



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 09:04 PM GMT

PDB ID : 4RVY  
Title : Serial Time resolved crystallography of Photosystem II using a femtosecond X-ray laser. The S state after two flashes (S3)  
Authors : Kupitz, C.; Basu, S.; Grotjohann, I.; Fromme, R.; Zatsepin, N.; Rendek, K.N.; Hunter, M.; Shoeman, R.L.; White, T.A.; Wang, D.; James, D.; Yang, J.-H.; Cobb, D.E.; Reeder, B.; Sierra, R.G.; Liu, H.; Barty, A.; Aquila, A.; Deponte, D.; Kirian, R.; Bari, S.; Bergkamp, J.J.; Beyerlein, K.; Bogan, M.J.; Caleman, C.; Chao, T.-C.; Conrad, C.E.; Davis, K.M.; Fleckenstein, H.; Galli, L.; Hau-Riege, S.P.; Kassemeyer, S.; Laksmono, H.; Liang, M.; Lomb, L.; Marchesini, S.; Martin, A.V.; Messerschmidt, M.; Milathianaki, D.; Nass, K.; Ros, A.; Roy-Chowdhury, S.; Schmidt, K.; Seibert, M.; Steinbrener, J.; Stellato, F.; Yan, L.; Yoon, C.; Moore, T.A.; Moore, A.L.; Pushkar, Y.; Williams, G.J.; Boutet, S.; Doak, R.B.; Weierstall, U.; Frank, M.; Chapman, H.N.; Spence, J.C.H.; Fromme, P.  
Deposited on : 2014-11-29  
Resolution : 5.50 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-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135

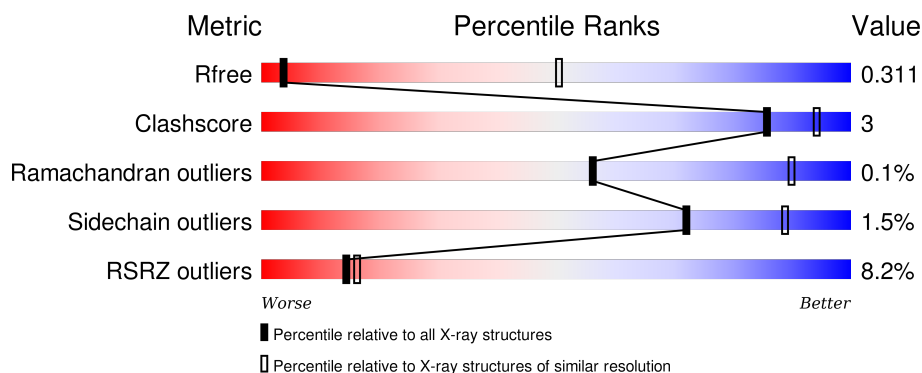
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 5.50 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	1015 (7.38-3.62)
Clashscore	102246	1020 (7.10-3.70)
Ramachandran outliers	100387	1014 (7.36-3.64)
Sidechain outliers	100360	1013 (7.38-3.62)
RSRZ outliers	91569	1014 (7.38-3.62)

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	
1	a	334	

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CCP4 : 6.5.0  
 Ideal geometry (proteins) : Engh & Huber (2001)  
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : rb-20026982

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Mol	Chain	Length	Quality of chain
2	B	504	
2	b	504	
3	C	461	
3	c	461	
4	D	342	
4	d	342	
5	E	81	
5	e	81	
6	F	34	
6	f	34	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	34	
12	m	34	
13	O	243	
13	o	243	
14	T	30	

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Mol	Chain	Length	Quality of chain
14	t	30	
15	U	97	
15	u	97	
16	V	137	
16	v	137	
17	X	39	
17	x	39	
18	Y	29	
18	y	29	
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
20	OEX	a	601	-	-	-	X
22	CLA	A	603	X	-	-	X
22	CLA	A	604	X	-	-	X
22	CLA	A	607	X	-	-	X
22	CLA	B	602	X	-	-	X
22	CLA	B	603	X	-	-	X
22	CLA	B	604	X	-	-	X
22	CLA	B	605	X	-	-	X
22	CLA	B	606	X	-	-	X
22	CLA	B	607	X	-	-	X
22	CLA	B	608	X	-	-	X
22	CLA	B	609	X	-	-	X
22	CLA	B	610	X	-	-	X
22	CLA	B	611	X	-	-	X
22	CLA	B	612	X	-	-	X
22	CLA	B	613	X	-	-	X
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	616	X	-	-	X
22	CLA	B	617	X	-	-	X
22	CLA	C	501	X	-	-	X
22	CLA	C	502	X	-	-	X
22	CLA	C	503	X	-	-	X
22	CLA	C	504	X	-	-	X
22	CLA	C	505	X	-	-	X
22	CLA	C	506	X	-	-	X
22	CLA	C	507	X	-	-	X
22	CLA	C	508	X	-	-	X
22	CLA	C	509	X	-	-	X
22	CLA	C	510	X	-	-	X
22	CLA	C	511	X	-	-	X
22	CLA	C	512	X	-	-	X
22	CLA	C	513	X	-	-	X
22	CLA	D	401	X	-	-	X
22	CLA	D	402	X	-	-	X
22	CLA	D	403	X	-	-	X
22	CLA	a	603	X	-	-	X
22	CLA	a	604	X	-	-	X
22	CLA	a	607	X	-	-	X
22	CLA	b	602	X	-	-	X
22	CLA	b	603	X	-	-	X
22	CLA	b	604	X	-	-	X
22	CLA	b	605	X	-	-	X
22	CLA	b	606	X	-	-	X
22	CLA	b	607	X	-	-	X
22	CLA	b	608	X	-	-	X
22	CLA	b	609	X	-	-	X
22	CLA	b	610	X	-	-	X
22	CLA	b	611	X	-	-	X
22	CLA	b	612	X	-	-	X
22	CLA	b	613	X	-	-	X
22	CLA	b	614	X	-	-	X
22	CLA	b	615	X	-	-	X
22	CLA	b	616	X	-	-	X
22	CLA	b	617	X	-	-	X
22	CLA	c	501	X	-	-	X
22	CLA	c	502	X	-	-	X
22	CLA	c	503	X	-	-	X
22	CLA	c	504	X	-	-	X
22	CLA	c	505	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	506	X	-	-	X
22	CLA	c	507	X	-	-	X
22	CLA	c	508	X	-	-	X
22	CLA	c	509	X	-	-	X
22	CLA	c	510	X	-	-	X
22	CLA	c	511	X	-	-	X
22	CLA	c	512	X	-	-	X
22	CLA	c	513	X	-	-	X
22	CLA	d	401	X	-	-	X
22	CLA	d	402	X	-	-	X
22	CLA	d	403	X	-	-	X
23	PHO	A	605	-	-	-	X
23	PHO	A	606	-	-	-	X
23	PHO	a	605	-	-	-	X
23	PHO	a	606	-	-	-	X
24	BCR	A	608	-	-	-	X
24	BCR	B	622	-	-	-	X
24	BCR	C	514	-	-	-	X
24	BCR	C	515	-	-	-	X
24	BCR	D	404	-	-	-	X
24	BCR	H	101	-	-	-	X
24	BCR	K	101	-	-	-	X
24	BCR	K	102	-	-	-	X
24	BCR	T	102	-	-	-	X
24	BCR	a	608	-	-	-	X
24	BCR	b	618	-	-	-	X
24	BCR	b	622	-	-	-	X
24	BCR	c	514	-	-	-	X
24	BCR	c	515	-	-	-	X
24	BCR	d	404	-	-	-	X
24	BCR	h	101	-	-	-	X
24	BCR	k	101	-	-	-	X
24	BCR	k	102	-	-	-	X
24	BCR	t	101	-	-	-	X
25	SQD	A	609	-	-	-	X
25	SQD	D	411	-	-	-	X
25	SQD	L	101	-	-	-	X
25	SQD	a	609	-	-	-	X
25	SQD	b	601	-	-	-	X
25	SQD	b	621	-	-	-	X
25	SQD	d	411	-	-	-	X
26	CL	A	610	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CL	a	610	-	-	-	X
27	BCT	A	612	-	-	-	X
27	BCT	a	612	-	-	-	X
28	PL9	A	613	-	-	-	X
28	PL9	D	408	-	-	-	X
28	PL9	a	613	-	-	-	X
29	LMG	A	614	-	-	-	X
29	LMG	C	519	-	-	-	X
29	LMG	C	520	-	-	-	X
29	LMG	D	406	-	-	-	X
29	LMG	Z	101	-	-	-	X
29	LMG	a	614	-	-	-	X
29	LMG	c	519	-	-	-	X
29	LMG	c	520	-	-	-	X
29	LMG	d	406	-	-	-	X
29	LMG	z	101	-	-	-	X
31	DGD	C	516	-	-	-	X
31	DGD	C	517	-	-	-	X
31	DGD	C	518	-	-	-	X
31	DGD	D	410	-	-	-	X
31	DGD	H	102	-	-	-	X
31	DGD	c	516	-	-	-	X
31	DGD	c	518	-	-	-	X
31	DGD	d	410	-	-	-	X
31	DGD	h	102	-	-	-	X
32	LHG	D	407	-	-	-	X
32	LHG	D	409	-	-	-	X
32	LHG	E	101	-	-	-	X
32	LHG	d	405	-	-	-	X
32	LHG	d	409	-	-	-	X
32	LHG	e	101	-	-	-	X
33	HEM	F	101	-	-	-	X
33	HEM	V	201	-	-	-	X
33	HEM	f	101	-	-	-	X
33	HEM	v	201	-	-	-	X

## 2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 49594 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	0	0
			2620	1716	431	458	15			
1	a	334	Total	C	N	O	S	0	0	0
			2620	1716	431	458	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	0	0
			3969	2605	661	690	13			
2	b	504	Total	C	N	O	S	0	0	0
			3969	2605	661	690	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	0	0
			3486	2281	584	608	13			
3	c	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	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	0	0
			662	432	107	123				
5	e	81	Total	C	N	O		0	0	0
			662	432	107	123				

- 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
			511	341	82	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	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	0	0
			312	210	48	53	1			
8	i	38	Total	C	N	O	S	0	0	0
			312	210	48	53	1			

- 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	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	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	4			
13	o	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	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
			256	180	36	38	2			
14	t	30	Total	C	N	O	S	0	0	0
			256	180	36	38	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	0	0
			1064	675	177	208	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	39	Total	C	N	O	0	0	0
			287	191	46	50			
17	x	39	Total	C	N	O	0	0	0
			287	191	46	50			

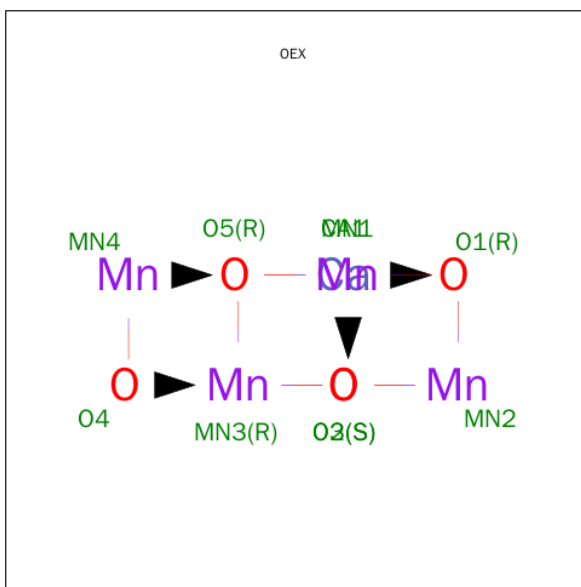
- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

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

- 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:  $\text{CaMn}_4\text{O}_5$ ).

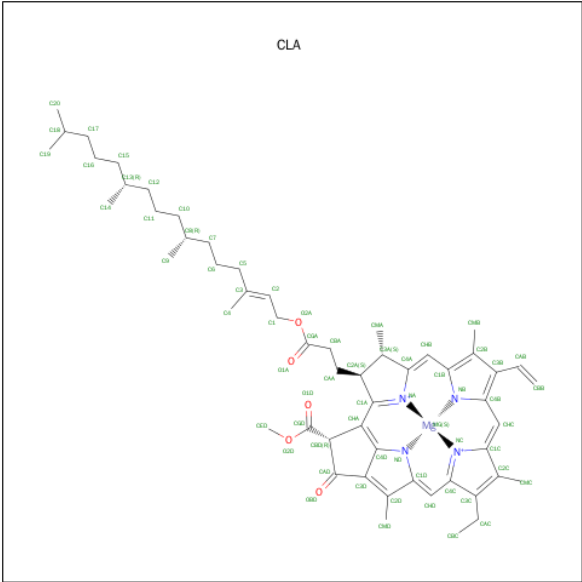


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
20	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- 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 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
22	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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

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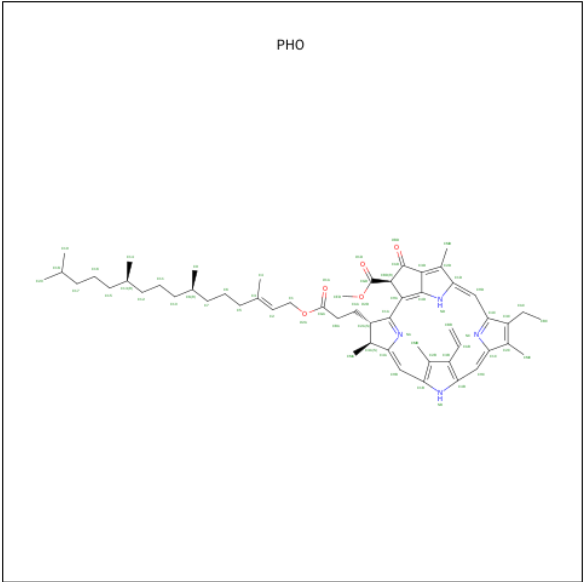
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N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

