
30	LHG	l	102	-	48,48,48	1.16	2 (4%)	49,54,54	0.94	2 (4%)
26	BCR	t	101	-	41,41,41	9.10	29 (70%)	56,56,56	6.04	34 (60%)
33	HEM	v	201	16	24,50,50	2.35	7 (29%)	16,82,82	1.49	3 (18%)
28	SQD	x	101	-	42,43,54	1.69	3 (7%)	51,54,65	1.78	8 (15%)
29	LMG	z	101	-	37,37,55	1.38	4 (10%)	45,45,63	1.25	3 (6%)

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
20	OEX	A	601	1,3	-	0/0/68/68	0/0/6/6
23	BCT	A	605	21	-	0/0/0/0	0/0/0/0
24	CLA	A	606	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	A	607	-	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	PHO	A	608	-	-	0/53/103/103	0/1/6/6
24	CLA	A	609	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	A	610	-	-	1/29/63/63	0/2/2/2
27	PL9	A	611	-	-	0/53/73/73	0/1/1/1
28	SQD	A	612	-	-	0/49/69/69	0/1/1/1
29	LMG	A	613	-	-	0/46/66/70	0/1/1/1
28	SQD	A	614	-	-	0/49/69/69	0/1/1/1
30	LHG	A	615	-	-	0/53/53/53	0/0/0/0
24	CLA	B	602	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	604	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	607[A]	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	607[B]	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	609	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	610	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	613	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	617	-	2/2/20/25	0/37/135/135	0/0/9/9
26	BCR	B	618	-	-	1/29/63/63	0/2/2/2
26	BCR	B	619	-	-	4/29/63/63	0/2/2/2
26	BCR	B	620	-	-	2/29/63/63	0/2/2/2
29	LMG	B	621	-	-	0/46/66/70	0/1/1/1
28	SQD	B	622	-	-	0/49/69/69	0/1/1/1
24	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	505	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	508	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	510	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	C	511	3	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	C	512	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	C	513	-	2/2/20/25	0/37/135/135	0/0/9/9
26	BCR	C	514	-	-	1/29/63/63	0/2/2/2
32	DGD	C	515	-	-	0/51/91/95	0/2/2/2
32	DGD	C	516	-	-	0/51/91/95	0/2/2/2
32	DGD	C	517	-	-	0/51/91/95	0/2/2/2
29	LMG	C	518	-	-	0/46/66/70	0/1/1/1
29	LMG	C	519	-	-	0/46/66/70	0/1/1/1
25	PHO	D	401	-	-	0/53/103/103	0/1/6/6
24	CLA	D	402	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	D	403	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	D	404	-	3/3/20/25	0/37/135/135	0/0/9/9
27	PL9	D	405	-	-	0/53/73/73	0/1/1/1
30	LHG	D	406	-	-	0/53/53/53	0/0/0/0
30	LHG	D	407	-	-	0/53/53/53	0/0/0/0
