



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2017 – 07:39 AM EDT

PDB ID : 5H2F
Title : Crystal structure of the PsbM-deletion mutant of photosystem II
Authors : Uto, S.; Kawakami, K.; Umena, Y.; Iwai, M.; Ikeuchi, M.; Shen, J.R.; Kamiya, N.
Deposited on : unknown
Resolution : 2.20 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

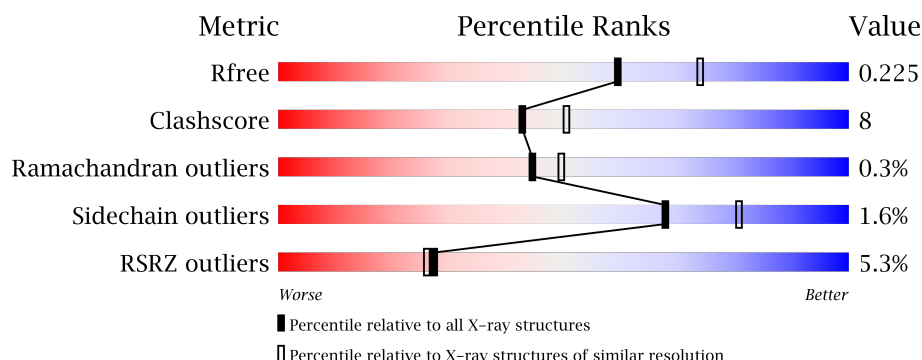
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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>4%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	a	334	<div> <div>10%</div> <div>98%</div> <div>.</div> </div>
2	B	505	<div> <div>7%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
2	b	505	<div> <div>4%</div> <div>94%</div> <div>.</div> <div>.</div> </div>
3	C	455	<div> <div>3%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	c	455	96% .
4	D	342	78% 21% .
4	d	342	97% .
5	E	80	13% 75% 23% ..
5	e	80	15% 94% 5% .
6	F	33	12% 76% 24%
6	f	33	3% 88% 6% 6%
7	H	63	2% 67% 32% .
7	h	63	13% 94% 5% .
8	I	36	3% 72% 22% . .
8	i	36	100%
9	J	40	5% 70% 20% 10%
9	j	40	15% 98% .
10	K	37	65% 32% .
10	k	37	3% 95% 5%
11	L	35	20% 86% 14%
11	l	35	11% 97% .
12	O	243	3% 78% 21%
12	o	243	6% 98% .
13	T	30	73% 27%
13	t	30	7% 93% 7%
14	U	97	82% 18%
14	u	97	99% .
15	V	137	84% 15% .
15	v	137	2% 97% ..

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Mol	Chain	Length	Quality of chain
16	Y	29	
16	y	29	
17	X	37	
17	x	37	
18	Z	62	
18	z	62	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	405	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	A	408	X	-	-	-
22	CLA	B	602	X	-	-	X
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	B	617	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	C	514	X	-	-	-
22	CLA	D	401	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	a	407	X	-	-	-
22	CLA	a	408	X	-	-	-
22	CLA	a	409	X	-	-	-
22	CLA	b	602	X	-	-	X
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	c	902	X	-	-	-
22	CLA	c	903	X	-	-	-
22	CLA	c	904	X	-	-	-
22	CLA	c	905	X	-	-	-
22	CLA	c	906	X	-	-	-
22	CLA	c	907	X	-	-	-
22	CLA	c	908	X	-	-	-
22	CLA	c	909	X	-	-	-
22	CLA	c	910	X	-	-	-
22	CLA	c	911	X	-	-	-
22	CLA	c	912	X	-	-	-
22	CLA	c	913	X	-	-	-
22	CLA	c	914	X	-	-	-
22	CLA	d	402	X	-	-	-
22	CLA	d	403	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	BCR	B	618	-	-	-	X
24	BCR	D	405	-	-	-	X
24	BCR	b	618	-	-	-	X
24	BCR	b	619	-	-	-	X
25	LMG	B	621	-	-	-	X
25	LMG	C	531	-	-	-	X
25	LMG	J	101	-	-	-	X
25	LMG	b	622	-	-	-	X
27	LHG	A	412	-	-	-	X
28	SQD	A	413	-	-	-	X
29	LMT	A	414	-	-	-	X
29	LMT	E	101	-	-	-	X
29	LMT	I	102	-	-	-	X
29	LMT	T	102	-	-	-	X
29	LMT	Z	101	-	-	-	X
29	LMT	a	419	-	-	-	X
29	LMT	c	921	-	-	-	X
29	LMT	c	931	-	-	-	X
29	LMT	f	102	-	-	-	X
29	LMT	t	101	-	-	-	X
30	UNL	A	415	-	-	-	X
30	UNL	B	624	-	-	-	X
30	UNL	D	413	-	-	-	X
30	UNL	I	104	-	-	-	X
30	UNL	J	103	-	-	-	X
30	UNL	T	101	-	-	-	X
30	UNL	U	201	-	-	-	X
30	UNL	a	417	-	-	-	X
30	UNL	a	420	-	-	-	X
30	UNL	i	104	-	-	-	X
30	UNL	j	103	-	-	-	X
30	UNL	t	102	-	-	-	X
30	UNL	u	201	-	-	-	X
31	DMS	B	628	-	-	-	X
31	DMS	B	631	-	-	-	X
31	DMS	B	638	-	-	X	-
31	DMS	B	640	-	-	-	X
31	DMS	C	528	-	-	-	X
31	DMS	C	530	-	-	-	X
31	DMS	C	535	-	-	-	X
31	DMS	C	536	-	-	-	X
31	DMS	C	540	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	DMS	D	417	-	-	-	X
31	DMS	F	101	-	-	-	X
31	DMS	L	102	-	-	-	X
31	DMS	O	304	-	-	X	X
31	DMS	O	307	-	-	-	X
31	DMS	O	310	-	-	X	X
31	DMS	O	312	-	-	-	X
31	DMS	O	313	-	-	-	X
31	DMS	U	203	-	-	-	X
31	DMS	V	204	-	-	-	X
31	DMS	V	209	-	-	-	X
31	DMS	V	211	-	-	-	X
31	DMS	V	212	-	-	X	-
31	DMS	a	424	-	-	-	X
31	DMS	a	425	-	-	-	X
31	DMS	b	629	-	-	-	X
31	DMS	b	630	-	-	-	X
31	DMS	b	638	-	-	-	X
31	DMS	c	924	-	-	-	X
31	DMS	c	925	-	-	-	X
31	DMS	c	926	-	-	-	X
31	DMS	c	927	-	-	-	X
31	DMS	c	929	-	-	-	X
31	DMS	c	934	-	-	-	X
31	DMS	c	935	-	-	-	X
31	DMS	c	939	-	-	-	X
31	DMS	f	103	-	-	-	X
31	DMS	i	106	-	-	-	X
31	DMS	o	302	-	-	-	X
31	DMS	o	303	-	-	-	X
31	DMS	o	305	-	-	-	X
31	DMS	o	307	-	-	-	X
31	DMS	u	205	-	-	-	X
31	DMS	v	210	-	-	-	X
31	DMS	v	211	-	-	-	X
34	HTG	B	626	-	-	-	X
34	HTG	D	414	-	-	-	X
34	HTG	D	415	-	-	-	X
34	HTG	V	203	-	-	-	X
34	HTG	b	632	-	-	-	X
35	DGD	C	519	-	-	-	X
35	DGD	D	407	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	DGD	d	406	-	-	-	X

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 51892 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	1	0
			2598	1706	428	449	15			
1	a	334	Total	C	N	O	S	0	1	0
			2555	1675	427	438	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	3	0
			3950	2596	661	680	13			
2	b	483	Total	C	N	O	S	0	1	0
			3780	2484	631	652	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	0	0
			3470	2274	580	603	13			
3	c	455	Total	C	N	O	S	0	1	0
			3521	2305	589	614	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	3	0
			2732	1814	442	464	12			
4	d	341	Total	C	N	O	S	0	2	0
			2717	1805	441	459	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	79	Total	C	N	O	0	0	0
			635	417	101	117			
5	e	79	Total	C	N	O	0	0	0
			636	418	101	117			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			
6	f	31	Total	C	N	O	S	0	0	0
			250	170	42	37	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	3	0
			522	347	87	86	2			
7	h	62	Total	C	N	O	S	0	1	0
			501	335	82	82	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			288	196	45	46	1			
8	i	36	Total	C	N	O	S	0	0	0
			293	199	46	47	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	40	Total	C	N	O	S	0	0	0
			277	186	41	49	1			

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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total	C	N	O	0	0	0
			286	198	42	46			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	35	Total	C	N	O	0	0	0
			287	192	46	49			
11	l	35	Total	C	N	O	0	0	0
			287	192	46	49			

- Molecule 12 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	O	243	Total	C	N	O	S	0	1	0
			1853	1160	311	378	4			
12	o	243	Total	C	N	O	S	0	0	0
			1833	1149	305	375	4			

- Molecule 13 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	T	30	Total	C	N	O	S	0	0	0
			253	177	36	38	2			
13	t	30	Total	C	N	O	S	0	0	0
			253	177	36	38	2			

- Molecule 14 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	U	97	Total	C	N	O	0	1	0
			782	496	132	154			
14	u	97	Total	C	N	O	0	0	0
			766	487	129	150			

- Molecule 15 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	V	137	Total	C	N	O	S	0	1	0
			1066	677	177	208	4			
15	v	137	Total	C	N	O	S	0	1	0
			1058	671	175	208	4			

- Molecule 16 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
16	y	29	Total	C	N	O	S	0	0	0
			207	134	37	33	3			

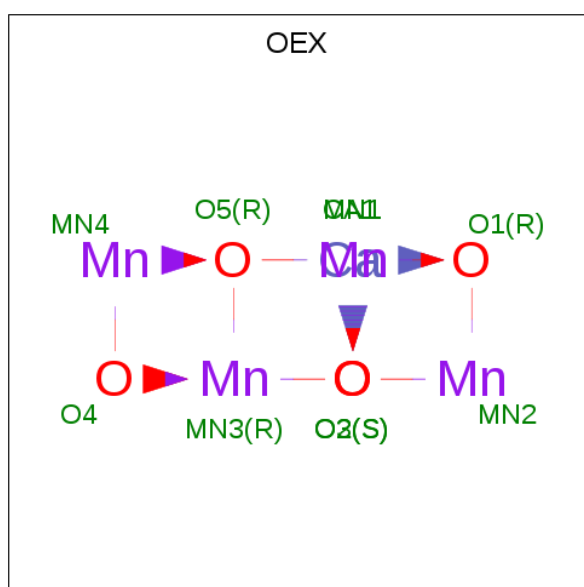
- Molecule 17 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	37	Total	C	N	O	0	1	0
			269	183	40	46			
17	x	36	Total	C	N	O	0	0	0
			253	172	37	44			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Z	62	Total	C	N	O	S	0	0	0
			453	311	68	72	2			
18	z	61	Total	C	N	O	S	0	0	0
			436	299	67	69	1			

- Molecule 19 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

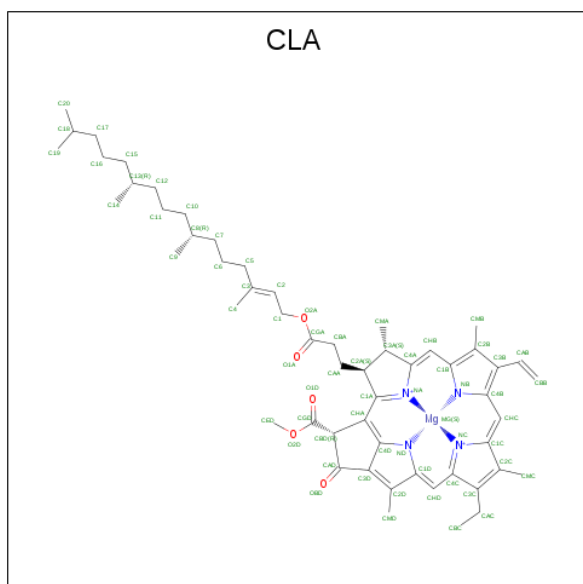
- Molecule 20 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 21 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
22	B	1	Total 53	C 43	Mg 1	N 4	O 5	0	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 56	C 46	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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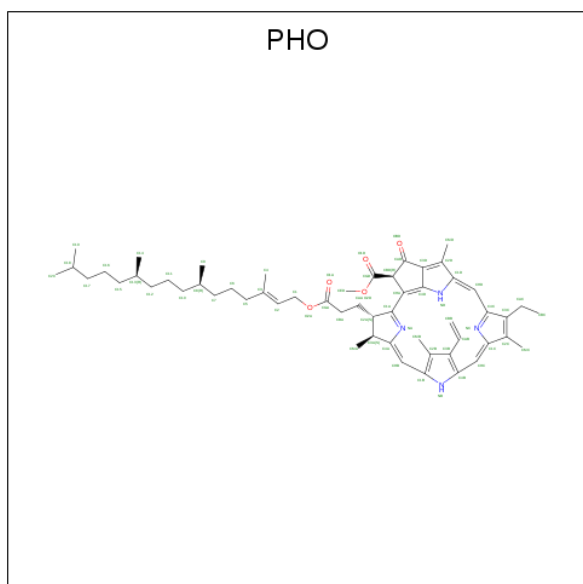
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 59	C 49	Mg 1	N 4	O 5	0	0
22	b	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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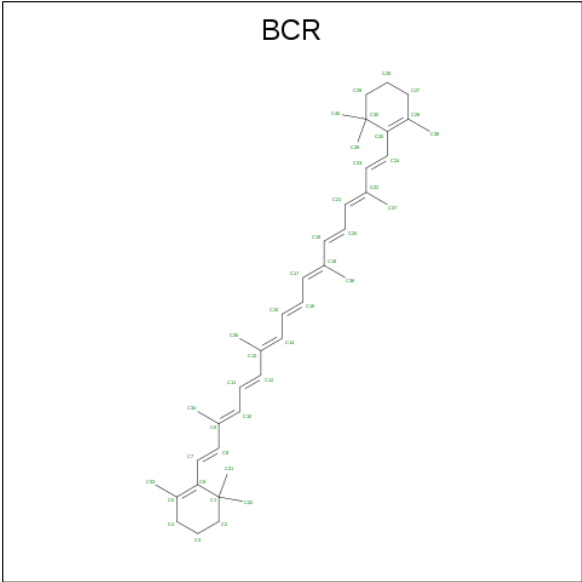
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