*Continued on next page...*

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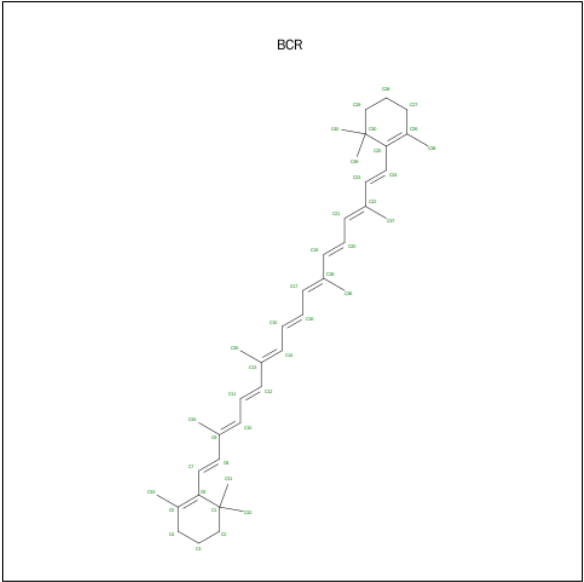
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N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

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



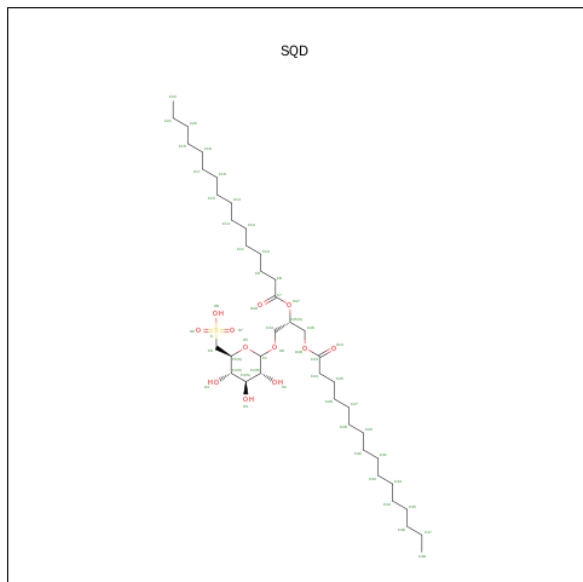
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	a	1	Total	C	N	O	0	0
			64	55	4	5		
23	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	d	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	h	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	k	1	Total C 40 40	0	0
24	k	1	Total C 40 40	0	0
24	T	1	Total C 40 40	0	0
24	T	1	Total C 40 40	0	0
24	t	1	Total C 40 40	0	0

- Molecule 25 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).

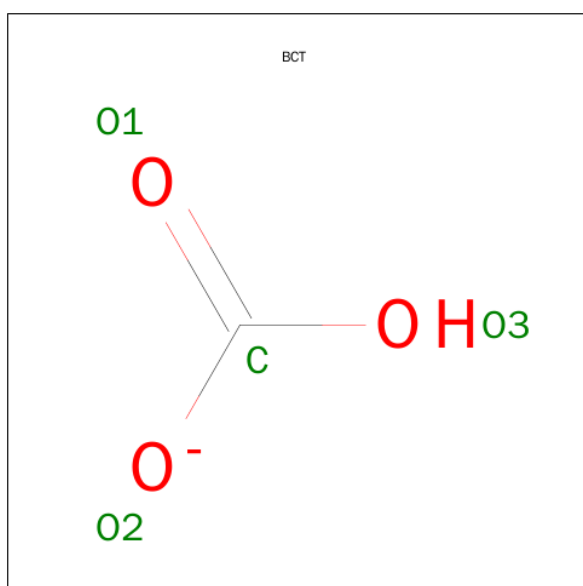


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	O	S	0	0
			54	41	12	1		
25	a	1	Total	C	O	S	0	0
			54	41	12	1		
25	B	1	Total	C	O	S	0	0
			54	41	12	1		
25	b	1	Total	C	O	S	0	0
			54	41	12	1		
25	b	1	Total	C	O	S	0	0
			54	41	12	1		
25	D	1	Total	C	O	S	0	0
			43	30	12	1		
25	d	1	Total	C	O	S	0	0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

- Molecule 26 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

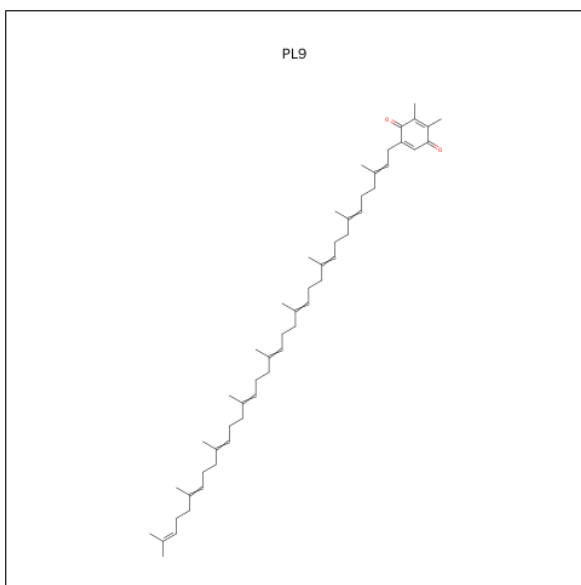
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	2	Total Cl 2 2	0	0
26	u	1	Total Cl 1 1	0	0
26	a	2	Total Cl 2 2	0	0
26	U	1	Total Cl 1 1	0	0

- Molecule 27 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



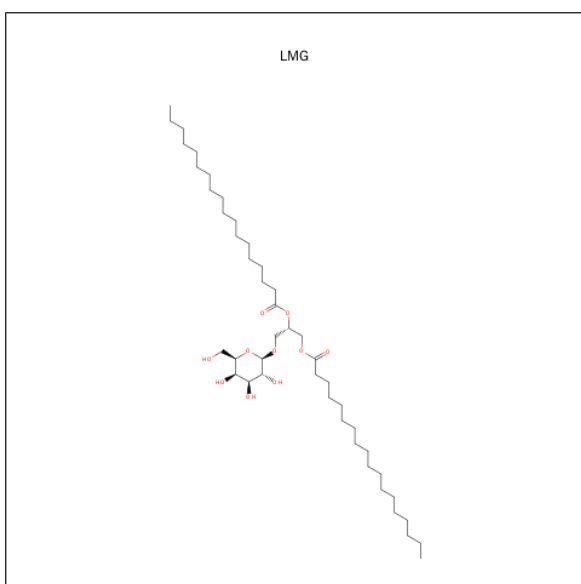
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 4 1 3	0	0
27	a	1	Total C O 4 1 3	0	0

- 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:  $\text{C}_{53}\text{H}_{80}\text{O}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			55	53	2		
28	a	1	Total	C	O	0	0
			55	53	2		
28	D	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-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).

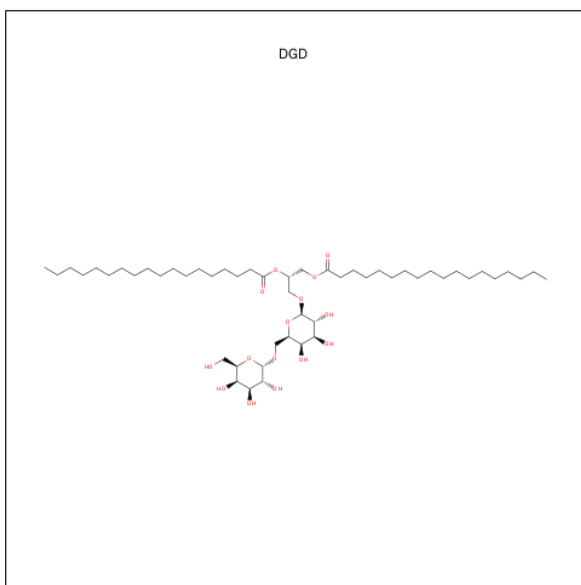


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 51 41 10	0	0
29	a	1	Total C O 51 41 10	0	0
29	B	1	Total C O 51 41 10	0	0
29	b	1	Total C O 51 41 10	0	0
29	C	1	Total C O 51 41 10	0	0
29	C	1	Total C O 51 41 10	0	0
29	c	1	Total C O 51 41 10	0	0
29	c	1	Total C O 51 41 10	0	0
29	D	1	Total C O 51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

- Molecule 30 is CALCIUM ION (three-letter code: CA) (formula: Ca).

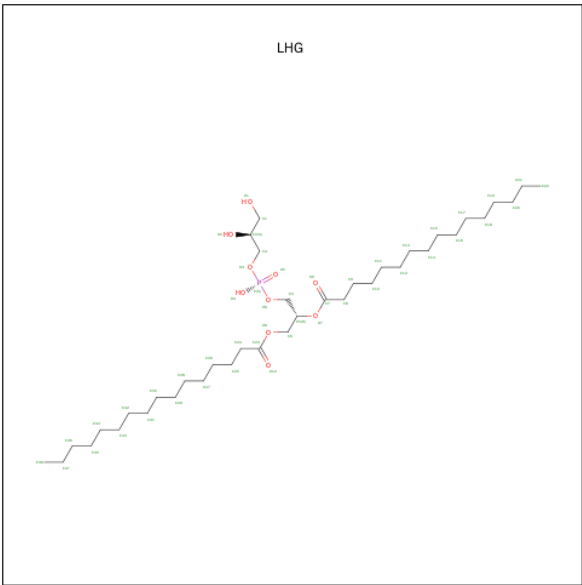
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	B	1	Total Ca 1 1	0	0
30	F	1	Total Ca 1 1	0	0
30	o	1	Total Ca 1 1	0	0
30	O	1	Total Ca 1 1	0	0
30	b	1	Total Ca 1 1	0	0
30	f	1	Total Ca 1 1	0	0

- Molecule 31 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
31	C	1	Total	C	O	0	0
			62	47	15		
31	C	1	Total	C	O	0	0
			62	47	15		
31	C	1	Total	C	O	0	0
			62	47	15		
31	c	1	Total	C	O	0	0
			62	47	15		
31	c	1	Total	C	O	0	0
			62	47	15		
31	c	1	Total	C	O	0	0
			62	47	15		
31	D	1	Total	C	O	0	0
			62	47	15		
31	d	1	Total	C	O	0	0
			62	47	15		
31	H	1	Total	C	O	0	0
			62	47	15		
31	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



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

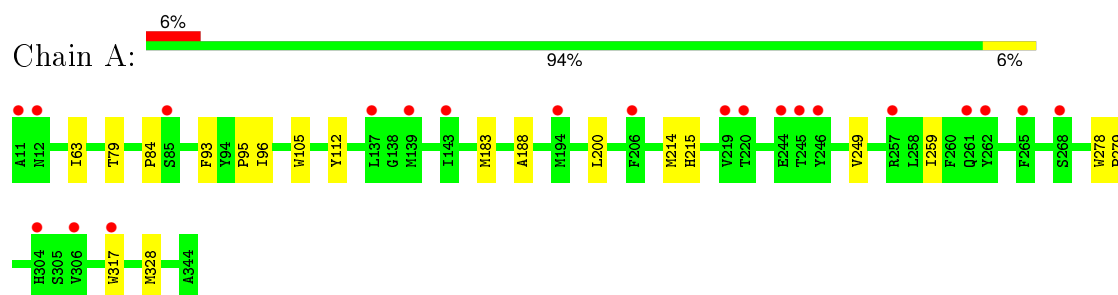
- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



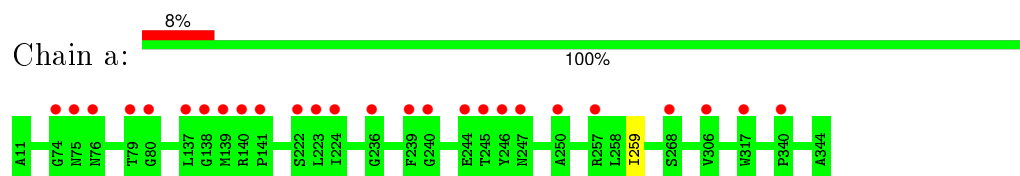
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

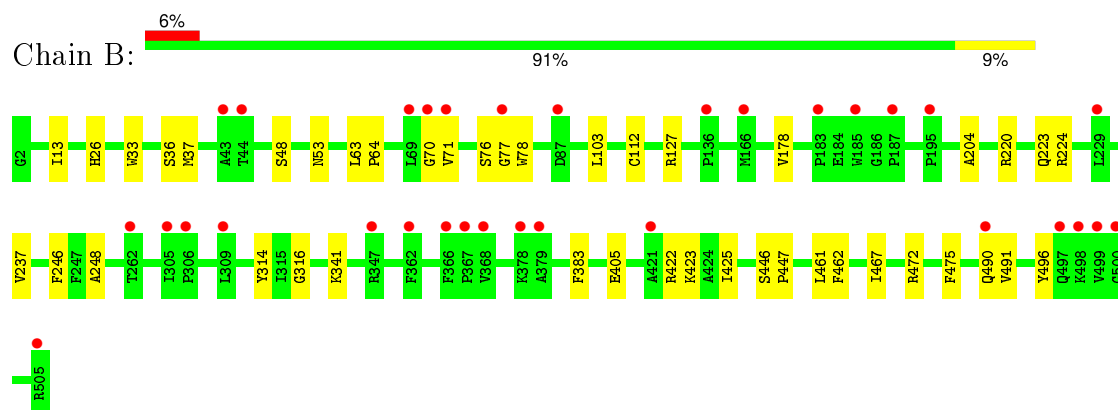
- Molecule 1: Photosystem II protein D1 1



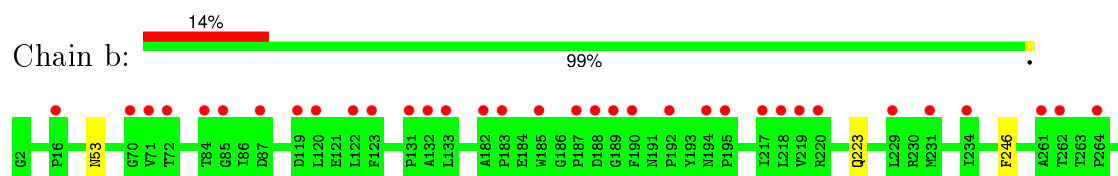
- Molecule 1: Photosystem II protein D1 1