29	LMG	D	408	-	-	0/46/66/70	0/1/1/1
32	DGD	E	101	-	-	0/51/91/95	0/2/2/2
30	LHG	E	102	-	-	0/46/46/53	0/0/0/0
33	HEM	E	103	5,6	-	0/6/54/54	0/0/8/8
26	BCR	F	101	-	-	1/29/63/63	0/2/2/2
26	BCR	H	101	-	-	2/29/63/63	0/2/2/2
32	DGD	H	102	-	-	0/51/91/95	0/2/2/2
26	BCR	I	101	-	-	1/29/63/63	0/2/2/2
26	BCR	K	101	-	-	2/29/63/63	0/2/2/2
26	BCR	K	102	-	-	0/29/63/63	0/2/2/2
30	LHG	L	101	-	-	0/53/53/53	0/0/0/0
28	SQD	L	102	-	-	0/49/69/69	0/1/1/1
26	BCR	T	101	-	-	0/29/63/63	0/2/2/2
33	HEM	V	201	16	-	0/6/54/54	0/0/8/8
28	SQD	X	101	-	-	0/38/58/69	0/1/1/1
29	LMG	Z	101	-	-	1/31/51/70	0/1/1/1
20	OEX	a	601	1,3	-	0/0/68/68	0/0/6/6
23	BCT	a	605	21	-	0/0/0/0	0/0/0/0
24	CLA	a	606	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	a	607	-	3/3/20/25	0/37/135/135	0/0/9/9
25	PHO	a	608	-	-	0/53/103/103	0/1/6/6
24	CLA	a	609	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	a	610	-	-	1/29/63/63	0/2/2/2
27	PL9	a	611	-	-	0/53/73/73	0/1/1/1
28	SQD	a	612	-	-	0/49/69/69	0/1/1/1
29	LMG	a	613	-	-	0/46/66/70	0/1/1/1
28	SQD	a	614	-	-	0/49/69/69	0/1/1/1
24	CLA	a	615	-	3/3/20/25	0/37/135/135	0/0/9/9
30	LHG	a	616	-	-	0/53/53/53	0/0/0/0
28	SQD	b	601	-	-	0/49/69/69	0/1/1/1
24	CLA	b	603	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	604	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	608[A]	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	608[B]	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	609	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	610	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	612	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	617	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	618	-	2/2/20/25	0/37/135/135	0/0/9/9
26	BCR	b	619	-	-	1/29/63/63	0/2/2/2
26	BCR	b	620	-	-	3/29/63/63	0/2/2/2
26	BCR	b	621	-	-	1/29/63/63	0/2/2/2
29	LMG	b	622	-	-	0/46/66/70	0/1/1/1
24	CLA	c	501	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	c	502	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	504	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	505	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	506	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	507	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	508	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	510	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	511	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	512	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	c	513	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	c	514	-	-	1/29/63/63	0/2/2/2