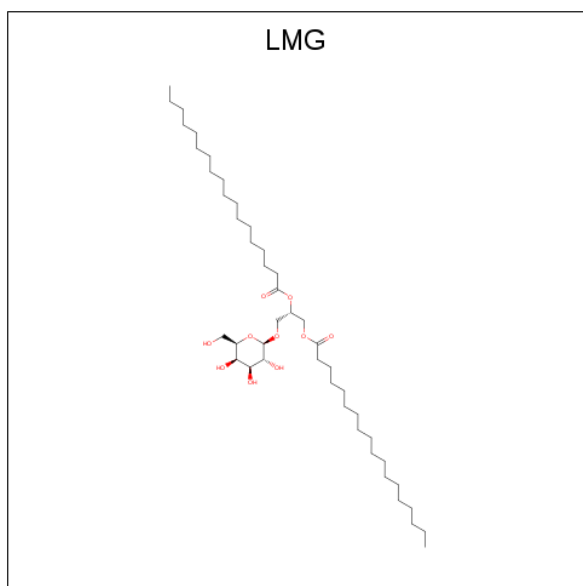
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 19 19	0	0
24	B	1	Total C 30 30	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	Y	1	Total C 39 39	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 20 20	0	0
24	b	1	Total C 31 31	0	0
24	b	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	c	1	Total C 40 40	0	0
24	d	1	Total C 40 40	0	0
24	k	1	Total C 40 40	0	0
24	y	1	Total C 40 40	0	0

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



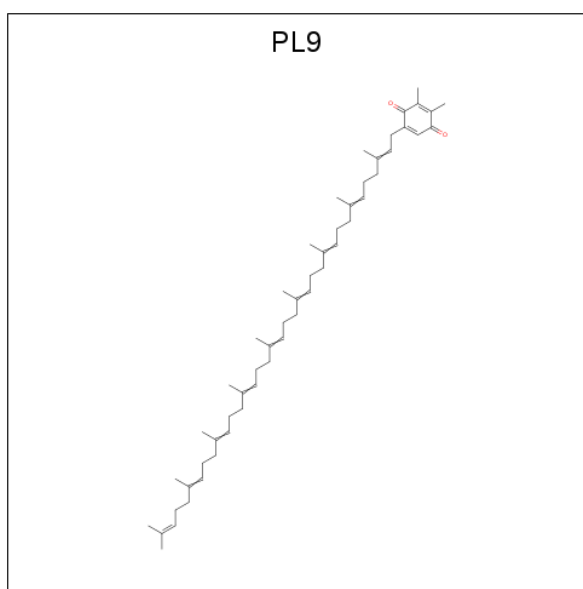
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 51 41 10	0	0
25	B	1	Total C O 40 30 10	0	0
25	C	1	Total C O 51 41 10	0	0
25	C	1	Total C O 40 30 10	0	0
25	D	1	Total C O 46 36 10	0	0
25	J	1	Total C O 45 35 10	0	0
25	b	1	Total C O 43 33 10	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	c	1	Total	C	O	0	0
			51	41	10		
25	c	1	Total	C	O	0	0
			49	39	10		
25	d	1	Total	C	O	0	0
			47	37	10		
25	i	1	Total	C	O	0	0
			51	41	10		
25	j	1	Total	C	O	0	0
			47	37	10		

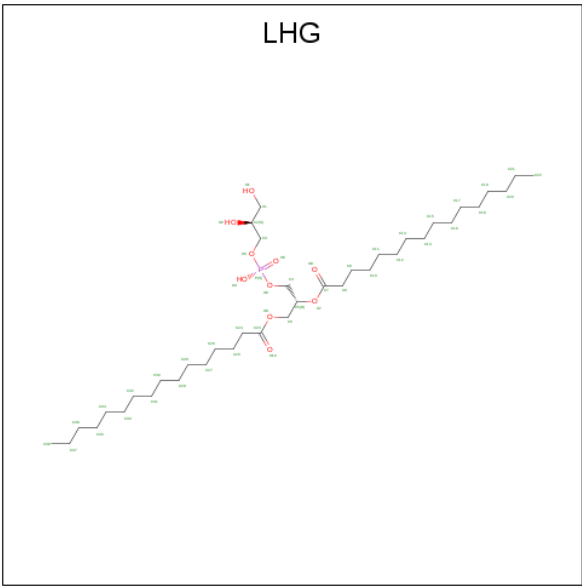
- Molecule 26 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



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

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code:

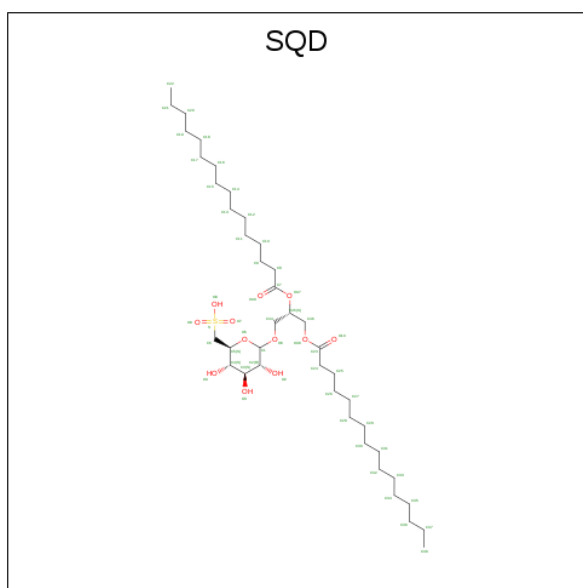
LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	P	0	0
			31	22	8	1		
27	C	1	Total	C	O	P	0	0
			30	21	8	1		
27	D	1	Total	C	O	P	0	0
			49	38	10	1		
27	D	1	Total	C	O	P	0	0
			49	38	10	1		
27	D	1	Total	C	O	P	0	0
			45	34	10	1		
27	L	1	Total	C	O	P	0	0
			40	29	10	1		
27	a	1	Total	C	O	P	0	0
			49	38	10	1		
27	a	1	Total	C	O	P	0	0
			45	34	10	1		
27	d	1	Total	C	O	P	0	0
			33	24	8	1		
27	d	1	Total	C	O	P	0	0
			49	38	10	1		
27	d	1	Total	C	O	P	0	0
			46	35	10	1		
27	l	1	Total	C	O	P	0	0
			49	38	10	1		

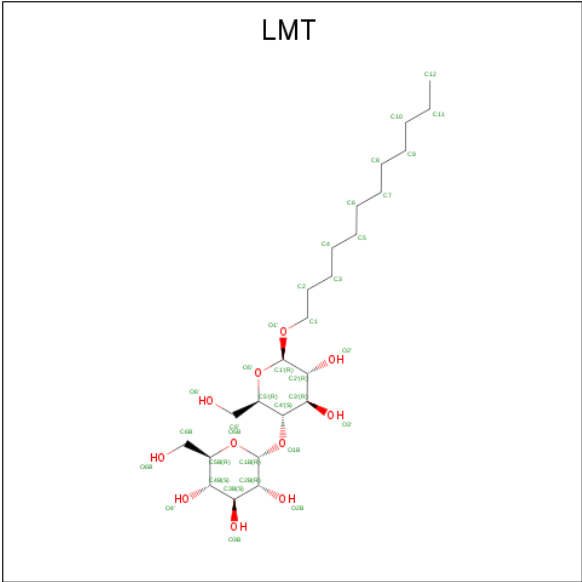
- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-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
			49	36	12	1		
28	C	1	Total	C	O	S	0	0
			54	41	12	1		
28	D	1	Total	C	O	S	0	0
			20	9	10	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			51	38	12	1		
28	b	1	Total	C	O	S	0	0
			38	26	11	1		
28	f	1	Total	C	O	S	0	0
			14	6	7	1		
28	l	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			35	24	11		
29	B	1	Total	C	O	0	0
			24	18	6		
29	E	1	Total	C	O	0	0
			24	18	6		
29	I	1	Total	C	O	0	0
			35	24	11		
29	T	1	Total	C	O	0	0
			24	18	6		
29	Z	1	Total	C	O	0	0
			35	24	11		
29	a	1	Total	C	O	0	0
			35	24	11		
29	c	1	Total	C	O	0	0
			35	24	11		
29	c	1	Total	C	O	0	0
			24	18	6		
29	f	1	Total	C	O	0	0
			25	19	6		
29	t	1	Total	C	O	0	0
			24	18	6		

- Molecule 30 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

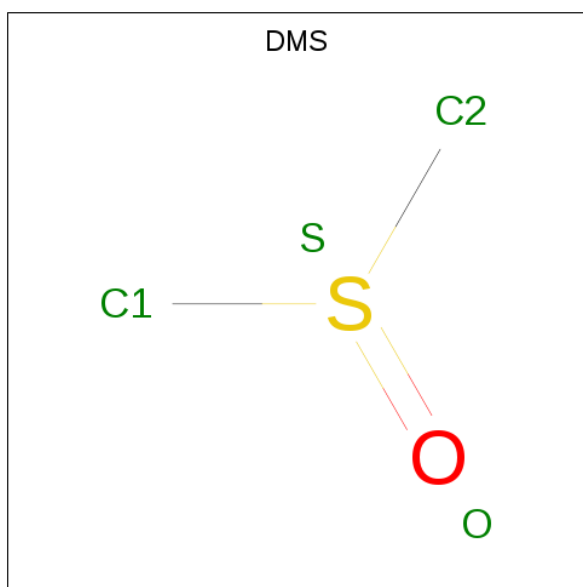
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	J	1	Total	C	0	0
			16	16		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	i	4	Total C 58 58	0	0
30	D	1	Total C 16 16	0	0
30	d	1	Total C 16 16	0	0
30	B	2	Total C 23 23	0	0
30	I	3	Total C 45 45	0	0
30	c	1	Total C 10 10	0	0
30	a	2	Total C 16 16	0	0
30	j	1	Total C 16 16	0	0
30	x	1	Total C 15 15	0	0
30	Z	1	Total C 9 9	0	0
30	A	1	Total C 5 5	0	0
30	T	1	Total C 13 13	0	0
30	U	1	Total C 14 14	0	0
30	X	1	Total C 16 16	0	0
30	O	1	Total C 16 16	0	0
30	t	1	Total C 16 16	0	0
30	u	1	Total C 11 11	0	0
30	b	2	Total C 27 27	0	0

- Molecule 31 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	F	1	Total 4	C 2	O 1	S 1	0	0
31	H	1	Total 4	C 2	O 1	S 1	0	0
31	I	1	Total 4	C 2	O 1	S 1	0	0
31	I	1	Total 4	C 2	O 1	S 1	0	0
31	L	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	U	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	U	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0