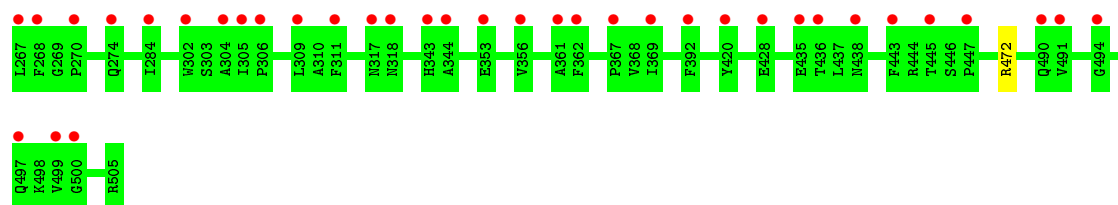


- Molecule 2: Photosystem II CP47 reaction center protein

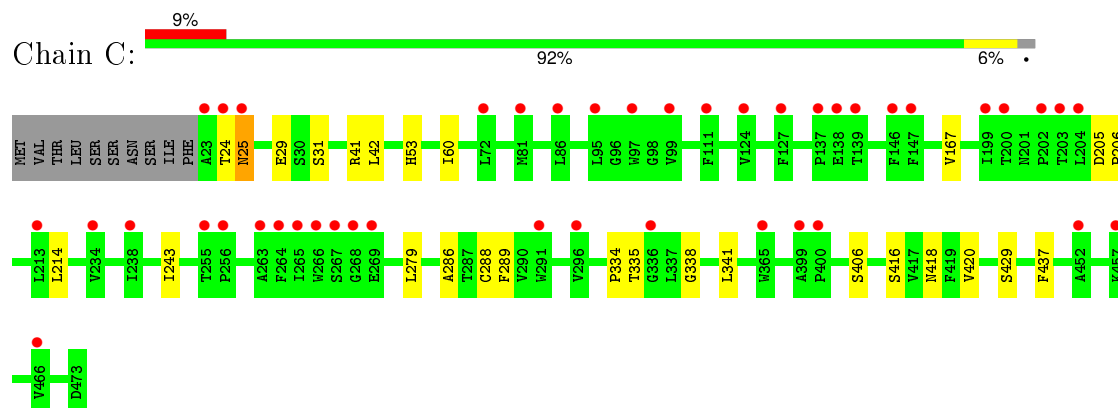


- Molecule 2: Photosystem II CP47 reaction center protein

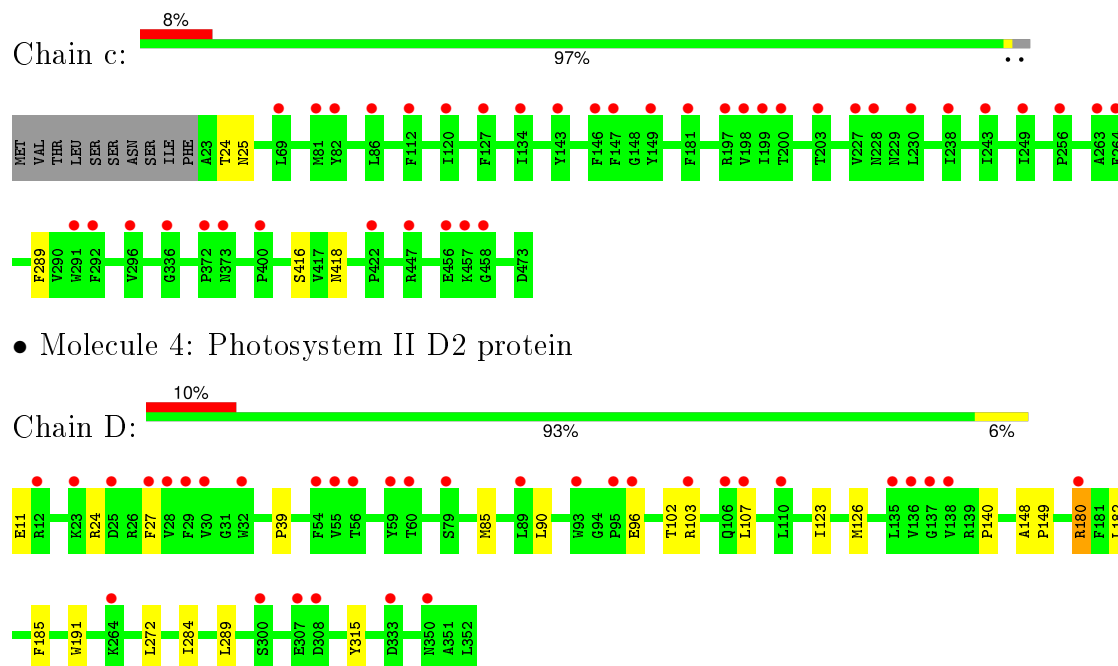




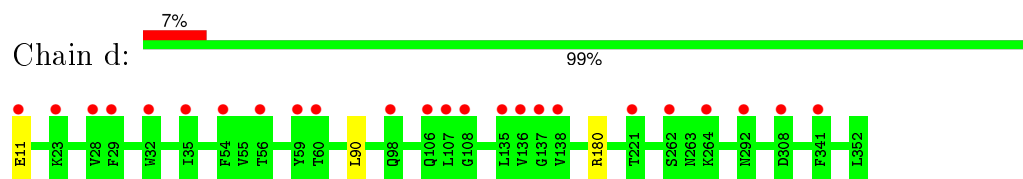
• Molecule 3: Photosystem II CP43 reaction center protein



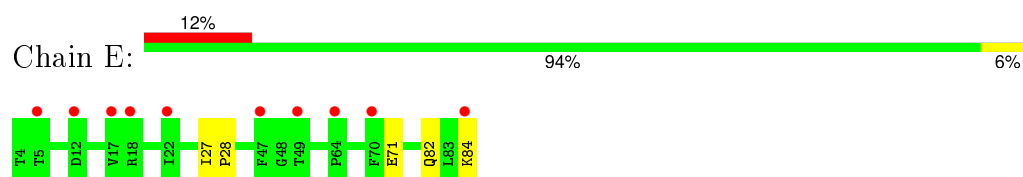
• Molecule 4: Photosystem II D2 protein



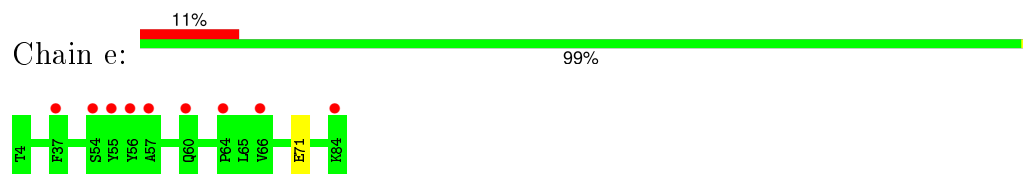
• Molecule 4: Photosystem II D2 protein



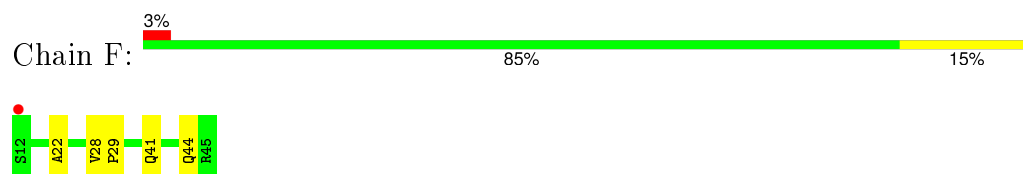
• Molecule 5: Cytochrome b559 subunit alpha



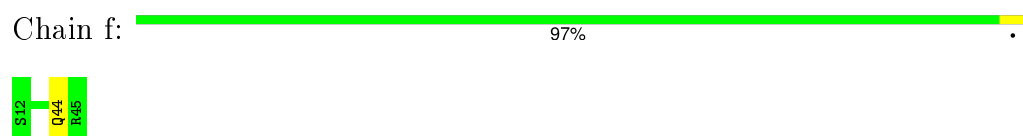
- Molecule 5: Cytochrome b559 subunit alpha



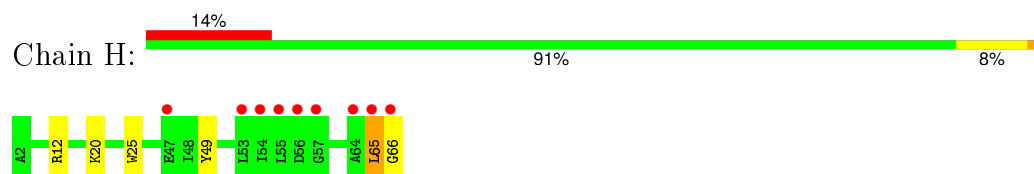
- Molecule 6: Cytochrome b559 subunit beta



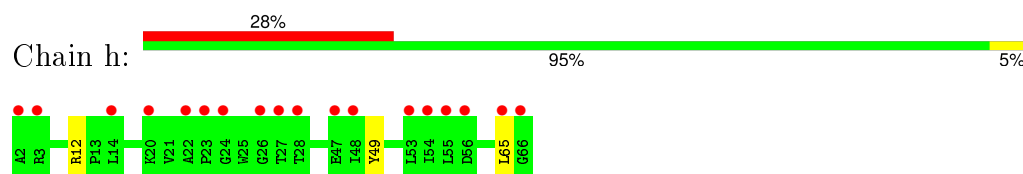
- Molecule 6: Cytochrome b559 subunit beta



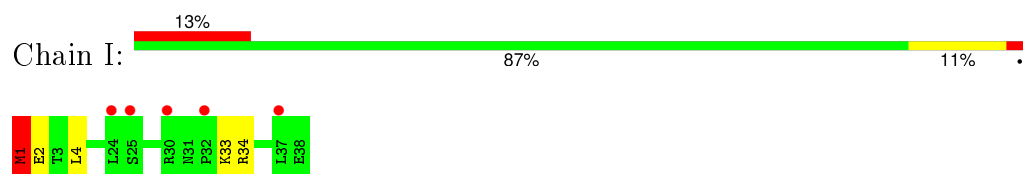
- Molecule 7: Photosystem II reaction center protein H



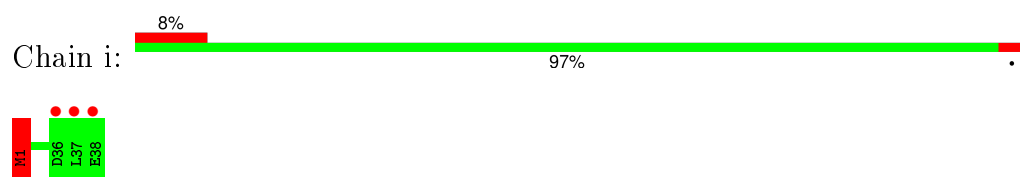
- Molecule 7: Photosystem II reaction center protein H



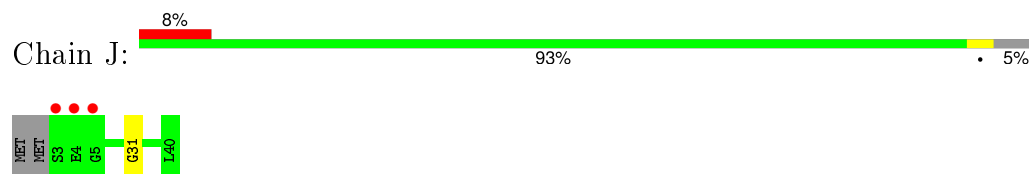
- Molecule 8: Photosystem II reaction center protein I



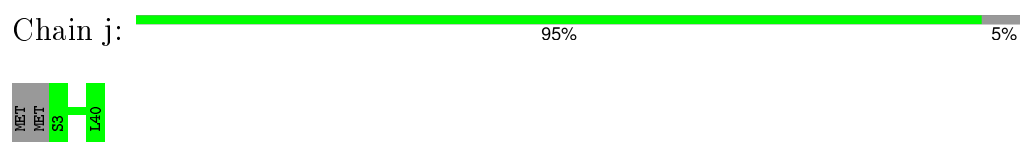
- Molecule 8: Photosystem II reaction center protein I



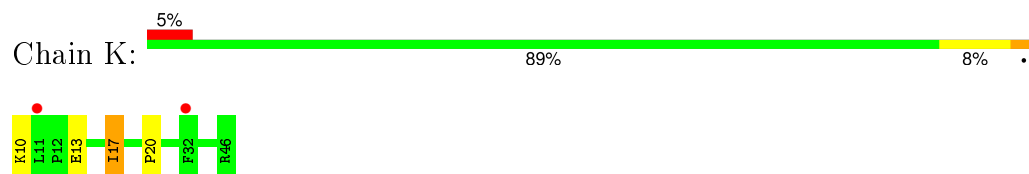
- Molecule 9: Photosystem II reaction center protein J



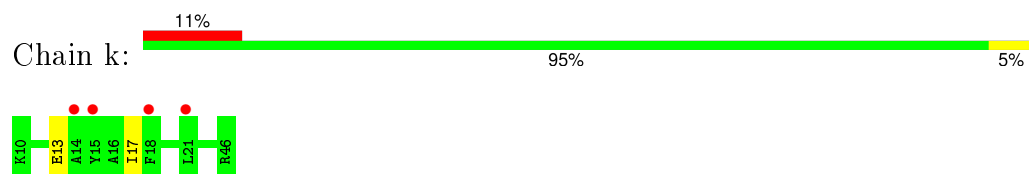
- Molecule 9: Photosystem II reaction center protein J



