



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:40 PM GMT

PDB ID : 4IL6
Title : Structure of Sr-substituted photosystem II
Authors : Koua, F.H.M.; Umena, Y.; Kawakami, K.; Kamiya, N.; Shen, J.R.
Deposited on : 2012-12-29
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

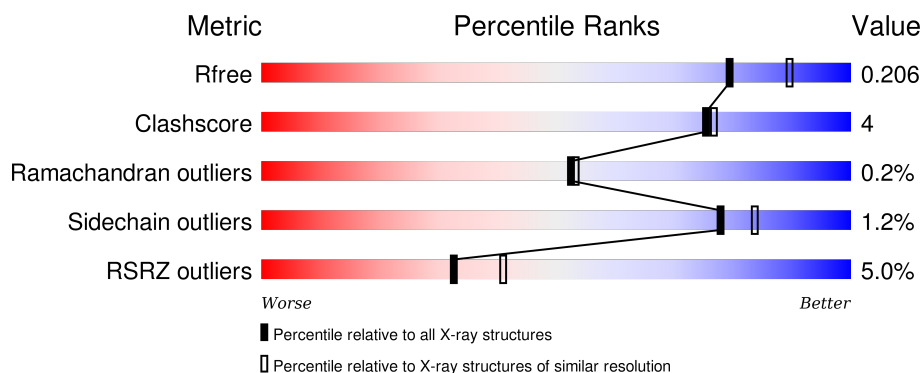
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	334	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>10%</div> </div> </div>
1	a	334	<div> <div>2%</div> <div> <div></div> <div>99%</div> <div>.</div> </div> </div>
2	B	505	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>10%</div> </div> </div>
2	b	505	<div> <div>5%</div> <div> <div></div> <div>98%</div> <div>.</div> </div> </div>
3	C	451	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>13%</div> </div> </div>

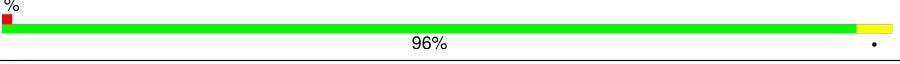
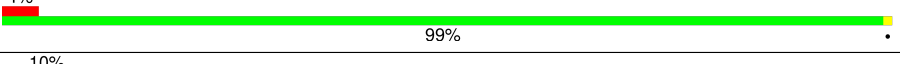
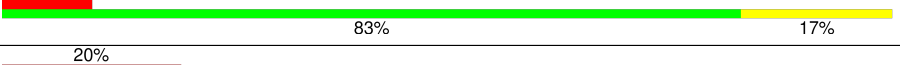
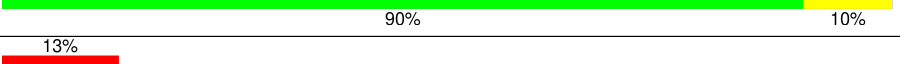
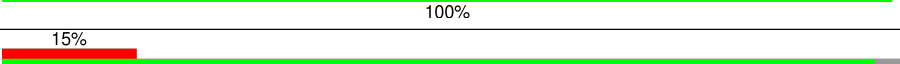
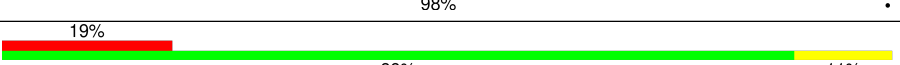
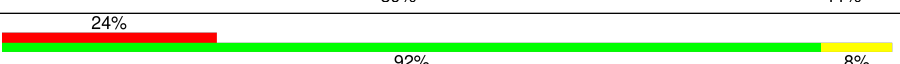


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Mol	Chain	Length	Quality of chain
3	c	451	
4	D	342	
4	d	342	
5	E	80	
5	e	80	
6	F	34	
6	f	34	
7	H	63	
7	h	63	
8	I	36	
8	i	36	
9	J	37	
9	j	37	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	34	
12	m	34	
13	O	244	
13	o	244	
14	T	31	
14	t	31	
15	U	97	
15	u	97	

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Mol	Chain	Length	Quality of chain
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	
20	R	34	

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
24	CLA	A	1005	X	-	-	-
24	CLA	A	1006	X	-	-	-
24	CLA	A	1008	X	-	-	-
24	CLA	B	601	X	-	-	X
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	D	405	X	-	-	-
24	CLA	a	407	X	-	-	-
24	CLA	a	408	X	-	-	-
24	CLA	a	409	X	-	-	X
24	CLA	a	412	X	-	-	X
24	CLA	b	604	X	-	-	X
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	c	501	X	-	-	-
24	CLA	c	502	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	403	X	-	-	-
26	BCR	B	618	-	-	-	X
27	PL9	A	1010	-	-	-	X
27	PL9	a	414	-	-	-	X
28	SQD	B	620[A]	-	-	-	X
28	SQD	B	620[B]	-	-	-	X
28	SQD	a	401	-	-	-	X
28	SQD	b	623[A]	-	-	-	X
28	SQD	b	623[B]	-	-	-	X
29	LMG	A	1012	-	-	-	X
29	LMG	B	622	-	-	-	X
29	LMG	C	519	-	-	-	X
29	LMG	D	412	-	-	-	X
29	LMG	Z	101	-	-	-	X
29	LMG	c	519	-	-	-	X
29	LMG	c	521	-	-	-	X
29	LMG	d	409	-	-	-	X
29	LMG	m	102	-	-	-	X
30	DMS	A	1014	-	-	-	X
30	DMS	B	627	-	-	-	X
30	DMS	B	632	-	-	-	X
30	DMS	B	634	-	-	-	X
30	DMS	C	524	-	-	-	X
30	DMS	D	416	-	-	-	X
30	DMS	D	417	-	-	-	X
30	DMS	O	301	-	-	-	X
30	DMS	O	302	-	-	-	X
30	DMS	V	203	-	-	-	X
30	DMS	b	629	-	-	-	X
30	DMS	b	634	-	-	-	X
30	DMS	b	635	-	-	-	X
30	DMS	c	526	-	-	-	X
30	DMS	c	529	-	-	-	X
30	DMS	d	413	-	-	-	X
30	DMS	v	202	-	-	-	X
31	UNL	B	630	-	-	-	X
31	UNL	D	414	-	-	-	X
31	UNL	D	415	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	UNL	I	101	-	-	-	X
31	UNL	K	103	-	-	-	X
31	UNL	b	603	-	-	-	X
31	UNL	c	523	-	-	-	X
31	UNL	d	412	-	-	-	X
31	UNL	l	101	-	-	-	X
31	UNL	t	102	-	-	-	X
31	UNL	x	101	-	-	-	X
32	LMT	A	1017	-	-	-	X
32	LMT	A	1018	-	-	-	X
32	LMT	C	520	-	-	-	X
32	LMT	M	101	-	-	-	X
32	LMT	a	402	-	-	-	X
32	LMT	a	416	-	-	-	X
32	LMT	b	631	-	-	-	X
32	LMT	f	103	-	-	-	X
32	LMT	i	102	-	-	-	X
32	LMT	m	103	-	-	-	X
32	LMT	t	103	-	-	-	X
33	GOL	V	204	-	-	-	X
33	GOL	V	206	-	-	-	X
34	LHG	D	411	-	-	-	X
34	LHG	E	101	-	-	-	X
34	LHG	d	406	-	-	-	X
34	LHG	d	408	-	-	-	X
34	LHG	e	101	-	-	-	X
35	HTG	B	628	-	-	-	X
35	HTG	C	522	-	-	-	X
35	HTG	D	413	-	-	-	X
35	HTG	V	202	-	-	-	X
35	HTG	b	626	-	-	-	X
35	HTG	d	410	-	-	-	X
35	HTG	d	416	-	-	-	X
35	HTG	o	301	-	-	-	X
36	DGD	C	516	-	-	-	X
36	DGD	c	516	-	-	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 53568 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	5	0
			2643	1733	431	464	15			
1	a	334	Total	C	N	O	S	0	4	0
			2637	1729	431	462	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	SEE REMARK 999	UNP P51765
a	279	PRO	ARG	SEE REMARK 999	UNP P51765

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	10	0
			4040	2652	674	701	13			
2	b	505	Total	C	N	O	S	0	9	0
			4033	2646	676	698	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	3	0
			3500	2292	584	611	13			
3	c	450	Total	C	N	O	S	0	2	0
			3492	2287	583	609	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	80	Total	C	N	O		0	2	0
			660	431	105	124				
5	e	78	Total	C	N	O		0	0	0
			638	418	103	117				

- 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	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total	C	N	O	S	0	1	0
			506	338	83	83	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	37	Total	C	N	O	S	0	0	0
			266	179	41	45	1			
9	j	37	Total	C	N	O	S	0	0	0
			266	179	41	45	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	1	0
			274	184	40	49	1			
12	m	34	Total	C	N	O	S	0	1	0
			274	184	40	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	2	0
			1883	1176	317	386	4			
13	o	243	Total	C	N	O	S	0	1	0
			1868	1167	315	382	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	31	Total	C	N	O	S	0	0	0
			267	187	38	40	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	1	0
			780	495	129	156			
15	u	97	Total	C	N	O	0	1	0
			780	495	129	156			

- 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	3	0
			1081	687	179	211	4			
16	v	137	Total	C	N	O	S	0	2	0
			1076	683	177	212	4			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	40	Total	C	N	O	0	0	0
			296	197	47	52			
18	x	39	Total	C	N	O	0	0	0
			287	191	46	50			

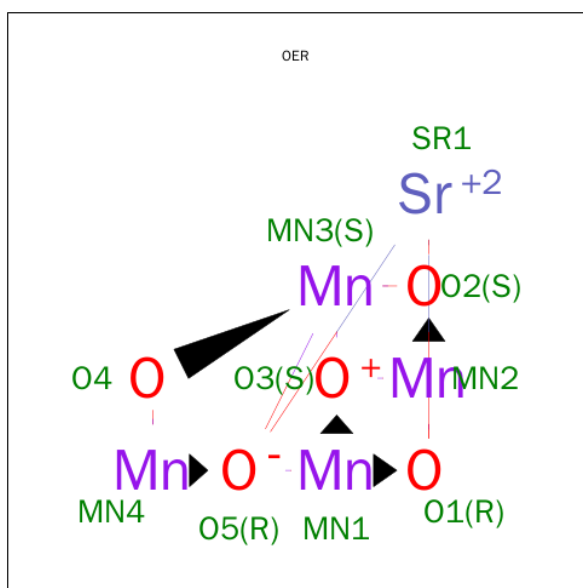
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			481	329	72	78	2			
19	z	62	Total	C	N	O	S	0	0	0
			481	329	72	78	2			

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

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

- Molecule 21 is SR-MN4-O5 CLUSTER (three-letter code: OER) (formula: $\text{Mn}_4\text{O}_5\text{Sr}$).



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

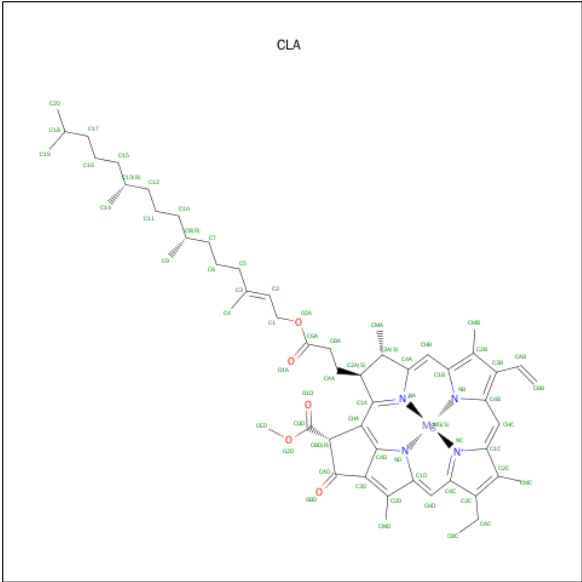
- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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

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

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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
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

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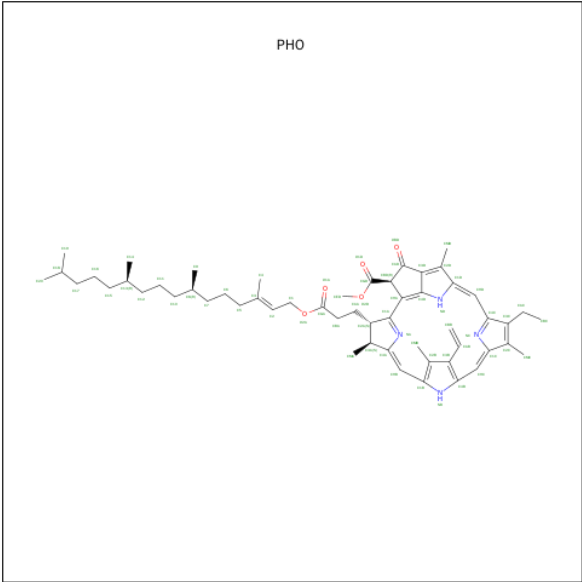
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N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

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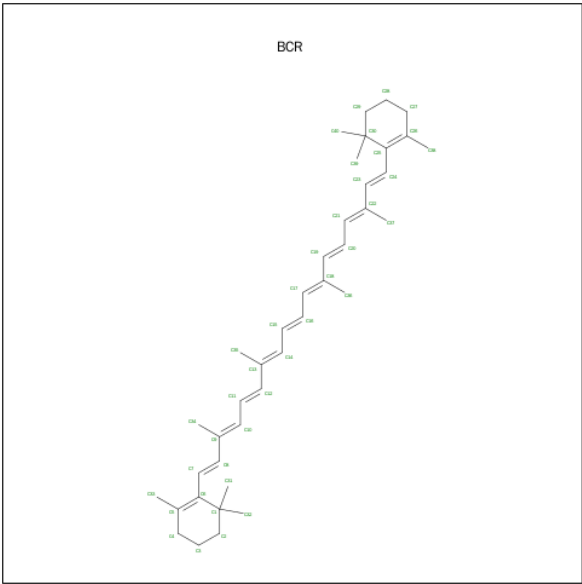
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	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	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: C₅₅H₇₄N₄O₅).



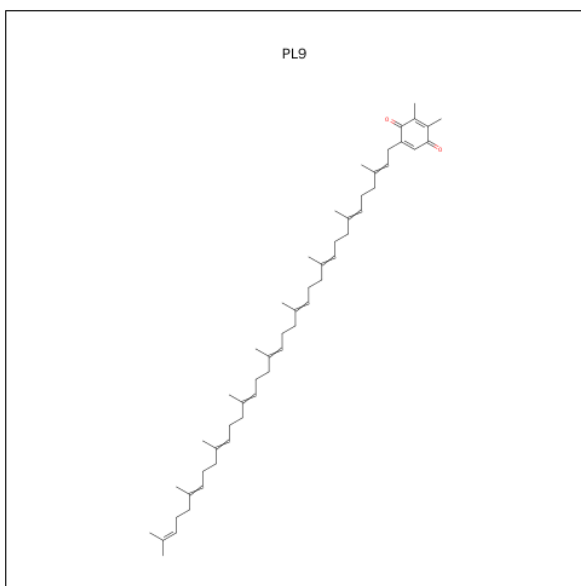
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	D	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



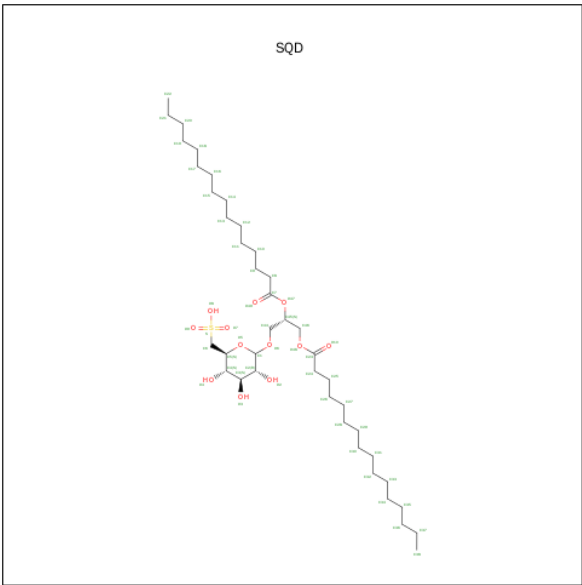
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	J	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total 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
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	d	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	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0
26	y	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: $C_{53}H_{80}O_2$).