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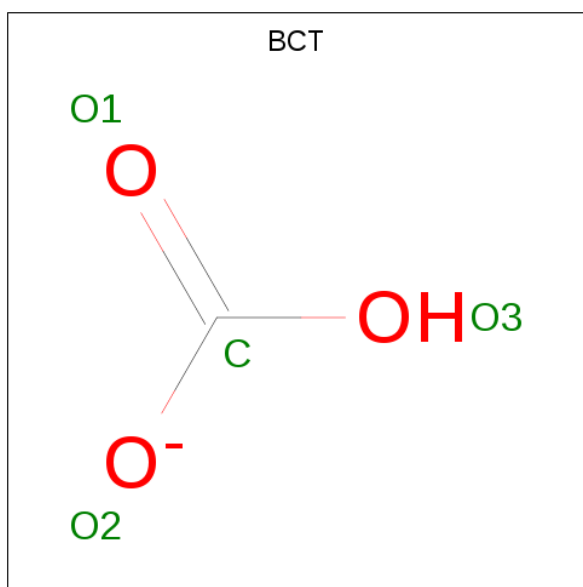
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	f	1	Total 4	C 2	O 1	S 1	0	0
31	i	1	Total 4	C 2	O 1	S 1	0	0
31	l	1	Total 4	C 2	O 1	S 1	0	0
31	l	1	Total 4	C 2	O 1	S 1	0	0
31	l	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	t	1	Total 4	C 2	O 1	S 1	0	0
31	t	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	t	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0

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

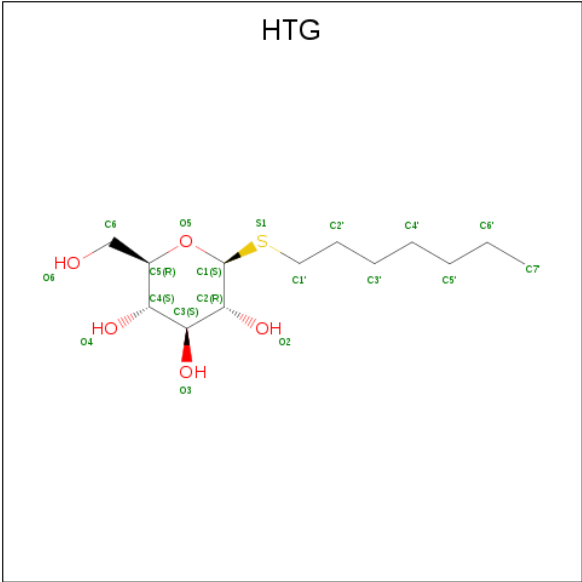


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	1
			8	2	6		
32	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	o	1	Total	Ca	0	0
			1	1		
33	O	1	Total	Ca	0	0
			1	1		
33	B	1	Total	Ca	0	0
			1	1		
33	b	1	Total	Ca	0	0
			1	1		
33	c	1	Total	Ca	0	0
			1	1		

- Molecule 34 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).



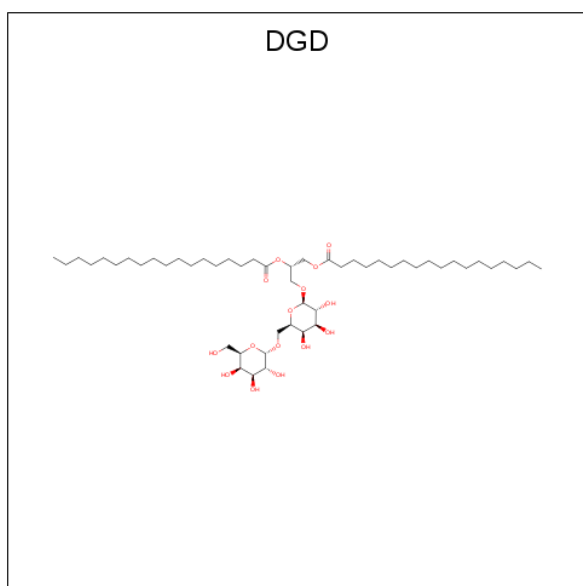
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	C	1	Total	C	O	S	0	0
			19	13	5	1		
34	C	1	Total	C	S		0	0
			9	8	1			
34	C	1	Total	C	O	S	0	0
			19	13	5	1		
34	D	1	Total	C	O	S	0	0
			19	13	5	1		
34	D	1	Total	C	O	S	0	0
			19	13	5	1		
34	V	1	Total	C	O	S	0	0
			14	8	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	c	1	Total	C	O	S	0	0
			19	13	5	1		
34	l	1	Total	C	O	S	0	0
			19	13	5	1		
34	v	1	Total	C	O	S	0	0
			16	10	5	1		

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



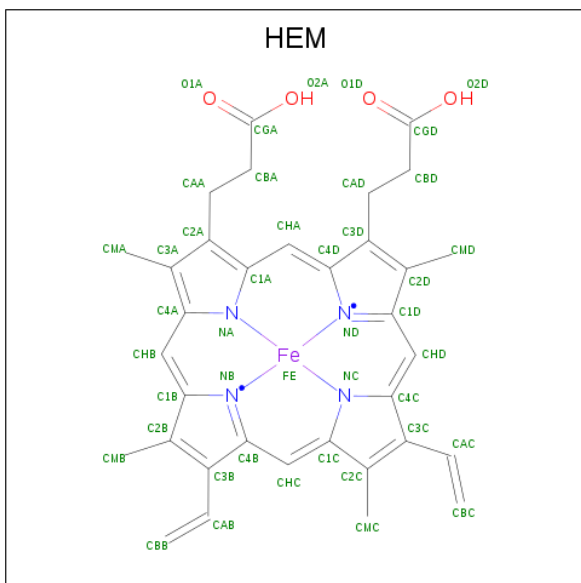
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	C	1	Total	C	O		0	0
			62	47	15			
35	C	1	Total	C	O		0	0
			62	47	15			
35	C	1	Total	C	O		0	0
			62	47	15			
35	D	1	Total	C	O		0	0
			50	41	9			
35	H	1	Total	C	O		0	0
			62	47	15			
35	c	1	Total	C	O		0	0
			62	47	15			
35	c	1	Total	C	O		0	0
			62	47	15			
35	c	1	Total	C	O		0	0
			62	47	15			

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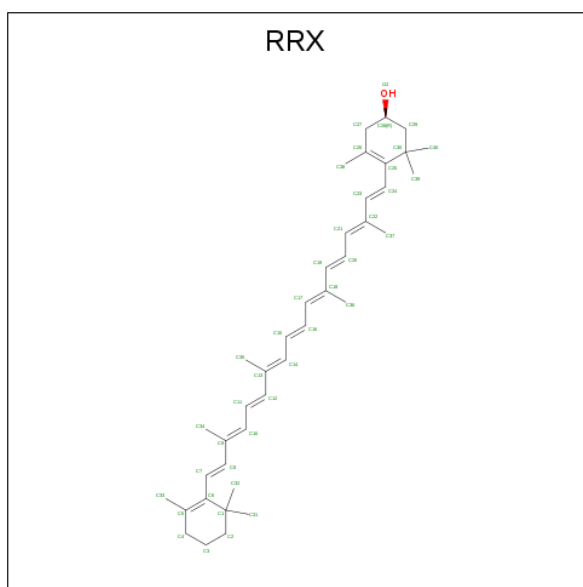
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	d	1	Total	C	O	0	0
			43	37	6		
35	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 36 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
36	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
36	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
36	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
36	v	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 37 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: C₄₀H₅₆O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	H	1	Total	C	O	0	0
			41	40	1		
37	h	1	Total	C	O	0	0
			41	40	1		

- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	A	132	Total	O	0	0
			132	132		
39	B	256	Total	O	0	6
			262	262		
39	C	174	Total	O	0	4
			178	178		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	D	130	Total O 131 131	0	1
39	E	33	Total O 35 35	0	2
39	F	4	Total O 4 4	0	0
39	H	39	Total O 39 39	0	0
39	I	5	Total O 5 5	0	0
39	J	15	Total O 16 16	0	1
39	K	7	Total O 7 7	0	0
39	L	18	Total O 19 19	0	1
39	O	161	Total O 166 166	0	5
39	T	12	Total O 12 12	0	0
39	U	72	Total O 74 74	0	2
39	V	110	Total O 113 113	0	3
39	Y	7	Total O 8 8	0	1
39	X	15	Total O 16 16	0	1
39	Z	5	Total O 5 5	0	0
39	a	122	Total O 123 123	0	1
39	b	251	Total O 261 261	0	10
39	c	216	Total O 220 220	0	4
39	d	115	Total O 115 115	0	0
39	e	16	Total O 17 17	0	1
39	f	4	Total O 4 4	0	0

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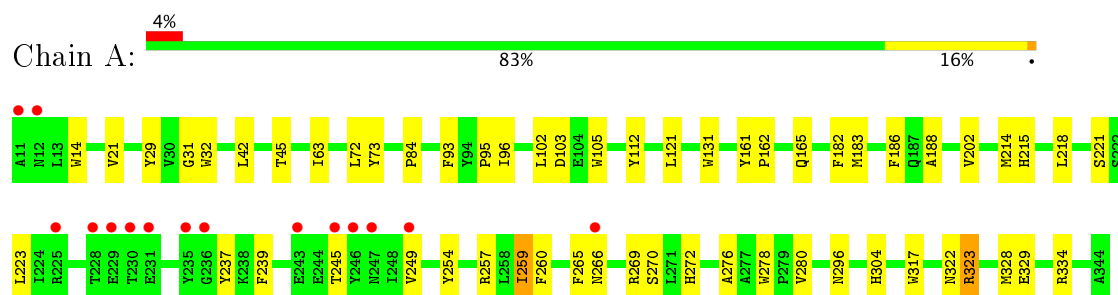
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	h	31	Total 31	O 31	0	0
39	i	5	Total 5	O 5	0	0
39	j	10	Total 10	O 10	0	0
39	k	9	Total 10	O 10	0	1
39	l	14	Total 15	O 15	0	1
39	o	153	Total 156	O 156	0	3
39	t	10	Total 10	O 10	0	0
39	u	75	Total 75	O 75	0	0
39	v	77	Total 82	O 82	0	5
39	y	1	Total 1	O 1	0	0
39	x	5	Total 5	O 5	0	0
39	z	8	Total 8	O 8	0	0

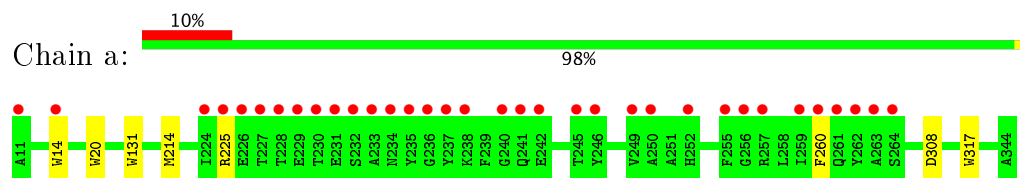
3 Residue-property plots [i](#)

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

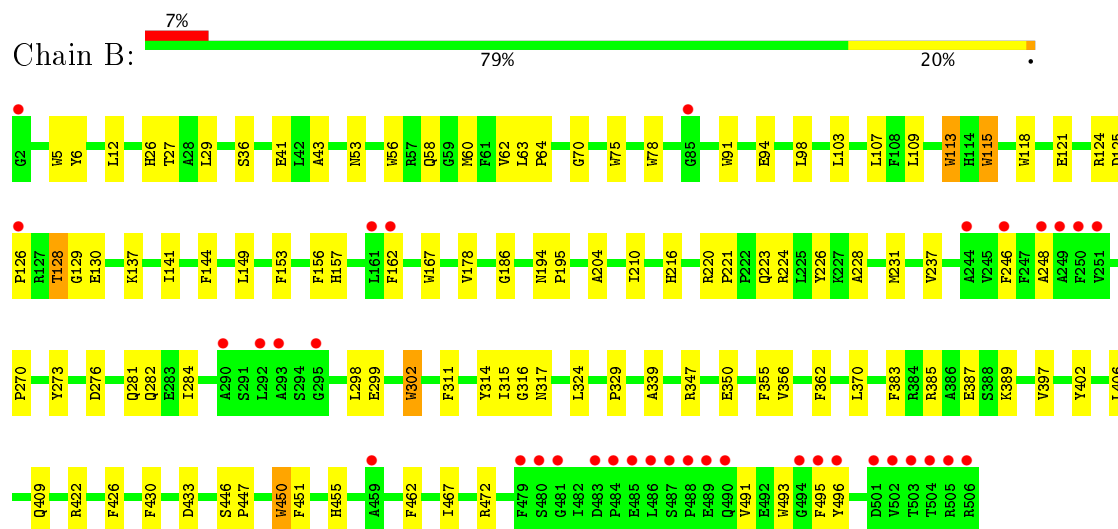
- Molecule 1: Photosystem II protein D1 1