26	BCR	c	515	-	-	1/29/63/63	0/2/2/2
32	DGD	c	516	-	-	0/51/91/95	0/2/2/2
32	DGD	c	517	-	-	0/51/91/95	0/2/2/2
32	DGD	c	518	-	-	0/51/91/95	0/2/2/2
29	LMG	c	519	-	-	0/46/66/70	0/1/1/1
29	LMG	c	520	-	-	0/46/66/70	0/1/1/1
26	BCR	c	521	-	-	0/29/63/63	0/2/2/2
25	PHO	d	401	-	-	0/53/103/103	0/1/6/6
24	CLA	d	402	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	d	403	-	3/3/20/25	0/37/135/135	0/0/9/9
27	PL9	d	404	-	-	0/53/73/73	0/1/1/1
32	DGD	d	405	-	-	0/51/91/95	0/2/2/2
30	LHG	d	406	-	-	0/53/53/53	0/0/0/0
30	LHG	d	407	-	-	0/53/53/53	0/0/0/0
30	LHG	e	101	-	-	0/46/46/53	0/0/0/0
33	HEM	e	102	5,6	-	0/6/54/54	0/0/8/8
26	BCR	f	101	-	-	0/29/63/63	0/2/2/2
26	BCR	h	101	-	-	3/29/63/63	0/2/2/2
32	DGD	h	102	-	-	0/51/91/95	0/2/2/2
29	LMG	j	101	34	-	0/46/66/70	0/1/1/1
26	BCR	k	101	-	-	1/29/63/63	0/2/2/2
28	SQD	l	101	-	-	0/49/69/69	0/1/1/1
30	LHG	l	102	-	-	0/53/53/53	0/0/0/0
26	BCR	t	101	-	-	1/29/63/63	0/2/2/2
33	HEM	v	201	16	-	0/6/54/54	0/0/8/8
28	SQD	x	101	-	-	0/38/58/69	0/1/1/1
29	LMG	z	101	-	-	1/31/51/70	0/1/1/1

The worst 5 of 2600 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	620	BCR	C21-C22	-21.97	1.06	1.35
26	T	101	BCR	C21-C22	-21.78	1.06	1.35
26	H	101	BCR	C21-C22	-21.34	1.06	1.35
26	h	101	BCR	C21-C22	-21.33	1.07	1.35
26	b	619	BCR	C21-C22	-20.94	1.07	1.35

The worst 5 of 1981 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	F	101	BCR	C33-C5-C6	-16.30	107.26	124.62
26	B	618	BCR	C33-C5-C6	-15.99	107.59	124.62
26	T	101	BCR	C38-C26-C25	-15.84	107.75	124.62
26	B	618	BCR	C38-C26-C25	-15.46	108.15	124.62
26	b	619	BCR	C33-C5-C6	-15.27	108.36	124.62

5 of 205 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	C	508	CLA	NA
24	C	508	CLA	NC
24	C	508	CLA	ND
24	b	607	CLA	NA
24	b	607	CLA	NC

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	t	101	BCR	C21-C20-C19-C18
26	b	620	BCR	C17-C16-C15-C14
26	a	610	BCR	C21-C20-C19-C18
26	C	514	BCR	C16-C17-C18-C19
26	c	514	BCR	C20-C21-C22-C23

There are no ring outliers.

73 monomers are involved in 571 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	601	OEX	1	0
24	A	606	CLA	9	0
24	A	607	CLA	7	0
25	A	608	PHO	4	0
24	A	609	CLA	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	610	BCR	19	0
27	A	611	PL9	17	0
28	A	612	SQD	2	0
29	A	613	LMG	3	0
28	A	614	SQD	2	0
30	A	615	LHG	10	0
24	B	602	CLA	6	0
24	B	603	CLA	7	0
24	B	604	CLA	10	0
24	B	605	CLA	11	0
24	B	606	CLA	14	0