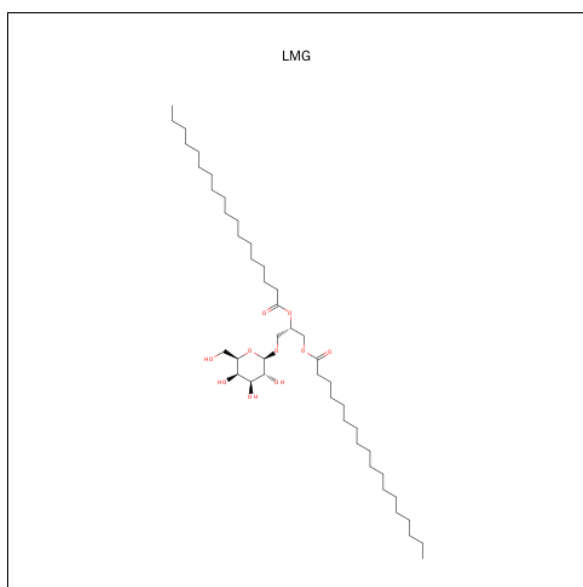
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			55	53	2		
27	D	1	Total	C	O	0	0
			55	53	2		
27	a	1	Total	C	O	0	0
			55	53	2		
27	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



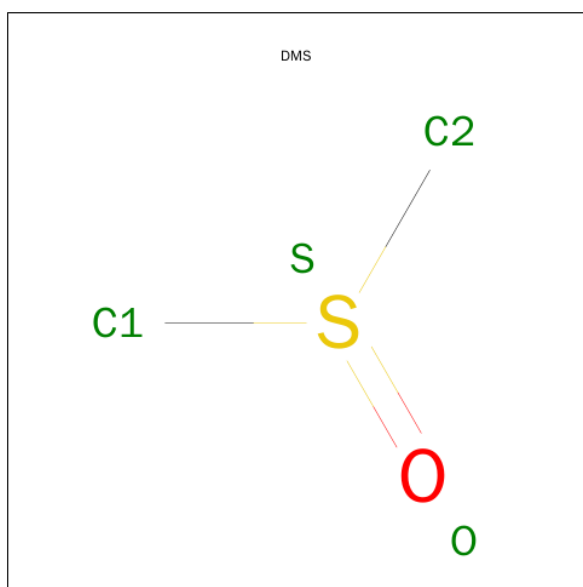
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	B	1	Total	C	O	S	0	1
			108	82	24	2		
28	D	1	Total	C	O	S	0	0
			43	30	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	b	1	Total	C	O	S	0	1
			108	82	24	2		
28	c	1	Total	C	O	S	0	0
			54	41	12	1		
28	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



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
			51	41	10		
29	a	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	c	1	Total	C	O	0	0
			51	41	10		
29	d	1	Total	C	O	0	0
			51	41	10		
29	m	1	Total	C	O	0	0
			51	41	10		

- Molecule 30 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			4	2	1	1		
30	A	1	Total	C	O	S	0	0
			4	2	1	1		
30	B	1	Total	C	O	S	0	0
			4	2	1	1		
30	B	1	Total	C	O	S	0	0
			4	2	1	1		
30	B	1	Total	C	O	S	0	0
			4	2	1	1		
30	B	1	Total	C	O	S	0	0
			4	2	1	1		
30	C	1	Total	C	O	S	0	0
			4	2	1	1		
30	C	1	Total	C	O	S	0	0
			4	2	1	1		
30	C	1	Total	C	O	S	0	0
			4	2	1	1		
30	C	1	Total	C	O	S	0	0
			4	2	1	1		
30	D	1	Total	C	O	S	0	0
			4	2	1	1		
30	D	1	Total	C	O	S	0	0
			4	2	1	1		

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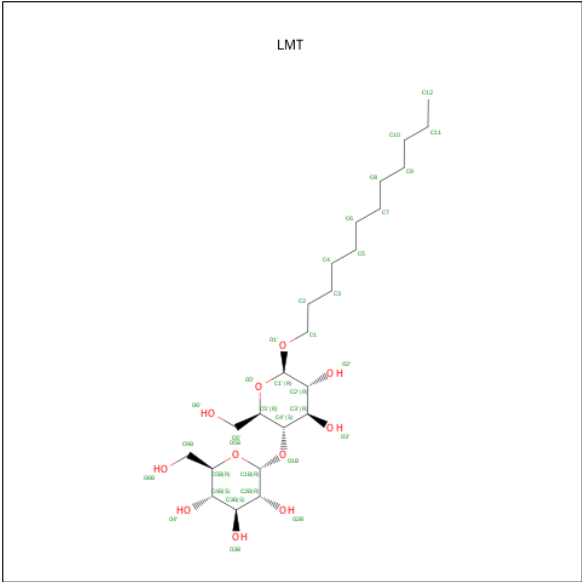
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	O	1	Total 4	C 2	O 1	S 1	0	0
30	O	1	Total 4	C 2	O 1	S 1	0	0
30	U	1	Total 4	C 2	O 1	S 1	0	0
30	V	1	Total 4	C 2	O 1	S 1	0	0
30	V	1	Total 4	C 2	O 1	S 1	0	0
30	a	1	Total 4	C 2	O 1	S 1	0	0
30	a	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	b	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	c	1	Total 4	C 2	O 1	S 1	0	0
30	d	1	Total 4	C 2	O 1	S 1	0	0
30	d	1	Total 4	C 2	O 1	S 1	0	0
30	u	1	Total 4	C 2	O 1	S 1	0	0
30	v	1	Total 4	C 2	O 1	S 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	J	1	Total C 16 16	0	0
31	i	1	Total C 16 16	0	0
31	D	2	Total C O 56 51 5	0	0
31	K	1	Total C O 34 29 5	0	0
31	y	1	Total C 16 16	0	0
31	l	1	Total C 16 16	0	0
31	B	2	Total C 32 32	0	0
31	I	2	Total C 26 26	0	0
31	c	1	Total C O 32 27 5	0	0
31	a	1	Total C O 30 25 5	0	0
31	x	1	Total C 16 16	0	0
31	A	1	Total C O 28 23 5	0	0
31	j	1	Total C 16 16	0	0
31	X	1	Total C 16 16	0	0
31	d	2	Total C O 52 47 5	0	0
31	t	1	Total C 16 16	0	0
31	Y	1	Total C 16 16	0	0
31	L	1	Total C 16 16	0	0
31	b	2	Total C 32 32	0	0

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



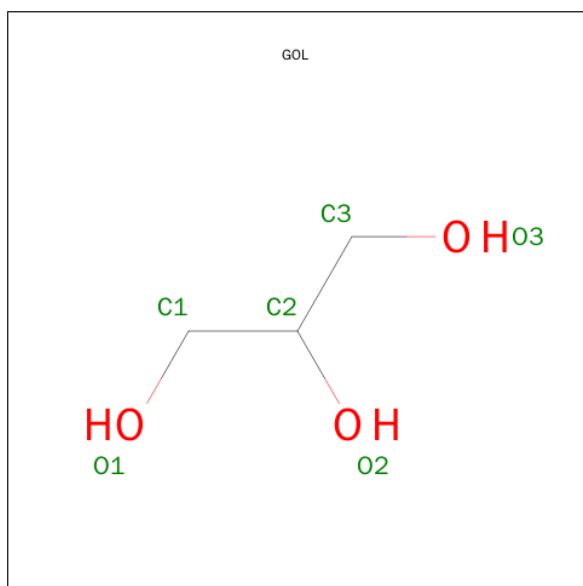
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			35	24	11		
32	A	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	C	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	a	1	Total	C	O	0	0
			35	24	11		
32	a	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			35	24	11		
32	f	1	Total	C	O	0	0
			35	24	11		
32	i	1	Total	C	O	0	0
			35	24	11		
32	m	1	Total	C	O	0	0
			35	24	11		
32	m	1	Total	C	O	0	0
			35	24	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	t	1	Total	C	O	0	0
			35	24	11		

- Molecule 33 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



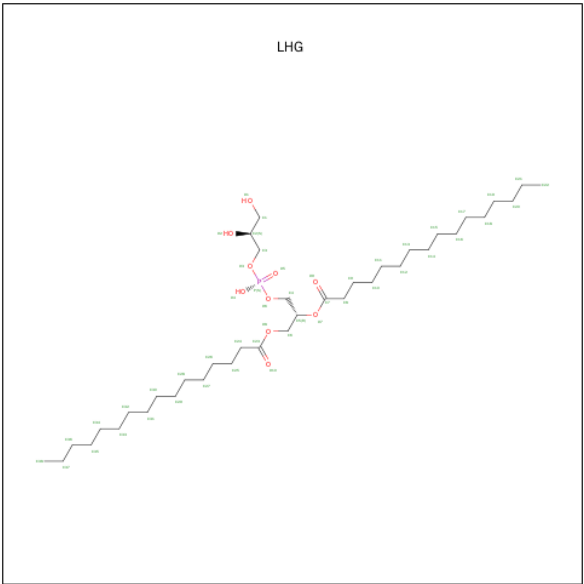
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	A	1	Total	C	O	0	0
			6	3	3		
33	B	1	Total	C	O	0	0
			6	3	3		
33	D	1	Total	C	O	0	0
			6	3	3		
33	V	1	Total	C	O	0	0
			6	3	3		
33	V	1	Total	C	O	0	0
			6	3	3		
33	V	1	Total	C	O	0	0
			6	3	3		
33	a	1	Total	C	O	0	0
			6	3	3		
33	b	1	Total	C	O	0	0
			6	3	3		
33	d	1	Total	C	O	0	0
			6	3	3		
33	d	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	v	1	Total	C	O	0	0
			6	3	3		
33	v	1	Total	C	O	0	0
			6	3	3		

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



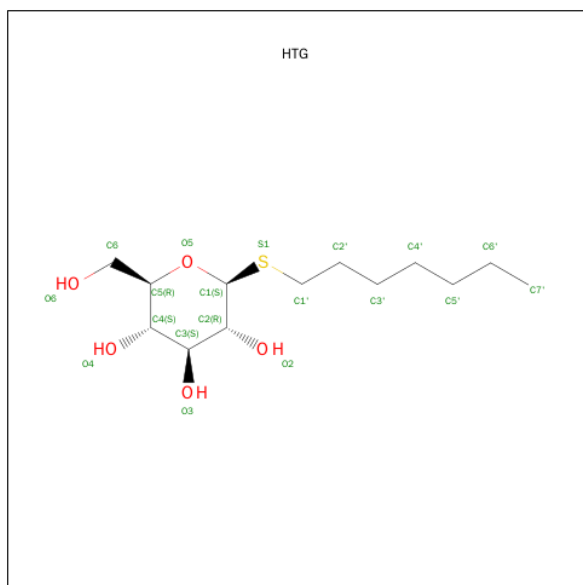
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	P	0	0
			49	38	10	1		
34	D	1	Total	C	O	P	0	0
			49	38	10	1		
34	D	1	Total	C	O	P	0	0
			49	38	10	1		
34	D	1	Total	C	O	P	0	0
			49	38	10	1		
34	E	1	Total	C	O	P	0	0
			49	38	10	1		
34	b	1	Total	C	O	P	0	0
			49	38	10	1		
34	d	1	Total	C	O	P	0	0
			49	38	10	1		
34	d	1	Total	C	O	P	0	0
			49	38	10	1		
34	d	1	Total	C	O	P	0	0
			49	38	10	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	e	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 35 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



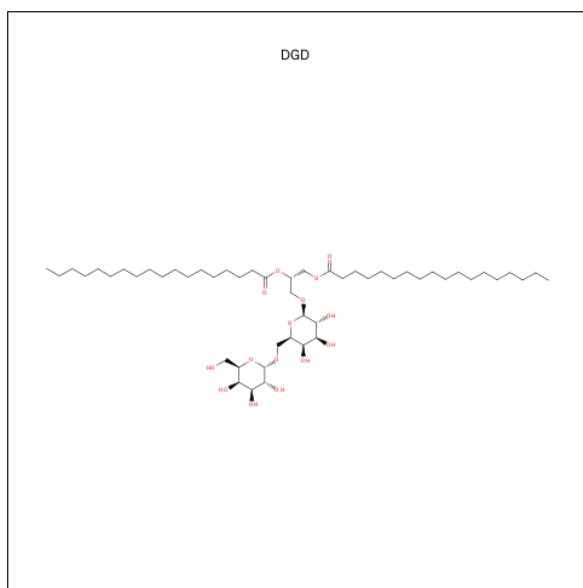
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			19	13	5	1		
35	V	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	d	1	Total	C	O	S	0	0
			19	13	5	1		
35	d	1	Total	C	O	S	0	0
			19	13	5	1		
35	o	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



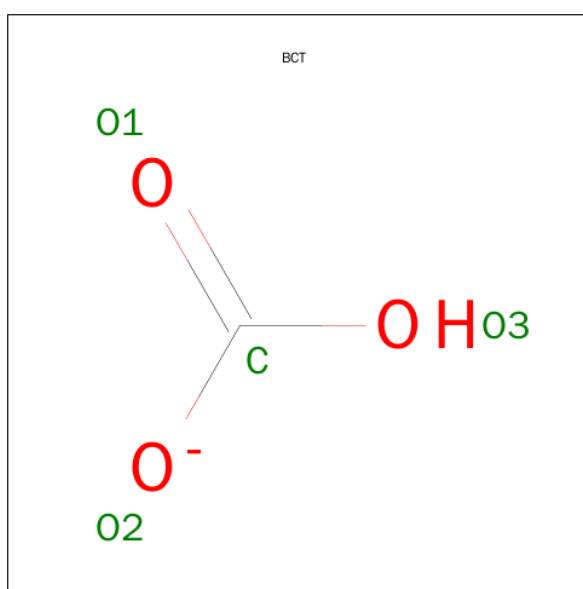
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			62	47	15		
36	H	1	Total	C	O	0	0
			62	47	15		

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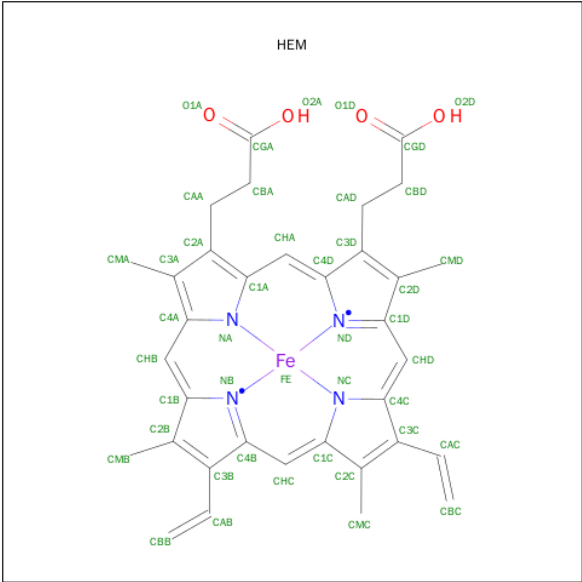
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 37 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	D	1	Total	C	O	0	0
			4	1	3		
37	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	F	1	Total	C	Fe	N	O	
			43	34	1	4	4	
38	V	1	Total	C	Fe	N	O	
			43	34	1	4	4	
38	f	1	Total	C	Fe	N	O	
			43	34	1	4	4	
38	v	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	J	1	Total	Mg		
			1	1	0	0
39	j	1	Total	Mg		
			1	1	0	0
39	K	1	Total	Mg		
			1	1	0	0
39	k	1	Total	Mg		
			1	1	0	0

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	A	134	Total	O		
			134	134	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	B	252	Total 253	O 253	0	1
40	C	168	Total 168	O 168	0	0
40	D	132	Total 132	O 132	0	0
40	E	22	Total 22	O 22	0	0
40	F	6	Total 6	O 6	0	0
40	H	31	Total 31	O 31	0	0
40	I	4	Total 4	O 4	0	0
40	J	7	Total 7	O 7	0	0
40	K	7	Total 7	O 7	0	0
40	L	11	Total 11	O 11	0	0
40	M	6	Total 6	O 6	0	0
40	O	119	Total 119	O 119	0	0
40	T	10	Total 10	O 10	0	0
40	U	63	Total 63	O 63	0	0
40	V	96	Total 96	O 96	0	0
40	Y	1	Total 1	O 1	0	0
40	X	8	Total 8	O 8	0	0
40	Z	1	Total 1	O 1	0	0
40	R	1	Total 1	O 1	0	0
40	a	118	Total 118	O 118	0	0
40	b	209	Total 209	O 209	0	0

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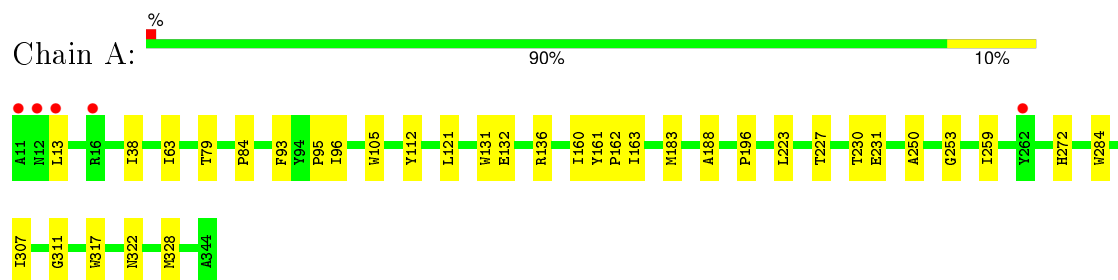
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	c	169	Total 169	O 169	0	0
40	d	121	Total 121	O 121	0	0
40	e	9	Total 9	O 9	0	0
40	f	5	Total 5	O 5	0	0
40	h	23	Total 23	O 23	0	0
40	i	4	Total 4	O 4	0	0
40	j	5	Total 5	O 5	0	0
40	k	3	Total 3	O 3	0	0
40	l	8	Total 8	O 8	0	0
40	m	10	Total 10	O 10	0	0
40	o	112	Total 112	O 112	0	0
40	t	13	Total 13	O 13	0	0
40	u	74	Total 74	O 74	0	0
40	v	65	Total 65	O 65	0	0
40	y	1	Total 1	O 1	0	0
40	x	9	Total 9	O 9	0	0

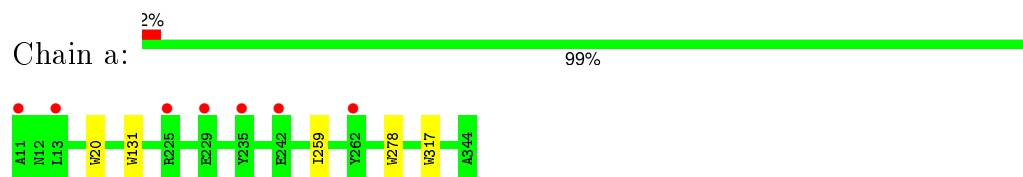
3 Residue-property plots [i](#)