- Molecule 1: Photosystem II protein D1 1

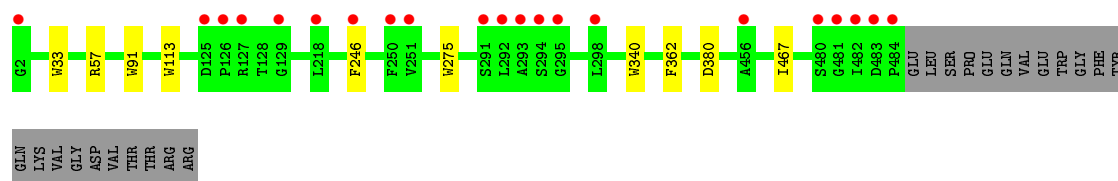


- Molecule 2: Photosystem II CP47 reaction center protein

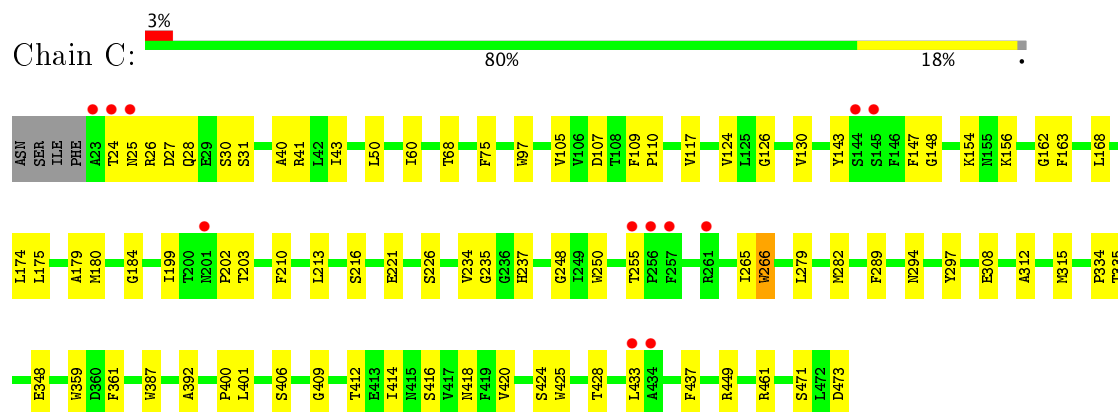


- Molecule 2: Photosystem II CP47 reaction center protein

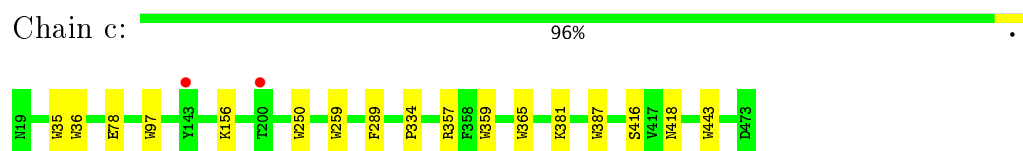




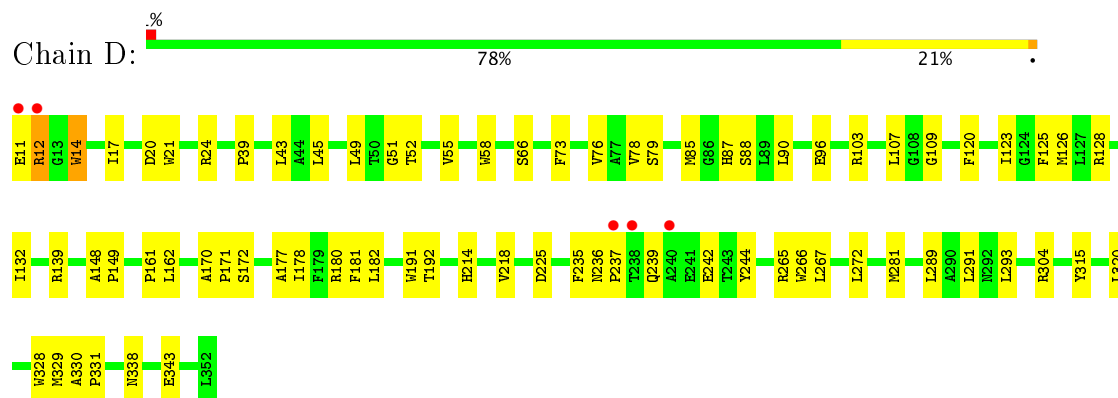
- Molecule 3: Photosystem II CP43 reaction center protein



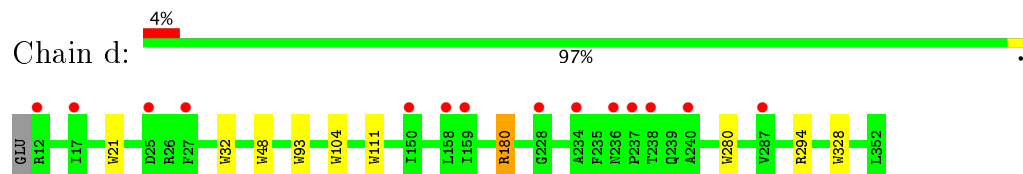
- Molecule 3: Photosystem II CP43 reaction center protein



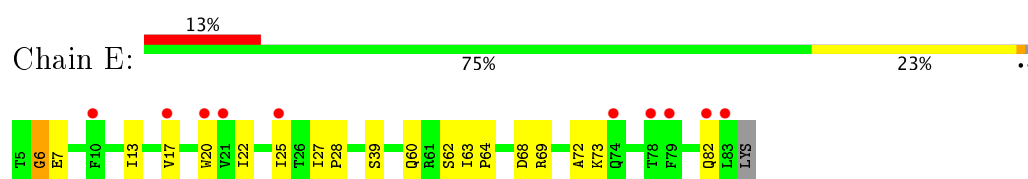
- Molecule 4: Photosystem II D2 protein



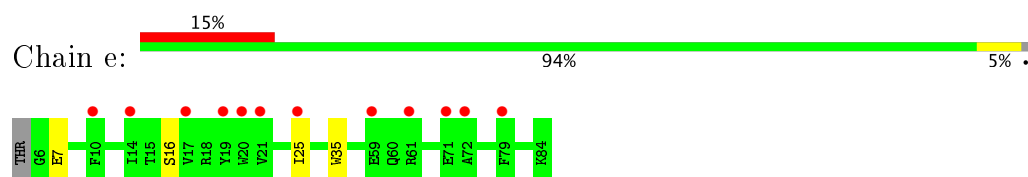
- Molecule 4: Photosystem II D2 protein



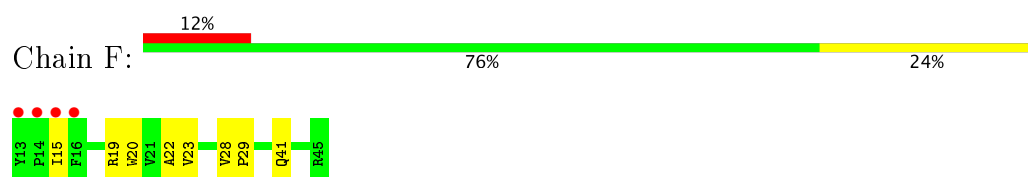
- Molecule 5: Cytochrome b559 subunit alpha



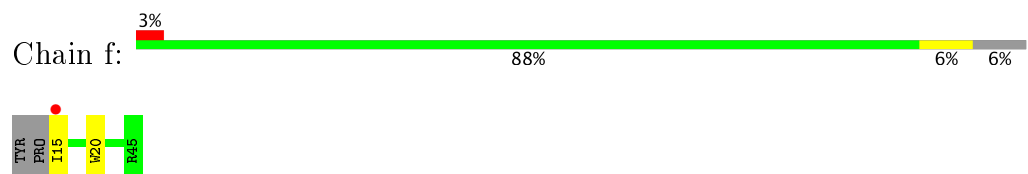
- Molecule 5: Cytochrome b559 subunit alpha



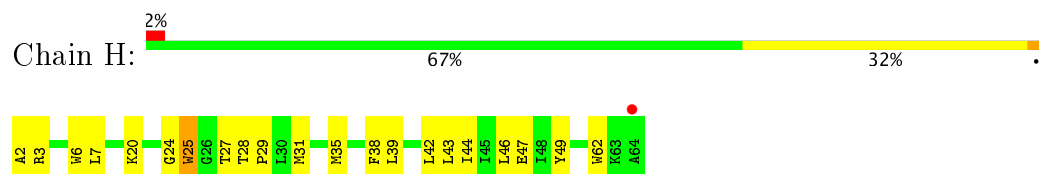
- Molecule 6: Cytochrome b559 subunit beta



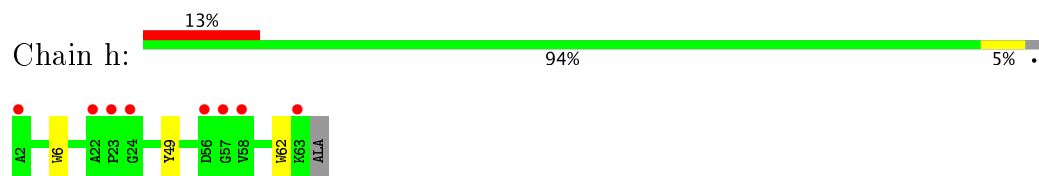
- Molecule 6: Cytochrome b559 subunit beta



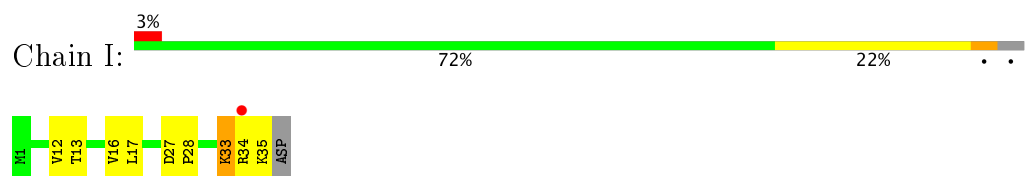
- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I

Chain i:  100%

There are no outlier residues recorded for this chain.

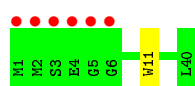
- Molecule 9: Photosystem II reaction center protein J

Chain J:  5% 70% 20% 10%



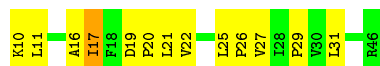
- Molecule 9: Photosystem II reaction center protein J

Chain j:  15% 98% .



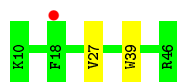
- Molecule 10: Photosystem II reaction center protein K

Chain K:  65% 32% .




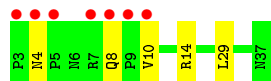
- Molecule 10: Photosystem II reaction center protein K

Chain k:  3% 95% 5%



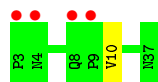
- Molecule 11: Photosystem II reaction center protein L

Chain L:  20% 86% 14%




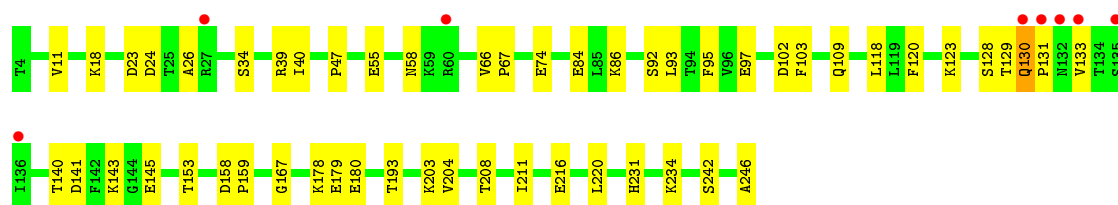
- Molecule 11: Photosystem II reaction center protein L

Chain l:  11% 97% .