24	B	607[A]	CLA	2	0
24	B	607[B]	CLA	6	0
24	B	608	CLA	5	0
24	B	609	CLA	8	0
24	B	610	CLA	5	0
24	B	611	CLA	5	0
24	B	612	CLA	5	0
24	B	613	CLA	8	0
24	B	614	CLA	11	0
24	B	615	CLA	10	0
24	B	616	CLA	9	0
24	B	617	CLA	9	0
26	B	618	BCR	24	0
26	B	619	BCR	36	0
26	B	620	BCR	25	0
29	B	621	LMG	2	0
28	B	622	SQD	6	0
24	C	501	CLA	13	0
24	C	502	CLA	5	0
24	C	503	CLA	11	0
24	C	504	CLA	6	0
24	C	505	CLA	9	0
24	C	506	CLA	10	0
24	C	507	CLA	7	0
24	C	508	CLA	6	0
24	C	509	CLA	4	0
24	C	510	CLA	9	0
24	C	511	CLA	3	0
24	C	512	CLA	4	0
24	C	513	CLA	5	0
26	C	514	BCR	21	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	C	516	DGD	3	0
32	C	517	DGD	7	0
29	C	518	LMG	2	0
29	C	519	LMG	4	0
25	D	401	PHO	12	0
24	D	402	CLA	6	0
24	D	403	CLA	8	0
24	D	404	CLA	6	0
27	D	405	PL9	14	0
30	D	406	LHG	6	0
30	D	407	LHG	4	0
29	D	408	LMG	7	0
32	E	101	DGD	1	0
33	E	103	HEM	6	0
26	F	101	BCR	28	0
26	H	101	BCR	25	0
32	H	102	DGD	11	0
26	I	101	BCR	18	0
26	K	101	BCR	21	0
26	K	102	BCR	15	0
30	L	101	LHG	6	0
28	L	102	SQD	6	0
26	T	101	BCR	29	0
33	V	201	HEM	10	0
28	X	101	SQD	4	0
29	Z	101	LMG	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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(Å²)	Q<0.9	
1	A	334/334 (100%)	0.96	20 (5%)	25	19	57, 63, 84, 93	0
1	a	334/334 (100%)	0.88	24 (7%)	18	15	78, 84, 104, 114	0
2	B	504/504 (100%)	0.76	16 (3%)	51	42	59, 68, 89, 111	0
2	b	504/504 (100%)	0.94	46 (9%)	11	10	80, 88, 110, 131	0
3	C	451/451 (100%)	0.88	27 (5%)	25	19	61, 72, 85, 97	0
3	c	451/451 (100%)	0.85	39 (8%)	13	12	82, 93, 105, 118	0
4	D	342/342 (100%)	0.92	16 (4%)	35	28	57, 64, 80, 102	0
4	d	342/342 (100%)	0.93	25 (7%)	18	14	78, 85, 101, 123	0
5	E	81/81 (100%)	0.75	5 (6%)	24	19	68, 81, 98, 104	0
5	e	81/81 (100%)	0.84	8 (9%)	9	9	89, 102, 119, 125	0
6	F	34/34 (100%)	0.85	1 (2%)	55	45	68, 74, 99, 102	0
6	f	34/34 (100%)	0.93	4 (11%)	6	6	89, 95, 120, 122	0
7	H	65/65 (100%)	0.74	4 (6%)	24	19	64, 74, 81, 99	0
7	h	65/65 (100%)	0.85	8 (12%)	5	6	85, 95, 102, 120	0
8	I	38/38 (100%)	0.56	1 (2%)	59	49	70, 74, 105, 109	0
8	i	38/38 (100%)	0.73	2 (5%)	30	23	90, 95, 126, 130	0
9	J	38/38 (100%)	0.72	2 (5%)	30	23	66, 78, 109, 112	0
9	j	38/38 (100%)	0.69	2 (5%)	30	23	87, 99, 129, 133	0
10	K	37/37 (100%)	0.75	1 (2%)	58	47	74, 79, 86, 88	0
10	k	37/37 (100%)	1.02	4 (10%)	8	7	94, 100, 107, 108	0
11	L	37/37 (100%)	0.69	2 (5%)	29	23	58, 62, 90, 99	0
11	l	37/37 (100%)	0.78	2 (5%)	29	23	79, 83, 111, 120	0
12	M	34/34 (100%)	0.79	2 (5%)	26	20	62, 64, 77, 93	0