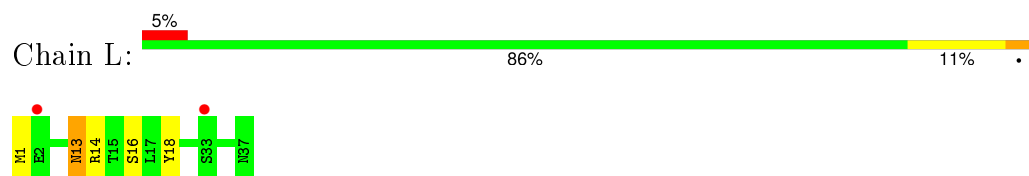
- Molecule 10: Photosystem II reaction center protein K



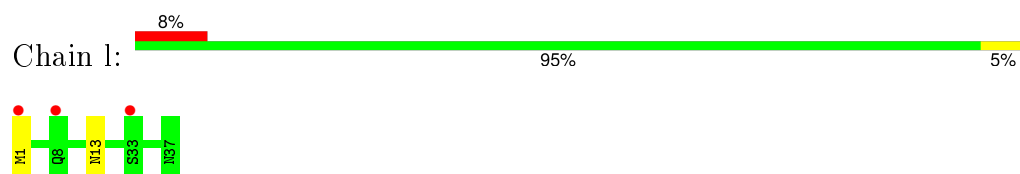
- Molecule 10: Photosystem II reaction center protein K



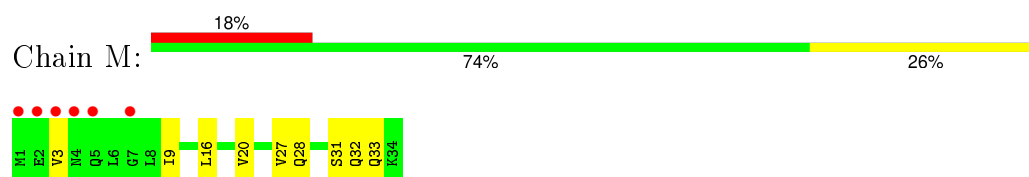
- Molecule 11: Photosystem II reaction center protein L



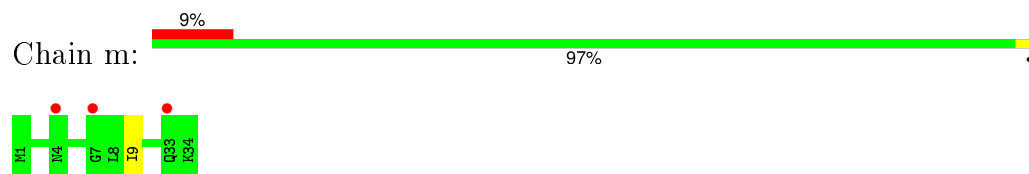
- Molecule 11: Photosystem II reaction center protein L



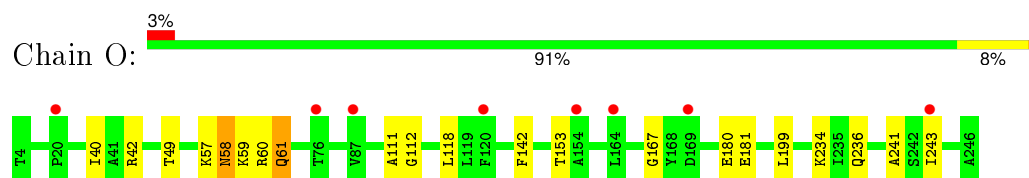
- Molecule 12: Photosystem II reaction center protein M



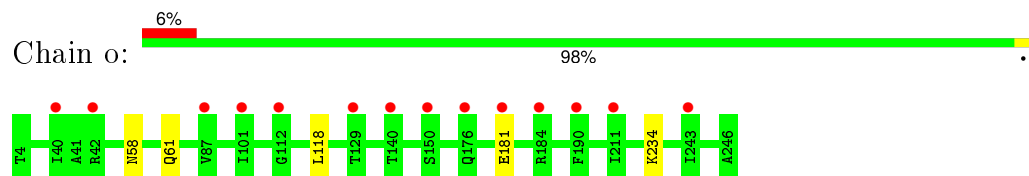
- Molecule 12: Photosystem II reaction center protein M



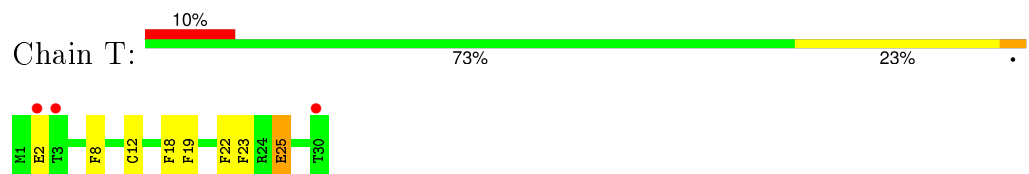
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



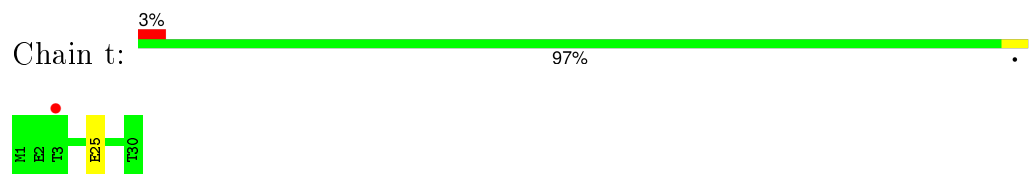
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



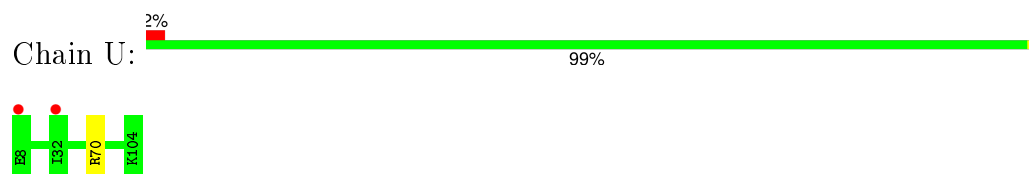
- Molecule 14: Photosystem II reaction center protein T



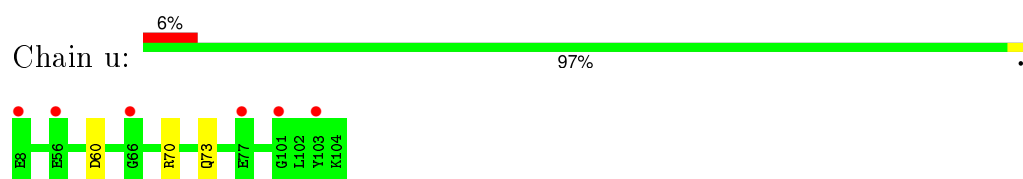
- Molecule 14: Photosystem II reaction center protein T



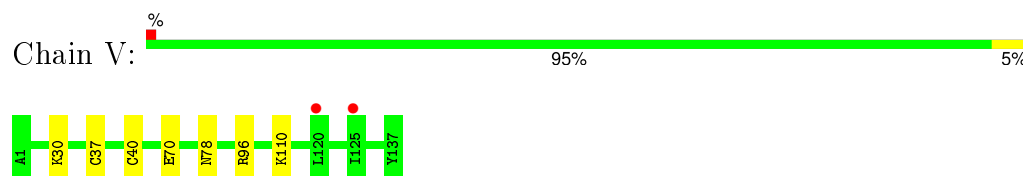
- Molecule 15: Photosystem II 12 kDa extrinsic protein



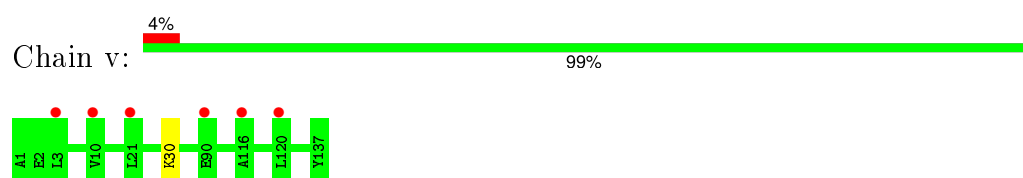
- Molecule 15: Photosystem II 12 kDa extrinsic protein



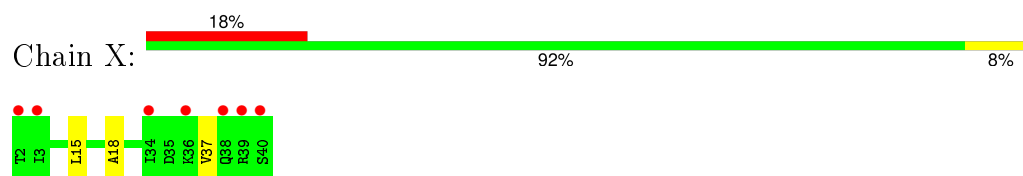
- Molecule 16: Cytochrome c-550



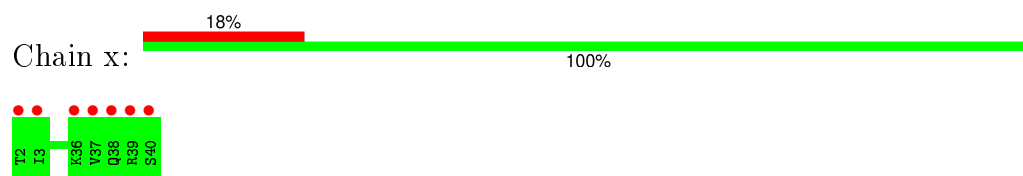
- Molecule 16: Cytochrome c-550



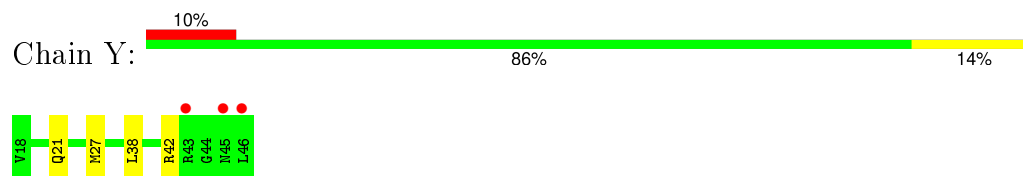
- Molecule 17: Photosystem II reaction center X protein



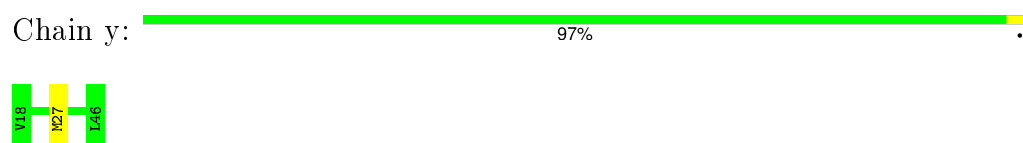
- Molecule 17: Photosystem II reaction center X protein



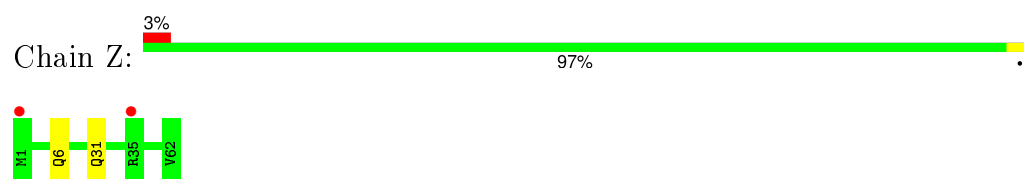
- Molecule 18: Photosystem II reaction center protein Ycf12



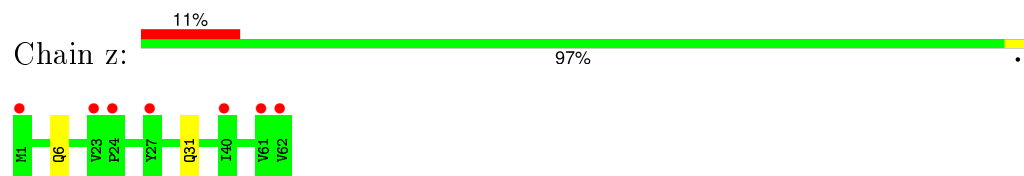
- Molecule 18: Photosystem II reaction center protein Ycf12



- 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 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.61Å 228.09Å 308.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.30 – 5.50 102.29 – 5.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (102.30-5.50) 100.0 (102.29-5.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 5.42Å)	Xtriage
Refinement program	Phenix (phenix.refine: 1.8.2_1336)	Depositor
R, $R_{free}$	0.281 , 0.291 0.303 , 0.311	Depositor DCC
$R_{free}$ test set	1626 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	357.8	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 62.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 32105 reflections	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	49594	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.53	0/2705	0.55	0/3689
1	a	0.53	0/2705	0.55	0/3689
2	B	0.50	0/4109	0.54	0/5600
2	b	0.50	0/4109	0.54	0/5600
3	C	0.46	0/3599	0.51	0/4900
3	c	0.46	0/3599	0.51	0/4900
4	D	0.53	0/2821	0.55	0/3844
4	d	0.53	0/2821	0.55	0/3844
5	E	0.43	0/681	0.51	0/928
5	e	0.43	0/681	0.51	0/928
6	F	0.49	0/284	0.45	0/387
6	f	0.49	0/284	0.45	0/387
7	H	0.47	0/524	0.50	0/713
7	h	0.47	0/524	0.50	0/713
8	I	2.22	2/319 (0.6%)	1.25	4/429 (0.9%)
8	i	2.22	2/319 (0.6%)	1.25	4/429 (0.9%)
9	J	0.46	0/278	0.43	0/376
9	j	0.46	0/278	0.43	0/376
10	K	0.42	0/303	0.50	0/416
10	k	0.43	0/303	0.50	0/416
11	L	0.55	0/311	0.51	0/422
11	l	0.55	0/311	0.51	0/422
12	M	0.47	0/270	0.59	0/367
12	m	0.47	0/270	0.59	0/367
13	O	0.45	0/1896	0.58	0/2571
13	o	0.45	0/1896	0.58	0/2571
14	T	0.53	0/265	0.54	0/359
14	t	0.53	0/265	0.54	0/359
15	U	0.46	0/785	0.55	0/1064
15	u	0.46	0/785	0.55	0/1064
16	V	0.47	0/1085	0.53	0/1473
16	v	0.47	0/1085	0.53	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	X	0.43	0/290	0.47	0/392
17	x	0.43	0/290	0.47	0/392
18	Y	0.41	0/216	0.45	0/289
18	y	0.41	0/216	0.45	0/289
19	Z	0.41	0/490	0.45	0/669
19	z	0.41	0/490	0.45	0/669
All	All	0.55	4/42462 (0.0%)	0.55	8/57776 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	I	1	1
8	i	1	1
All	All	2	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	1	MET	N-CA	36.97	2.20	1.46
8	I	1	MET	N-CA	36.95	2.20	1.46
8	I	1	MET	CA-C	12.27	1.84	1.52
8	i	1	MET	CA-C	12.26	1.84	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	MET	N-CA-CB	-17.88	78.41	110.60
8	I	1	MET	N-CA-CB	-17.86	78.45	110.60
8	I	1	MET	N-CA-C	-12.99	75.92	111.00
8	i	1	MET	N-CA-C	-12.98	75.94	111.00
8	I	1	MET	CA-C-N	-6.32	103.29	117.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	I	1	MET	CA
8	i	1	MET	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	I	1	MET	Mainchain
8	i	1	MET	Mainchain