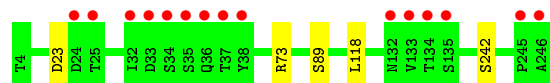


- Molecule 12: Photosystem II manganese-stabilizing polypeptide

Chain O:  3% 78% 21%



- Molecule 12: Photosystem II manganese-stabilizing polypeptide



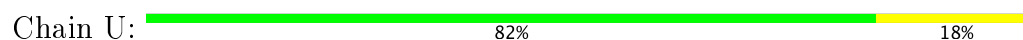
- Molecule 13: Photosystem II reaction center protein T



- Molecule 13: Photosystem II reaction center protein T



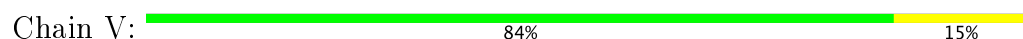
- Molecule 14: Photosystem II 12 kDa extrinsic protein



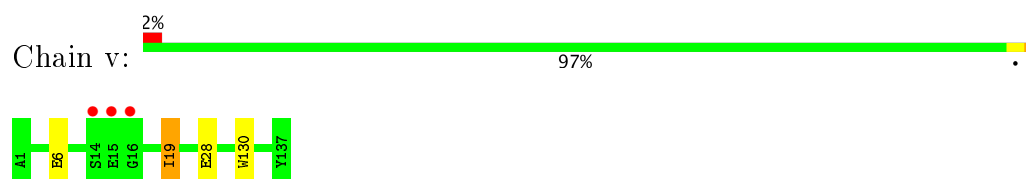
- Molecule 14: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Cytochrome c-550



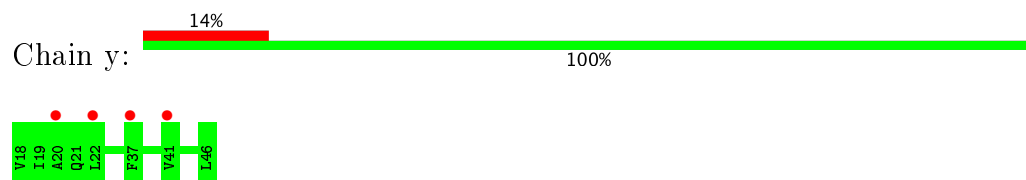
- Molecule 15: Cytochrome c-550



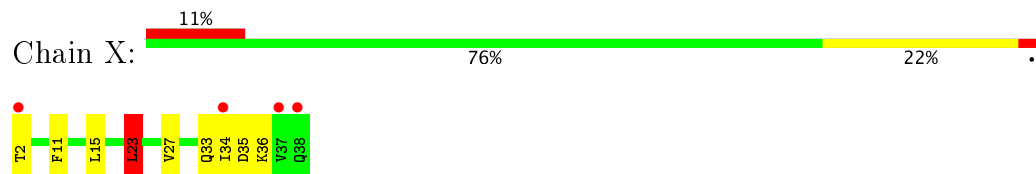
- Molecule 16: Photosystem II reaction center protein Ycf12



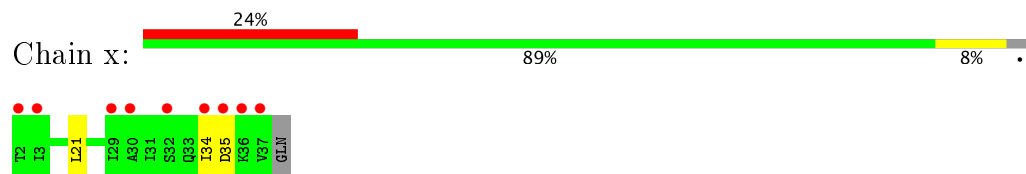
- Molecule 16: Photosystem II reaction center protein Ycf12



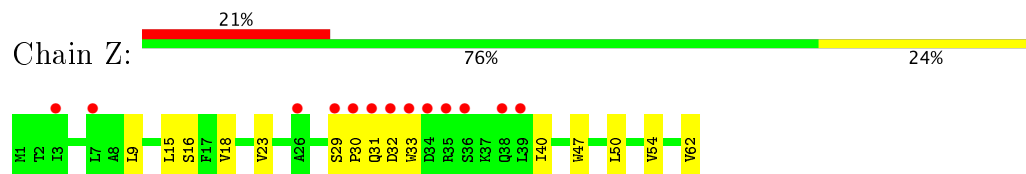
- Molecule 17: Photosystem II reaction center X protein



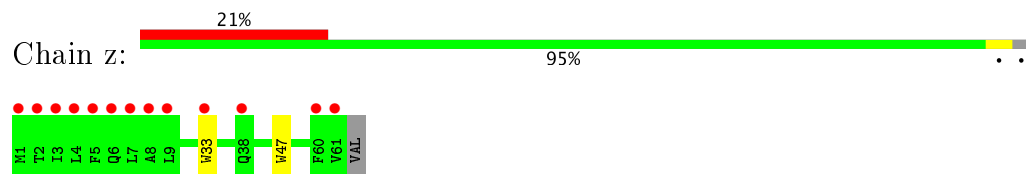
- Molecule 17: Photosystem II reaction center X protein



- Molecule 18: Photosystem II reaction center protein Z



- Molecule 18: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.95Å 226.99Å 285.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 46.79 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.00-2.20) 96.3 (46.79-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.174 , 0.226 0.174 , 0.225	Depositor DCC
R_{free} test set	19307 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	51892	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, HTG, MG, OEX, PHO, DGD, CL, CA, SQD, LMT, CLA, PL9, DMS, FE2, RRX, BCT, HEM, FME, UNL, BCR, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.86	3/2686 (0.1%)	0.76	2/3666 (0.1%)
1	a	0.87	4/2640 (0.2%)	0.77	1/3604 (0.0%)
2	B	0.87	10/4099 (0.2%)	0.77	5/5591 (0.1%)
2	b	0.85	5/3917 (0.1%)	0.78	3/5342 (0.1%)
3	C	0.85	6/3583 (0.2%)	0.76	1/4880 (0.0%)
3	c	0.83	9/3638 (0.2%)	0.76	1/4953 (0.0%)
4	D	0.91	5/2836 (0.2%)	0.77	0/3866
4	d	0.88	8/2818 (0.3%)	0.75	2/3842 (0.1%)
5	E	0.73	0/654	0.73	0/895
5	e	0.71	1/655 (0.2%)	0.72	0/896
6	F	0.83	1/278 (0.4%)	0.62	0/379
6	f	0.78	1/257 (0.4%)	0.66	0/349
7	H	0.83	3/541 (0.6%)	0.74	0/737
7	h	0.80	2/517 (0.4%)	0.68	0/704
8	I	0.67	0/285	0.67	0/385
8	i	0.63	0/290	0.64	0/392
9	J	0.80	1/257 (0.4%)	0.72	0/349
9	j	0.79	1/283 (0.4%)	0.67	0/384
10	K	0.71	0/303	0.73	0/416
10	k	0.74	1/296 (0.3%)	0.70	0/408
11	L	0.74	0/294	0.73	0/399
11	l	0.72	0/294	0.71	0/399
12	O	0.69	0/1887	0.80	0/2561
12	o	0.63	0/1864	0.78	1/2535 (0.0%)
13	T	0.79	0/252	0.72	0/342
13	t	0.74	0/252	0.69	0/342
14	U	0.76	0/796	0.82	0/1078
14	u	0.71	0/777	0.79	0/1054
15	V	0.78	0/1090	0.78	0/1480
15	v	0.69	1/1082 (0.1%)	0.75	0/1472
16	Y	0.54	0/216	0.72	0/289

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	y	0.48	0/208	0.67	0/278
17	X	0.55	0/275	0.68	1/373 (0.3%)
17	x	0.56	0/256	0.65	0/349
18	Z	0.69	1/463 (0.2%)	0.67	0/636
18	z	0.65	2/447 (0.4%)	0.62	0/614
All	All	0.81	65/41286 (0.2%)	0.76	17/56239 (0.0%)

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	387	TRP	CD2-CE2	7.25	1.50	1.41
2	B	78	TRP	CD2-CE2	6.94	1.49	1.41
1	A	317	TRP	CD2-CE2	6.86	1.49	1.41
3	c	365	TRP	CD2-CE2	6.65	1.49	1.41
1	A	278	TRP	CD2-CE2	6.57	1.49	1.41

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	57	ARG	NE-CZ-NH2	-7.02	116.79	120.30
2	b	57	ARG	NE-CZ-NH1	6.84	123.72	120.30
3	C	473	ASP	CB-CG-OD1	6.78	124.40	118.30
4	d	180	ARG	NE-CZ-NH1	-5.99	117.31	120.30
2	B	433	ASP	CB-CG-OD1	5.78	123.50	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2598	0	2484	59	0
1	a	2555	0	2420	0	0
2	B	3950	0	3776	99	0
2	b	3780	0	3636	0	0
3	C	3470	0	3380	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3521	0	3439	0	0
4	D	2732	0	2640	74	0
4	d	2717	0	2628	0	0
5	E	635	0	613	14	0
5	e	636	0	609	0	0
6	F	269	0	277	7	0
6	f	250	0	261	0	0
7	H	522	0	547	20	0
7	h	501	0	526	0	0
8	I	288	0	307	5	0
8	i	293	0	309	0	0
9	J	251	0	257	10	0
9	j	277	0	277	0	0
10	K	293	0	305	15	0
10	k	286	0	285	0	0
11	L	287	0	299	5	0
11	l	287	0	299	0	0
12	O	1853	0	1819	48	0
12	o	1833	0	1783	0	0
13	T	253	0	247	5	0
13	t	253	0	247	0	0
14	U	782	0	786	12	0
14	u	766	0	765	0	0
15	V	1066	0	1075	26	0
15	v	1058	0	1053	0	0
16	Y	215	0	246	12	0
16	y	207	0	221	0	0
17	X	269	0	297	6	0
17	x	253	0	274	0	0
18	Z	453	0	471	8	0
18	z	436	0	431	0	0
19	A	10	0	0	0	0
19	a	10	0	0	0	0
20	A	1	0	0	0	0
20	a	1	0	0	0	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	185	0	193	15	0
22	B	1014	0	1091	73	0
22	C	836	0	915	39	0
22	D	195	0	216	7	0
22	a	256	0	277	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	b	1016	0	1096	0	0
22	c	845	0	936	0	0
22	d	130	0	144	0	0
23	A	64	0	74	1	0
23	D	64	0	74	5	0
23	a	128	0	148	0	0
24	A	40	0	56	0	0
24	B	89	0	121	8	0
24	C	80	0	112	5	0
24	D	40	0	56	1	0
24	K	40	0	56	2	0
24	Y	39	0	53	4	0
24	a	40	0	56	0	0
24	b	91	0	123	0	0
24	c	80	0	112	0	0
24	d	40	0	56	0	0
24	k	40	0	56	0	0
24	y	40	0	56	0	0
25	A	51	0	72	2	0
25	B	40	0	50	3	0
25	C	91	0	122	3	0
25	D	46	0	62	5	0
25	J	45	0	60	2	0
25	b	43	0	56	0	0
25	c	100	0	140	0	0
25	d	47	0	64	0	0
25	i	51	0	72	0	0
25	j	47	0	64	0	0
26	A	55	0	80	11	0
26	D	55	0	80	5	0
26	a	55	0	80	0	0
26	d	55	0	80	0	0
27	A	31	0	36	1	0
27	C	30	0	33	1	0
27	D	143	0	211	18	0
27	L	40	0	53	7	0
27	a	94	0	137	0	0
27	d	128	0	178	0	0
27	l	49	0	74	0	0
28	A	49	0	64	2	0
28	C	54	0	78	6	0
28	D	20	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	a	105	0	147	0	0
28	b	38	0	47	0	0
28	f	14	0	8	0	0
28	l	54	0	78	0	0
29	A	35	0	46	6	0
29	B	24	0	35	3	0
29	E	24	0	35	1	0
29	I	35	0	46	0	0
29	T	24	0	35	1	0
29	Z	35	0	46	1	0
29	a	35	0	46	0	0
29	c	59	0	81	0	0
29	f	25	0	35	0	0
29	t	24	0	35	0	0
30	A	5	0	0	0	0
30	B	23	0	0	0	0
30	D	16	0	0	0	0
30	I	45	0	0	1	0
30	J	16	0	0	1	0
30	O	16	0	0	0	0
30	T	13	0	0	0	0
30	U	14	0	0	1	0
30	X	16	0	0	1	0
30	Z	9	0	0	0	0
30	a	16	0	0	0	0
30	b	27	0	0	0	0
30	c	10	0	0	0	0
30	d	16	0	0	0	0
30	i	58	0	0	0	0
30	j	16	0	0	0	0
30	t	16	0	0	0	0
30	u	11	0	0	0	0
30	x	15	0	0	0	0
31	A	20	0	30	2	0
31	B	60	0	90	15	0
31	C	60	0	90	3	0
31	D	12	0	18	0	0
31	F	4	0	6	0	0
31	H	4	0	6	0	0
31	I	8	0	12	0	0
31	L	4	0	6	0	0
31	O	48	0	72	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	U	8	0	12	1	0
31	V	40	0	60	19	0
31	a	20	0	30	0	0
31	b	36	0	54	0	0
31	c	76	0	114	0	0
31	d	20	0	30	0	0
31	f	4	0	6	0	0
31	i	4	0	6	0	0
31	l	12	0	18	0	0
31	o	28	0	42	0	0
31	t	12	0	18	0	0
31	u	16	0	24	0	0
31	v	36	0	54	0	0
32	A	8	0	0	1	0
32	a	4	0	0	0	0
33	B	1	0	0	0	0
33	O	1	0	0	0	0
33	b	1	0	0	0	0
33	c	1	0	0	0	0
33	o	1	0	0	0	0
34	B	57	0	78	4	0
34	C	47	0	67	2	0
34	D	38	0	52	10	0
34	V	14	0	13	0	0
34	b	95	0	130	0	0
34	c	19	0	26	0	0
34	l	19	0	26	0	0
34	v	16	0	17	0	0
35	C	186	0	246	3	0
35	D	50	0	69	0	0
35	H	62	0	82	4	0
35	c	186	0	246	0	0
35	d	43	0	62	0	0
35	h	62	0	82	0	0
36	E	43	0	30	1	0
36	V	43	0	30	1	0
36	e	43	0	30	0	0
36	v	43	0	30	0	0
37	H	41	0	56	12	0
37	h	41	0	56	0	0
38	J	1	0	0	0	0
38	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	j	1	0	0	0	0
38	k	1	0	0	0	0
39	A	132	0	0	1	0
39	B	262	0	0	13	0
39	C	178	0	0	3	0
39	D	131	0	0	5	0
39	E	35	0	0	1	0
39	F	4	0	0	0	0
39	H	39	0	0	1	0
39	I	5	0	0	0	0
39	J	16	0	0	0	0
39	K	7	0	0	0	0
39	L	19	0	0	0	0
39	O	166	0	0	13	0
39	T	12	0	0	0	0
39	U	74	0	0	3	0
39	V	113	0	0	5	0
39	X	16	0	0	0	0
39	Y	8	0	0	0	0
39	Z	5	0	0	1	0
39	a	123	0	0	0	0
39	b	261	0	0	0	0
39	c	220	0	0	0	0
39	d	115	0	0	0	0
39	e	17	0	0	0	0
39	f	4	0	0	0	0
39	h	31	0	0	0	0
39	i	5	0	0	0	0
39	j	10	0	0	0	0
39	k	10	0	0	0	0
39	l	15	0	0	0	0
39	o	156	0	0	0	0
39	t	10	0	0	0	0
39	u	75	0	0	0	0
39	v	82	0	0	0	0
39	x	5	0	0	0	0
39	y	1	0	0	0	0
39	z	8	0	0	0	0
All	All	51892	0	50274	587	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 8.