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

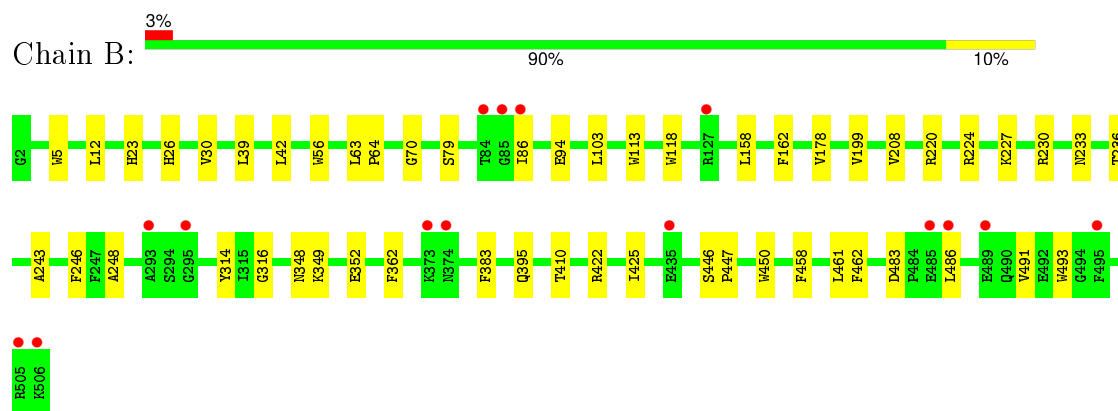
- Molecule 1: Photosystem Q(B) protein



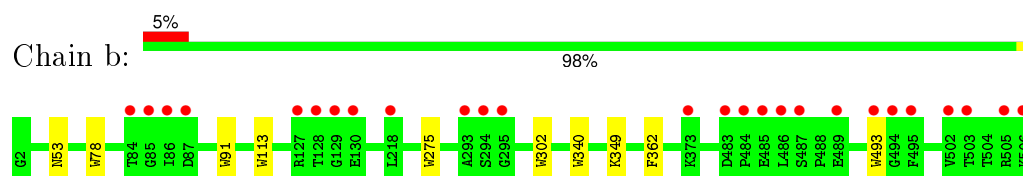
- Molecule 1: Photosystem Q(B) protein



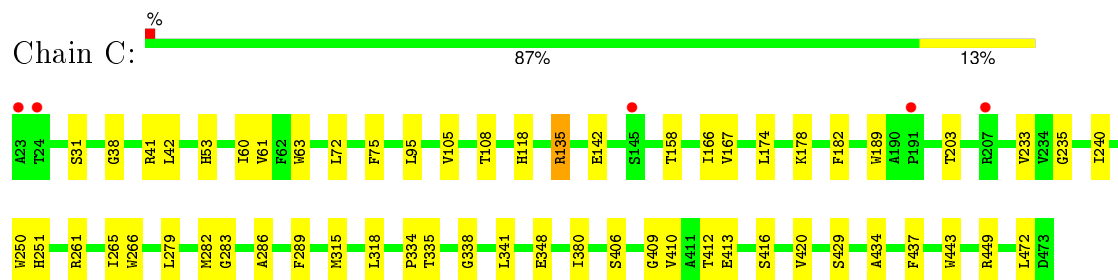
- Molecule 2: Photosystem II core light harvesting protein



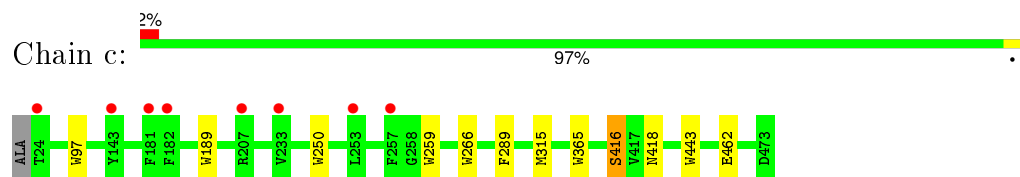
- Molecule 2: Photosystem II core light harvesting protein



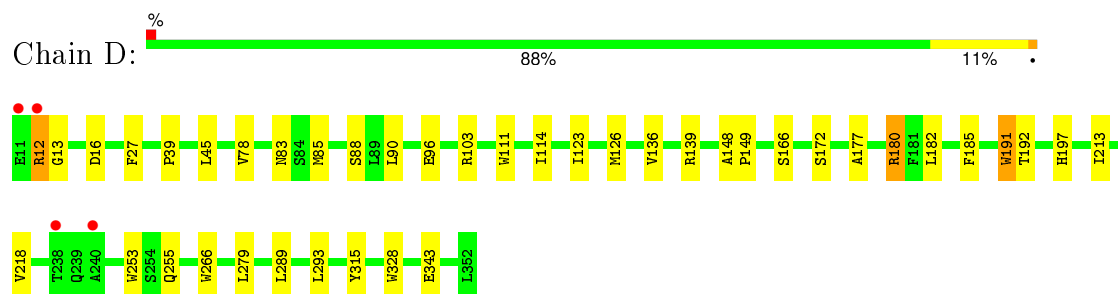
- Molecule 3: Photosystem II CP43 protein



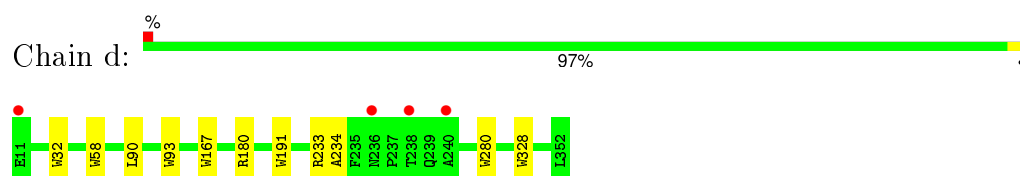
- Molecule 3: Photosystem II CP43 protein



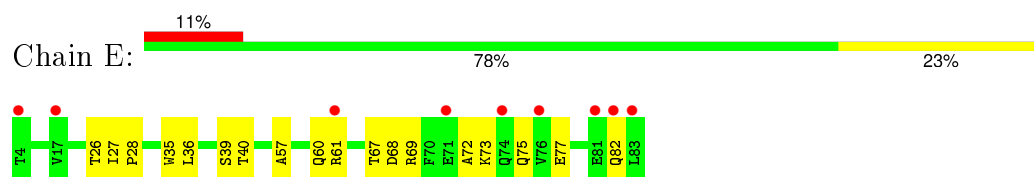
- Molecule 4: Photosystem II D2 protein



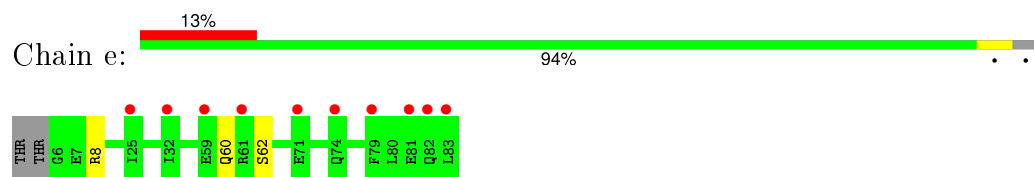
- Molecule 4: Photosystem II D2 protein



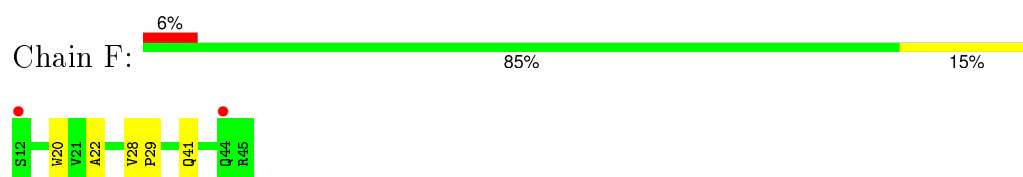
- Molecule 5: Cytochrome b559 subunit alpha



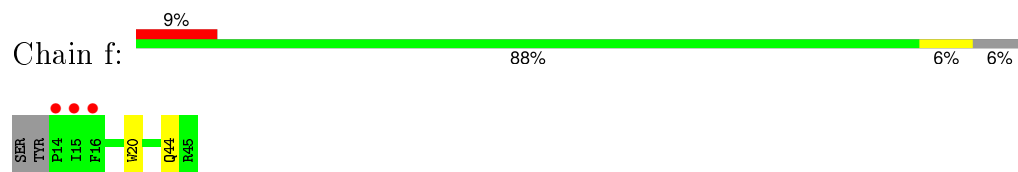
- Molecule 5: Cytochrome b559 subunit alpha



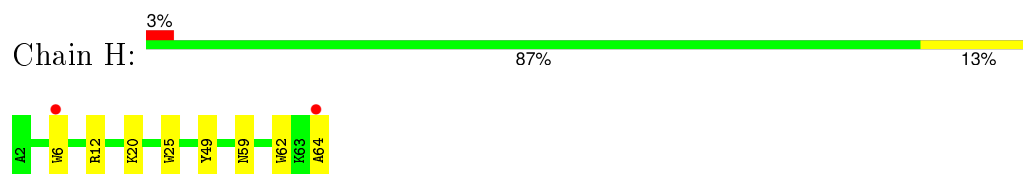
- Molecule 6: Cytochrome b559 subunit beta



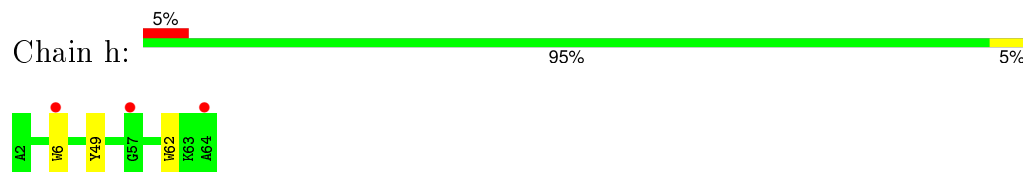
- Molecule 6: Cytochrome b559 subunit beta



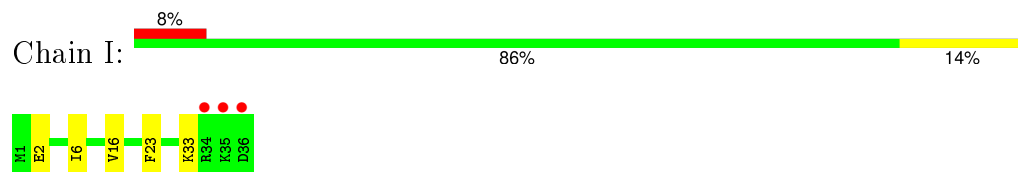
- Molecule 7: Photosystem II reaction center protein H



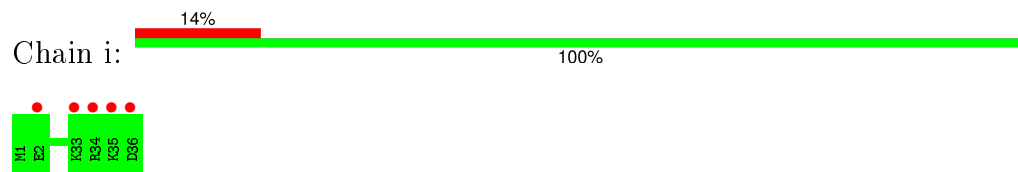
- Molecule 7: Photosystem II reaction center protein H



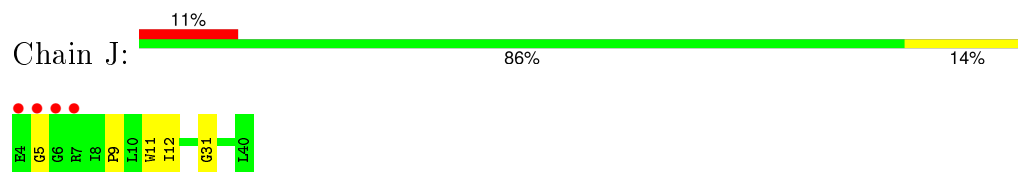
- Molecule 8: Photosystem II reaction center protein I



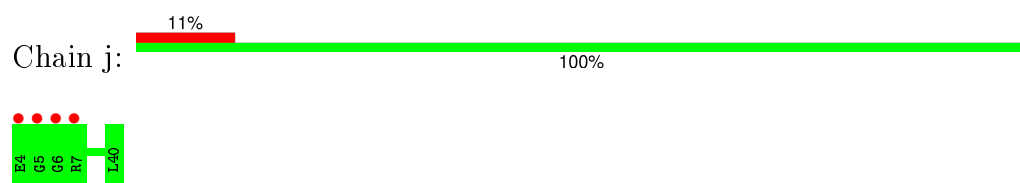
- Molecule 8: Photosystem II reaction center protein I



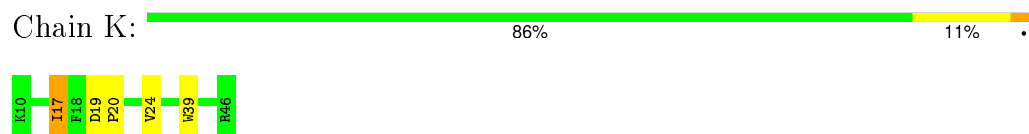
- Molecule 9: Photosystem II reaction center protein J



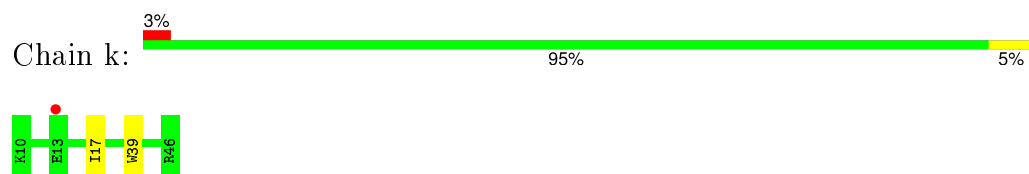
- Molecule 9: Photosystem II reaction center protein J



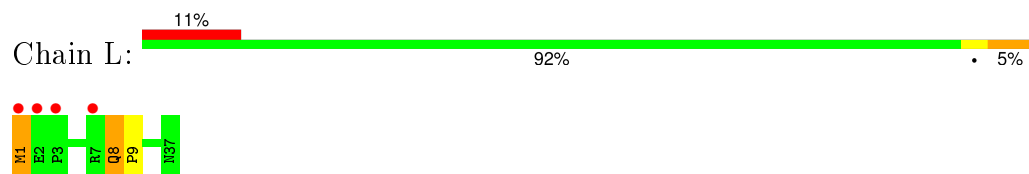
- Molecule 10: Photosystem II reaction center protein K



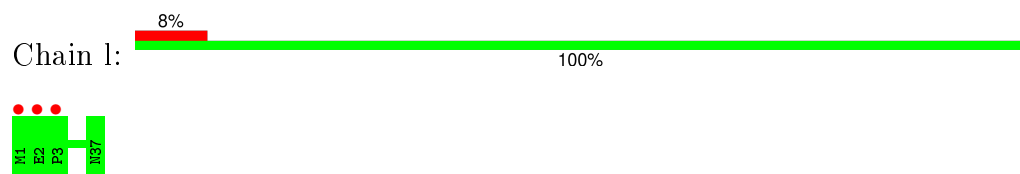
- Molecule 10: Photosystem II reaction center protein K



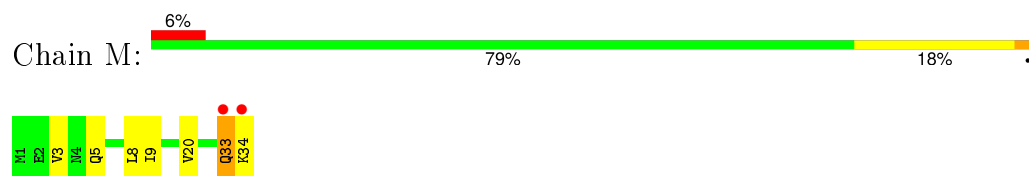
- Molecule 11: Photosystem II reaction center protein L



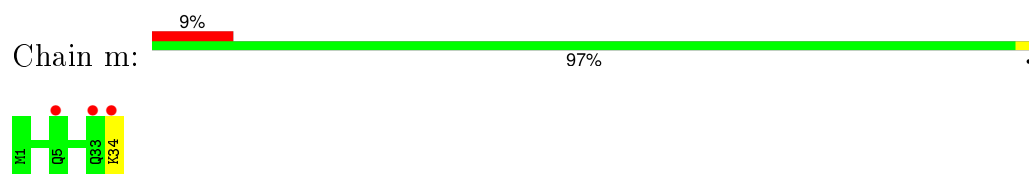
- Molecule 11: Photosystem II reaction center protein L



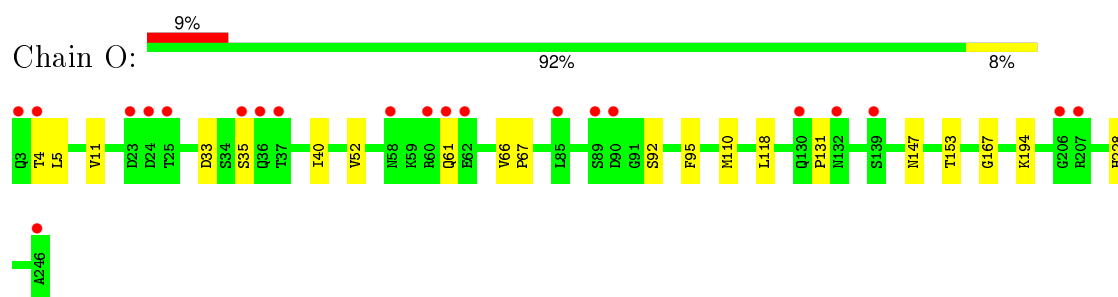
- Molecule 12: Photosystem II reaction center protein M



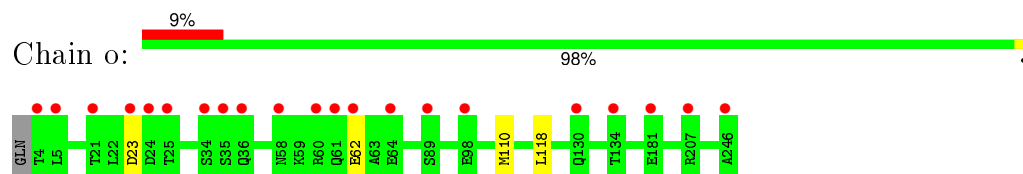
- Molecule 12: Photosystem II reaction center protein M



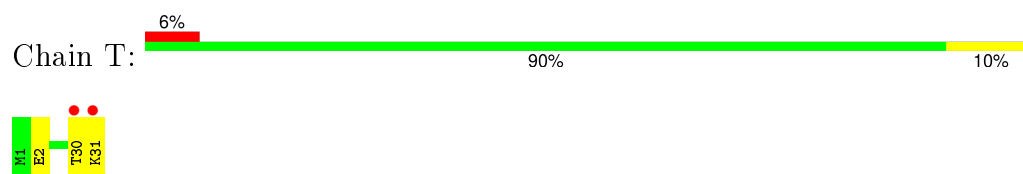
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