12	m	34/34 (100%)	0.87	2 (5%)	26	20	83, 84, 98, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/243 (100%)	0.77	15 (6%) 24 19	59, 73, 95, 111	0
13	o	243/243 (100%)	0.96	27 (11%) 7 7	79, 94, 116, 132	0
14	T	30/30 (100%)	0.50	0 100 100	60, 64, 85, 93	0
14	t	30/30 (100%)	0.58	0 100 100	80, 85, 105, 114	0
15	U	97/97 (100%)	0.77	3 (3%) 52 43	64, 71, 89, 90	0
15	u	97/97 (100%)	0.85	6 (6%) 24 19	84, 92, 110, 111	0
16	V	137/137 (100%)	0.84	9 (6%) 22 16	64, 69, 80, 88	0
16	v	137/137 (100%)	0.79	10 (7%) 18 14	84, 89, 101, 109	0
17	Y	29/29 (100%)	0.75	1 (3%) 49 40	82, 89, 115, 118	0
17	y	29/29 (100%)	0.70	5 (17%) 2 2	103, 110, 136, 138	0
18	X	39/39 (100%)	0.55	1 (2%) 59 49	74, 80, 107, 108	0
18	x	39/39 (100%)	0.52	0 100 100	95, 101, 127, 129	0
19	Z	62/62 (100%)	0.56	2 (3%) 51 42	80, 89, 109, 112	0
19	z	62/62 (100%)	0.50	3 (4%) 34 27	101, 110, 129, 133	0
All	All	5264/5264 (100%)	0.84	345 (6%) 22 16	57, 83, 107, 138	0

The worst 5 of 345 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	d	11	GLU	5.3
9	j	3	SER	5.0
16	v	77	LYS	4.7
1	a	137	LEU	4.6
3	c	293	ASN	4.5

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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(Å <sup>2</sup> )	Q<0.9
26	BCR	H	101	40/40	0.73	0.78	6.73	67,74,83,83	0
29	LMG	C	519	51/55	0.67	0.77	6.56	83,117,122,123	0
28	SQD	a	614	54/54	0.69	0.70	5.98	111,124,129,130	0
30	LHG	E	102	42/49	0.50	0.79	5.80	110,124,127,127	0
32	DGD	d	405	62/66	0.55	0.81	5.40	138,151,164,165	0
27	PL9	A	611	55/55	0.51	0.93	5.36	93,109,118,119	0
29	LMG	b	622	51/55	0.69	0.60	5.11	91,100,112,116	0
29	LMG	c	520	51/55	0.60	0.87	5.07	104,137,142,143	0
29	LMG	z	101	37/55	0.74	0.96	4.54	117,145,149,150	0
26	BCR	K	102	40/40	0.84	0.83	4.10	70,74,78,78	0
29	LMG	B	621	51/55	0.77	0.56	3.90	70,80,92,95	0
26	BCR	C	514	40/40	0.76	0.71	3.88	78,84,87,88	0
28	SQD	x	101	43/54	0.59	0.83	3.81	128,136,140,140	0
29	LMG	A	613	51/55	0.77	0.73	3.70	94,100,105,105	0
26	BCR	k	101	40/40	0.76	0.69	3.62	95,99,100,100	0
26	BCR	t	101	40/40	0.79	0.54	3.60	86,99,106,106	0
28	SQD	L	102	54/54	0.78	0.58	3.54	119,131,146,147	0
22	CL	A	604	1/1	0.82	0.64	3.54	62,62,62,62	0
26	BCR	c	521	40/40	0.76	0.78	3.50	91,95,98,99	0
28	SQD	X	101	43/54	0.76	0.68	3.47	108,115,119,119	0
29	LMG	c	519	51/55	0.62	0.71	3.40	92,118,134,135	0
32	DGD	E	101	62/66	0.56	0.78	3.34	118,130,143,144	0
24	CLA	B	606	65/65	0.87	0.68	3.33	59,64,75,76	0
24	CLA	c	509	65/65	0.89	0.80	3.21	91,93,108,108	0
26	BCR	b	619	40/40	0.83	0.54	3.16	84,88,90,90	0