The worst 5 of 587 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)
22:B:608:CLA:H52	22:B:608:CLA:H92	2.73	1.10
22:B:608:CLA:H52	22:B:608:CLA:C9	3.21	1.05
2:B:125:ASP:HB3	2:B:128:THR:CG2	4.42	1.05
12:O:66:VAL:HG13	12:O:67:PRO:HD2	1.37	1.05
26:D:406:PL9:C33	27:L:101:LHG:H223	1.87	1.04

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	333/334 (100%)	326 (98%)	6 (2%)	1 (0%)	44	49
1	a	333/334 (100%)	321 (96%)	11 (3%)	1 (0%)	44	49
2	B	506/505 (100%)	495 (98%)	11 (2%)	0	100	100
2	b	482/505 (95%)	465 (96%)	17 (4%)	0	100	100
3	C	449/455 (99%)	434 (97%)	13 (3%)	2 (0%)	38	41
3	c	454/455 (100%)	435 (96%)	18 (4%)	1 (0%)	51	58
4	D	343/342 (100%)	336 (98%)	6 (2%)	1 (0%)	44	49
4	d	341/342 (100%)	333 (98%)	8 (2%)	0	100	100
5	E	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	14	11
5	e	77/80 (96%)	75 (97%)	2 (3%)	0	100	100
6	F	31/33 (94%)	31 (100%)	0	0	100	100
6	f	29/33 (88%)	29 (100%)	0	0	100	100
7	H	64/63 (102%)	60 (94%)	4 (6%)	0	100	100
7	h	61/63 (97%)	58 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	I	33/36 (92%)	31 (94%)	2 (6%)	0	100	100
8	i	34/36 (94%)	30 (88%)	4 (12%)	0	100	100
9	J	34/40 (85%)	33 (97%)	0	1 (3%)	5	2
9	j	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	33/35 (94%)	33 (100%)	0	0	100	100
11	l	33/35 (94%)	33 (100%)	0	0	100	100
12	O	242/243 (100%)	228 (94%)	12 (5%)	2 (1%)	22	21
12	o	241/243 (99%)	231 (96%)	10 (4%)	0	100	100
13	T	28/30 (93%)	28 (100%)	0	0	100	100
13	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	U	96/97 (99%)	92 (96%)	4 (4%)	0	100	100
14	u	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
15	V	136/137 (99%)	131 (96%)	5 (4%)	0	100	100
15	v	136/137 (99%)	126 (93%)	9 (7%)	1 (1%)	25	24
16	Y	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
16	y	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
17	X	36/37 (97%)	35 (97%)	1 (3%)	0	100	100
17	x	34/37 (92%)	31 (91%)	1 (3%)	2 (6%)	2	0
18	Z	60/62 (97%)	56 (93%)	1 (2%)	3 (5%)	2	1
18	z	59/62 (95%)	55 (93%)	4 (7%)	0	100	100
All	All	5100/5190 (98%)	4921 (96%)	163 (3%)	16 (0%)	44	49

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	12	ARG
3	C	24	THR
3	C	416	SER
5	E	6	GLY
18	Z	31	GLN

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	263/270 (97%)	263 (100%)	0	100	100
1	a	252/270 (93%)	250 (99%)	2 (1%)	85	92
2	B	391/403 (97%)	386 (99%)	5 (1%)	73	85
2	b	378/403 (94%)	375 (99%)	3 (1%)	85	92
3	C	347/356 (98%)	341 (98%)	6 (2%)	66	79
3	c	356/356 (100%)	350 (98%)	6 (2%)	66	79
4	D	278/277 (100%)	276 (99%)	2 (1%)	87	93
4	d	276/277 (100%)	275 (100%)	1 (0%)	93	97
5	E	68/71 (96%)	67 (98%)	1 (2%)	70	82
5	e	67/71 (94%)	64 (96%)	3 (4%)	32	39
6	F	27/27 (100%)	27 (100%)	0	100	100
6	f	25/27 (93%)	24 (96%)	1 (4%)	36	45
7	H	56/53 (106%)	55 (98%)	1 (2%)	64	77
7	h	54/53 (102%)	53 (98%)	1 (2%)	62	76
8	I	31/32 (97%)	30 (97%)	1 (3%)	44	56
8	i	31/32 (97%)	31 (100%)	0	100	100
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	25/28 (89%)	25 (100%)	0	100	100
10	K	30/30 (100%)	27 (90%)	3 (10%)	9	8
10	k	28/30 (93%)	27 (96%)	1 (4%)	40	50
11	L	33/33 (100%)	32 (97%)	1 (3%)	46	58
11	l	33/33 (100%)	32 (97%)	1 (3%)	46	58
12	O	203/206 (98%)	197 (97%)	6 (3%)	46	58
12	o	199/206 (97%)	195 (98%)	4 (2%)	60	74
13	T	24/26 (92%)	23 (96%)	1 (4%)	34	43
13	t	24/26 (92%)	22 (92%)	2 (8%)	13	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	U	85/84 (101%)	85 (100%)	0	100	100
14	u	82/84 (98%)	81 (99%)	1 (1%)	75	86
15	V	117/117 (100%)	113 (97%)	4 (3%)	42	53
15	v	115/117 (98%)	112 (97%)	3 (3%)	51	64
16	Y	22/22 (100%)	19 (86%)	3 (14%)	4	3
16	y	19/22 (86%)	19 (100%)	0	100	100
17	X	29/30 (97%)	27 (93%)	2 (7%)	18	19
17	x	27/30 (90%)	26 (96%)	1 (4%)	39	49
18	Z	45/52 (86%)	45 (100%)	0	100	100
18	z	40/52 (77%)	40 (100%)	0	100	100
All	All	4103/4234 (97%)	4037 (98%)	66 (2%)	68	81

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	V	129[A]	LYS
1	a	214	MET
13	t	28	ARG
15	V	129[B]	LYS
16	Y	43	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	315	ASN
2	b	179	GLN
15	v	34	GLN
2	b	53	ASN
2	b	281	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	9,9,10	0.90	0	7,9,11	1.33	2 (28%)
13	FME	T	1	13	9,9,10	0.89	1 (11%)	7,9,11	1.35	2 (28%)
8	FME	i	1	8	9,9,10	0.50	0	7,9,11	1.42	1 (14%)
13	FME	t	1	13	9,9,10	1.17	1 (11%)	7,9,11	1.78	2 (28%)

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
13	FME	T	1	13	-	0/6/9/11	0/0/0/0
8	FME	i	1	8	-	0/6/9/11	0/0/0/0
13	FME	t	1	13	-	0/6/9/11	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	1	FME	CA-C	2.05	1.52	1.50
13	t	1	FME	CA-C	3.10	1.54	1.50

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	O-C-CA	-2.77	118.69	125.15
8	I	1	FME	O-C-CA	-2.40	119.54	125.15
13	T	1	FME	O-C-CA	-2.20	120.02	125.15
13	t	1	FME	O-C-CA	-2.11	120.23	125.15
13	T	1	FME	CE-SD-CG	2.16	108.08	100.35