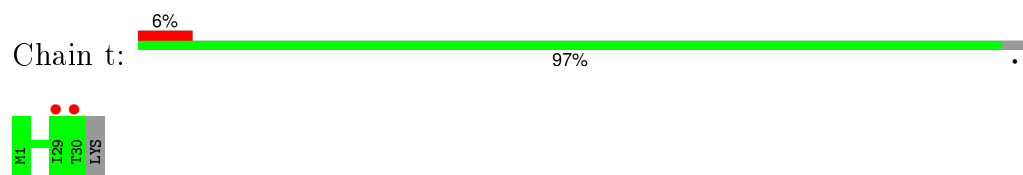
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



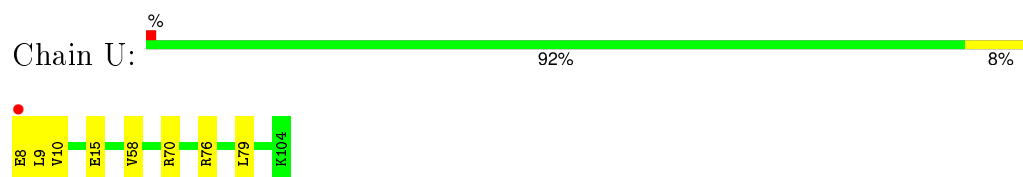
- Molecule 14: Photosystem II reaction center protein T



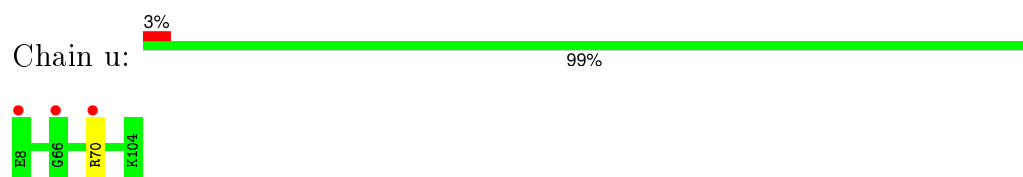
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein

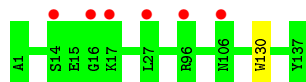


- Molecule 16: Cytochrome c-550

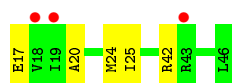
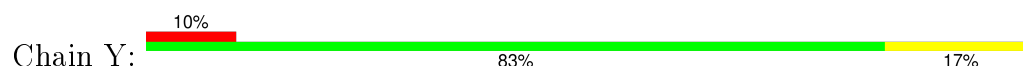




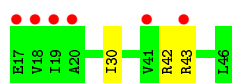
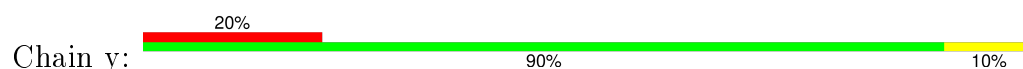
- Molecule 16: Cytochrome c-550



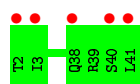
- Molecule 17: Photosystem II reaction center protein ycf12



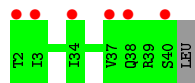
- Molecule 17: Photosystem II reaction center protein ycf12



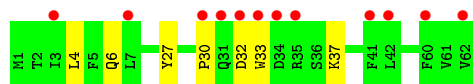
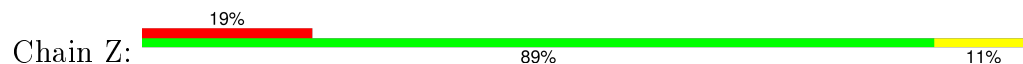
- Molecule 18: Photosystem II reaction center protein X



- Molecule 18: Photosystem II reaction center protein X

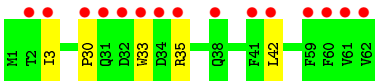


- Molecule 19: Photosystem II reaction center protein Z

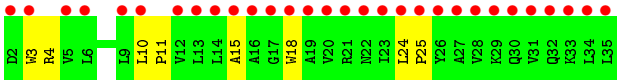
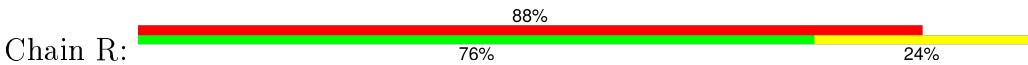


- Molecule 19: Photosystem II reaction center protein Z





● Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.86 Å 228.79 Å 285.76 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.10 19.96 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.96-2.10) 99.9 (19.96-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.09 Å)	Xtriage
Refinement program	REFMAC5.6.0117	Depositor
R, R_{free}	0.176 , 0.205 0.177 , 0.206	Depositor DCC
R_{free} test set	23034 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 460677 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	53568	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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, GOL, MG, PHO, DGD, CL, OER, LMT, CLA, PL9, DMS, FE2, SQD, BCT, HEM, FME, UNL, HTG, 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	0.57	1/2743 (0.0%)	0.52	0/3740
1	a	0.56	4/2734 (0.1%)	0.52	0/3728
2	B	0.58	6/4210 (0.1%)	0.53	0/5731
2	b	0.58	7/4200 (0.2%)	0.52	0/5719
3	C	0.58	4/3622 (0.1%)	0.52	0/4931
3	c	0.58	7/3611 (0.2%)	0.51	0/4916
4	D	0.62	3/2821 (0.1%)	0.54	0/3844
4	d	0.60	7/2821 (0.2%)	0.53	0/3844
5	E	0.51	1/685 (0.1%)	0.51	0/936
5	e	0.49	0/657	0.49	0/897
6	F	0.57	1/284 (0.4%)	0.46	0/387
6	f	0.56	1/265 (0.4%)	0.47	0/360
7	H	0.60	2/522 (0.4%)	0.52	0/712
7	h	0.60	2/511 (0.4%)	0.53	0/697
8	I	0.34	0/293	0.42	0/396
8	i	0.35	0/293	0.44	0/396
9	J	0.54	1/272 (0.4%)	0.49	0/368
9	j	0.51	0/272	0.49	0/368
10	K	0.52	1/303 (0.3%)	0.49	0/416
10	k	0.51	1/303 (0.3%)	0.52	0/416
11	L	0.38	0/311	0.46	0/422
11	l	0.36	0/311	0.47	0/422
12	M	0.30	0/270	0.48	0/368
12	m	0.33	0/270	0.47	0/368
13	O	0.34	0/1920	0.53	0/2603
13	o	0.33	0/1902	0.52	0/2579
14	T	0.40	0/266	0.45	0/360
14	t	0.38	0/257	0.45	0/349
15	U	0.36	0/794	0.51	0/1076
15	u	0.34	0/794	0.51	0/1076
16	V	0.40	0/1111	0.49	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.40	1/1103 (0.1%)	0.48	0/1497
17	Y	0.33	0/225	0.49	0/301
17	y	0.30	0/225	0.48	0/301
18	X	0.32	0/299	0.43	0/403
18	x	0.33	0/290	0.42	0/392
19	Z	0.52	1/482 (0.2%)	0.46	0/659
19	z	0.51	1/482 (0.2%)	0.46	0/659
20	R	0.65	2/279 (0.7%)	0.52	0/383
All	All	0.53	54/43013 (0.1%)	0.51	0/58527

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	317	TRP	CD2-CE2	5.39	1.47	1.41
4	d	167	TRP	CD2-CE2	5.37	1.47	1.41
4	d	191	TRP	CD2-CE2	5.34	1.47	1.41
2	b	91	TRP	CD2-CE2	5.32	1.47	1.41
2	B	56	TRP	CD2-CE2	5.26	1.47	1.41

There are no bond angle outliers.

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	2643	0	2550	30	0
1	a	2637	0	2544	0	0
2	B	4040	0	3928	47	0
2	b	4033	0	3921	0	0
3	C	3500	0	3429	41	0
3	c	3492	0	3419	0	0
4	D	2726	0	2627	38	0
4	d	2726	0	2627	0	0
5	E	660	0	644	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	e	638	0	621	0	0
6	F	275	0	282	3	0
6	f	257	0	269	0	0
7	H	506	0	531	3	0
7	h	498	0	518	0	0
8	I	296	0	311	4	0
8	i	296	0	311	0	0
9	J	266	0	274	2	0
9	j	266	0	274	0	0
10	K	293	0	305	5	0
10	k	293	0	305	0	0
11	L	304	0	316	5	0
11	l	304	0	316	0	0
12	M	274	0	299	5	0
12	m	274	0	299	0	0
13	O	1883	0	1857	11	0
13	o	1868	0	1843	0	0
14	T	267	0	274	2	0
14	t	258	0	261	0	0
15	U	780	0	779	4	0
15	u	780	0	779	0	0
16	V	1081	0	1100	10	0
16	v	1076	0	1087	0	0
17	Y	224	0	252	6	0
17	y	224	0	252	0	0
18	X	296	0	328	0	0
18	x	287	0	317	0	0
19	Z	481	0	515	1	0
19	z	481	0	515	0	0
20	R	273	0	305	4	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	2	0	0	0	0
23	a	2	0	0	0	0
24	A	195	0	216	10	0
24	B	1040	0	1152	52	0
24	C	845	0	936	46	0
24	D	195	0	216	9	0
24	a	260	0	288	0	0
24	b	1040	0	1152	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	c	845	0	936	0	0
24	d	130	0	144	0	0
25	A	64	0	74	1	0
25	D	64	0	74	4	0
25	a	128	0	148	0	0
26	A	40	0	48	0	0
26	B	120	0	140	2	0
26	C	40	0	46	3	0
26	D	40	0	46	1	0
26	H	40	0	46	0	0
26	J	40	0	48	1	0
26	K	80	0	95	2	0
26	T	40	0	47	0	0
26	a	40	0	46	0	0
26	b	120	0	141	0	0
26	c	40	0	47	0	0
26	d	40	0	47	0	0
26	h	40	0	48	0	0
26	k	80	0	94	0	0
26	t	40	0	47	0	0
26	y	40	0	46	0	0
27	A	55	0	80	5	0
27	D	55	0	80	0	0
27	a	55	0	80	0	0
27	d	55	0	80	0	0
28	A	108	0	156	3	0
28	B	108	0	156	21	0
28	D	43	0	53	1	0
28	a	54	0	78	0	0
28	b	108	0	156	0	0
28	c	54	0	78	0	0
28	f	43	0	53	0	0
29	A	51	0	72	0	0
29	B	51	0	72	2	0
29	C	102	0	144	2	0
29	D	51	0	72	1	0
29	Z	51	0	72	1	0
29	a	51	0	72	0	0
29	c	153	0	216	0	0
29	d	51	0	72	0	0
29	m	51	0	72	0	0
30	A	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B	20	0	30	2	0
30	C	20	0	30	0	0
30	D	8	0	12	0	0
30	O	8	0	12	0	0
30	U	4	0	6	0	0
30	V	8	0	12	0	0
30	a	8	0	12	0	0
30	b	20	0	30	0	0
30	c	20	0	30	0	0
30	d	8	0	12	0	0
30	u	4	0	6	0	0
30	v	4	0	6	0	0
31	A	28	0	0	0	0
31	B	32	0	0	0	0
31	D	56	0	0	0	0
31	I	26	0	0	0	0
31	J	16	0	0	0	0
31	K	34	0	0	0	0
31	L	16	0	0	0	0
31	X	16	0	0	0	0
31	Y	16	0	0	0	0
31	a	30	0	0	0	0
31	b	32	0	0	0	0
31	c	32	0	0	0	0
31	d	52	0	0	0	0
31	i	16	0	0	0	0
31	j	16	0	0	0	0
31	l	16	0	0	0	0
31	t	16	0	0	0	0
31	x	16	0	0	0	0
31	y	16	0	0	0	0
32	A	70	0	92	3	0
32	B	35	0	46	0	0
32	C	35	0	46	0	0
32	M	70	0	92	3	0
32	a	70	0	92	0	0
32	b	70	0	92	0	0
32	f	35	0	46	0	0
32	i	35	0	46	0	0
32	m	70	0	92	0	0
32	t	35	0	46	0	0
33	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	B	6	0	8	1	0
33	D	6	0	8	0	0
33	V	18	0	24	0	0
33	a	6	0	8	0	0
33	b	6	0	8	0	0
33	d	12	0	16	0	0
33	v	12	0	16	0	0
34	B	49	0	74	1	0
34	D	147	0	222	13	0
34	E	49	0	74	3	0
34	b	49	0	74	0	0
34	d	147	0	222	0	0
34	e	49	0	74	0	0
35	B	57	0	78	1	0
35	C	38	0	52	0	0
35	D	38	0	52	1	0
35	V	19	0	26	0	0
35	b	76	0	104	0	0
35	c	38	0	52	0	0
35	d	38	0	52	0	0
35	o	19	0	26	0	0
36	C	186	0	246	5	0
36	H	62	0	82	3	0
36	c	186	0	246	0	0
36	h	62	0	82	0	0
37	D	4	0	0	0	0
37	d	4	0	0	0	0
38	F	43	0	30	3	0
38	V	43	0	30	8	0
38	f	43	0	30	0	0
38	v	43	0	30	0	0
39	J	1	0	0	0	0
39	K	1	0	0	0	0
39	j	1	0	0	0	0
39	k	1	0	0	0	0
40	A	134	0	0	1	0
40	B	253	0	0	0	0
40	C	168	0	0	2	0
40	D	132	0	0	0	0
40	E	22	0	0	1	0
40	F	6	0	0	0	0
40	H	31	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	I	4	0	0	0	0
40	J	7	0	0	0	0
40	K	7	0	0	0	0
40	L	11	0	0	0	0
40	M	6	0	0	0	0
40	O	119	0	0	1	0
40	R	1	0	0	0	0
40	T	10	0	0	0	0
40	U	63	0	0	0	0
40	V	96	0	0	0	0
40	X	8	0	0	0	0
40	Y	1	0	0	0	0
40	Z	1	0	0	0	0
40	a	118	0	0	0	0
40	b	209	0	0	0	0
40	c	169	0	0	0	0
40	d	121	0	0	0	0
40	e	9	0	0	0	0
40	f	5	0	0	0	0
40	h	23	0	0	0	0
40	i	4	0	0	0	0
40	j	5	0	0	0	0
40	k	3	0	0	0	0
40	l	8	0	0	0	0
40	m	10	0	0	0	0
40	o	112	0	0	0	0
40	t	13	0	0	0	0
40	u	74	0	0	0	0
40	v	65	0	0	0	0
40	x	9	0	0	0	0
40	y	1	0	0	0	0
All	All	53568	0	52620	319	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 319 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	38:V:201:HEM:HAB	1.58	1.53
28:B:620[B]:SQD:H141	28:B:620[B]:SQD:C38	1.48	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:620[B]:SQD:C14	28:B:620[B]:SQD:H382	1.52	1.39
16:V:40:CYS:SG	38:V:201:HEM:CAC	2.14	1.35
16:V:37:CYS:SG	38:V:201:HEM:CAB	2.13	1.35

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	337/334 (101%)	333 (99%)	3 (1%)	1 (0%)	46	45
1	a	336/334 (101%)	331 (98%)	4 (1%)	1 (0%)	46	45
2	B	513/505 (102%)	505 (98%)	8 (2%)	0	100	100
2	b	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
3	C	452/451 (100%)	442 (98%)	9 (2%)	1 (0%)	52	53
3	c	450/451 (100%)	441 (98%)	8 (2%)	1 (0%)	52	53
4	D	340/342 (99%)	331 (97%)	9 (3%)	0	100	100
4	d	340/342 (99%)	333 (98%)	6 (2%)	1 (0%)	46	45
5	E	80/80 (100%)	79 (99%)	1 (1%)	0	100	100
5	e	76/80 (95%)	74 (97%)	2 (3%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	30/34 (88%)	30 (100%)	0	0	100	100
7	H	62/63 (98%)	59 (95%)	3 (5%)	0	100	100
7	h	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
8	I	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
8	i	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
9	J	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	6	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	j	35/37 (95%)	35 (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	33/34 (97%)	33 (100%)	0	0	100	100
12	m	33/34 (97%)	33 (100%)	0	0	100	100
13	O	244/244 (100%)	240 (98%)	4 (2%)	0	100	100
13	o	242/244 (99%)	234 (97%)	8 (3%)	0	100	100
14	T	29/31 (94%)	29 (100%)	0	0	100	100
14	t	28/31 (90%)	28 (100%)	0	0	100	100
15	U	96/97 (99%)	93 (97%)	3 (3%)	0	100	100
15	u	96/97 (99%)	94 (98%)	2 (2%)	0	100	100
16	V	138/137 (101%)	134 (97%)	4 (3%)	0	100	100
16	v	137/137 (100%)	134 (98%)	3 (2%)	0	100	100
17	Y	28/30 (93%)	28 (100%)	0	0	100	100
17	y	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
18	X	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	37 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	11	5
19	z	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	11	5
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	5258/5296 (99%)	5151 (98%)	99 (2%)	8 (0%)	52	53