## 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	2620	0	2517	16	0
1	a	2620	0	2517	0	0
2	B	3969	0	3828	47	0
2	b	3969	0	3828	0	0
3	C	3486	0	3407	20	0
3	c	3486	0	3407	0	0
4	D	2726	0	2627	21	0
4	d	2726	0	2627	0	0
5	E	662	0	648	3	0
5	e	662	0	648	0	0
6	F	275	0	282	3	0
6	f	275	0	282	0	0
7	H	511	0	532	4	0
7	h	511	0	532	0	0
8	I	312	0	329	16	0
8	i	312	0	329	0	0
9	J	272	0	279	1	0
9	j	272	0	279	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	267	0	288	21	0
12	m	267	0	287	0	0
13	O	1865	0	1838	21	0
13	o	1865	0	1838	0	0
14	T	256	0	262	12	0
14	t	256	0	262	0	0
15	U	774	0	773	0	0
15	u	774	0	773	0	7
16	V	1064	0	1073	10	7
16	v	1064	0	1073	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	X	287	0	317	3	0
17	x	287	0	317	0	0
18	Y	215	0	246	2	0
18	y	215	0	246	0	0
19	Z	479	0	516	0	0
19	z	479	0	516	0	0
20	A	10	0	0	0	0
20	a	10	0	0	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	195	0	216	10	0
22	B	1040	0	1152	32	0
22	C	845	0	936	29	0
22	D	195	0	216	8	0
22	a	195	0	216	0	0
22	b	1040	0	1152	0	0
22	c	845	0	936	0	0
22	d	195	0	216	0	0
23	A	128	0	148	6	0
23	a	128	0	148	0	0
24	A	40	0	48	1	0
24	B	120	0	140	8	0
24	C	80	0	93	0	0
24	D	40	0	48	3	0
24	H	40	0	46	1	0
24	K	80	0	93	1	0
24	T	80	0	95	9	0
24	a	40	0	48	0	0
24	b	80	0	92	0	0
24	c	80	0	93	0	0
24	d	40	0	48	0	0
24	h	40	0	46	0	0
24	k	80	0	93	0	0
24	t	40	0	47	0	0
25	A	54	0	78	2	0
25	B	54	0	78	4	0
25	D	43	0	53	0	0
25	L	54	0	34	5	0
25	a	54	0	78	0	0
25	b	108	0	112	0	0
25	d	43	0	53	0	0
25	l	108	0	59	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A	2	0	0	0	0
26	U	1	0	0	0	0
26	a	2	0	0	0	0
26	u	1	0	0	0	0
27	A	4	0	0	0	0
27	a	4	0	0	0	0
28	A	55	0	80	8	0
28	D	55	0	80	0	0
28	a	55	0	80	0	0
28	d	55	0	80	0	0
29	A	51	0	72	3	0
29	B	51	0	72	3	0
29	C	102	0	144	1	0
29	D	51	0	72	2	0
29	Z	37	0	44	1	0
29	a	51	0	72	0	0
29	b	51	0	72	0	0
29	c	102	0	144	0	0
29	d	51	0	72	0	0
29	z	37	0	44	0	0
30	B	1	0	0	0	0
30	F	1	0	0	0	0
30	O	1	0	0	0	0
30	b	1	0	0	0	0
30	f	1	0	0	0	0
30	o	1	0	0	0	0
31	C	186	0	246	5	0
31	D	62	0	82	3	0
31	H	62	0	82	1	0
31	c	186	0	246	0	0
31	d	62	0	82	0	0
31	h	62	0	82	0	0
32	D	147	0	222	13	0
32	E	42	0	57	2	0
32	L	49	0	74	1	0
32	d	147	0	222	0	0
32	e	42	0	57	0	0
32	l	49	0	74	0	0
33	F	43	0	30	1	0
33	V	43	0	30	9	0
33	f	43	0	30	0	0
33	v	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	J	1	0	0	0	0
34	j	1	0	0	0	0
All	All	49594	0	50450	263	7

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 3.

The worst 5 of 263 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)
16:V:37:CYS:SG	33:V:201:HEM:HAB	1.52	1.48
16:V:37:CYS:SG	33:V:201:HEM:CAB	2.02	1.47
16:V:40:CYS:SG	33:V:201:HEM:CAC	2.04	1.46
16:V:40:CYS:SG	33:V:201:HEM:HAC	1.57	1.44
8:I:1:MET:CA	8:I:1:MET:C	1.84	1.44

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:u:73:GLN:OE1	16:V:70:GLU:CD[3_544]	0.80	1.40
15:u:73:GLN:OE1	16:V:70:GLU:OE1[3_544]	1.22	0.98
15:u:73:GLN:OE1	16:V:70:GLU:OE2[3_544]	1.45	0.75
15:u:73:GLN:CD	16:V:70:GLU:OE1[3_544]	1.79	0.41
15:u:73:GLN:CD	16:V:70:GLU:CD[3_544]	1.89	0.31

## 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	332/334 (99%)	328 (99%)	3 (1%)	1 (0%)	46 83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	332/334 (99%)	328 (99%)	3 (1%)	1 (0%)	46	83
2	B	502/504 (100%)	497 (99%)	5 (1%)	0	100	100
2	b	502/504 (100%)	496 (99%)	6 (1%)	0	100	100
3	C	449/461 (97%)	440 (98%)	8 (2%)	1 (0%)	52	86
3	c	449/461 (97%)	440 (98%)	8 (2%)	1 (0%)	52	86
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	79/81 (98%)	78 (99%)	1 (1%)	0	100	100
5	e	79/81 (98%)	78 (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	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
7	h	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	36/40 (90%)	36 (100%)	0	0	100	100
9	j	36/40 (90%)	36 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	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	32/34 (94%)	32 (100%)	0	0	100	100
12	m	32/34 (94%)	32 (100%)	0	0	100	100
13	O	241/243 (99%)	233 (97%)	7 (3%)	1 (0%)	39	80
13	o	241/243 (99%)	233 (97%)	7 (3%)	1 (0%)	39	80
14	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	t	28/30 (93%)	27 (96%)	1 (4%)	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	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
16	v	135/137 (98%)	132 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	X	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
17	x	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
18	Y	27/29 (93%)	27 (100%)	0	0	100	100
18	y	27/29 (93%)	27 (100%)	0	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	5188/5288 (98%)	5085 (98%)	97 (2%)	6 (0%)	56	90

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	58	ASN
13	o	58	ASN
3	C	416	SER
3	c	416	SER
1	A	259	ILE

### 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	269/269 (100%)	269 (100%)	0	100	100
1	a	269/269 (100%)	269 (100%)	0	100	100
2	B	402/402 (100%)	398 (99%)	4 (1%)	82	92
2	b	402/402 (100%)	398 (99%)	4 (1%)	82	92
3	C	352/362 (97%)	348 (99%)	4 (1%)	80	91
3	c	352/362 (97%)	348 (99%)	4 (1%)	80	91
4	D	277/277 (100%)	274 (99%)	3 (1%)	80	91
4	d	277/277 (100%)	274 (99%)	3 (1%)	80	91
5	E	72/72 (100%)	71 (99%)	1 (1%)	74	89
5	e	72/72 (100%)	71 (99%)	1 (1%)	74	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	28/28 (100%)	27 (96%)	1 (4%)	42	74
6	f	28/28 (100%)	27 (96%)	1 (4%)	42	74
7	H	54/54 (100%)	51 (94%)	3 (6%)	26	63
7	h	54/54 (100%)	51 (94%)	3 (6%)	26	63
8	I	35/35 (100%)	34 (97%)	1 (3%)	50	78
8	i	35/35 (100%)	34 (97%)	1 (3%)	50	78
9	J	26/28 (93%)	26 (100%)	0	100	100
9	j	26/28 (93%)	26 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	20	57
10	k	30/30 (100%)	28 (93%)	2 (7%)	20	57
11	L	35/35 (100%)	33 (94%)	2 (6%)	25	62
11	l	35/35 (100%)	33 (94%)	2 (6%)	25	62
12	M	31/31 (100%)	30 (97%)	1 (3%)	46	77
12	m	31/31 (100%)	30 (97%)	1 (3%)	46	77
13	O	206/206 (100%)	202 (98%)	4 (2%)	65	86
13	o	206/206 (100%)	202 (98%)	4 (2%)	65	86
14	T	27/27 (100%)	26 (96%)	1 (4%)	41	74
14	t	27/27 (100%)	26 (96%)	1 (4%)	41	74
15	U	84/84 (100%)	83 (99%)	1 (1%)	78	90
15	u	84/84 (100%)	83 (99%)	1 (1%)	78	90
16	V	117/117 (100%)	116 (99%)	1 (1%)	84	93
16	v	117/117 (100%)	116 (99%)	1 (1%)	84	93
17	X	32/32 (100%)	32 (100%)	0	100	100
17	x	32/32 (100%)	32 (100%)	0	100	100
18	Y	22/22 (100%)	21 (96%)	1 (4%)	34	69
18	y	22/22 (100%)	21 (96%)	1 (4%)	34	69
19	Z	52/52 (100%)	50 (96%)	2 (4%)	40	73
19	z	52/52 (100%)	50 (96%)	2 (4%)	40	73
All	All	4302/4326 (99%)	4238 (98%)	64 (2%)	72	89