26	BCR	T	101	40/40	0.78	0.49	3.06	65,78,85,86	0
30	LHG	d	407	49/49	0.84	0.63	3.02	85,89,98,102	0
28	SQD	b	601	54/54	0.72	0.55	2.98	99,107,121,121	0
29	LMG	a	613	51/55	0.82	0.71	2.93	114,121,126,126	0
30	LHG	e	101	42/49	0.56	0.82	2.86	131,145,147,148	0
28	SQD	A	614	54/54	0.72	0.56	2.86	91,103,109,109	0
24	CLA	B	608	65/65	0.85	0.54	2.80	58,61,73,74	0
24	CLA	b	603	65/65	0.77	0.67	2.70	94,102,127,128	0
27	PL9	a	611	55/55	0.52	0.71	2.69	113,130,139,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	BCR	B	618	40/40	0.80	0.55	2.66	63,68,69,70	0
30	LHG	a	616	49/49	0.73	0.74	2.49	87,94,124,125	0
26	BCR	K	101	40/40	0.83	0.63	2.48	75,78,79,80	0
24	CLA	c	508	65/65	0.83	0.52	2.47	87,90,115,119	0
30	LHG	D	406	49/49	0.80	0.61	2.46	70,75,81,82	0
26	BCR	h	101	40/40	0.72	0.60	2.40	87,94,103,104	0
24	CLA	B	602	65/65	0.80	0.55	2.36	73,82,107,107	0
24	CLA	B	611	65/65	0.89	0.60	2.33	62,65,73,77	0
30	LHG	d	406	49/49	0.80	0.63	2.30	91,96,102,102	0
27	PL9	d	404	55/55	0.74	0.67	2.30	80,84,91,93	0
24	CLA	b	615	65/65	0.87	0.48	2.29	80,84,106,108	0
26	BCR	f	101	40/40	0.73	0.56	2.27	87,91,109,110	0
24	CLA	b	609	65/65	0.82	0.51	2.27	79,82,94,95	0
26	BCR	c	514	40/40	0.74	0.63	2.18	99,105,108,108	0
32	DGD	h	102	62/66	0.84	0.62	2.15	87,93,99,101	0
30	LHG	D	407	49/49	0.82	0.55	2.12	64,69,78,81	0
24	CLA	b	612	65/65	0.88	0.61	2.05	82,86,94,98	0
29	LMG	Z	101	37/55	0.55	0.67	2.01	96,124,129,129	0
24	CLA	C	510	65/65	0.90	0.55	1.97	65,69,76,78	0
32	DGD	H	102	62/66	0.85	0.57	1.90	66,72,79,81	0
24	CLA	C	509	65/65	0.88	0.65	1.86	70,72,87,88	0
24	CLA	B	613	65/65	0.87	0.58	1.84	61,64,71,72	0
24	CLA	C	511	65/65	0.89	0.61	1.82	70,75,78,79	0
24	CLA	C	513	65/65	0.79	0.57	1.81	80,85,105,105	0
26	BCR	I	101	40/40	0.74	0.63	1.79	71,78,81,82	0
24	CLA	B	607[B]	65/65	0.81	0.54	1.78	63,67,72,75	65
24	CLA	D	403	65/65	0.88	0.56	1.77	54,59,75,76	0
24	CLA	C	512	65/65	0.90	0.54	1.76	78,82,103,104	0
26	BCR	b	621	40/40	0.78	0.47	1.74	89,94,100,101	0
26	BCR	B	620	40/40	0.79	0.47	1.73	68,74,80,80	0
27	PL9	D	405	55/55	0.80	0.56	1.70	60,64,70,72	0
26	BCR	c	515	40/40	0.76	0.61	1.69	92,98,102,102	0
24	CLA	B	607[A]	65/65	0.81	0.54	1.68	65,69,81,82	65
28	SQD	A	612	54/54	0.83	0.47	1.68	90,98,107,108	0
26	BCR	b	620	40/40	0.81	0.44	1.65	83,89,101,101	0
24	CLA	c	510	65/65	0.86	0.52	1.62	86,90,96,99	0
24	CLA	b	604	65/65	0.89	0.55	1.58	85,88,93,94	0
24	CLA	b	608[A]	65/65	0.78	0.57	1.54	85,90,102,103	65
24	CLA	B	605	65/65	0.88	0.54	1.54	60,63,91,91	0