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
3	c	416	SER
9	J	5	GLY
4	d	234	ALA
19	z	30	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/269 (102%)	274 (100%)	0	100	100
1	a	273/269 (102%)	273 (100%)	0	100	100
2	B	413/403 (102%)	412 (100%)	1 (0%)	95	97
2	b	412/403 (102%)	409 (99%)	3 (1%)	88	92
3	C	355/352 (101%)	352 (99%)	3 (1%)	86	91
3	c	354/352 (101%)	349 (99%)	5 (1%)	74	80
4	D	277/277 (100%)	274 (99%)	3 (1%)	80	85
4	d	277/277 (100%)	274 (99%)	3 (1%)	80	85
5	E	73/71 (103%)	72 (99%)	1 (1%)	74	80
5	e	69/71 (97%)	66 (96%)	3 (4%)	35	34
6	F	28/28 (100%)	28 (100%)	0	100	100
6	f	26/28 (93%)	25 (96%)	1 (4%)	40	40
7	H	54/53 (102%)	51 (94%)	3 (6%)	26	22
7	h	53/53 (100%)	52 (98%)	1 (2%)	65	70
8	I	32/32 (100%)	32 (100%)	0	100	100
8	i	32/32 (100%)	32 (100%)	0	100	100
9	J	25/25 (100%)	25 (100%)	0	100	100
9	j	25/25 (100%)	25 (100%)	0	100	100
10	K	30/30 (100%)	29 (97%)	1 (3%)	45	47
10	k	30/30 (100%)	29 (97%)	1 (3%)	45	47
11	L	35/35 (100%)	33 (94%)	2 (6%)	25	22
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	31/30 (103%)	29 (94%)	2 (6%)	21	17
12	m	31/30 (103%)	30 (97%)	1 (3%)	46	48
13	O	209/207 (101%)	207 (99%)	2 (1%)	82	87
13	o	207/207 (100%)	203 (98%)	4 (2%)	65	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	27/27 (100%)	27 (100%)	0	100	100
14	t	26/27 (96%)	26 (100%)	0	100	100
15	U	85/84 (101%)	84 (99%)	1 (1%)	78	84
15	u	85/84 (101%)	84 (99%)	1 (1%)	78	84
16	V	120/117 (103%)	119 (99%)	1 (1%)	86	91
16	v	119/117 (102%)	119 (100%)	0	100	100
17	Y	23/23 (100%)	22 (96%)	1 (4%)	35	34
17	y	23/23 (100%)	20 (87%)	3 (13%)	5	2
18	X	33/33 (100%)	33 (100%)	0	100	100
18	x	32/33 (97%)	32 (100%)	0	100	100
19	Z	51/51 (100%)	47 (92%)	4 (8%)	16	11
19	z	51/51 (100%)	48 (94%)	3 (6%)	24	20
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4364/4323 (101%)	4310 (99%)	54 (1%)	78	84

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	Z	37	LYS
3	c	416	SER
17	y	42	ARG
2	b	53	ASN
2	b	362	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
13	O	147	ASN
19	Z	58	ASN
16	v	34	GLN
16	V	34	GLN
2	B	331	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FME	I	1	8	8,9,10	0.52	0	6,9,11	1.60	3 (50%)
12	FME	M	1	12	8,9,10	0.47	0	6,9,11	2.01	3 (50%)
14	FME	T	1	14	8,9,10	0.52	0	6,9,11	1.76	2 (33%)
19	FME	Z	1	19	8,9,10	0.59	0	6,9,11	2.15	3 (50%)
8	FME	i	1	8	8,9,10	0.48	0	6,9,11	1.57	3 (50%)
12	FME	m	1	12	8,9,10	0.47	0	6,9,11	2.07	2 (33%)
14	FME	t	1	14	8,9,10	0.46	0	6,9,11	1.84	3 (50%)
19	FME	z	1	19	8,9,10	0.46	0	6,9,11	2.09	3 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	0/6/9/11	0/0/0/0
12	FME	M	1	12	-	0/6/9/11	0/0/0/0
14	FME	T	1	14	-	0/6/9/11	0/0/0/0
19	FME	Z	1	19	-	0/6/9/11	0/0/0/0
8	FME	i	1	8	-	0/6/9/11	0/0/0/0
12	FME	m	1	12	-	0/6/9/11	0/0/0/0
14	FME	t	1	14	-	0/6/9/11	0/0/0/0
19	FME	z	1	19	-	0/6/9/11	0/0/0/0