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	H	65	LEU
10	K	17	ILE
18	y	27	MET
7	h	12	ARG
8	I	1	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	83	ASN
6	F	44	GLN
16	v	34	GLN
4	d	83	ASN
6	f	44	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 166 ligands modelled in this entry, 16 are monoatomic - leaving 150 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	-
22	CLA	A	603	-	57,73,73	1.81	10 (17%)	61,113,113	1.90	14 (22%)
22	CLA	A	604	-	57,73,73	1.73	10 (17%)	61,113,113	2.19	15 (24%)
23	PHO	A	605	-	67,69,69	1.88	13 (19%)	86,99,99	1.94	21 (24%)
23	PHO	A	606	-	67,69,69	1.99	15 (22%)	86,99,99	1.95	22 (25%)
22	CLA	A	607	-	57,73,73	1.84	10 (17%)	61,113,113	2.01	15 (24%)
24	BCR	A	608	-	41,41,41	3.76	14 (34%)	56,56,56	7.62	39 (69%)
25	SQD	A	609	-	53,54,54	1.49	3 (5%)	62,65,65	1.78	12 (19%)
27	BCT	A	612	21	0,3,3	0.00	-	0,3,3	0.00	-
28	PL9	A	613	-	54,55,55	0.66	2 (3%)	68,69,69	1.62	12 (17%)
29	LMG	A	614	-	51,51,55	0.92	2 (3%)	59,59,63	1.01	3 (5%)
25	SQD	B	601	-	53,54,54	1.50	3 (5%)	62,65,65	1.42	6 (9%)
22	CLA	B	602	-	57,73,73	1.91	11 (19%)	61,113,113	2.02	15 (24%)
22	CLA	B	603	-	57,73,73	1.89	11 (19%)	61,113,113	1.82	13 (21%)
22	CLA	B	604	-	57,73,73	1.83	12 (21%)	61,113,113	2.15	15 (24%)
22	CLA	B	605	-	57,73,73	1.72	12 (21%)	61,113,113	2.13	14 (22%)
22	CLA	B	606	-	57,73,73	1.77	10 (17%)	61,113,113	1.97	14 (22%)
22	CLA	B	607	-	57,73,73	1.85	11 (19%)	61,113,113	2.02	14 (22%)
22	CLA	B	608	-	57,73,73	1.80	10 (17%)	61,113,113	1.92	13 (21%)
22	CLA	B	609	-	57,73,73	1.76	10 (17%)	61,113,113	2.20	19 (31%)
22	CLA	B	610	-	57,73,73	1.79	10 (17%)	61,113,113	1.97	13 (21%)
22	CLA	B	611	-	57,73,73	1.82	11 (19%)	61,113,113	1.90	12 (19%)
22	CLA	B	612	-	57,73,73	1.66	10 (17%)	61,113,113	2.02	13 (21%)
22	CLA	B	613	-	57,73,73	1.80	11 (19%)	61,113,113	2.00	15 (24%)
22	CLA	B	614	-	57,73,73	1.80	11 (19%)	61,113,113	1.88	14 (22%)
22	CLA	B	615	-	57,73,73	1.77	12 (21%)	61,113,113	2.04	16 (26%)
22	CLA	B	616	-	57,73,73	1.83	11 (19%)	61,113,113	1.88	14 (22%)
22	CLA	B	617	-	57,73,73	1.85	10 (17%)	61,113,113	1.96	17 (27%)
24	BCR	B	618	-	41,41,41	3.70	14 (34%)	56,56,56	7.34	38 (67%)
24	BCR	B	619	-	41,41,41	3.70	14 (34%)	56,56,56	7.60	42 (75%)
29	LMG	B	620	-	51,51,55	0.91	2 (3%)	59,59,63	1.01	3 (5%)
24	BCR	B	622	-	41,41,41	3.85	14 (34%)	56,56,56	6.92	38 (67%)
22	CLA	C	501	-	57,73,73	1.85	11 (19%)	61,113,113	2.08	16 (26%)
22	CLA	C	502	-	57,73,73	1.79	11 (19%)	61,113,113	1.92	13 (21%)
22	CLA	C	503	-	57,73,73	1.87	11 (19%)	61,113,113	1.87	13 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	C	504	-	57,73,73	1.85	10 (17%)	61,113,113	2.02	13 (21%)
22	CLA	C	505	-	57,73,73	1.85	12 (21%)	61,113,113	1.91	13 (21%)
22	CLA	C	506	-	57,73,73	1.88	11 (19%)	61,113,113	2.04	15 (24%)
22	CLA	C	507	-	57,73,73	1.94	11 (19%)	61,113,113	1.99	15 (24%)
22	CLA	C	508	-	57,73,73	1.91	12 (21%)	61,113,113	1.91	10 (16%)
22	CLA	C	509	-	57,73,73	1.85	12 (21%)	61,113,113	2.04	15 (24%)
22	CLA	C	510	-	57,73,73	1.82	11 (19%)	61,113,113	1.95	15 (24%)
22	CLA	C	511	3	57,73,73	1.88	11 (19%)	61,113,113	1.93	13 (21%)
22	CLA	C	512	-	57,73,73	1.90	12 (21%)	61,113,113	1.96	17 (27%)
22	CLA	C	513	-	57,73,73	1.97	12 (21%)	61,113,113	1.85	14 (22%)
24	BCR	C	514	-	41,41,41	3.91	14 (34%)	56,56,56	8.26	35 (62%)
24	BCR	C	515	-	41,41,41	3.87	14 (34%)	56,56,56	8.04	39 (69%)
31	DGD	C	516	-	63,63,67	0.85	2 (3%)	77,77,81	0.99	3 (3%)
31	DGD	C	517	-	63,63,67	0.85	2 (3%)	77,77,81	0.86	3 (3%)
31	DGD	C	518	-	63,63,67	0.77	2 (3%)	77,77,81	0.90	2 (2%)
29	LMG	C	519	-	51,51,55	0.91	2 (3%)	59,59,63	1.03	4 (6%)
29	LMG	C	520	-	51,51,55	0.98	3 (5%)	59,59,63	1.00	2 (3%)
22	CLA	D	401	-	57,73,73	1.82	13 (22%)	61,113,113	2.04	18 (29%)
22	CLA	D	402	-	57,73,73	1.76	11 (19%)	61,113,113	2.20	16 (26%)
22	CLA	D	403	-	57,73,73	1.87	12 (21%)	61,113,113	1.85	13 (21%)
24	BCR	D	404	-	41,41,41	3.86	14 (34%)	56,56,56	7.66	40 (71%)
32	LHG	D	405	-	48,48,48	0.84	2 (4%)	49,54,54	1.01	3 (6%)
29	LMG	D	406	34	51,51,55	0.85	2 (3%)	59,59,63	0.80	3 (5%)
32	LHG	D	407	-	48,48,48	0.87	2 (4%)	49,54,54	0.85	2 (4%)
28	PL9	D	408	-	54,55,55	0.76	1 (1%)	68,69,69	1.37	8 (11%)
32	LHG	D	409	-	48,48,48	0.92	2 (4%)	49,54,54	0.91	3 (6%)
31	DGD	D	410	-	63,63,67	0.96	3 (4%)	77,77,81	1.08	5 (6%)
25	SQD	D	411	-	42,43,54	1.70	3 (7%)	51,54,65	1.78	8 (15%)
32	LHG	E	101	-	41,41,48	1.03	2 (4%)	42,47,54	1.10	3 (7%)
33	HEM	F	101	5,6	24,50,50	2.26	6 (25%)	16,82,82	2.14	2 (12%)
24	BCR	H	101	-	41,41,41	3.84	14 (34%)	56,56,56	8.08	41 (73%)
31	DGD	H	102	-	63,63,67	0.90	3 (4%)	77,77,81	0.94	5 (6%)
24	BCR	K	101	-	41,41,41	3.88	14 (34%)	56,56,56	7.89	36 (64%)
24	BCR	K	102	-	41,41,41	3.81	14 (34%)	56,56,56	7.59	40 (71%)
25	SQD	L	101	-	53,54,54	1.43	3 (5%)	62,65,65	1.63	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	LHG	L	102	-	48,48,48	0.87	2 (4%)	49,54,54	0.99	2 (4%)
24	BCR	T	101	-	41,41,41	3.70	14 (34%)	56,56,56	7.34	38 (67%)
24	BCR	T	102	-	41,41,41	3.77	14 (34%)	56,56,56	8.25	42 (75%)
33	HEM	V	201	16	24,50,50	2.27	5 (20%)	16,82,82	1.88	3 (18%)
29	LMG	Z	101	-	37,37,55	0.98	3 (8%)	45,45,63	1.39	3 (6%)
20	OEX	a	601	1,3	0,15,15	0.00	-	0,32,32	0.00	-
22	CLA	a	603	-	57,73,73	1.81	10 (17%)	61,113,113	1.89	14 (22%)
22	CLA	a	604	-	57,73,73	1.72	10 (17%)	61,113,113	2.18	15 (24%)
23	PHO	a	605	-	67,69,69	1.88	13 (19%)	86,99,99	1.95	21 (24%)
23	PHO	a	606	-	67,69,69	1.99	15 (22%)	86,99,99	1.95	22 (25%)
22	CLA	a	607	-	57,73,73	1.83	10 (17%)	61,113,113	2.00	15 (24%)
24	BCR	a	608	-	41,41,41	3.76	14 (34%)	56,56,56	7.62	39 (69%)
25	SQD	a	609	-	53,54,54	1.49	3 (5%)	62,65,65	1.78	12 (19%)
27	BCT	a	612	21	0,3,3	0.00	-	0,3,3	0.00	-
28	PL9	a	613	-	54,55,55	0.66	2 (3%)	68,69,69	1.62	12 (17%)
29	LMG	a	614	-	51,51,55	0.92	2 (3%)	59,59,63	1.01	3 (5%)
25	SQD	b	601	-	53,54,54	1.51	3 (5%)	62,65,65	1.42	6 (9%)
22	CLA	b	602	-	57,73,73	1.91	11 (19%)	61,113,113	2.02	15 (24%)
22	CLA	b	603	-	57,73,73	1.89	11 (19%)	61,113,113	1.83	13 (21%)
22	CLA	b	604	-	57,73,73	1.84	12 (21%)	61,113,113	2.16	15 (24%)
22	CLA	b	605	-	57,73,73	1.73	12 (21%)	61,113,113	2.12	14 (22%)
22	CLA	b	606	-	57,73,73	1.77	11 (19%)	61,113,113	1.96	14 (22%)
22	CLA	b	607	-	57,73,73	1.85	11 (19%)	61,113,113	2.02	14 (22%)
22	CLA	b	608	-	57,73,73	1.80	10 (17%)	61,113,113	1.91	13 (21%)
22	CLA	b	609	-	57,73,73	1.77	10 (17%)	61,113,113	2.20	19 (31%)
22	CLA	b	610	-	57,73,73	1.79	10 (17%)	61,113,113	1.96	13 (21%)
22	CLA	b	611	-	57,73,73	1.81	11 (19%)	61,113,113	1.90	12 (19%)
22	CLA	b	612	-	57,73,73	1.66	10 (17%)	61,113,113	2.02	13 (21%)
22	CLA	b	613	-	57,73,73	1.80	11 (19%)	61,113,113	2.00	15 (24%)
22	CLA	b	614	-	57,73,73	1.80	11 (19%)	61,113,113	1.88	14 (22%)
22	CLA	b	615	-	57,73,73	1.76	12 (21%)	61,113,113	2.04	16 (26%)
22	CLA	b	616	-	57,73,73	1.83	11 (19%)	61,113,113	1.88	14 (22%)
22	CLA	b	617	-	57,73,73	1.85	10 (17%)	61,113,113	1.96	16 (26%)
24	BCR	b	618	-	41,41,41	3.70	14 (34%)	56,56,56	7.61	42 (75%)
29	LMG	b	619	-	51,51,55	0.92	2 (3%)	59,59,63	1.01	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	SQD	b	621	-	53,54,54	1.48	3 (5%)	62,65,65	1.73	9 (14%)
24	BCR	b	622	-	41,41,41	3.85	14 (34%)	56,56,56	6.92	38 (67%)
22	CLA	c	501	-	57,73,73	1.85	11 (19%)	61,113,113	2.08	16 (26%)
22	CLA	c	502	-	57,73,73	1.79	11 (19%)	61,113,113	1.92	13 (21%)
22	CLA	c	503	-	57,73,73	1.87	11 (19%)	61,113,113	1.86	13 (21%)
22	CLA	c	504	-	57,73,73	1.85	10 (17%)	61,113,113	2.01	13 (21%)
22	CLA	c	505	-	57,73,73	1.86	12 (21%)	61,113,113	1.91	13 (21%)
22	CLA	c	506	-	57,73,73	1.88	11 (19%)	61,113,113	2.03	15 (24%)
22	CLA	c	507	-	57,73,73	1.94	11 (19%)	61,113,113	1.99	15 (24%)
22	CLA	c	508	-	57,73,73	1.92	12 (21%)	61,113,113	1.91	11 (18%)
22	CLA	c	509	-	57,73,73	1.86	12 (21%)	61,113,113	2.04	15 (24%)
22	CLA	c	510	-	57,73,73	1.82	11 (19%)	61,113,113	1.95	15 (24%)
22	CLA	c	511	3	57,73,73	1.87	11 (19%)	61,113,113	1.93	13 (21%)
22	CLA	c	512	-	57,73,73	1.90	12 (21%)	61,113,113	1.96	17 (27%)
22	CLA	c	513	-	57,73,73	1.97	12 (21%)	61,113,113	1.85	14 (22%)
24	BCR	c	514	-	41,41,41	3.91	15 (36%)	56,56,56	8.26	35 (62%)
24	BCR	c	515	-	41,41,41	3.87	14 (34%)	56,56,56	8.03	39 (69%)
31	DGD	c	516	-	63,63,67	0.85	2 (3%)	77,77,81	0.99	3 (3%)
31	DGD	c	517	-	63,63,67	0.85	2 (3%)	77,77,81	0.86	3 (3%)
31	DGD	c	518	-	63,63,67	0.77	2 (3%)	77,77,81	0.90	2 (2%)
29	LMG	c	519	-	51,51,55	0.92	2 (3%)	59,59,63	1.03	4 (6%)
29	LMG	c	520	-	51,51,55	0.98	3 (5%)	59,59,63	1.00	2 (3%)
22	CLA	d	401	-	57,73,73	1.81	12 (21%)	61,113,113	2.04	18 (29%)
22	CLA	d	402	-	57,73,73	1.76	11 (19%)	61,113,113	2.20	15 (24%)
22	CLA	d	403	-	57,73,73	1.87	13 (22%)	61,113,113	1.86	13 (21%)
24	BCR	d	404	-	41,41,41	3.86	14 (34%)	56,56,56	7.65	40 (71%)
32	LHG	d	405	-	48,48,48	0.84	2 (4%)	49,54,54	1.00	3 (6%)
29	LMG	d	406	34	51,51,55	0.85	2 (3%)	59,59,63	0.80	3 (5%)
32	LHG	d	407	-	48,48,48	0.88	2 (4%)	49,54,54	0.85	2 (4%)
28	PL9	d	408	-	54,55,55	0.76	1 (1%)	68,69,69	1.37	8 (11%)
32	LHG	d	409	-	48,48,48	0.92	2 (4%)	49,54,54	0.90	2 (4%)
31	DGD	d	410	-	63,63,67	0.96	4 (6%)	77,77,81	1.08	5 (6%)
25	SQD	d	411	-	42,43,54	1.70	3 (7%)	51,54,65	1.78	8 (15%)
32	LHG	e	101	-	41,41,48	1.03	2 (4%)	42,47,54	1.10	3 (7%)
33	HEM	f	101	5,6	24,50,50	2.26	6 (25%)	16,82,82	2.13	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	BCR	h	101	-	41,41,41	3.84	14 (34%)	56,56,56	8.08	41 (73%)
31	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	0.94	5 (6%)
24	BCR	k	101	-	41,41,41	3.88	14 (34%)	56,56,56	7.89	36 (64%)
24	BCR	k	102	-	41,41,41	3.81	14 (34%)	56,56,56	7.59	40 (71%)
25	SQD	l	101	-	53,54,54	1.43	4 (7%)	62,65,65	1.62	7 (11%)
25	SQD	l	102	-	53,54,54	1.48	4 (7%)	62,65,65	1.73	9 (14%)
32	LHG	l	103	-	48,48,48	0.87	2 (4%)	49,54,54	0.99	2 (4%)
24	BCR	t	101	-	41,41,41	3.77	14 (34%)	56,56,56	8.25	42 (75%)
33	HEM	v	201	16	24,50,50	2.27	6 (25%)	16,82,82	1.88	3 (18%)
29	LMG	z	101	-	37,37,55	0.98	3 (8%)	45,45,63	1.40	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
22	CLA	A	603	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	A	604	-	2/2/20/25	0/37/135/135	0/0/9/9
23	PHO	A	605	-	-	0/53/103/103	0/1/6/6
23	PHO	A	606	-	-	0/53/103/103	0/1/6/6
22	CLA	A	607	-	1/1/20/25	0/37/135/135	0/0/9/9
24	BCR	A	608	-	-	0/29/63/63	0/2/2/2
25	SQD	A	609	-	-	0/49/69/69	0/1/1/1
27	BCT	A	612	21	-	0/0/0/0	0/0/0/0
28	PL9	A	613	-	-	0/53/73/73	0/1/1/1
29	LMG	A	614	-	-	0/46/66/70	0/1/1/1
25	SQD	B	601	-	-	0/49/69/69	0/1/1/1
22	CLA	B	602	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	607	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	609	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	B	610	-	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	612	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	617	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	B	618	-	-	0/29/63/63	0/2/2/2
24	BCR	B	619	-	-	0/29/63/63	0/2/2/2
29	LMG	B	620	-	-	0/46/66/70	0/1/1/1
24	BCR	B	622	-	-	0/29/63/63	0/2/2/2
22	CLA	C	501	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	C	502	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	505	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	508	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	511	3	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	C	512	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	513	-	2/2/20/25	0/37/135/135	0/0/9/9
24	BCR	C	514	-	-	0/29/63/63	0/2/2/2
24	BCR	C	515	-	-	0/29/63/63	0/2/2/2
31	DGD	C	516	-	-	0/51/91/95	0/2/2/2
31	DGD	C	517	-	-	0/51/91/95	0/2/2/2
31	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
22	CLA	D	401	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	D	402	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	D	403	-	2/2/20/25	0/37/135/135	0/0/9/9
24	BCR	D	404	-	-	0/29/63/63	0/2/2/2
32	LHG	D	405	-	-	0/53/53/53	0/0/0/0
29	LMG	D	406	34	-	0/46/66/70	0/1/1/1
32	LHG	D	407	-	-	0/53/53/53	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PL9	D	408	-	-	0/53/73/73	0/1/1/1
32	LHG	D	409	-	-	0/53/53/53	0/0/0/0
31	DGD	D	410	-	-	0/51/91/95	0/2/2/2
25	SQD	D	411	-	-	0/38/58/69	0/1/1/1
32	LHG	E	101	-	-	0/46/46/53	0/0/0/0
33	HEM	F	101	5,6	-	0/6/54/54	0/0/8/8
24	BCR	H	101	-	-	0/29/63/63	0/2/2/2
31	DGD	H	102	-	-	0/51/91/95	0/2/2/2
24	BCR	K	101	-	-	0/29/63/63	0/2/2/2
24	BCR	K	102	-	-	0/29/63/63	0/2/2/2
25	SQD	L	101	-	-	0/49/69/69	0/1/1/1
32	LHG	L	102	-	-	0/53/53/53	0/0/0/0
24	BCR	T	101	-	-	0/29/63/63	0/2/2/2
24	BCR	T	102	-	-	0/29/63/63	0/2/2/2
33	HEM	V	201	16	-	0/6/54/54	0/0/8/8
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
22	CLA	a	603	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	a	604	-	2/2/20/25	0/37/135/135	0/0/9/9
23	PHO	a	605	-	-	0/53/103/103	0/1/6/6
23	PHO	a	606	-	-	0/53/103/103	0/1/6/6
22	CLA	a	607	-	1/1/20/25	0/37/135/135	0/0/9/9
24	BCR	a	608	-	-	0/29/63/63	0/2/2/2
25	SQD	a	609	-	-	0/49/69/69	0/1/1/1
27	BCT	a	612	21	-	0/0/0/0	0/0/0/0
28	PL9	a	613	-	-	0/53/73/73	0/1/1/1
29	LMG	a	614	-	-	0/46/66/70	0/1/1/1
25	SQD	b	601	-	-	0/49/69/69	0/1/1/1
22	CLA	b	602	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	b	603	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	604	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	607	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	609	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	b	610	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	612	-	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	b	618	-	-	0/29/63/63	0/2/2/2
29	LMG	b	619	-	-	0/46/66/70	0/1/1/1
25	SQD	b	621	-	-	0/49/69/69	0/1/1/1
24	BCR	b	622	-	-	0/29/63/63	0/2/2/2
22	CLA	c	501	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	c	502	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	504	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	505	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	c	506	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	507	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	508	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	510	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	511	3	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	c	512	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	513	-	2/2/20/25	0/37/135/135	0/0/9/9
24	BCR	c	514	-	-	0/29/63/63	0/2/2/2
24	BCR	c	515	-	-	0/29/63/63	0/2/2/2
31	DGD	c	516	-	-	0/51/91/95	0/2/2/2
31	DGD	c	517	-	-	0/51/91/95	0/2/2/2
31	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
22	CLA	d	401	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	d	402	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	d	403	-	2/2/20/25	0/37/135/135	0/0/9/9
24	BCR	d	404	-	-	0/29/63/63	0/2/2/2
32	LHG	d	405	-	-	0/53/53/53	0/0/0/0
29	LMG	d	406	34	-	0/46/66/70	0/1/1/1
32	LHG	d	407	-	-	0/53/53/53	0/0/0/0
28	PL9	d	408	-	-	0/53/73/73	0/1/1/1
32	LHG	d	409	-	-	0/53/53/53	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DGD	d	410	-	-	0/51/91/95	0/2/2/2
25	SQD	d	411	-	-	0/38/58/69	0/1/1/1
32	LHG	e	101	-	-	0/46/46/53	0/0/0/0
33	HEM	f	101	5,6	-	0/6/54/54	0/0/8/8
24	BCR	h	101	-	-	0/29/63/63	0/2/2/2
31	DGD	h	102	-	-	0/51/91/95	0/2/2/2
24	BCR	k	101	-	-	0/29/63/63	0/2/2/2
24	BCR	k	102	-	-	0/29/63/63	0/2/2/2
25	SQD	l	101	-	-	0/49/69/69	0/1/1/1
25	SQD	l	102	-	-	0/49/69/69	0/1/1/1
32	LHG	l	103	-	-	0/53/53/53	0/0/0/0
24	BCR	t	101	-	-	0/29/63/63	0/2/2/2
33	HEM	v	201	16	-	0/6/54/54	0/0/8/8
29	LMG	z	101	-	-	1/31/51/70	0/1/1/1