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 352 ligands modelled in this entry, 27 are unknown and 15 are monoatomic - leaving 310 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$
19	OEX	A	401	1,3,39	0,15,15	0.00	-	0,32,32	0.00	-
22	CLA	A	405	-	56,73,73	1.85	12 (21%)	65,113,113	1.90	18 (27%)
22	CLA	A	406	39	46,63,73	1.83	11 (23%)	53,101,113	2.53	23 (43%)
23	PHO	A	407	-	67,69,69	2.05	15 (22%)	87,99,99	1.93	22 (25%)
22	CLA	A	408	-	56,73,73	1.79	11 (19%)	65,113,113	1.88	14 (21%)
24	BCR	A	409	-	41,41,41	1.06	2 (4%)	56,56,56	1.25	5 (8%)
25	LMG	A	410	-	51,51,55	0.94	2 (3%)	59,59,63	1.12	5 (8%)
26	PL9	A	411	-	55,55,55	0.95	3 (5%)	69,69,69	1.67	13 (18%)
27	LHG	A	412	-	30,30,48	1.37	2 (6%)	32,35,54	1.47	4 (12%)
28	SQD	A	413	-	48,49,54	1.06	3 (6%)	58,60,65	2.06	11 (18%)
29	LMT	A	414	-	36,36,36	0.80	0	47,47,47	1.20	5 (10%)
31	DMS	A	416	-	3,3,3	2.65	1 (33%)	3,3,3	1.02	0
31	DMS	A	417	-	3,3,3	2.65	1 (33%)	3,3,3	0.46	0
31	DMS	A	418	-	3,3,3	2.40	1 (33%)	3,3,3	1.22	0
31	DMS	A	419	-	3,3,3	2.65	1 (33%)	3,3,3	0.79	0
31	DMS	A	420	-	3,3,3	2.73	1 (33%)	3,3,3	1.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	BCT	A	421[A]	20	0,3,3	0.00	-	0,3,3	0.00	-
32	BCT	A	421[B]	20	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	B	602	39	56,73,73	2.05	13 (23%)	65,113,113	1.92	14 (21%)
22	CLA	B	603	-	56,73,73	1.89	13 (23%)	65,113,113	2.16	23 (35%)
22	CLA	B	604	-	56,73,73	1.80	11 (19%)	65,113,113	2.12	20 (30%)
22	CLA	B	605	-	56,73,73	1.72	12 (21%)	65,113,113	2.09	20 (30%)
22	CLA	B	606	-	56,73,73	1.71	12 (21%)	65,113,113	1.96	17 (26%)
22	CLA	B	607	-	56,73,73	1.89	11 (19%)	65,113,113	2.25	19 (29%)
22	CLA	B	608	39	56,73,73	1.77	12 (21%)	65,113,113	1.98	20 (30%)
22	CLA	B	609	-	56,73,73	1.86	12 (21%)	65,113,113	2.17	19 (29%)
22	CLA	B	610	-	56,73,73	1.77	11 (19%)	65,113,113	1.88	15 (23%)
22	CLA	B	611	39	56,73,73	1.91	12 (21%)	65,113,113	2.09	15 (23%)
22	CLA	B	612	-	56,73,73	1.84	10 (17%)	65,113,113	1.77	16 (24%)
22	CLA	B	613	-	56,73,73	1.81	11 (19%)	65,113,113	1.72	16 (24%)
22	CLA	B	614	-	52,69,73	1.90	12 (23%)	60,108,113	1.65	15 (25%)
22	CLA	B	615	-	44,61,73	2.30	14 (31%)	50,98,113	2.34	19 (38%)
22	CLA	B	616	-	56,73,73	1.89	11 (19%)	65,113,113	1.77	16 (24%)
22	CLA	B	617	-	46,63,73	1.95	11 (23%)	53,101,113	2.56	20 (37%)
24	BCR	B	618	-	18,19,41	0.86	1 (5%)	24,26,56	1.39	4 (16%)
24	BCR	B	619	-	30,30,41	0.91	0	38,39,56	1.33	7 (18%)
24	BCR	B	620	-	41,41,41	0.95	2 (4%)	56,56,56	1.48	11 (19%)
25	LMG	B	621	-	40,40,55	1.24	3 (7%)	48,48,63	1.43	9 (18%)
29	LMT	B	622	-	24,24,36	0.63	1 (4%)	29,29,47	0.85	1 (3%)
34	HTG	B	623	-	19,19,19	1.14	1 (5%)	23,24,24	2.06	3 (13%)
34	HTG	B	626	-	19,19,19	0.71	0	23,24,24	2.04	5 (21%)
34	HTG	B	627	-	19,19,19	0.98	1 (5%)	23,24,24	2.26	4 (17%)
31	DMS	B	628	-	3,3,3	2.79	1 (33%)	3,3,3	0.76	0
31	DMS	B	629	-	3,3,3	2.53	1 (33%)	3,3,3	1.15	0
31	DMS	B	630	-	3,3,3	2.80	1 (33%)	3,3,3	0.88	0
31	DMS	B	631	-	3,3,3	2.55	1 (33%)	3,3,3	0.60	0
31	DMS	B	632	-	3,3,3	2.64	1 (33%)	3,3,3	0.58	0
31	DMS	B	633	-	3,3,3	2.65	1 (33%)	3,3,3	0.45	0
31	DMS	B	634	-	3,3,3	2.79	1 (33%)	3,3,3	0.63	0
31	DMS	B	635	-	3,3,3	2.76	1 (33%)	3,3,3	0.67	0
31	DMS	B	636	-	3,3,3	2.59	1 (33%)	3,3,3	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	B	637	-	3,3,3	2.77	1 (33%)	3,3,3	0.69	0
31	DMS	B	638	-	3,3,3	2.63	1 (33%)	3,3,3	0.38	0
31	DMS	B	639	-	3,3,3	2.75	1 (33%)	3,3,3	0.69	0
31	DMS	B	640	-	3,3,3	2.62	1 (33%)	3,3,3	0.60	0
31	DMS	B	641	-	3,3,3	2.74	1 (33%)	3,3,3	0.81	0
31	DMS	B	642	-	3,3,3	2.65	1 (33%)	3,3,3	1.03	0
28	SQD	C	501	-	53,54,54	1.02	3 (5%)	63,65,65	2.22	14 (22%)
22	CLA	C	502	-	56,73,73	1.79	12 (21%)	65,113,113	2.14	17 (26%)
22	CLA	C	503	-	56,73,73	1.84	12 (21%)	65,113,113	1.79	15 (23%)
22	CLA	C	504	-	56,73,73	2.04	13 (23%)	65,113,113	1.89	19 (29%)
22	CLA	C	505	39	56,73,73	1.86	12 (21%)	65,113,113	1.76	14 (21%)
22	CLA	C	506	-	56,73,73	1.95	12 (21%)	65,113,113	1.72	16 (24%)
22	CLA	C	507	-	56,73,73	1.89	13 (23%)	65,113,113	1.83	15 (23%)
22	CLA	C	508	39	56,73,73	1.90	12 (21%)	65,113,113	1.93	15 (23%)
22	CLA	C	509	-	56,73,73	1.88	13 (23%)	65,113,113	1.75	14 (21%)
22	CLA	C	510	-	56,73,73	1.89	10 (17%)	65,113,113	2.18	18 (27%)
22	CLA	C	511	-	56,73,73	1.95	12 (21%)	65,113,113	1.93	15 (23%)
22	CLA	C	512	3	56,73,73	1.98	12 (21%)	65,113,113	1.85	17 (26%)
22	CLA	C	513	-	47,64,73	2.14	12 (25%)	54,102,113	1.99	14 (25%)
22	CLA	C	514	-	56,73,73	2.04	13 (23%)	65,113,113	1.78	15 (23%)
24	BCR	C	515	-	41,41,41	0.79	1 (2%)	56,56,56	1.48	10 (17%)
24	BCR	C	516	-	41,41,41	0.89	0	56,56,56	1.35	8 (14%)
35	DGD	C	517	-	63,63,67	0.84	3 (4%)	77,77,81	1.37	12 (15%)
35	DGD	C	518	-	63,63,67	0.95	3 (4%)	77,77,81	1.33	11 (14%)
35	DGD	C	519	-	63,63,67	0.81	2 (3%)	77,77,81	1.24	10 (12%)
25	LMG	C	520	-	51,51,55	1.06	2 (3%)	59,59,63	1.28	5 (8%)
34	HTG	C	521	-	19,19,19	0.92	2 (10%)	23,24,24	1.91	2 (8%)
27	LHG	C	522	-	29,29,48	1.28	2 (6%)	33,34,54	1.42	4 (12%)
34	HTG	C	523	-	8,8,19	0.37	0	7,7,24	1.36	1 (14%)
31	DMS	C	524	-	3,3,3	2.47	1 (33%)	3,3,3	0.85	0
31	DMS	C	525	-	3,3,3	2.43	1 (33%)	3,3,3	0.60	0
31	DMS	C	526	-	3,3,3	2.58	1 (33%)	3,3,3	0.54	0
31	DMS	C	527	-	3,3,3	2.64	1 (33%)	3,3,3	0.55	0
31	DMS	C	528	-	3,3,3	2.62	1 (33%)	3,3,3	0.57	0
31	DMS	C	529	-	3,3,3	2.67	1 (33%)	3,3,3	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	C	530	-	3,3,3	2.66	1 (33%)	3,3,3	0.84	0
25	LMG	C	531	-	40,40,55	1.17	3 (7%)	48,48,63	1.18	4 (8%)
34	HTG	C	532	-	19,19,19	1.13	2 (10%)	23,24,24	2.31	1 (4%)
31	DMS	C	533	-	3,3,3	2.72	1 (33%)	3,3,3	0.72	0
31	DMS	C	534	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
31	DMS	C	535	-	3,3,3	2.72	1 (33%)	3,3,3	0.76	0
31	DMS	C	536	-	3,3,3	2.67	1 (33%)	3,3,3	0.44	0
31	DMS	C	537	-	3,3,3	2.74	1 (33%)	3,3,3	0.68	0
31	DMS	C	538	-	3,3,3	2.65	1 (33%)	3,3,3	0.57	0
31	DMS	C	539	-	3,3,3	2.68	1 (33%)	3,3,3	0.60	0
31	DMS	C	540	-	3,3,3	2.77	1 (33%)	3,3,3	0.86	0
22	CLA	D	401	39	56,73,73	1.74	10 (17%)	65,113,113	2.28	19 (29%)
23	PHO	D	402	-	67,69,69	2.07	16 (23%)	87,99,99	2.03	20 (22%)
22	CLA	D	403	-	56,73,73	1.61	13 (23%)	65,113,113	2.46	22 (33%)
22	CLA	D	404	-	56,73,73	1.95	12 (21%)	65,113,113	1.70	15 (23%)
24	BCR	D	405	-	41,41,41	0.98	1 (2%)	56,56,56	1.97	15 (26%)
26	PL9	D	406	-	55,55,55	0.91	3 (5%)	69,69,69	1.52	15 (21%)
35	DGD	D	407	-	50,50,67	1.17	3 (6%)	58,58,81	1.35	6 (10%)
28	SQD	D	408	-	19,20,54	0.94	2 (10%)	27,29,65	2.09	8 (29%)
27	LHG	D	409	-	48,48,48	1.01	2 (4%)	49,54,54	1.42	5 (10%)
27	LHG	D	410	-	48,48,48	0.78	2 (4%)	49,54,54	1.13	5 (10%)
27	LHG	D	411	-	44,44,48	0.96	2 (4%)	45,50,54	1.09	3 (6%)
25	LMG	D	412	-	46,46,55	1.12	3 (6%)	54,54,63	1.16	2 (3%)
34	HTG	D	414	-	19,19,19	0.85	1 (5%)	23,24,24	2.23	1 (4%)
34	HTG	D	415	-	19,19,19	1.15	1 (5%)	23,24,24	2.88	8 (34%)
31	DMS	D	416	-	3,3,3	2.49	1 (33%)	3,3,3	0.62	0
31	DMS	D	417	-	3,3,3	2.74	1 (33%)	3,3,3	0.58	0
31	DMS	D	418	-	3,3,3	2.39	1 (33%)	3,3,3	0.65	0
29	LMT	E	101	-	24,24,36	0.63	0	29,29,47	1.01	1 (3%)
36	HEM	E	102	5,6	28,50,50	2.14	7 (25%)	17,82,82	2.67	7 (41%)
31	DMS	F	101	-	3,3,3	2.65	1 (33%)	3,3,3	0.59	0
37	RRX	H	101	-	42,42,42	0.80	0	56,58,58	1.49	8 (14%)
35	DGD	H	102	-	63,63,67	1.01	3 (4%)	77,77,81	1.19	6 (7%)
31	DMS	H	103	-	3,3,3	2.90	1 (33%)	3,3,3	1.15	0
31	DMS	I	101	-	3,3,3	2.70	1 (33%)	3,3,3	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMT	I	102	-	36,36,36	0.68	1 (2%)	47,47,47	1.46	5 (10%)
31	DMS	I	106	-	3,3,3	2.67	1 (33%)	3,3,3	0.73	0
25	LMG	J	101	38	45,45,55	0.97	2 (4%)	53,53,63	1.07	6 (11%)
24	BCR	K	101	-	41,41,41	0.84	0	56,56,56	1.19	4 (7%)
27	LHG	L	101	-	39,39,48	1.03	2 (5%)	40,45,54	1.25	5 (12%)
31	DMS	L	102	-	3,3,3	2.73	1 (33%)	3,3,3	0.93	0
31	DMS	O	303	-	3,3,3	2.73	1 (33%)	3,3,3	0.74	0
31	DMS	O	304	-	3,3,3	2.56	1 (33%)	3,3,3	0.41	0
31	DMS	O	305	-	3,3,3	2.88	1 (33%)	3,3,3	0.82	0
31	DMS	O	306	-	3,3,3	2.69	1 (33%)	3,3,3	0.73	0
31	DMS	O	307	-	3,3,3	2.78	1 (33%)	3,3,3	0.90	0
31	DMS	O	308	-	3,3,3	2.77	1 (33%)	3,3,3	0.61	0
31	DMS	O	309	-	3,3,3	2.52	1 (33%)	3,3,3	0.57	0
31	DMS	O	310	-	3,3,3	2.61	1 (33%)	3,3,3	0.84	0
31	DMS	O	311	-	3,3,3	2.96	1 (33%)	3,3,3	0.89	0
31	DMS	O	312	-	3,3,3	2.61	1 (33%)	3,3,3	0.93	0
31	DMS	O	313	-	3,3,3	2.61	1 (33%)	3,3,3	0.46	0
31	DMS	O	314	-	3,3,3	2.72	1 (33%)	3,3,3	0.74	0
29	LMT	T	102	-	24,24,36	0.72	1 (4%)	29,29,47	1.34	3 (10%)