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	1	FME	O1-CN-N	-3.44	119.80	124.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	m	1	FME	O1-CN-N	-3.44	119.81	124.76
19	Z	1	FME	O1-CN-N	-3.35	119.93	124.76
19	z	1	FME	O1-CN-N	-3.00	120.43	124.76
14	t	1	FME	O1-CN-N	-2.44	121.25	124.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 261 ligands modelled in this entry, 24 are unknown and 10 are monoatomic - leaving 227 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	OER	A	1001	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
24	CLA	A	1005	-	55,73,73	1.87	11 (20%)	61,113,113	1.80	13 (21%)
24	CLA	A	1006	40	55,73,73	1.84	11 (20%)	61,113,113	1.87	14 (22%)
25	PHO	A	1007	-	67,69,69	1.99	15 (22%)	84,99,99	1.94	17 (20%)
24	CLA	A	1008	-	55,73,73	1.87	11 (20%)	61,113,113	1.82	14 (22%)
26	BCR	A	1009	-	41,41,41	3.77	14 (34%)	56,56,56	8.02	40 (71%)
27	PL9	A	1010	-	55,55,55	0.68	2 (3%)	68,69,69	1.71	17 (25%)
28	SQD	A	1011	-	53,54,54	1.36	3 (5%)	61,65,65	1.45	7 (11%)
29	LMG	A	1012	-	51,51,55	0.91	2 (3%)	59,59,63	0.93	2 (3%)
30	DMS	A	1013	-	3,3,3	2.49	1 (33%)	3,3,3	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	DMS	A	1014	-	3,3,3	2.63	1 (33%)	3,3,3	0.49	0
28	SQD	A	1016	-	53,54,54	1.38	3 (5%)	61,65,65	1.27	5 (8%)
32	LMT	A	1017	-	36,36,36	0.52	1 (2%)	47,47,47	0.88	1 (2%)
32	LMT	A	1018	-	36,36,36	0.52	0	47,47,47	1.03	5 (10%)
33	GOL	A	1019	-	5,5,5	0.22	0	5,5,5	0.26	0
24	CLA	B	601	40	55,73,73	1.90	12 (21%)	61,113,113	1.91	16 (26%)
24	CLA	B	602	-	55,73,73	1.88	12 (21%)	61,113,113	1.78	13 (21%)
24	CLA	B	603	-	55,73,73	1.82	11 (20%)	61,113,113	2.07	15 (24%)
24	CLA	B	604	-	55,73,73	1.84	10 (18%)	61,113,113	1.89	15 (24%)
24	CLA	B	605	-	55,73,73	1.83	11 (20%)	61,113,113	1.79	14 (22%)
24	CLA	B	606	-	55,73,73	1.89	12 (21%)	61,113,113	1.88	14 (22%)
24	CLA	B	607	40	55,73,73	1.78	11 (20%)	61,113,113	1.90	14 (22%)
24	CLA	B	608	-	55,73,73	1.85	12 (21%)	61,113,113	1.86	15 (24%)
24	CLA	B	609	-	55,73,73	1.86	11 (20%)	61,113,113	1.76	11 (18%)
24	CLA	B	610	40	55,73,73	1.84	11 (20%)	61,113,113	1.80	13 (21%)
24	CLA	B	611	-	55,73,73	1.90	11 (20%)	61,113,113	1.73	13 (21%)
24	CLA	B	612	-	55,73,73	1.90	11 (20%)	61,113,113	1.75	14 (22%)
24	CLA	B	613	-	55,73,73	1.85	11 (20%)	61,113,113	1.71	13 (21%)
24	CLA	B	614	-	55,73,73	1.89	11 (20%)	61,113,113	1.93	14 (22%)
24	CLA	B	615	-	55,73,73	1.92	12 (21%)	61,113,113	1.78	14 (22%)
24	CLA	B	616	-	55,73,73	1.84	11 (20%)	61,113,113	1.87	16 (26%)
26	BCR	B	617	-	41,41,41	3.76	15 (36%)	56,56,56	7.95	39 (69%)
26	BCR	B	618	-	41,41,41	3.76	14 (34%)	56,56,56	8.23	42 (75%)
26	BCR	B	619	-	41,41,41	3.81	15 (36%)	56,56,56	7.78	36 (64%)
28	SQD	B	620[A]	-	53,54,54	1.36	3 (5%)	61,65,65	1.17	5 (8%)
28	SQD	B	620[B]	-	53,54,54	1.35	3 (5%)	61,65,65	1.22	6 (9%)
34	LHG	B	621	-	48,48,48	0.90	2 (4%)	49,54,54	0.95	2 (4%)
29	LMG	B	622	-	51,51,55	0.94	2 (3%)	59,59,63	0.92	2 (3%)
32	LMT	B	623	-	36,36,36	0.47	0	47,47,47	1.04	2 (4%)
35	HTG	B	624	-	19,19,19	0.96	2 (10%)	22,24,24	1.94	1 (4%)
30	DMS	B	626	-	3,3,3	2.50	1 (33%)	3,3,3	0.31	0
30	DMS	B	627	-	3,3,3	2.53	1 (33%)	3,3,3	0.41	0
35	HTG	B	628	-	19,19,19	0.98	2 (10%)	22,24,24	1.60	1 (4%)
35	HTG	B	629	-	19,19,19	0.95	2 (10%)	22,24,24	1.68	1 (4%)
33	GOL	B	631	-	5,5,5	0.21	0	5,5,5	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	DMS	B	632	-	3,3,3	2.61	1 (33%)	3,3,3	0.44	0
30	DMS	B	633	-	3,3,3	2.64	1 (33%)	3,3,3	0.51	0
30	DMS	B	634	-	3,3,3	2.63	1 (33%)	3,3,3	0.44	0
24	CLA	C	501	-	55,73,73	1.87	12 (21%)	61,113,113	1.82	14 (22%)
24	CLA	C	502	-	55,73,73	1.84	11 (20%)	61,113,113	1.81	14 (22%)
24	CLA	C	503	-	55,73,73	1.92	11 (20%)	61,113,113	1.68	13 (21%)
24	CLA	C	504	40	55,73,73	1.89	12 (21%)	61,113,113	1.84	13 (21%)
24	CLA	C	505	-	55,73,73	1.87	12 (21%)	61,113,113	1.79	11 (18%)
24	CLA	C	506	-	55,73,73	1.91	12 (21%)	61,113,113	1.78	14 (22%)
24	CLA	C	507	40	55,73,73	1.93	11 (20%)	61,113,113	1.89	13 (21%)
24	CLA	C	508	-	55,73,73	1.91	11 (20%)	61,113,113	1.64	11 (18%)
24	CLA	C	509	-	55,73,73	1.87	11 (20%)	61,113,113	1.90	13 (21%)
24	CLA	C	510	-	55,73,73	1.85	11 (20%)	61,113,113	1.90	12 (19%)
24	CLA	C	511	3	55,73,73	1.93	11 (20%)	61,113,113	1.71	11 (18%)
24	CLA	C	512	-	55,73,73	1.92	12 (21%)	61,113,113	1.76	15 (24%)
24	CLA	C	513	-	55,73,73	1.96	12 (21%)	61,113,113	1.68	14 (22%)
26	BCR	C	514	-	41,41,41	3.87	15 (36%)	56,56,56	8.06	39 (69%)
36	DGD	C	515	-	63,63,67	0.84	2 (3%)	77,77,81	0.88	2 (2%)
36	DGD	C	516	-	63,63,67	0.88	3 (4%)	77,77,81	0.96	5 (6%)
36	DGD	C	517	-	63,63,67	0.82	2 (3%)	77,77,81	0.88	3 (3%)
29	LMG	C	518	-	51,51,55	0.94	2 (3%)	59,59,63	0.88	2 (3%)
29	LMG	C	519	-	51,51,55	0.96	2 (3%)	59,59,63	1.06	4 (6%)
32	LMT	C	520	-	36,36,36	0.50	0	47,47,47	1.05	2 (4%)
35	HTG	C	521	-	19,19,19	0.98	2 (10%)	22,24,24	1.59	1 (4%)
35	HTG	C	522	-	19,19,19	0.94	1 (5%)	22,24,24	2.14	5 (22%)
30	DMS	C	523	-	3,3,3	2.50	1 (33%)	3,3,3	0.34	0
30	DMS	C	524	-	3,3,3	2.54	1 (33%)	3,3,3	0.42	0
30	DMS	C	525	-	3,3,3	2.62	1 (33%)	3,3,3	0.49	0
30	DMS	C	526	-	3,3,3	2.61	1 (33%)	3,3,3	0.45	0
30	DMS	C	527	-	3,3,3	2.61	1 (33%)	3,3,3	0.50	0
37	BCT	D	401	22	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	D	402	-	55,73,73	1.84	11 (20%)	61,113,113	1.88	15 (24%)
24	CLA	D	403	40	55,73,73	1.81	10 (18%)	61,113,113	2.00	16 (26%)
25	PHO	D	404	-	67,69,69	2.06	16 (23%)	84,99,99	1.95	22 (26%)
24	CLA	D	405	-	55,73,73	1.90	12 (21%)	61,113,113	1.68	14 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	D	406	-	41,41,41	3.81	14 (34%)	56,56,56	7.95	45 (80%)
27	PL9	D	407	-	55,55,55	0.75	2 (3%)	68,69,69	1.53	15 (22%)
28	SQD	D	408	-	42,43,54	1.48	3 (7%)	50,54,65	1.87	9 (18%)
34	LHG	D	409	-	48,48,48	0.88	2 (4%)	49,54,54	0.98	4 (8%)
34	LHG	D	410	-	48,48,48	0.85	2 (4%)	49,54,54	0.98	3 (6%)
34	LHG	D	411	-	48,48,48	0.91	2 (4%)	49,54,54	0.95	2 (4%)
29	LMG	D	412	39	51,51,55	0.87	2 (3%)	59,59,63	0.81	1 (1%)
35	HTG	D	413	-	19,19,19	0.97	2 (10%)	22,24,24	1.63	1 (4%)
30	DMS	D	416	-	3,3,3	2.66	1 (33%)	3,3,3	0.68	0
30	DMS	D	417	-	3,3,3	2.63	1 (33%)	3,3,3	0.39	0
33	GOL	D	418	-	5,5,5	0.24	0	5,5,5	0.29	0
35	HTG	D	419	-	19,19,19	0.94	1 (5%)	22,24,24	2.04	1 (4%)
34	LHG	E	101	-	48,48,48	0.93	2 (4%)	49,54,54	0.98	2 (4%)
38	HEM	F	101	5,6	30,50,50	2.18	7 (23%)	24,82,82	2.39	10 (41%)
26	BCR	H	101	-	41,41,41	3.78	15 (36%)	56,56,56	8.18	41 (73%)
36	DGD	H	102	-	63,63,67	0.84	3 (4%)	77,77,81	0.83	3 (3%)
26	BCR	J	101	-	41,41,41	3.83	14 (34%)	56,56,56	8.55	40 (71%)
26	BCR	K	101	-	41,41,41	3.80	15 (36%)	56,56,56	7.81	41 (73%)
26	BCR	K	102	-	41,41,41	3.88	15 (36%)	56,56,56	8.27	41 (73%)
32	LMT	M	101	-	36,36,36	0.47	0	47,47,47	0.91	0
32	LMT	M	102	-	36,36,36	0.48	0	47,47,47	0.77	1 (2%)
30	DMS	O	301	-	3,3,3	2.64	1 (33%)	3,3,3	0.48	0
30	DMS	O	302	-	3,3,3	2.62	1 (33%)	3,3,3	0.55	0
26	BCR	T	101	-	41,41,41	3.85	15 (36%)	56,56,56	7.82	39 (69%)
30	DMS	U	201	-	3,3,3	2.59	1 (33%)	3,3,3	0.44	0
38	HEM	V	201	16	30,50,50	2.30	10 (33%)	24,82,82	2.50	13 (54%)
35	HTG	V	202	-	19,19,19	0.92	2 (10%)	22,24,24	1.81	3 (13%)
30	DMS	V	203	-	3,3,3	2.63	1 (33%)	3,3,3	0.46	0
33	GOL	V	204	-	5,5,5	0.24	0	5,5,5	0.20	0
30	DMS	V	205	-	3,3,3	2.62	1 (33%)	3,3,3	0.47	0
33	GOL	V	206	-	5,5,5	0.23	0	5,5,5	0.22	0
33	GOL	V	207	-	5,5,5	0.20	0	5,5,5	0.31	0
29	LMG	Z	101	-	51,51,55	0.95	2 (3%)	59,59,63	1.02	3 (5%)
28	SQD	a	401	-	53,54,54	1.39	3 (5%)	61,65,65	1.28	5 (8%)
32	LMT	a	402	-	36,36,36	0.57	1 (2%)	47,47,47	0.88	3 (6%)
21	OER	a	403	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	a	407	-	55,73,73	1.88	10 (18%)	61,113,113	1.67	10 (16%)
24	CLA	a	408	40	55,73,73	1.87	10 (18%)	61,113,113	1.84	13 (21%)
24	CLA	a	409	40	55,73,73	1.79	10 (18%)	61,113,113	1.79	14 (22%)
25	PHO	a	410	-	67,69,69	2.04	15 (22%)	84,99,99	1.91	19 (22%)
25	PHO	a	411	-	67,69,69	2.06	16 (23%)	84,99,99	2.01	21 (25%)
24	CLA	a	412	-	55,73,73	1.84	11 (20%)	61,113,113	1.88	16 (26%)
26	BCR	a	413	-	41,41,41	3.69	14 (34%)	56,56,56	8.30	41 (73%)
27	PL9	a	414	-	55,55,55	0.70	2 (3%)	68,69,69	1.56	15 (22%)
29	LMG	a	415	-	51,51,55	0.92	2 (3%)	59,59,63	0.99	3 (5%)
32	LMT	a	416	-	36,36,36	0.49	0	47,47,47	0.78	1 (2%)
30	DMS	a	417	-	3,3,3	2.51	1 (33%)	3,3,3	0.35	0
30	DMS	a	418	-	3,3,3	2.64	1 (33%)	3,3,3	0.53	0
33	GOL	a	420	-	5,5,5	0.24	0	5,5,5	0.24	0
35	HTG	b	601	-	19,19,19	0.94	1 (5%)	22,24,24	1.68	1 (4%)
35	HTG	b	602	-	19,19,19	0.95	2 (10%)	22,24,24	1.79	1 (4%)
24	CLA	b	604	40	55,73,73	1.97	12 (21%)	61,113,113	1.79	14 (22%)
24	CLA	b	605	-	55,73,73	1.92	12 (21%)	61,113,113	1.69	13 (21%)
24	CLA	b	606	-	55,73,73	1.88	11 (20%)	61,113,113	1.85	14 (22%)
24	CLA	b	607	-	55,73,73	1.87	11 (20%)	61,113,113	1.88	13 (21%)
24	CLA	b	608	-	55,73,73	1.82	11 (20%)	61,113,113	1.85	13 (21%)
24	CLA	b	609	-	55,73,73	1.94	12 (21%)	61,113,113	1.84	12 (19%)
24	CLA	b	610	40	55,73,73	1.84	12 (21%)	61,113,113	1.91	16 (26%)
24	CLA	b	611	-	55,73,73	1.86	11 (20%)	61,113,113	1.88	15 (24%)
24	CLA	b	612	-	55,73,73	1.87	12 (21%)	61,113,113	1.78	12 (19%)
24	CLA	b	613	40	55,73,73	1.88	11 (20%)	61,113,113	1.69	11 (18%)
24	CLA	b	614	-	55,73,73	1.82	11 (20%)	61,113,113	1.70	14 (22%)
24	CLA	b	615	-	55,73,73	1.89	11 (20%)	61,113,113	1.84	13 (21%)
24	CLA	b	616	-	55,73,73	1.84	11 (20%)	61,113,113	1.80	13 (21%)
24	CLA	b	617	-	55,73,73	1.84	11 (20%)	61,113,113	1.92	16 (26%)
24	CLA	b	618	-	55,73,73	1.89	11 (20%)	61,113,113	1.71	14 (22%)
24	CLA	b	619	-	55,73,73	1.88	11 (20%)	61,113,113	1.80	12 (19%)
26	BCR	b	620	-	41,41,41	3.76	14 (34%)	56,56,56	7.90	41 (73%)
26	BCR	b	621	-	41,41,41	3.79	14 (34%)	56,56,56	8.23	43 (76%)
26	BCR	b	622	-	41,41,41	3.85	15 (36%)	56,56,56	7.94	36 (64%)
28	SQD	b	623[A]	-	53,54,54	1.36	3 (5%)	61,65,65	1.21	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	SQD	b	623[B]	-	53,54,54	1.35	3 (5%)	61,65,65	1.14	5 (8%)
34	LHG	b	624	-	48,48,48	0.88	2 (4%)	49,54,54	0.98	2 (4%)
32	LMT	b	625	-	36,36,36	0.50	0	47,47,47	1.26	5 (10%)
35	HTG	b	626	-	19,19,19	0.92	1 (5%)	22,24,24	1.45	2 (9%)
30	DMS	b	628	-	3,3,3	2.47	1 (33%)	3,3,3	0.45	0
30	DMS	b	629	-	3,3,3	2.61	1 (33%)	3,3,3	0.40	0
35	HTG	b	630	-	19,19,19	1.00	2 (10%)	22,24,24	2.09	2 (9%)
32	LMT	b	631	-	36,36,36	0.49	0	47,47,47	0.85	2 (4%)
33	GOL	b	632	-	5,5,5	0.18	0	5,5,5	0.23	0
30	DMS	b	633	-	3,3,3	2.62	1 (33%)	3,3,3	0.59	0
30	DMS	b	634	-	3,3,3	2.67	1 (33%)	3,3,3	0.57	0
30	DMS	b	635	-	3,3,3	2.62	1 (33%)	3,3,3	0.40	0
24	CLA	c	501	-	55,73,73	1.89	12 (21%)	61,113,113	1.86	13 (21%)
24	CLA	c	502	-	55,73,73	1.89	11 (20%)	61,113,113	1.77	14 (22%)
24	CLA	c	503	-	55,73,73	1.93	12 (21%)	61,113,113	1.65	12 (19%)
24	CLA	c	504	40	55,73,73	1.89	12 (21%)	61,113,113	1.84	14 (22%)
24	CLA	c	505	-	55,73,73	1.91	12 (21%)	61,113,113	1.84	14 (22%)
24	CLA	c	506	-	55,73,73	1.92	12 (21%)	61,113,113	1.77	13 (21%)
24	CLA	c	507	40	55,73,73	1.93	11 (20%)	61,113,113	1.91	13 (21%)
24	CLA	c	508	-	55,73,73	1.93	12 (21%)	61,113,113	1.71	13 (21%)
24	CLA	c	509	-	55,73,73	1.92	12 (21%)	61,113,113	1.81	15 (24%)
24	CLA	c	510	-	55,73,73	1.89	12 (21%)	61,113,113	1.80	14 (22%)
24	CLA	c	511	3	55,73,73	1.93	11 (20%)	61,113,113	1.67	13 (21%)
24	CLA	c	512	-	55,73,73	1.94	12 (21%)	61,113,113	1.83	13 (21%)
24	CLA	c	513	-	55,73,73	1.94	12 (21%)	61,113,113	1.76	16 (26%)
26	BCR	c	514	-	41,41,41	3.85	15 (36%)	56,56,56	8.52	41 (73%)
36	DGD	c	515	-	63,63,67	0.86	3 (4%)	77,77,81	0.91	2 (2%)
36	DGD	c	516	-	63,63,67	0.89	2 (3%)	77,77,81	0.94	4 (5%)
36	DGD	c	517	-	63,63,67	0.86	2 (3%)	77,77,81	0.82	3 (3%)
28	SQD	c	518	-	53,54,54	1.36	3 (5%)	61,65,65	1.48	8 (13%)
29	LMG	c	519	-	51,51,55	0.94	2 (3%)	59,59,63	0.89	2 (3%)
29	LMG	c	520	-	51,51,55	0.96	3 (5%)	59,59,63	1.07	4 (6%)
29	LMG	c	521	-	51,51,55	0.97	2 (3%)	59,59,63	1.07	2 (3%)
35	HTG	c	522	-	19,19,19	0.93	2 (10%)	22,24,24	1.54	1 (4%)
30	DMS	c	524	-	3,3,3	2.54	1 (33%)	3,3,3	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	HTG	c	525	-	19,19,19	0.98	2 (10%)	22,24,24	1.51	1 (4%)
30	DMS	c	526	-	3,3,3	2.61	1 (33%)	3,3,3	0.41	0
30	DMS	c	527	-	3,3,3	2.64	1 (33%)	3,3,3	0.53	0
30	DMS	c	528	-	3,3,3	2.62	1 (33%)	3,3,3	0.49	0
30	DMS	c	529	-	3,3,3	2.56	1 (33%)	3,3,3	0.44	0
37	BCT	d	401	22	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	d	402	-	55,73,73	1.83	11 (20%)	61,113,113	1.81	14 (22%)
24	CLA	d	403	-	55,73,73	1.93	12 (21%)	61,113,113	1.62	11 (18%)
26	BCR	d	404	-	41,41,41	3.86	15 (36%)	56,56,56	8.03	42 (75%)
27	PL9	d	405	-	55,55,55	0.74	2 (3%)	68,69,69	1.46	12 (17%)
34	LHG	d	406	-	48,48,48	0.91	2 (4%)	49,54,54	0.94	3 (6%)
34	LHG	d	407	-	48,48,48	0.85	2 (4%)	49,54,54	0.93	3 (6%)
34	LHG	d	408	-	48,48,48	0.92	2 (4%)	49,54,54	0.95	2 (4%)
29	LMG	d	409	39	51,51,55	0.91	2 (3%)	59,59,63	0.87	2 (3%)
35	HTG	d	410	-	19,19,19	0.98	1 (5%)	22,24,24	1.68	1 (4%)
30	DMS	d	413	-	3,3,3	2.64	1 (33%)	3,3,3	0.54	0
30	DMS	d	414	-	3,3,3	2.61	1 (33%)	3,3,3	0.38	0
33	GOL	d	415	-	5,5,5	0.23	0	5,5,5	0.30	0
35	HTG	d	416	-	19,19,19	0.94	1 (5%)	22,24,24	2.07	1 (4%)
33	GOL	d	417	-	5,5,5	0.27	0	5,5,5	0.15	0
34	LHG	e	101	-	48,48,48	0.94	2 (4%)	49,54,54	1.01	2 (4%)
38	HEM	f	101	5,6	30,50,50	2.13	10 (33%)	24,82,82	2.43	9 (37%)
28	SQD	f	102	-	42,43,54	1.55	4 (9%)	50,54,65	1.46	7 (14%)
32	LMT	f	103	-	36,36,36	0.51	0	47,47,47	0.68	0
26	BCR	h	101	-	41,41,41	3.81	14 (34%)	56,56,56	8.27	42 (75%)
36	DGD	h	102	-	63,63,67	0.88	3 (4%)	77,77,81	0.85	2 (2%)
32	LMT	i	102	-	36,36,36	0.50	0	47,47,47	1.04	2 (4%)
26	BCR	k	101	-	41,41,41	3.81	15 (36%)	56,56,56	8.42	41 (73%)
26	BCR	k	102	-	41,41,41	3.75	15 (36%)	56,56,56	8.19	38 (67%)
32	LMT	m	101	-	36,36,36	0.46	0	47,47,47	0.71	0
29	LMG	m	102	-	51,51,55	0.95	2 (3%)	59,59,63	1.12	4 (6%)
32	LMT	m	103	-	36,36,36	0.51	1 (2%)	47,47,47	0.84	1 (2%)
35	HTG	o	301	-	19,19,19	0.96	1 (5%)	22,24,24	1.62	1 (4%)
26	BCR	t	101	-	41,41,41	3.83	15 (36%)	56,56,56	7.88	40 (71%)
32	LMT	t	103	-	36,36,36	0.44	0	47,47,47	1.06	2 (4%)
30	DMS	u	201	-	3,3,3	2.59	1 (33%)	3,3,3	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	HEM	v	201	16	30,50,50	2.30	9 (30%)	24,82,82	2.37	8 (33%)
30	DMS	v	202	-	3,3,3	2.58	1 (33%)	3,3,3	0.46	0
33	GOL	v	203	-	5,5,5	0.28	0	5,5,5	0.31	0
33	GOL	v	204	-	5,5,5	0.21	0	5,5,5	0.26	0
26	BCR	y	101	-	41,41,41	3.85	15 (36%)	56,56,56	8.63	44 (78%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	OER	A	1001	1,3,40	-	0/0/68/68	0/0/6/6
24	CLA	A	1005	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	A	1006	40	2/2/20/25	0/37/135/135	0/0/9/9
25	PHO	A	1007	-	-	0/53/103/103	0/1/6/6
24	CLA	A	1008	-	1/1/20/25	0/37/135/135	0/0/9/9
26	BCR	A	1009	-	-	1/29/63/63	0/2/2/2
27	PL9	A	1010	-	-	0/53/73/73	0/1/1/1
28	SQD	A	1011	-	-	0/49/69/69	0/1/1/1
29	LMG	A	1012	-	-	0/46/66/70	0/1/1/1
30	DMS	A	1013	-	-	0/0/0/0	0/0/0/0
30	DMS	A	1014	-	-	0/0/0/0	0/0/0/0
28	SQD	A	1016	-	-	0/49/69/69	0/1/1/1
32	LMT	A	1017	-	-	0/21/61/61	0/2/2/2
32	LMT	A	1018	-	-	0/21/61/61	0/2/2/2
33	GOL	A	1019	-	-	0/4/4/4	0/0/0/0
24	CLA	B	601	40	3/3/20/25	0/37/135/135	0/0/9/9
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	-	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	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	608	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	B	609	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	610	40	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
26	BCR	B	617	-	-	0/29/63/63	0/2/2/2
26	BCR	B	618	-	-	0/29/63/63	0/2/2/2
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
28	SQD	B	620[A]	-	-	2/49/69/69	0/1/1/1
28	SQD	B	620[B]	-	-	0/49/69/69	0/1/1/1
34	LHG	B	621	-	-	0/53/53/53	0/0/0/0
29	LMG	B	622	-	-	0/46/66/70	0/1/1/1
32	LMT	B	623	-	-	0/21/61/61	0/2/2/2
35	HTG	B	624	-	-	0/10/30/30	0/1/1/1
30	DMS	B	626	-	-	0/0/0/0	0/0/0/0
30	DMS	B	627	-	-	0/0/0/0	0/0/0/0
35	HTG	B	628	-	-	0/10/30/30	0/1/1/1
35	HTG	B	629	-	-	0/10/30/30	0/1/1/1
33	GOL	B	631	-	-	0/4/4/4	0/0/0/0
30	DMS	B	632	-	-	0/0/0/0	0/0/0/0
30	DMS	B	633	-	-	0/0/0/0	0/0/0/0
30	DMS	B	634	-	-	0/0/0/0	0/0/0/0
24	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	502	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	C	503	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	C	504	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	505	-	1/1/20/25	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	40	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	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	C	512	-	3/3/20/25	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	-	-	0/29/63/63	0/2/2/2
36	DGD	C	515	-	-	0/51/91/95	0/2/2/2
36	DGD	C	516	-	-	0/51/91/95	0/2/2/2
36	DGD	C	517	-	-	0/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	C	518	-	-	0/46/66/70	0/1/1/1
29	LMG	C	519	-	-	0/46/66/70	0/1/1/1
32	LMT	C	520	-	-	0/21/61/61	0/2/2/2
35	HTG	C	521	-	-	0/10/30/30	0/1/1/1
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1
30	DMS	C	523	-	-	0/0/0/0	0/0/0/0
30	DMS	C	524	-	-	0/0/0/0	0/0/0/0
30	DMS	C	525	-	-	0/0/0/0	0/0/0/0
30	DMS	C	526	-	-	0/0/0/0	0/0/0/0
30	DMS	C	527	-	-	0/0/0/0	0/0/0/0
37	BCT	D	401	22	-	0/0/0/0	0/0/0/0
24	CLA	D	402	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	D	403	40	1/1/20/25	0/37/135/135	0/0/9/9
25	PHO	D	404	-	-	0/53/103/103	0/1/6/6
24	CLA	D	405	-	2/2/20/25	0/37/135/135	0/0/9/9
26	BCR	D	406	-	-	0/29/63/63	0/2/2/2
27	PL9	D	407	-	-	0/53/73/73	0/1/1/1
28	SQD	D	408	-	-	0/38/58/69	0/1/1/1
34	LHG	D	409	-	-	0/53/53/53	0/0/0/0
34	LHG	D	410	-	-	0/53/53/53	0/0/0/0
34	LHG	D	411	-	-	0/53/53/53	0/0/0/0
29	LMG	D	412	39	-	0/46/66/70	0/1/1/1
35	HTG	D	413	-	-	0/10/30/30	0/1/1/1
30	DMS	D	416	-	-	0/0/0/0	0/0/0/0
30	DMS	D	417	-	-	0/0/0/0	0/0/0/0
33	GOL	D	418	-	-	0/4/4/4	0/0/0/0
35	HTG	D	419	-	-	0/10/30/30	0/1/1/1
34	LHG	E	101	-	-	0/53/53/53	0/0/0/0
38	HEM	F	101	5,6	-	0/10/54/54	0/0/8/8
26	BCR	H	101	-	-	2/29/63/63	0/2/2/2
36	DGD	H	102	-	-	0/51/91/95	0/2/2/2
26	BCR	J	101	-	-	0/29/63/63	0/2/2/2
26	BCR	K	101	-	-	0/29/63/63	0/2/2/2
26	BCR	K	102	-	-	1/29/63/63	0/2/2/2
32	LMT	M	101	-	-	0/21/61/61	0/2/2/2
32	LMT	M	102	-	-	0/21/61/61	0/2/2/2
30	DMS	O	301	-	-	0/0/0/0	0/0/0/0
30	DMS	O	302	-	-	0/0/0/0	0/0/0/0
26	BCR	T	101	-	-	0/29/63/63	0/2/2/2
30	DMS	U	201	-	-	0/0/0/0	0/0/0/0
38	HEM	V	201	16	-	0/10/54/54	0/0/8/8
35	HTG	V	202	-	-	0/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DMS	V	203	-	-	0/0/0/0	0/0/0/0
33	GOL	V	204	-	-	0/4/4/4	0/0/0/0
30	DMS	V	205	-	-	0/0/0/0	0/0/0/0
33	GOL	V	206	-	-	0/4/4/4	0/0/0/0
33	GOL	V	207	-	-	0/4/4/4	0/0/0/0
29	LMG	Z	101	-	-	0/46/66/70	0/1/1/1
28	SQD	a	401	-	-	0/49/69/69	0/1/1/1
32	LMT	a	402	-	-	0/21/61/61	0/2/2/2
21	OER	a	403	1,3,40	-	0/0/68/68	0/0/6/6
24	CLA	a	407	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	a	408	40	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	a	409	40	2/2/20/25	0/37/135/135	0/0/9/9
25	PHO	a	410	-	-	0/53/103/103	0/1/6/6
25	PHO	a	411	-	-	0/53/103/103	0/1/6/6
24	CLA	a	412	-	1/1/20/25	0/37/135/135	0/0/9/9
26	BCR	a	413	-	-	0/29/63/63	0/2/2/2
27	PL9	a	414	-	-	0/53/73/73	0/1/1/1
29	LMG	a	415	-	-	0/46/66/70	0/1/1/1
32	LMT	a	416	-	-	0/21/61/61	0/2/2/2
30	DMS	a	417	-	-	0/0/0/0	0/0/0/0
30	DMS	a	418	-	-	0/0/0/0	0/0/0/0
33	GOL	a	420	-	-	0/4/4/4	0/0/0/0
35	HTG	b	601	-	-	0/10/30/30	0/1/1/1
35	HTG	b	602	-	-	0/10/30/30	0/1/1/1
24	CLA	b	604	40	1/1/20/25	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	-	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	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	611	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	b	612	-	-	0/37/135/135	0/0/9/9
24	CLA	b	613	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	614	-	1/1/20/25	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	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	618	-	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	b	619	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	b	620	-	-	0/29/63/63	0/2/2/2
26	BCR	b	621	-	-	0/29/63/63	0/2/2/2
26	BCR	b	622	-	-	1/29/63/63	0/2/2/2
28	SQD	b	623[A]	-	-	0/49/69/69	0/1/1/1
28	SQD	b	623[B]	-	-	1/49/69/69	0/1/1/1
34	LHG	b	624	-	-	0/53/53/53	0/0/0/0
32	LMT	b	625	-	-	0/21/61/61	0/2/2/2
35	HTG	b	626	-	-	0/10/30/30	0/1/1/1
30	DMS	b	628	-	-	0/0/0/0	0/0/0/0
30	DMS	b	629	-	-	0/0/0/0	0/0/0/0
35	HTG	b	630	-	-	0/10/30/30	0/1/1/1
32	LMT	b	631	-	-	0/21/61/61	0/2/2/2
33	GOL	b	632	-	-	0/4/4/4	0/0/0/0
30	DMS	b	633	-	-	0/0/0/0	0/0/0/0
30	DMS	b	634	-	-	0/0/0/0	0/0/0/0
30	DMS	b	635	-	-	0/0/0/0	0/0/0/0
24	CLA	c	501	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	502	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	c	503	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	c	504	40	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	c	505	-	2/2/20/25	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	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	508	-	2/2/20/25	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	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	c	512	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	513	-	1/1/20/25	0/37/135/135	0/0/9/9
26	BCR	c	514	-	-	1/29/63/63	0/2/2/2
36	DGD	c	515	-	-	0/51/91/95	0/2/2/2
36	DGD	c	516	-	-	0/51/91/95	0/2/2/2
36	DGD	c	517	-	-	0/51/91/95	0/2/2/2
28	SQD	c	518	-	-	0/49/69/69	0/1/1/1
29	LMG	c	519	-	-	0/46/66/70	0/1/1/1
29	LMG	c	520	-	-	0/46/66/70	0/1/1/1
29	LMG	c	521	-	-	0/46/66/70	0/1/1/1
35	HTG	c	522	-	-	0/10/30/30	0/1/1/1
30	DMS	c	524	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HTG	c	525	-	-	0/10/30/30	0/1/1/1
30	DMS	c	526	-	-	0/0/0/0	0/0/0/0
30	DMS	c	527	-	-	0/0/0/0	0/0/0/0
30	DMS	c	528	-	-	0/0/0/0	0/0/0/0
30	DMS	c	529	-	-	0/0/0/0	0/0/0/0
37	BCT	d	401	22	-	0/0/0/0	0/0/0/0
24	CLA	d	402	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	d	403	-	2/2/20/25	0/37/135/135	0/0/9/9
26	BCR	d	404	-	-	0/29/63/63	0/2/2/2
27	PL9	d	405	-	-	0/53/73/73	0/1/1/1
34	LHG	d	406	-	-	0/53/53/53	0/0/0/0
34	LHG	d	407	-	-	0/53/53/53	0/0/0/0
34	LHG	d	408	-	-	0/53/53/53	0/0/0/0
29	LMG	d	409	39	-	0/46/66/70	0/1/1/1
35	HTG	d	410	-	-	0/10/30/30	0/1/1/1
30	DMS	d	413	-	-	0/0/0/0	0/0/0/0
30	DMS	d	414	-	-	0/0/0/0	0/0/0/0
33	GOL	d	415	-	-	0/4/4/4	0/0/0/0
35	HTG	d	416	-	-	0/10/30/30	0/1/1/1
33	GOL	d	417	-	-	0/4/4/4	0/0/0/0
34	LHG	e	101	-	-	0/53/53/53	0/0/0/0
38	HEM	f	101	5,6	-	0/10/54/54	0/0/8/8
28	SQD	f	102	-	-	0/38/58/69	0/1/1/1
32	LMT	f	103	-	-	0/21/61/61	0/2/2/2
26	BCR	h	101	-	-	0/29/63/63	0/2/2/2
36	DGD	h	102	-	-	0/51/91/95	0/2/2/2
32	LMT	i	102	-	-	0/21/61/61	0/2/2/2
26	BCR	k	101	-	-	0/29/63/63	0/2/2/2
26	BCR	k	102	-	-	1/29/63/63	0/2/2/2
32	LMT	m	101	-	-	0/21/61/61	0/2/2/2
29	LMG	m	102	-	-	0/46/66/70	0/1/1/1
32	LMT	m	103	-	-	0/21/61/61	0/2/2/2
35	HTG	o	301	-	-	0/10/30/30	0/1/1/1
26	BCR	t	101	-	-	0/29/63/63	0/2/2/2
32	LMT	t	103	-	-	0/21/61/61	0/2/2/2
30	DMS	u	201	-	-	0/0/0/0	0/0/0/0
38	HEM	v	201	16	-	0/10/54/54	0/0/8/8
30	DMS	v	202	-	-	0/0/0/0	0/0/0/0
33	GOL	v	203	-	-	0/4/4/4	0/0/0/0
33	GOL	v	204	-	-	0/4/4/4	0/0/0/0
26	BCR	y	101	-	-	1/29/63/63	0/2/2/2