The worst 5 of 1272 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	609	SQD	C6-S	-8.73	1.67	1.77
25	a	609	SQD	C6-S	-8.71	1.67	1.77
24	C	514	BCR	C8-C9	-8.55	1.27	1.45
24	c	514	BCR	C8-C9	-8.51	1.27	1.45
25	b	601	SQD	C6-S	-8.50	1.67	1.77

The worst 5 of 2184 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	T	102	BCR	C36-C18-C17	-10.18	108.08	122.89
24	t	101	BCR	C36-C18-C17	-10.18	108.09	122.89
24	D	404	BCR	C30-C25-C26	-9.49	109.80	122.50
24	d	404	BCR	C30-C25-C26	-9.48	109.82	122.50
24	a	608	BCR	C37-C22-C21	-9.38	109.26	122.89

5 of 166 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	B	617	CLA	NC
22	B	617	CLA	ND
22	B	617	CLA	NA
22	c	513	CLA	NC
22	c	513	CLA	NA

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	z	101	LMG	C7-O1-C1-O6
29	Z	101	LMG	C7-O1-C1-O6

There are no ring outliers.

62 monomers are involved in 148 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	603	CLA	5	0
22	A	604	CLA	3	0
23	A	605	PHO	2	0
23	A	606	PHO	4	0
22	A	607	CLA	2	0
24	A	608	BCR	1	0
25	A	609	SQD	2	0
28	A	613	PL9	8	0
29	A	614	LMG	3	0
25	B	601	SQD	4	0
22	B	603	CLA	1	0
22	B	604	CLA	2	0
22	B	605	CLA	2	0
22	B	606	CLA	5	0
22	B	607	CLA	2	0
22	B	609	CLA	2	0
22	B	611	CLA	4	0
22	B	612	CLA	2	0
22	B	613	CLA	3	0
22	B	614	CLA	5	0
22	B	615	CLA	3	0
22	B	616	CLA	2	0
22	B	617	CLA	4	0
24	B	618	BCR	3	0
24	B	619	BCR	1	0
29	B	620	LMG	3	0
24	B	622	BCR	4	0
22	C	501	CLA	2	0
22	C	502	CLA	3	0
22	C	503	CLA	3	0
22	C	504	CLA	1	0
22	C	505	CLA	2	0
22	C	506	CLA	4	0
22	C	507	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	508	CLA	3	0
22	C	509	CLA	2	0
22	C	510	CLA	6	0
22	C	511	CLA	2	0
22	C	512	CLA	3	0
22	C	513	CLA	1	0
31	C	516	DGD	2	0
31	C	517	DGD	2	0
31	C	518	DGD	1	0
29	C	519	LMG	1	0
22	D	401	CLA	1	0
22	D	402	CLA	4	0
22	D	403	CLA	3	0
24	D	404	BCR	3	0
29	D	406	LMG	2	0
32	D	409	LHG	13	0
31	D	410	DGD	3	0
32	E	101	LHG	2	0
33	F	101	HEM	1	0
24	H	101	BCR	1	0
31	H	102	DGD	1	0
24	K	102	BCR	1	0
25	L	101	SQD	5	0
32	L	102	LHG	1	0
24	T	101	BCR	7	0
24	T	102	BCR	2	0
33	V	201	HEM	9	0
29	Z	101	LMG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	334/334 (100%)	0.59	21 (6%) 23 22	16, 22, 43, 53	0
1	a	334/334 (100%)	0.60	26 (7%) 16 17	16, 22, 43, 53	0
2	B	504/504 (100%)	0.47	32 (6%) 23 22	18, 27, 49, 70	0
2	b	504/504 (100%)	0.76	70 (13%) 4 8	18, 27, 49, 70	0
3	C	451/461 (97%)	0.64	43 (9%) 10 13	21, 31, 44, 56	0
3	c	451/461 (97%)	0.52	39 (8%) 13 16	21, 31, 44, 56	0
4	D	342/342 (100%)	0.78	33 (9%) 10 13	17, 23, 39, 61	0
4	d	342/342 (100%)	0.70	24 (7%) 19 20	17, 23, 39, 61	0
5	E	81/81 (100%)	0.82	10 (12%) 5 9	27, 40, 57, 63	0
5	e	81/81 (100%)	0.42	9 (11%) 7 11	27, 40, 57, 63	0
6	F	34/34 (100%)	0.36	1 (2%) 55 49	28, 33, 58, 61	0
6	f	34/34 (100%)	-0.00	0 100 100	28, 33, 58, 61	0
7	H	65/65 (100%)	0.65	9 (13%) 4 8	23, 34, 40, 58	0
7	h	65/65 (100%)	1.42	18 (27%) 1 4	23, 34, 40, 58	0
8	I	38/38 (100%)	0.54	5 (13%) 4 8	30, 34, 65, 68	0
8	i	38/38 (100%)	0.08	3 (7%) 15 17	30, 34, 65, 68	0
9	J	38/40 (95%)	0.56	3 (7%) 15 17	26, 37, 68, 72	0
9	j	38/40 (95%)	-0.14	0 100 100	26, 37, 68, 72	0
10	K	37/37 (100%)	0.52	2 (5%) 29 29	33, 38, 45, 47	0
10	k	37/37 (100%)	0.60	4 (10%) 8 11	33, 38, 45, 47	0
11	L	37/37 (100%)	0.60	2 (5%) 29 29	17, 22, 50, 59	0
11	l	37/37 (100%)	0.59	3 (8%) 15 17	17, 22, 50, 59	0
12	M	34/34 (100%)	1.02	6 (17%) 2 6	21, 23, 36, 52	0
12	m	34/34 (100%)	0.74	3 (8%) 12 15	21, 23, 36, 52	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/243 (100%)	0.38	8 (3%) 50 44	18, 32, 55, 71	0
13	o	243/243 (100%)	0.56	14 (5%) 26 25	18, 32, 55, 71	0
14	T	30/30 (100%)	0.87	3 (10%) 9 12	19, 23, 44, 52	0
14	t	30/30 (100%)	0.85	1 (3%) 50 44	19, 23, 44, 52	0
15	U	97/97 (100%)	0.30	2 (2%) 67 61	23, 30, 48, 50	0
15	u	97/97 (100%)	0.55	6 (6%) 24 23	23, 30, 48, 50	0
16	V	137/137 (100%)	0.22	2 (1%) 76 70	23, 28, 39, 48	0
16	v	137/137 (100%)	0.38	6 (4%) 38 35	23, 28, 39, 48	0
17	X	39/39 (100%)	0.99	7 (17%) 2 6	33, 40, 66, 68	0
17	x	39/39 (100%)	1.00	7 (17%) 2 6	33, 40, 66, 68	0
18	Y	29/29 (100%)	0.69	3 (10%) 9 12	42, 48, 75, 77	0
18	y	29/29 (100%)	0.29	0 100 100	42, 48, 75, 77	0
19	Z	62/62 (100%)	0.48	2 (3%) 51 45	39, 48, 68, 72	0
19	z	62/62 (100%)	0.69	7 (11%) 7 10	39, 48, 68, 72	0
All	All	5264/5288 (99%)	0.59	434 (8%) 14 16	16, 29, 51, 77	0

The worst 5 of 434 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	X	2	THR	7.2
4	D	59	TYR	6.8
9	J	3	SER	6.5
4	D	56	THR	5.7
4	d	136	VAL	5.4