24	CLA	B	617	65/65	0.84	0.50	1.52	63,69,118,119	0
24	CLA	b	608[B]	65/65	0.78	0.57	1.51	83,87,93,95	65
24	CLA	b	605	65/65	0.89	0.56	1.50	79,84,92,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
30	LHG	A	615	49/49	0.82	0.56	1.44	67,74,103,104	0
24	CLA	b	607	65/65	0.91	0.59	1.35	80,84,95,97	0
24	CLA	B	614	65/65	0.88	0.46	1.34	60,63,85,87	0
26	BCR	a	610	40/40	0.85	0.49	1.33	83,89,93,94	0
24	CLA	B	610	65/65	0.91	0.50	1.28	64,69,72,73	0
24	CLA	c	513	65/65	0.72	0.56	1.27	101,106,125,126	0
24	CLA	b	614	65/65	0.86	0.62	1.26	81,85,91,92	0
24	CLA	C	505	65/65	0.86	0.54	1.24	69,71,85,85	0
24	CLA	c	507	65/65	0.89	0.56	1.23	91,94,113,115	0
26	BCR	F	101	40/40	0.81	0.49	1.22	66,71,88,90	0
24	CLA	C	504	65/65	0.86	0.53	1.19	66,68,95,95	0
28	SQD	a	612	54/54	0.68	0.44	1.15	110,119,128,128	0
24	CLA	B	604	65/65	0.90	0.54	1.14	58,63,72,76	0
24	CLA	b	606	65/65	0.89	0.53	1.11	81,84,111,112	0
24	CLA	c	506	65/65	0.85	0.48	1.07	93,100,136,136	0
24	CLA	B	603	65/65	0.88	0.53	1.05	64,67,72,73	0
24	CLA	c	505	65/65	0.87	0.52	1.05	89,92,106,106	0
29	LMG	D	408	51/55	0.76	0.50	1.03	66,76,106,108	0
24	CLA	b	617	65/65	0.82	0.55	1.03	86,89,107,108	0
25	PHO	a	608	64/64	0.88	0.51	1.02	78,83,86,87	0
32	DGD	c	517	62/66	0.83	0.46	1.01	84,96,124,124	0
24	CLA	b	613	65/65	0.89	0.49	1.00	80,83,94,96	0
26	BCR	A	610	40/40	0.84	0.48	0.99	63,68,73,73	0
24	CLA	a	615	65/65	0.93	0.47	0.97	75,79,91,96	0
24	CLA	C	503	65/65	0.89	0.52	0.96	68,72,76,77	0
24	CLA	c	504	65/65	0.86	0.46	0.94	86,89,115,116	0
24	CLA	B	616	65/65	0.86	0.51	0.91	65,68,86,87	0
24	CLA	C	501	65/65	0.85	0.53	0.91	69,73,85,87	0
33	HEM	V	201	43/43	0.92	0.54	0.90	63,65,68,69	0
29	LMG	C	518	51/55	0.64	0.54	0.90	72,98,113,114	0
24	CLA	c	511	65/65	0.88	0.55	0.90	90,95,99,99	0
24	CLA	a	609	65/65	0.88	0.47	0.89	83,85,133,133	0
24	CLA	c	503	65/65	0.87	0.53	0.89	89,93,96,97	0
24	CLA	A	606	65/65	0.91	0.52	0.89	56,59,66,75	0
24	CLA	B	612	65/65	0.89	0.49	0.88	60,62,73,75	0
32	DGD	c	516	62/66	0.70	0.55	0.86	84,94,122,124	0
24	CLA	a	606	65/65	0.88	0.52	0.85	77,80,87,95	0
33	HEM	E	103	43/43	0.92	0.46	0.79	80,82,86,87	0
24	CLA	A	609	65/65	0.90	0.46	0.79	62,65,112,113	0
24	CLA	b	618	65/65	0.88	0.54	0.78	83,90,139,139	0
24	CLA	c	502	65/65	0.90	0.50	0.77	85,87,101,103	0
24	CLA	b	616	65/65	0.84	0.56	0.76	82,86,121,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	CLA	b	611	65/65	0.88	0.52	0.73	85,90,92,93	0
24	CLA	D	402	65/65	0.91	0.47	0.72	54,59,70,76	0