The worst 5 of 1382 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	514	BCR	C8-C9	-8.68	1.26	1.45
26	t	101	BCR	C8-C9	-8.61	1.26	1.45
26	k	102	BCR	C12-C13	-8.59	1.26	1.45
26	K	101	BCR	C8-C9	-8.59	1.26	1.45
26	D	406	BCR	C19-C18	-8.58	1.26	1.45

The worst 5 of 2212 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	617	BCR	C36-C18-C17	-9.42	108.99	122.90
26	J	101	BCR	C36-C18-C17	-9.27	109.20	122.90
26	a	413	BCR	C36-C18-C17	-8.55	110.27	122.90
26	B	619	BCR	C36-C18-C17	-8.34	110.58	122.90
26	J	101	BCR	C33-C5-C4	-8.34	97.62	113.43

5 of 166 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	C	503	CLA	NC
24	C	503	CLA	NA
24	B	612	CLA	NA
24	B	612	CLA	NC
24	B	612	CLA	ND

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	y	101	BCR	C21-C20-C19-C18
26	H	101	BCR	C21-C20-C19-C18
26	b	622	BCR	C17-C16-C15-C14
26	H	101	BCR	C17-C16-C15-C14
26	k	102	BCR	C21-C20-C19-C18

There are no ring outliers.

71 monomers are involved in 191 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1005	CLA	5	0
24	A	1006	CLA	2	0
25	A	1007	PHO	1	0
24	A	1008	CLA	3	0
27	A	1010	PL9	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	A	1011	SQD	2	0
28	A	1016	SQD	1	0
32	A	1017	LMT	2	0
32	A	1018	LMT	1	0
24	B	601	CLA	1	0
24	B	603	CLA	2	0
24	B	604	CLA	5	0
24	B	605	CLA	7	0
24	B	606	CLA	6	0
24	B	607	CLA	7	0
24	B	608	CLA	4	0
24	B	609	CLA	2	0
24	B	610	CLA	4	0
24	B	611	CLA	4	0
24	B	612	CLA	4	0
24	B	613	CLA	7	0
24	B	614	CLA	3	0
24	B	615	CLA	6	0
24	B	616	CLA	5	0
26	B	617	BCR	1	0
26	B	618	BCR	1	0
28	B	620[A]	SQD	9	0
28	B	620[B]	SQD	12	0
34	B	621	LHG	1	0
29	B	622	LMG	2	0
35	B	629	HTG	1	0
33	B	631	GOL	1	0
30	B	634	DMS	2	0
24	C	501	CLA	3	0
24	C	502	CLA	4	0
24	C	503	CLA	3	0
24	C	504	CLA	4	0
24	C	505	CLA	6	0
24	C	506	CLA	5	0
24	C	507	CLA	5	0
24	C	508	CLA	3	0
24	C	509	CLA	2	0
24	C	510	CLA	10	0
24	C	511	CLA	3	0
24	C	512	CLA	5	0
24	C	513	CLA	2	0
26	C	514	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	C	515	DGD	3	0
36	C	516	DGD	1	0
36	C	517	DGD	1	0
29	C	519	LMG	2	0
24	D	402	CLA	4	0
24	D	403	CLA	4	0
25	D	404	PHO	4	0
24	D	405	CLA	1	0
26	D	406	BCR	1	0
28	D	408	SQD	1	0
34	D	409	LHG	4	0
34	D	410	LHG	1	0
34	D	411	LHG	8	0
29	D	412	LMG	1	0
35	D	413	HTG	1	0
34	E	101	LHG	3	0
38	F	101	HEM	3	0
36	H	102	DGD	3	0
26	J	101	BCR	1	0
26	K	102	BCR	2	0
32	M	101	LMT	2	0
32	M	102	LMT	1	0
38	V	201	HEM	8	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/334 (100%)	-0.69	5 (1%) 76 81	19, 25, 44, 64	0
1	a	334/334 (100%)	-0.55	7 (2%) 67 72	21, 28, 51, 72	0
2	B	505/505 (100%)	-0.49	15 (2%) 54 62	20, 29, 50, 69	0
2	b	505/505 (100%)	-0.30	26 (5%) 32 40	21, 31, 59, 88	0
3	C	451/451 (100%)	-0.50	5 (1%) 82 86	22, 33, 47, 72	0
3	c	450/451 (99%)	-0.34	8 (1%) 71 76	26, 38, 51, 68	0
4	D	342/342 (100%)	-0.67	4 (1%) 81 85	18, 26, 39, 88	0
4	d	342/342 (100%)	-0.63	4 (1%) 81 85	21, 29, 46, 80	0
5	E	80/80 (100%)	0.29	9 (11%) 7 9	29, 43, 65, 74	0
5	e	78/80 (97%)	0.58	10 (12%) 5 6	35, 47, 68, 75	0
6	F	34/34 (100%)	-0.32	2 (5%) 26 34	29, 34, 55, 67	0
6	f	32/34 (94%)	0.02	3 (9%) 11 14	33, 40, 69, 78	0
7	H	63/63 (100%)	-0.15	2 (3%) 51 60	27, 36, 45, 54	0
7	h	63/63 (100%)	-0.08	3 (4%) 34 43	30, 39, 49, 56	0
8	I	35/36 (97%)	0.02	3 (8%) 13 18	32, 37, 71, 87	0
8	i	35/36 (97%)	0.06	5 (14%) 4 5	32, 37, 71, 92	0
9	J	37/37 (100%)	-0.08	4 (10%) 8 10	28, 37, 84, 92	0
9	j	37/37 (100%)	0.20	4 (10%) 8 10	33, 44, 68, 75	0
10	K	37/37 (100%)	-0.50	0 100 100	33, 38, 50, 52	0
10	k	37/37 (100%)	0.00	1 (2%) 58 65	38, 44, 61, 71	0
11	L	37/37 (100%)	-0.31	4 (10%) 8 10	21, 24, 57, 73	0
11	l	37/37 (100%)	-0.21	3 (8%) 15 20	22, 25, 63, 88	0
12	M	33/34 (97%)	-0.25	2 (6%) 25 33	24, 27, 51, 76	0
12	m	33/34 (97%)	-0.31	3 (9%) 11 16	25, 29, 52, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/244 (100%)	0.13	21 (8%) 13 18	20, 37, 68, 88	0
13	o	243/244 (99%)	0.07	21 (8%) 13 18	24, 38, 68, 78	0
14	T	30/31 (96%)	-0.22	2 (6%) 21 28	22, 27, 56, 84	0
14	t	29/31 (93%)	-0.29	2 (6%) 20 27	23, 27, 53, 66	0
15	U	97/97 (100%)	-0.28	1 (1%) 84 87	25, 31, 48, 66	0
15	u	97/97 (100%)	-0.33	3 (3%) 52 61	28, 32, 42, 71	0
16	V	137/137 (100%)	-0.53	1 (0%) 89 91	24, 30, 43, 62	0
16	v	137/137 (100%)	-0.07	6 (4%) 38 47	30, 40, 57, 66	0
17	Y	30/30 (100%)	0.52	3 (10%) 9 13	40, 47, 58, 63	0
17	y	30/30 (100%)	0.71	6 (20%) 1 2	45, 56, 69, 75	0
18	X	40/40 (100%)	0.26	5 (12%) 5 7	33, 40, 65, 80	0
18	x	39/40 (97%)	0.43	6 (15%) 3 4	38, 47, 76, 83	0
19	Z	61/62 (98%)	0.59	12 (19%) 1 2	37, 45, 77, 86	0
19	z	61/62 (98%)	1.11	15 (24%) 1 1	49, 59, 90, 96	0
20	R	34/34 (100%)	4.14	30 (88%) 0 0	71, 86, 100, 101	0
All	All	5280/5296 (99%)	-0.27	266 (5%) 32 41	18, 33, 61, 101	0