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
24	BCR	K	102	40/40	0.81	2.30	11.02	29,33,37,37	0
28	PL9	A	613	55/55	0.34	1.95	7.12	52,69,78,78	0
24	BCR	k	102	40/40	0.70	2.17	6.57	29,33,37,37	0
29	LMG	Z	101	37/55	0.33	1.65	6.14	55,84,88,88	0
24	BCR	D	404	40/40	0.40	1.52	6.09	25,30,48,49	0
22	CLA	c	501	65/65	0.72	1.66	6.07	29,32,44,46	0
24	BCR	c	514	40/40	0.72	1.69	5.47	37,43,47,47	0
24	BCR	C	515	40/40	0.73	1.99	5.43	30,37,40,41	0
29	LMG	c	520	51/55	0.21	1.84	5.31	43,76,81,82	0
24	BCR	K	101	40/40	0.61	1.39	5.10	34,38,39,39	0
25	SQD	D	411	43/54	0.66	1.27	5.06	67,74,78,79	0
29	LMG	C	519	51/55	0.42	0.86	5.03	31,57,72,73	0
24	BCR	c	515	40/40	0.79	1.59	4.80	30,37,40,41	0
28	PL9	a	613	55/55	0.27	1.47	4.75	52,69,78,78	0
24	BCR	d	404	40/40	0.33	1.17	4.66	25,30,48,49	0
24	BCR	C	514	40/40	0.76	1.48	4.52	37,43,47,47	0
22	CLA	a	607	65/65	0.76	0.81	4.40	21,24,71,72	0
23	PHO	A	606	64/64	0.82	1.13	4.35	19,22,28,32	0
22	CLA	C	509	65/65	0.93	1.30	4.34	29,32,46,47	0
22	CLA	c	509	65/65	0.82	1.18	4.33	29,32,46,47	0
24	BCR	T	102	40/40	0.41	1.10	4.26	27,33,39,39	0
22	CLA	c	507	65/65	0.76	1.38	4.23	29,33,52,53	0
22	CLA	B	603	65/65	0.83	1.15	4.22	23,26,32,32	0
31	DGD	D	410	62/66	0.48	1.24	4.16	77,89,103,103	0
22	CLA	c	503	65/65	0.82	1.11	4.03	27,31,35,36	0
22	CLA	C	501	65/65	0.79	1.23	3.99	29,32,44,46	0
22	CLA	c	512	65/65	0.66	1.58	3.98	37,41,62,63	0
29	LMG	c	519	51/55	0.83	0.67	3.92	31,57,72,73	0
22	CLA	D	401	65/65	0.84	0.95	3.87	13,18,34,35	0
24	BCR	k	101	40/40	0.29	1.14	3.87	34,38,39,39	0
22	CLA	b	604	65/65	0.88	1.30	3.78	18,22,31,35	0
25	SQD	d	411	43/54	0.61	0.90	3.75	67,74,78,79	0
29	LMG	z	101	37/55	0.26	1.48	3.65	55,84,88,88	0
31	DGD	H	102	62/66	0.85	1.00	3.58	26,32,38,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	d	401	65/65	0.90	0.84	3.51	13,18,34,35	0
22	CLA	c	510	65/65	0.86	0.86	3.49	24,28,35,37	0
22	CLA	C	512	65/65	0.70	1.33	3.45	37,41,62,63	0
22	CLA	A	607	65/65	0.82	0.78	3.43	21,24,71,72	0
22	CLA	D	403	65/65	0.70	1.20	3.42	24,27,65,67	0
29	LMG	C	520	51/55	0.31	1.35	3.39	43,76,81,82	0
22	CLA	b	603	65/65	0.83	1.17	3.28	23,26,32,32	0
33	HEM	f	101	43/43	0.91	0.69	3.22	39,42,45,47	0
22	CLA	d	403	65/65	0.74	1.19	3.12	24,27,65,67	0
29	LMG	a	614	51/55	0.68	0.80	3.11	53,59,64,65	0
22	CLA	a	604	65/65	0.57	0.86	3.09	19,21,63,65	0
32	LHG	E	101	42/49	0.55	1.29	3.06	69,83,86,86	0
24	BCR	A	608	40/40	0.45	0.70	3.00	22,27,32,32	0
22	CLA	A	604	65/65	0.75	1.01	2.96	19,21,63,65	0
22	CLA	C	511	65/65	0.91	1.24	2.83	29,34,37,38	0
22	CLA	B	613	65/65	0.87	0.73	2.75	20,24,30,31	0
22	CLA	c	502	65/65	0.68	0.96	2.71	24,26,39,42	0
29	LMG	A	614	51/55	0.63	0.84	2.68	53,59,64,65	0
23	PHO	a	606	64/64	0.82	0.79	2.60	19,22,28,32	0
32	LHG	D	409	49/49	0.75	0.75	2.59	26,33,62,64	0
22	CLA	B	604	65/65	0.88	1.04	2.57	18,22,31,35	0
25	SQD	a	609	54/54	0.64	0.53	2.49	49,57,66,67	0
29	LMG	D	406	51/55	0.78	0.79	2.48	26,35,65,67	0
22	CLA	C	507	65/65	0.70	1.33	2.45	29,33,52,53	0
22	CLA	b	616	65/65	0.81	1.25	2.42	25,27,45,46	0
31	DGD	h	102	62/66	0.82	0.90	2.41	26,32,38,40	0
22	CLA	b	605	65/65	0.82	0.79	2.40	19,22,50,51	0
24	BCR	t	101	40/40	0.47	0.63	2.37	27,33,39,39	0
22	CLA	b	602	65/65	0.61	1.48	2.36	32,41,66,66	0
22	CLA	b	610	65/65	0.86	1.10	2.24	23,28,31,32	0
22	CLA	c	506	65/65	0.85	0.93	2.23	31,38,74,75	0
22	CLA	B	611	65/65	0.90	0.99	2.22	21,25,32,37	0
22	CLA	B	610	65/65	0.90	0.83	2.21	23,28,31,32	0
22	CLA	c	505	65/65	0.87	0.82	2.21	28,30,44,45	0
27	BCT	a	612	4/4	0.93	1.21	2.14	39,39,40,42	0
22	CLA	B	609	65/65	0.81	0.88	2.08	20,24,31,31	0
22	CLA	b	609	65/65	0.83	1.02	2.04	20,24,31,31	0
33	HEM	v	201	43/43	0.92	0.72	1.98	23,24,27,29	0
22	CLA	B	606	65/65	0.83	0.84	1.92	19,23,34,35	0
22	CLA	B	616	65/65	0.78	0.74	1.87	25,27,45,46	0
22	CLA	C	508	65/65	0.73	0.74	1.87	25,29,54,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	b	606	65/65	0.78	0.84	1.84	19,23,34,35	0
22	CLA	B	605	65/65	0.89	0.57	1.83	19,22,50,51	0
24	BCR	h	101	40/40	0.81	1.32	1.82	26,33,42,42	0
22	CLA	b	613	65/65	0.86	0.75	1.82	20,24,30,31	0
22	CLA	b	611	65/65	0.84	0.94	1.76	21,25,32,37	0
22	CLA	C	504	65/65	0.81	0.70	1.70	25,28,54,54	0
22	CLA	a	603	65/65	0.73	0.60	1.69	15,19,25,34	0
22	CLA	c	511	65/65	0.83	0.88	1.68	29,34,37,38	0
26	CL	a	610	1/1	0.57	0.55	1.68	24,24,24,24	0
24	BCR	H	101	40/40	0.67	1.32	1.66	26,33,42,42	0
33	HEM	V	201	43/43	0.91	0.69	1.65	23,24,27,29	0
31	DGD	d	410	62/66	0.53	0.76	1.65	77,89,103,103	0
27	BCT	A	612	4/4	0.88	1.02	1.63	39,39,40,42	0
22	CLA	c	508	65/65	0.87	0.60	1.60	25,29,54,58	0
33	HEM	F	101	43/43	0.89	0.79	1.56	39,42,45,47	0
22	CLA	C	510	65/65	0.83	0.81	1.55	24,28,35,37	0
22	CLA	C	513	65/65	0.66	1.10	1.52	39,45,64,64	0
22	CLA	c	513	65/65	0.68	1.02	1.49	39,45,64,64	0
22	CLA	C	502	65/65	0.86	0.79	1.47	24,26,39,42	0
22	CLA	b	617	65/65	0.67	0.91	1.45	22,29,77,78	0
22	CLA	C	505	65/65	0.90	0.90	1.44	28,30,44,45	0
25	SQD	A	609	54/54	0.65	0.63	1.42	49,57,66,67	0
22	CLA	A	603	65/65	0.77	0.67	1.41	15,19,25,34	0
22	CLA	B	602	65/65	0.62	1.02	1.37	32,41,66,66	0
22	CLA	b	607	65/65	0.51	0.88	1.34	24,28,40,41	0
31	DGD	C	518	62/66	0.75	0.64	1.25	22,31,52,56	0
31	DGD	C	516	62/66	0.85	0.58	1.25	23,33,61,62	0
23	PHO	A	605	64/64	0.77	0.59	1.22	16,21,25,26	0
22	CLA	C	506	65/65	0.76	0.97	1.21	31,38,74,75	0
22	CLA	C	503	65/65	0.90	0.80	1.13	27,31,35,36	0
32	LHG	d	409	49/49	0.77	0.71	1.09	26,33,62,64	0
24	BCR	a	608	40/40	0.39	0.47	1.07	22,27,32,32	0
32	LHG	e	101	42/49	0.52	0.61	1.06	69,83,86,86	0
31	DGD	c	518	62/66	0.81	0.53	1.02	22,31,52,56	0
23	PHO	a	605	64/64	0.81	0.52	0.99	16,21,25,26	0
24	BCR	b	618	40/40	0.75	0.41	0.98	21,28,40,40	0
25	SQD	b	601	54/54	0.73	0.49	0.84	50,63,68,68	0
32	LHG	D	407	49/49	0.81	0.49	0.82	24,28,37,40	0
22	CLA	B	617	65/65	0.69	0.51	0.78	22,29,77,78	0
28	PL9	D	408	55/55	0.70	0.51	0.75	19,23,29,32	0
29	LMG	d	406	51/55	0.76	0.50	0.75	26,35,65,67	0
22	CLA	B	607	65/65	0.61	0.62	0.70	24,28,40,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	B	612	65/65	0.85	0.44	0.61	19,21,32,34	0
31	DGD	C	517	62/66	0.82	0.54	0.59	23,35,62,63	0
31	DGD	c	516	62/66	0.87	0.55	0.51	23,33,61,62	0
22	CLA	D	402	65/65	0.78	0.53	0.49	14,18,29,35	0
22	CLA	c	504	65/65	0.91	0.51	0.46	25,28,54,54	0
22	CLA	b	612	65/65	0.77	0.43	0.27	19,21,32,34	0
20	OEX	a	601	10/10	0.93	0.41	0.19	22,23,26,26	0
22	CLA	b	614	65/65	0.73	0.45	0.13	19,22,45,47	0
24	BCR	T	101	40/40	0.79	0.40	0.07	23,27,28,29	0
24	BCR	b	622	40/40	0.69	0.48	0.02	25,37,44,45	0
31	DGD	c	517	62/66	0.89	0.40	-0.02	23,35,62,63	0
25	SQD	L	101	54/54	0.77	0.41	-0.04	57,69,84,85	0
22	CLA	d	402	65/65	0.78	0.47	-0.06	14,18,29,35	0
22	CLA	b	608	65/65	0.87	0.43	-0.09	17,20,32,34	0
25	SQD	b	621	54/54	0.77	0.40	-0.12	58,66,80,80	0
32	LHG	d	405	49/49	0.81	0.44	-0.13	29,34,41,41	0
26	CL	a	611	1/1	0.91	0.37	-0.22	21,21,21,21	0
34	MG	j	101	1/1	0.71	0.30	-0.25	27,27,27,27	0
28	PL9	d	408	55/55	0.78	0.40	-0.38	19,23,29,32	0
32	LHG	d	407	49/49	0.80	0.37	-0.39	24,28,37,40	0
22	CLA	b	615	65/65	0.67	0.44	-0.40	20,24,60,61	0
22	CLA	B	608	65/65	0.91	0.41	-0.51	17,20,32,34	0
22	CLA	B	614	65/65	0.91	0.38	-0.52	19,22,45,47	0
26	CL	A	610	1/1	0.80	0.45	-0.57	24,24,24,24	0
20	OEX	A	601	10/10	0.92	0.40	-0.57	22,23,26,26	0
29	LMG	b	619	51/55	0.67	0.38	-0.58	29,39,51,54	0
32	LHG	D	405	49/49	0.76	0.38	-0.62	29,34,41,41	0
32	LHG	L	102	49/49	0.84	0.35	-0.64	23,31,43,44	0
32	LHG	l	103	49/49	0.86	0.33	-0.73	23,31,43,44	0
29	LMG	B	620	51/55	0.58	0.38	-0.80	29,39,51,54	0
25	SQD	l	101	54/54	0.82	0.32	-0.82	57,69,84,85	0
25	SQD	l	102	54/54	0.82	0.32	-0.82	58,66,80,80	0
24	BCR	B	618	40/40	0.82	0.30	-0.85	23,27,28,29	0
22	CLA	B	615	65/65	0.74	0.38	-0.86	20,24,60,61	0
25	SQD	B	601	54/54	0.73	0.35	-0.86	50,63,68,68	0
24	BCR	B	622	40/40	0.67	0.43	-0.91	25,37,44,45	0
26	CL	A	611	1/1	0.85	0.35	-1.00	21,21,21,21	0
34	MG	J	101	1/1	0.87	0.11	-1.31	27,27,27,27	0
21	FE2	A	602	1/1	0.96	0.16	-1.50	26,26,26,26	0
30	CA	o	301	1/1	0.95	0.28	-1.83	49,49,49,49	0
24	BCR	B	619	40/40	0.73	0.31	-1.99	21,28,40,40	0
21	FE2	a	602	1/1	0.83	0.35	-1.99	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
30	CA	O	301	1/1	0.93	0.14	-2.63	49,49,49,49	0
30	CA	f	102	1/1	0.28	0.73	-	56,56,56,56	0
26	CL	U	201	1/1	0.02	0.17	-	50,50,50,50	0
30	CA	B	621	1/1	0.25	0.73	-	76,76,76,76	0
26	CL	u	201	1/1	0.03	0.36	-	50,50,50,50	0
30	CA	F	102	1/1	0.70	0.50	-	56,56,56,56	0
30	CA	b	620	1/1	0.53	1.24	-	76,76,76,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.