33	HEM	v	201	43/43	0.91	0.52	0.72	84,86,88,90	0
33	HEM	e	102	43/43	0.92	0.48	0.70	101,103,107,108	0
24	CLA	C	502	65/65	0.88	0.46	0.69	65,67,80,83	0
32	DGD	C	515	62/66	0.80	0.48	0.69	64,73,102,103	0
25	PHO	A	608	64/64	0.89	0.49	0.68	57,62,65,67	0
24	CLA	b	610	65/65	0.85	0.47	0.66	82,86,92,93	0
24	CLA	d	402	65/65	0.87	0.52	0.66	75,80,95,96	0
24	CLA	B	609	65/65	0.89	0.45	0.64	61,65,71,72	0
24	CLA	B	615	65/65	0.87	0.49	0.63	61,65,101,102	0
26	BCR	B	619	40/40	0.80	0.42	0.59	62,69,81,81	0
28	SQD	l	101	54/54	0.83	0.42	0.55	98,110,125,126	0
25	PHO	d	401	64/64	0.87	0.46	0.54	80,84,90,94	0
25	PHO	D	401	64/64	0.88	0.45	0.53	59,63,69,73	0
24	CLA	c	512	65/65	0.81	0.50	0.50	99,102,124,124	0
30	LHG	l	102	49/49	0.77	0.45	0.49	84,92,104,106	0
28	SQD	B	622	54/54	0.81	0.42	0.47	119,127,141,142	0
23	BCT	A	605	4/4	0.85	0.52	0.46	79,80,81,82	0
24	CLA	C	508	65/65	0.88	0.46	0.46	66,70,95,99	0
24	CLA	A	607	65/65	0.92	0.46	0.45	60,62,104,106	0
24	CLA	C	507	65/65	0.85	0.49	0.44	70,74,92,94	0
34	MG	j	102	1/1	0.97	0.43	0.41	89,89,89,89	0
24	CLA	a	607	65/65	0.87	0.47	0.41	80,83,124,126	0
32	DGD	c	518	62/66	0.79	0.47	0.33	83,93,113,117	0
29	LMG	j	101	51/55	0.71	0.44	0.32	87,96,126,129	0
24	CLA	c	501	65/65	0.85	0.51	0.31	90,93,106,108	0
24	CLA	D	404	65/65	0.91	0.42	0.30	65,68,106,107	0
22	CL	A	603	1/1	0.75	0.45	0.29	65,65,65,65	0
32	DGD	C	517	62/66	0.82	0.46	0.18	62,72,93,97	0
32	DGD	C	516	62/66	0.84	0.42	0.03	63,75,103,104	0
30	LHG	L	101	49/49	0.83	0.41	0.01	63,72,83,85	0
24	CLA	C	506	65/65	0.88	0.40	-0.00	72,79,115,115	0
24	CLA	d	403	65/65	0.89	0.40	0.00	86,89,126,128	0
23	BCT	a	605	4/4	0.95	0.48	-0.03	100,101,101,103	0
34	MG	J	101	1/1	0.95	0.38	-0.20	68,68,68,68	0
20	OEX	a	601	10/10	0.96	0.40	-0.26	83,84,87,88	0
22	CL	a	603	1/1	0.90	0.39	-0.31	86,86,86,86	0
22	CL	a	604	1/1	0.60	0.32	-0.80	83,83,83,83	0
31	CA	o	301	1/1	0.84	0.41	-1.00	110,110,110,110	0
21	FE2	a	602	1/1	0.95	0.30	-1.13	88,88,88,88	0
20	OEX	A	601	10/10	0.97	0.39	-1.28	63,64,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
21	FE2	A	602	1/1	0.94	0.32	-1.39	67,67,67,67	0
31	CA	f	102	1/1	0.86	0.15	-	118,118,118,118	0
31	CA	B	601	1/1	0.20	0.46	-	117,117,117,117	0
31	CA	O	301	1/1	0.47	0.21	-	90,90,90,90	0
31	CA	b	602	1/1	0.47	0.39	-	137,137,137,137	0
22	CL	U	201	1/1	0.67	0.53	-	91,91,91,91	0
31	CA	F	102	1/1	0.33	0.18	-	97,97,97,97	0
22	CL	u	201	1/1	0.34	0.61	-	112,112,112,112	0

## 6.5 Other polymers

There are no such residues in this entry.