The worst 5 of 266 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	494	GLY	9.0
19	z	62	VAL	8.5
18	x	2	THR	7.8
20	R	18	TRP	7.6
3	C	23	ALA	7.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	FME	Z	1	10/11	0.75	0.23	-	69,71,74,78	0
8	FME	I	1	10/11	0.97	0.07	-	34,39,40,40	0
12	FME	m	1	10/11	0.92	0.12	-	35,38,49,54	0
14	FME	T	1	10/11	0.95	0.09	-	27,29,44,46	0
8	FME	i	1	10/11	0.95	0.08	-	36,38,40,40	0
19	FME	z	1	10/11	0.71	0.34	-	87,91,94,95	0
12	FME	M	1	10/11	0.91	0.12	-	33,36,43,49	0
14	FME	t	1	10/11	0.89	0.14	-	28,30,46,49	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	LMT	a	402	35/35	0.50	0.31	15.44	52,65,69,70	0
32	LMT	A	1017	35/35	0.62	0.31	13.83	54,72,75,80	0
35	HTG	D	413	19/19	0.53	0.31	12.19	69,80,85,86	0
33	GOL	V	206	6/6	0.84	0.29	9.13	53,56,57,58	0
32	LMT	b	631	35/35	0.59	0.28	8.96	40,74,94,96	0
30	DMS	O	302	4/4	0.94	0.27	8.95	58,59,62,62	0
32	LMT	t	103	35/35	0.53	0.30	8.91	46,75,96,99	0
35	HTG	o	301	19/19	0.80	0.18	8.17	47,49,53,53	0
32	LMT	f	103	35/35	0.59	0.35	7.27	71,92,104,104	0
32	LMT	A	1018	35/35	0.24	0.44	7.08	51,93,113,116	0
30	DMS	D	416	4/4	0.91	0.26	6.94	55,55,56,59	0
31	UNL	t	102	16/-	0.74	0.18	6.66	68,72,74,74	0
28	SQD	a	401	54/54	0.84	0.16	6.43	42,60,74,76	0
27	PL9	a	414	55/55	0.80	0.21	5.54	53,63,77,78	0
28	SQD	b	623[A]	54/54	0.75	0.25	5.33	41,53,70,71	54
31	UNL	D	414	40/-	0.64	0.24	5.17	48,58,72,73	0
31	UNL	b	603	16/-	0.46	0.36	5.08	64,67,71,71	0
30	DMS	O	301	4/4	0.73	0.30	5.05	72,73,75,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
30	DMS	A	1014	4/4	0.92	0.20	4.84	54,54,55,61	0
30	DMS	c	529	4/4	0.96	0.20	4.80	51,51,53,54	0
28	SQD	b	623[B]	54/54	0.75	0.25	4.80	49,57,77,80	54
27	PL9	A	1010	55/55	0.82	0.20	4.66	43,55,72,72	0
33	GOL	V	204	6/6	0.70	0.34	4.65	57,58,59,60	0
31	UNL	d	412	16/-	0.89	0.18	4.48	48,53,62,63	0
29	LMG	c	521	51/55	0.57	0.30	4.48	53,81,93,97	0
35	HTG	d	416	19/19	0.69	0.33	4.10	70,92,94,96	0
30	DMS	d	413	4/4	0.88	0.21	4.09	57,62,62,63	0
35	HTG	V	202	19/19	0.81	0.29	4.00	56,63,77,77	0
30	DMS	D	417	4/4	0.91	0.20	3.99	57,58,62,64	0
35	HTG	d	410	19/19	0.58	0.33	3.81	74,84,91,91	0
24	CLA	B	601	65/65	0.84	0.16	3.62	34,42,66,69	0
29	LMG	Z	101	51/55	0.47	0.35	3.58	47,77,104,110	0
32	LMT	i	102	35/35	0.22	0.41	3.54	52,88,111,111	0
30	DMS	c	526	4/4	0.95	0.19	3.54	73,74,74,75	0
35	HTG	b	626	19/19	0.81	0.17	3.49	43,48,51,51	0
29	LMG	B	622	51/55	0.86	0.14	3.48	38,47,58,64	0
30	DMS	b	635	4/4	0.61	0.29	3.47	66,70,72,74	0
31	UNL	D	415	16/-	0.89	0.13	3.39	39,42,48,49	0
34	LHG	e	101	49/49	0.61	0.31	3.38	66,97,101,102	0
30	DMS	B	634	4/4	0.92	0.27	3.34	54,57,59,59	0
35	HTG	C	522	19/19	0.81	0.26	3.33	65,75,80,80	0
34	LHG	D	411	49/49	0.95	0.14	3.29	29,38,73,76	0
29	LMG	D	412	51/55	0.90	0.15	3.28	27,38,77,78	0
31	UNL	l	101	16/-	0.80	0.21	3.14	49,58,68,69	0
34	LHG	d	408	49/49	0.93	0.15	3.13	32,41,72,74	0
36	DGD	C	516	62/66	0.92	0.10	3.06	28,36,70,72	0
30	DMS	b	634	4/4	0.70	0.25	3.04	61,63,65,68	0
29	LMG	d	409	51/55	0.86	0.16	3.01	33,42,72,76	0
32	LMT	a	416	35/35	0.79	0.32	3.01	73,75,79,79	0
28	SQD	B	620[A]	54/54	0.78	0.24	2.92	42,56,75,76	54
31	UNL	K	103	34/-	0.57	0.24	2.90	57,76,82,83	0
29	LMG	A	1012	51/55	0.83	0.17	2.90	49,56,67,71	0
30	DMS	C	524	4/4	0.97	0.17	2.83	40,41,41,42	0
31	UNL	x	101	16/-	0.78	0.17	2.78	41,45,59,60	0
30	DMS	B	632	4/4	0.97	0.18	2.72	57,58,60,61	0
29	LMG	C	519	51/55	0.73	0.28	2.71	38,74,84,85	0
31	UNL	B	630	16/-	0.81	0.24	2.68	53,56,60,60	0
24	CLA	a	409	65/65	0.94	0.12	2.60	24,26,85,90	0
31	UNL	c	523	32/-	0.64	0.30	2.59	63,75,84,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	UNL	I	101	13/-	0.81	0.27	2.59	54,56,56,57	0
29	LMG	m	102	51/55	0.87	0.13	2.58	35,49,57,59	0
28	SQD	B	620[B]	54/54	0.78	0.24	2.54	40,54,66,66	54
29	LMG	c	519	51/55	0.80	0.18	2.46	45,62,77,80	0
34	LHG	E	101	49/49	0.66	0.26	2.45	51,77,83,85	0
30	DMS	b	629	4/4	0.96	0.12	2.44	48,49,52,53	0
32	LMT	M	101	35/35	0.55	0.29	2.41	52,85,95,97	0
30	DMS	V	203	4/4	0.96	0.14	2.40	50,51,51,52	0
24	CLA	b	604	65/65	0.83	0.17	2.36	40,48,69,70	0
32	LMT	m	103	35/35	0.52	0.29	2.34	55,90,100,101	0
36	DGD	c	516	62/66	0.90	0.12	2.32	36,42,75,79	0
24	CLA	a	412	65/65	0.93	0.15	2.32	26,28,90,92	0
30	DMS	v	202	4/4	0.95	0.14	2.21	55,56,58,58	0
26	BCR	B	618	40/40	0.93	0.09	2.21	27,32,41,41	0
35	HTG	B	628	19/19	0.77	0.20	2.20	45,68,72,74	0
32	LMT	C	520	35/35	0.78	0.27	2.07	68,75,79,79	0
30	DMS	B	627	4/4	0.97	0.09	2.05	41,41,42,44	0
34	LHG	d	406	49/49	0.94	0.13	2.01	38,41,46,46	0
24	CLA	d	403	65/65	0.89	0.14	1.99	31,34,76,77	0
37	BCT	D	401	4/4	0.97	0.16	1.98	37,38,38,41	0
36	DGD	C	515	62/66	0.94	0.11	1.97	27,36,63,64	0
31	UNL	d	411	36/-	0.65	0.21	1.96	46,56,78,79	0
24	CLA	A	1008	65/65	0.93	0.13	1.96	25,27,79,81	0
36	DGD	H	102	62/66	0.93	0.11	1.95	27,34,38,39	0
30	DMS	b	633	4/4	0.87	0.15	1.92	55,55,56,62	0
28	SQD	f	102	43/54	0.78	0.28	1.87	61,80,89,91	0
35	HTG	D	419	19/19	0.62	0.27	1.85	59,79,83,84	0
31	UNL	j	101	16/-	0.68	0.16	1.81	58,60,62,63	0
30	DMS	C	526	4/4	0.91	0.18	1.81	71,71,72,72	0
24	CLA	C	504	65/65	0.94	0.10	1.80	27,30,55,57	0
36	DGD	c	515	62/66	0.93	0.12	1.78	28,38,69,71	0
36	DGD	C	517	62/66	0.94	0.10	1.76	24,33,62,69	0
35	HTG	b	630	19/19	0.59	0.35	1.76	66,83,88,90	0
31	UNL	X	101	16/-	0.85	0.14	1.74	39,43,51,51	0
36	DGD	h	102	62/66	0.91	0.11	1.73	32,38,46,48	0
34	LHG	d	407	49/49	0.95	0.11	1.73	26,31,40,45	0
24	CLA	b	612	65/65	0.93	0.13	1.67	30,34,37,38	0
28	SQD	A	1016	54/54	0.82	0.17	1.63	46,60,72,73	0
26	BCR	K	101	40/40	0.91	0.13	1.60	32,35,37,38	0
34	LHG	D	410	49/49	0.96	0.11	1.57	26,30,38,41	0
29	LMG	a	415	51/55	0.81	0.17	1.56	50,60,70,71	0
24	CLA	A	1006	65/65	0.95	0.10	1.56	22,23,66,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	DGD	c	517	62/66	0.92	0.12	1.54	29,38,64,73	0
25	PHO	a	411	64/64	0.95	0.11	1.51	24,30,35,36	0
28	SQD	A	1011	54/54	0.91	0.15	1.48	43,57,69,69	0
31	UNL	Y	101	16/-	0.58	0.27	1.47	66,68,70,70	0
32	LMT	b	625	35/35	0.53	0.29	1.44	52,82,103,104	0
29	LMG	C	518	51/55	0.83	0.18	1.40	36,62,70,70	0
24	CLA	B	604	65/65	0.96	0.10	1.40	22,24,53,55	0
38	HEM	V	201	43/43	0.98	0.12	1.40	25,26,28,29	0
24	CLA	D	405	65/65	0.92	0.12	1.39	28,30,70,71	0
24	CLA	B	607	65/65	0.96	0.09	1.36	20,22,36,37	0
24	CLA	B	606	65/65	0.92	0.12	1.36	27,30,51,53	0
32	LMT	B	623	35/35	0.70	0.24	1.32	48,65,71,72	0
26	BCR	t	101	40/40	0.93	0.09	1.29	26,39,46,47	0
24	CLA	a	407	65/65	0.97	0.10	1.28	21,23,30,35	0
34	LHG	D	409	49/49	0.94	0.11	1.24	35,38,43,45	0
26	BCR	A	1009	40/40	0.93	0.10	1.21	25,29,32,32	0
24	CLA	A	1005	65/65	0.97	0.10	1.20	17,20,29,33	0
26	BCR	D	406	40/40	0.90	0.11	1.19	28,32,50,51	0
24	CLA	B	616	65/65	0.89	0.16	1.16	27,31,79,80	0
24	CLA	C	512	65/65	0.88	0.13	1.15	39,42,71,72	0
24	CLA	C	513	65/65	0.85	0.15	1.14	41,48,66,68	0
24	CLA	c	509	65/65	0.96	0.11	1.14	33,35,50,51	0
24	CLA	C	509	65/65	0.96	0.10	1.13	28,31,52,53	0
24	CLA	C	508	65/65	0.94	0.10	1.09	28,31,65,70	0
30	DMS	u	201	4/4	0.93	0.24	1.07	56,57,57,59	0
24	CLA	b	619	65/65	0.88	0.15	1.06	31,35,80,81	0
28	SQD	c	518	54/54	0.90	0.14	1.04	41,59,74,76	0
27	PL9	D	407	55/55	0.95	0.09	1.03	21,25,32,33	0
29	LMG	c	520	51/55	0.69	0.26	1.03	42,74,84,89	0
33	GOL	v	203	6/6	0.81	0.20	1.02	48,52,53,53	0
31	UNL	L	101	16/-	0.83	0.21	0.96	53,56,63,63	0
24	CLA	B	613	65/65	0.97	0.08	0.95	23,25,49,53	0
24	CLA	d	402	65/65	0.97	0.10	0.95	21,23,39,43	0
26	BCR	K	102	40/40	0.85	0.12	0.88	39,49,52,52	0
24	CLA	c	504	65/65	0.94	0.10	0.85	32,35,57,59	0
26	BCR	d	404	40/40	0.89	0.11	0.84	31,36,59,59	0
24	CLA	C	507	65/65	0.94	0.11	0.82	34,37,51,53	0
24	CLA	C	505	65/65	0.94	0.10	0.81	32,35,44,48	0
24	CLA	b	609	65/65	0.91	0.12	0.80	29,32,65,68	0
24	CLA	c	513	65/65	0.86	0.16	0.79	45,54,69,70	0
24	CLA	c	508	65/65	0.93	0.10	0.77	32,35,65,72	0
30	DMS	V	205	4/4	0.89	0.17	0.73	61,62,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
28	SQD	D	408	43/54	0.91	0.18	0.71	41,67,74,76	0
24	CLA	b	607	65/65	0.96	0.09	0.71	24,26,50,51	0
24	CLA	B	614	65/65	0.95	0.10	0.70	24,27,67,68	0
24	CLA	c	512	65/65	0.91	0.12	0.67	42,46,65,67	0
27	PL9	d	405	55/55	0.95	0.09	0.67	21,27,32,33	0
24	CLA	b	608	65/65	0.96	0.10	0.66	24,26,35,35	0
26	BCR	b	622	40/40	0.94	0.09	0.66	33,36,40,41	0
26	BCR	k	101	40/40	0.93	0.12	0.65	36,45,47,48	0
24	CLA	b	605	65/65	0.95	0.10	0.56	29,32,37,37	0
24	CLA	c	506	65/65	0.88	0.15	0.54	38,40,78,81	0
26	BCR	k	102	40/40	0.87	0.14	0.53	48,54,64,66	0
24	CLA	b	616	65/65	0.97	0.09	0.53	25,25,50,52	0
24	CLA	C	510	65/65	0.97	0.09	0.53	27,31,38,39	0
24	CLA	B	605	65/65	0.96	0.10	0.52	23,26,31,32	0
38	HEM	f	101	43/43	0.95	0.12	0.50	42,44,57,63	0
32	LMT	m	101	35/35	0.73	0.20	0.50	38,51,56,57	0
26	BCR	a	413	40/40	0.93	0.09	0.50	24,30,34,34	0
24	CLA	c	505	65/65	0.95	0.10	0.49	34,36,48,48	0
24	CLA	b	610	65/65	0.96	0.08	0.47	23,25,34,35	0
26	BCR	B	619	40/40	0.94	0.08	0.46	31,34,42,43	0
26	BCR	J	101	40/40	0.92	0.09	0.46	35,37,41,41	0
24	CLA	D	402	65/65	0.97	0.09	0.44	17,20,35,37	0
24	CLA	B	610	65/65	0.96	0.09	0.44	24,26,34,36	0
24	CLA	c	507	65/65	0.94	0.12	0.43	33,34,50,51	0
24	CLA	B	609	65/65	0.95	0.11	0.43	28,31,33,35	0
24	CLA	b	613	65/65	0.95	0.10	0.40	28,31,38,40	0
24	CLA	a	408	65/65	0.97	0.08	0.38	20,23,31,34	0
24	CLA	b	617	65/65	0.96	0.10	0.38	24,28,67,68	0
24	CLA	B	615	65/65	0.95	0.10	0.37	27,28,44,46	0
24	CLA	C	506	65/65	0.92	0.11	0.36	36,43,73,76	0
24	CLA	D	403	65/65	0.97	0.07	0.35	18,20,29,33	0
34	LHG	b	624	49/49	0.96	0.09	0.32	27,32,48,53	0
26	BCR	b	621	40/40	0.94	0.08	0.32	28,31,41,42	0
34	LHG	B	621	49/49	0.97	0.09	0.32	26,32,45,49	0
25	PHO	D	404	64/64	0.96	0.09	0.31	22,25,29,30	0
26	BCR	T	101	40/40	0.95	0.08	0.30	27,37,42,43	0
33	GOL	V	207	6/6	0.75	0.18	0.28	60,63,64,64	0
24	CLA	b	614	65/65	0.96	0.09	0.26	24,26,40,41	0
32	LMT	M	102	35/35	0.73	0.20	0.26	39,58,64,66	0
35	HTG	b	601	19/19	0.89	0.14	0.23	44,60,67,67	0
30	DMS	d	414	4/4	0.96	0.11	0.23	58,59,59,60	0
24	CLA	B	602	65/65	0.96	0.09	0.21	25,27,34,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
26	BCR	C	514	40/40	0.94	0.11	0.18	31,38,41,41	0
31	UNL	y	102	16/-	0.72	0.21	0.18	63,65,67,67	0
24	CLA	C	502	65/65	0.96	0.09	0.15	26,28,42,44	0
26	BCR	c	514	40/40	0.92	0.11	0.10	34,41,43,44	0
24	CLA	B	612	65/65	0.97	0.08	0.08	24,26,30,31	0
24	CLA	c	510	65/65	0.96	0.08	0.08	33,35,41,43	0
30	DMS	U	201	4/4	0.91	0.19	0.07	56,56,58,58	0
24	CLA	c	501	65/65	0.95	0.11	0.06	35,36,43,44	0
30	DMS	B	626	4/4	0.98	0.07	0.05	25,26,26,27	0
25	PHO	A	1007	64/64	0.97	0.08	0.05	21,24,26,28	0
26	BCR	b	620	40/40	0.96	0.09	0.05	28,34,35,35	0
38	HEM	v	201	43/43	0.97	0.10	0.00	31,32,36,37	0
24	CLA	B	611	65/65	0.97	0.09	-0.01	22,24,36,37	0
25	PHO	a	410	64/64	0.97	0.08	-0.03	22,24,29,31	0
24	CLA	b	611	65/65	0.96	0.08	-0.03	26,28,38,39	0
24	CLA	c	503	65/65	0.95	0.09	-0.04	33,39,42,44	0
26	BCR	B	617	40/40	0.95	0.08	-0.05	28,30,33,33	0
24	CLA	b	606	65/65	0.97	0.09	-0.06	26,29,35,39	0
24	CLA	c	502	65/65	0.96	0.09	-0.08	28,31,50,51	0
26	BCR	h	101	40/40	0.90	0.12	-0.10	32,39,47,48	0
24	CLA	B	603	65/65	0.97	0.08	-0.12	25,26,32,34	0
26	BCR	y	101	40/40	0.92	0.09	-0.14	40,44,46,47	0
24	CLA	b	615	65/65	0.95	0.08	-0.15	25,28,32,35	0
30	DMS	b	628	4/4	0.98	0.07	-0.19	30,31,31,32	0
24	CLA	C	511	65/65	0.95	0.10	-0.19	29,35,40,42	0
37	BCT	d	401	4/4	0.96	0.09	-0.22	40,40,41,42	0
26	BCR	H	101	40/40	0.93	0.09	-0.27	27,36,42,42	0
38	HEM	F	101	43/43	0.96	0.11	-0.33	39,41,44,46	0
24	CLA	C	501	65/65	0.96	0.08	-0.43	31,35,41,42	0
24	CLA	c	511	65/65	0.95	0.10	-0.53	36,39,43,46	0
24	CLA	B	608	65/65	0.97	0.08	-0.56	25,27,31,31	0
24	CLA	C	503	65/65	0.96	0.08	-0.58	28,33,36,38	0
24	CLA	b	618	65/65	0.96	0.08	-0.75	30,32,44,46	0
21	OER	A	1001	10/10	1.00	0.06	-1.06	24,25,28,28	1
22	FE2	a	404	1/1	1.00	0.05	-1.12	29,29,29,29	0
21	OER	a	403	10/10	1.00	0.05	-1.76	27,28,29,31	1
39	MG	j	102	1/1	0.94	0.06	-1.87	37,37,37,37	0
22	FE2	A	1002	1/1	1.00	0.03	-2.03	29,29,29,29	0
23	CL	a	406	1/1	1.00	0.05	-2.03	27,27,27,27	0
39	MG	J	103	1/1	0.98	0.04	-2.30	32,32,32,32	0
23	CL	A	1003	1/1	0.99	0.03	-2.53	25,25,25,25	0
23	CL	a	405	1/1	0.99	0.03	-3.06	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
23	CL	A	1004	1/1	1.00	0.02	-3.95	22,22,22,22	0
31	UNL	i	101	16/-	0.69	0.23	-	55,57,62,62	0
30	DMS	B	633	4/4	0.80	0.23	-	67,69,70,75	0
30	DMS	C	527	4/4	0.88	0.26	-	75,75,77,80	0
31	UNL	A	1015	28/-	0.61	0.27	-	62,73,78,78	0
31	UNL	I	102	13/-	0.85	0.14	-	55,57,60,60	0
35	HTG	C	521	19/19	0.85	0.23	-	69,71,74,75	0
33	GOL	B	631	6/6	0.89	0.24	-	56,57,60,62	0
33	GOL	A	1019	6/6	0.86	0.21	-	60,61,62,62	0
35	HTG	c	522	19/19	0.81	0.28	-	82,85,89,90	0
33	GOL	a	420	6/6	0.90	0.15	-	53,56,57,59	0
31	UNL	a	419	30/-	0.62	0.29	-	62,74,87,89	0
30	DMS	a	417	4/4	0.97	0.09	-	31,32,33,33	0
35	HTG	c	525	19/19	0.55	0.36	-	76,90,95,96	0
30	DMS	c	528	4/4	0.84	0.21	-	83,85,86,88	0
31	UNL	B	625	16/-	0.85	0.13	-	44,46,52,54	0
31	UNL	J	102	16/-	0.78	0.16	-	50,52,58,59	0
33	GOL	d	417	6/6	0.59	0.26	-	58,61,62,62	0
35	HTG	b	602	19/19	0.59	0.26	-	60,89,94,94	0
30	DMS	a	418	4/4	0.83	0.20	-	62,63,66,69	0
39	MG	K	104	1/1	0.93	0.08	-	48,48,48,48	0
35	HTG	B	624	19/19	0.53	0.42	-	58,86,92,92	0
30	DMS	c	524	4/4	0.98	0.18	-	43,43,43,43	0
33	GOL	v	204	6/6	0.75	0.24	-	74,75,76,76	0
33	GOL	D	418	6/6	0.46	0.31	-	70,72,73,74	0
30	DMS	C	525	4/4	0.87	0.24	-	71,73,73,74	0
33	GOL	d	415	6/6	0.70	0.20	-	63,66,66,67	0
31	UNL	b	627	16/-	0.79	0.13	-	47,48,50,50	0
39	MG	k	103	1/1	0.97	0.05	-	45,45,45,45	0
30	DMS	c	527	4/4	0.88	0.25	-	65,65,66,66	0
35	HTG	B	629	19/19	0.53	0.28	-	52,86,90,90	0
30	DMS	A	1013	4/4	0.98	0.09	-	29,29,30,31	0
30	DMS	C	523	4/4	0.99	0.10	-	36,37,38,38	0
33	GOL	b	632	6/6	0.71	0.26	-	51,56,61,63	0

6.5 Other polymers ⓘ

There are no such residues in this entry.