31	DMS	U	202	-	3,3,3	2.76	1 (33%)	3,3,3	1.26	0
31	DMS	U	203	-	3,3,3	2.76	1 (33%)	3,3,3	1.23	0
31	DMS	V	201	-	3,3,3	2.62	1 (33%)	3,3,3	0.87	0
36	HEM	V	202	15	28,50,50	2.28	8 (28%)	17,82,82	1.80	4 (23%)
34	HTG	V	203	-	14,14,19	0.67	0	18,19,24	3.13	7 (38%)
31	DMS	V	204	-	3,3,3	2.72	1 (33%)	3,3,3	0.79	0
31	DMS	V	205	-	3,3,3	2.61	1 (33%)	3,3,3	0.63	0
31	DMS	V	206	-	3,3,3	2.69	1 (33%)	3,3,3	0.55	0
31	DMS	V	207	-	3,3,3	2.74	1 (33%)	3,3,3	0.87	0
31	DMS	V	208	-	3,3,3	2.58	1 (33%)	3,3,3	0.39	0
31	DMS	V	209	-	3,3,3	2.63	1 (33%)	3,3,3	0.47	0
31	DMS	V	210	-	3,3,3	2.76	1 (33%)	3,3,3	0.87	0
31	DMS	V	211	-	3,3,3	2.80	1 (33%)	3,3,3	0.76	0
31	DMS	V	212	-	3,3,3	2.77	1 (33%)	3,3,3	1.15	0
24	BCR	Y	101	-	39,40,41	0.86	1 (2%)	51,54,56	1.70	16 (31%)
29	LMT	Z	101	-	36,36,36	0.67	1 (2%)	47,47,47	1.20	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	a	401	-	3,3,3	2.73	1 (33%)	3,3,3	0.78	0
31	DMS	a	402	-	3,3,3	2.37	1 (33%)	3,3,3	0.71	0
19	OEX	a	403	1,3,39	0,15,15	0.00	-	0,32,32	0.00	-
22	CLA	a	407	-	56,73,73	1.88	11 (19%)	65,113,113	1.89	20 (30%)
22	CLA	a	408	39	56,73,73	1.86	10 (17%)	65,113,113	2.01	17 (26%)
22	CLA	a	409	39	52,69,73	1.79	12 (23%)	60,108,113	2.49	21 (35%)
23	PHO	a	410	-	67,69,69	1.93	16 (23%)	87,99,99	1.90	22 (25%)
23	PHO	a	411	-	67,69,69	2.01	15 (22%)	87,99,99	2.20	22 (25%)
22	CLA	a	412	-	56,73,73	1.80	10 (17%)	65,113,113	2.18	20 (30%)
24	BCR	a	413	-	41,41,41	1.12	2 (4%)	56,56,56	1.14	6 (10%)
28	SQD	a	414	-	53,54,54	1.06	3 (5%)	63,65,65	2.26	13 (20%)
26	PL9	a	415	-	55,55,55	0.93	3 (5%)	69,69,69	1.46	9 (13%)
27	LHG	a	416	-	48,48,48	1.12	2 (4%)	49,54,54	1.23	4 (8%)
28	SQD	a	418	-	50,51,54	1.14	3 (6%)	60,62,65	1.65	10 (16%)
29	LMT	a	419	-	36,36,36	0.78	0	47,47,47	1.44	8 (17%)
31	DMS	a	421	-	3,3,3	2.64	1 (33%)	3,3,3	0.59	0
32	BCT	a	422	20	0,3,3	0.00	-	0,3,3	0.00	-
27	LHG	a	423	-	44,44,48	1.00	2 (4%)	45,50,54	1.14	4 (8%)
31	DMS	a	424	-	3,3,3	2.70	1 (33%)	3,3,3	0.99	0
31	DMS	a	425	-	3,3,3	3.00	1 (33%)	3,3,3	0.87	0
22	CLA	b	602	39	56,73,73	2.18	12 (21%)	65,113,113	1.97	17 (26%)
22	CLA	b	603	-	56,73,73	1.91	11 (19%)	65,113,113	2.00	18 (27%)
22	CLA	b	604	-	56,73,73	1.72	12 (21%)	65,113,113	2.32	20 (30%)
22	CLA	b	605	-	56,73,73	1.70	12 (21%)	65,113,113	1.91	16 (24%)
22	CLA	b	606	-	56,73,73	1.61	9 (16%)	65,113,113	2.09	16 (24%)
22	CLA	b	607	-	56,73,73	1.75	12 (21%)	65,113,113	2.18	17 (26%)
22	CLA	b	608	39	56,73,73	1.86	11 (19%)	65,113,113	1.78	14 (21%)
22	CLA	b	609	-	56,73,73	1.81	10 (17%)	65,113,113	1.91	17 (26%)
22	CLA	b	610	-	56,73,73	1.91	12 (21%)	65,113,113	1.85	16 (24%)
22	CLA	b	611	39	56,73,73	1.89	12 (21%)	65,113,113	2.10	17 (26%)
22	CLA	b	612	-	56,73,73	1.70	9 (16%)	65,113,113	1.83	14 (21%)
22	CLA	b	613	-	56,73,73	1.95	13 (23%)	65,113,113	2.10	21 (32%)
22	CLA	b	614	-	50,67,73	1.92	13 (26%)	57,105,113	2.00	15 (26%)
22	CLA	b	615	-	43,60,73	2.24	13 (30%)	49,97,113	2.12	18 (36%)
22	CLA	b	616	-	56,73,73	2.03	12 (21%)	65,113,113	1.81	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	b	617	-	51,68,73	2.10	11 (21%)	59,107,113	2.19	19 (32%)
24	BCR	b	618	-	19,20,41	0.68	0	27,27,56	1.73	5 (18%)
24	BCR	b	619	-	31,31,41	1.08	2 (6%)	40,40,56	1.32	7 (17%)
24	BCR	b	620	-	41,41,41	0.84	0	56,56,56	1.34	8 (14%)
28	SQD	b	621	-	37,38,54	1.03	2 (5%)	46,48,65	1.72	10 (21%)
25	LMG	b	622	-	43,43,55	1.34	4 (9%)	51,51,63	1.92	12 (23%)
34	HTG	b	623	-	19,19,19	1.08	1 (5%)	23,24,24	1.30	4 (17%)
34	HTG	b	624	-	19,19,19	1.03	1 (5%)	23,24,24	2.45	6 (26%)
34	HTG	b	626	-	19,19,19	0.82	1 (5%)	23,24,24	1.81	4 (17%)
34	HTG	b	627	-	19,19,19	1.00	1 (5%)	23,24,24	2.13	3 (13%)
31	DMS	b	629	-	3,3,3	2.27	1 (33%)	3,3,3	1.07	0
31	DMS	b	630	-	3,3,3	2.65	1 (33%)	3,3,3	0.29	0
31	DMS	b	631	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
34	HTG	b	632	-	19,19,19	1.05	2 (10%)	23,24,24	2.79	7 (30%)
31	DMS	b	633	-	3,3,3	2.65	1 (33%)	3,3,3	0.54	0
31	DMS	b	634	-	3,3,3	2.70	1 (33%)	3,3,3	0.57	0
31	DMS	b	635	-	3,3,3	2.74	1 (33%)	3,3,3	0.54	0
31	DMS	b	636	-	3,3,3	2.66	1 (33%)	3,3,3	0.68	0
31	DMS	b	637	-	3,3,3	2.70	1 (33%)	3,3,3	0.60	0
31	DMS	b	638	-	3,3,3	2.96	1 (33%)	3,3,3	0.67	0
22	CLA	c	902	-	56,73,73	1.84	12 (21%)	65,113,113	1.82	13 (20%)
22	CLA	c	903	-	56,73,73	1.76	11 (19%)	65,113,113	2.06	20 (30%)
22	CLA	c	904	-	56,73,73	1.92	12 (21%)	65,113,113	1.88	18 (27%)
22	CLA	c	905	39	56,73,73	1.82	11 (19%)	65,113,113	1.75	13 (20%)
22	CLA	c	906	-	56,73,73	1.98	13 (23%)	65,113,113	1.82	16 (24%)
22	CLA	c	907	-	56,73,73	1.85	11 (19%)	65,113,113	1.91	15 (23%)
22	CLA	c	908	39	56,73,73	2.09	12 (21%)	65,113,113	1.92	12 (18%)
22	CLA	c	909	-	56,73,73	2.07	15 (26%)	65,113,113	1.78	16 (24%)
22	CLA	c	910	-	56,73,73	1.98	12 (21%)	65,113,113	2.04	20 (30%)
22	CLA	c	911	-	56,73,73	1.86	11 (19%)	65,113,113	1.81	17 (26%)
22	CLA	c	912	3	56,73,73	1.97	13 (23%)	65,113,113	1.59	13 (20%)
22	CLA	c	913	-	56,73,73	1.98	12 (21%)	65,113,113	1.85	17 (26%)
22	CLA	c	914	-	56,73,73	1.94	12 (21%)	65,113,113	1.88	18 (27%)
24	BCR	c	915	-	41,41,41	0.83	1 (2%)	56,56,56	1.39	7 (12%)
24	BCR	c	916	-	41,41,41	0.84	0	56,56,56	1.54	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	DGD	c	917	-	63,63,67	0.96	3 (4%)	77,77,81	1.04	4 (5%)
35	DGD	c	918	-	63,63,67	0.93	4 (6%)	77,77,81	1.06	5 (6%)
35	DGD	c	919	-	63,63,67	0.97	3 (4%)	77,77,81	1.19	6 (7%)
25	LMG	c	920	-	51,51,55	0.98	2 (3%)	59,59,63	1.14	6 (10%)
29	LMT	c	921	-	36,36,36	0.67	1 (2%)	47,47,47	1.08	4 (8%)
34	HTG	c	922	-	19,19,19	0.82	1 (5%)	23,24,24	1.96	2 (8%)
31	DMS	c	923	-	3,3,3	2.49	1 (33%)	3,3,3	0.39	0
31	DMS	c	924	-	3,3,3	2.80	1 (33%)	3,3,3	1.28	1 (33%)
31	DMS	c	925	-	3,3,3	2.64	1 (33%)	3,3,3	1.07	0
31	DMS	c	926	-	3,3,3	2.59	1 (33%)	3,3,3	0.76	0
31	DMS	c	927	-	3,3,3	2.63	1 (33%)	3,3,3	0.41	0
31	DMS	c	928	-	3,3,3	2.68	1 (33%)	3,3,3	0.75	0
31	DMS	c	929	-	3,3,3	2.79	1 (33%)	3,3,3	0.82	0
25	LMG	c	930	-	49,49,55	1.09	3 (6%)	57,57,63	1.10	4 (7%)
29	LMT	c	931	-	24,24,36	0.78	1 (4%)	29,29,47	0.88	2 (6%)
31	DMS	c	933	-	3,3,3	2.82	1 (33%)	3,3,3	0.89	0
31	DMS	c	934	-	3,3,3	2.65	1 (33%)	3,3,3	0.66	0
31	DMS	c	935	-	3,3,3	2.65	1 (33%)	3,3,3	0.86	0
31	DMS	c	936	-	3,3,3	2.68	1 (33%)	3,3,3	0.57	0
31	DMS	c	937	-	3,3,3	2.86	1 (33%)	3,3,3	0.80	0
31	DMS	c	938	-	3,3,3	2.75	1 (33%)	3,3,3	0.81	0
31	DMS	c	939	-	3,3,3	2.75	1 (33%)	3,3,3	0.63	0
31	DMS	c	940	-	3,3,3	2.71	1 (33%)	3,3,3	0.56	0
31	DMS	c	941	-	3,3,3	2.59	1 (33%)	3,3,3	0.51	0
31	DMS	c	942	-	3,3,3	2.72	1 (33%)	3,3,3	0.70	0
31	DMS	c	943	-	3,3,3	2.68	1 (33%)	3,3,3	0.78	0
31	DMS	c	944	-	3,3,3	2.71	1 (33%)	3,3,3	0.76	0
27	LHG	d	401	-	32,32,48	1.22	2 (6%)	36,37,54	1.22	4 (11%)
22	CLA	d	402	-	56,73,73	1.83	12 (21%)	65,113,113	1.99	15 (23%)
22	CLA	d	403	-	56,73,73	2.14	13 (23%)	65,113,113	1.71	12 (18%)
24	BCR	d	404	-	41,41,41	1.03	3 (7%)	56,56,56	1.77	13 (23%)
26	PL9	d	405	-	55,55,55	1.00	4 (7%)	69,69,69	1.43	8 (11%)
35	DGD	d	406	-	42,42,67	1.23	3 (7%)	44,45,81	1.12	3 (6%)
27	LHG	d	407	-	48,48,48	0.74	2 (4%)	49,54,54	1.10	3 (6%)
27	LHG	d	408	-	45,45,48	1.02	2 (4%)	46,51,54	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LMG	d	409	-	47,47,55	1.08	3 (6%)	55,55,63	1.50	9 (16%)
31	DMS	d	411	-	3,3,3	2.70	1 (33%)	3,3,3	0.91	0
31	DMS	d	412	-	3,3,3	2.55	1 (33%)	3,3,3	0.81	0
31	DMS	d	413	-	3,3,3	2.53	1 (33%)	3,3,3	0.38	0
31	DMS	d	414	-	3,3,3	2.68	1 (33%)	3,3,3	0.56	0
31	DMS	d	415	-	3,3,3	2.61	1 (33%)	3,3,3	0.60	0
36	HEM	e	101	5,6	28,50,50	2.21	12 (42%)	17,82,82	2.17	4 (23%)
28	SQD	f	101	-	13,13,54	2.04	1 (7%)	15,16,65	1.64	3 (20%)
29	LMT	f	102	-	25,25,36	1.00	1 (4%)	30,30,47	1.27	6 (20%)
31	DMS	f	103	-	3,3,3	2.69	1 (33%)	3,3,3	0.88	0
37	RRX	h	101	-	42,42,42	0.95	0	56,58,58	1.19	5 (8%)
35	DGD	h	102	-	63,63,67	0.96	2 (3%)	77,77,81	1.18	6 (7%)
25	LMG	i	101	-	51,51,55	0.97	2 (3%)	59,59,63	1.21	7 (11%)
31	DMS	i	106	-	3,3,3	2.61	1 (33%)	3,3,3	0.55	0
25	LMG	j	101	38	47,47,55	1.00	2 (4%)	55,55,63	1.23	9 (16%)
24	BCR	k	101	-	41,41,41	0.89	0	56,56,56	1.23	6 (10%)
28	SQD	l	101	-	53,54,54	1.11	4 (7%)	63,65,65	1.65	9 (14%)
27	LHG	l	102	-	48,48,48	0.92	2 (4%)	49,54,54	1.13	3 (6%)
31	DMS	l	103	-	3,3,3	2.69	1 (33%)	3,3,3	0.64	0
31	DMS	l	104	-	3,3,3	2.75	1 (33%)	3,3,3	0.56	0
31	DMS	l	105	-	3,3,3	2.73	1 (33%)	3,3,3	0.70	0
34	HTG	l	106	-	19,19,19	0.99	2 (10%)	23,24,24	2.46	3 (13%)
31	DMS	o	302	-	3,3,3	2.66	1 (33%)	3,3,3	0.94	0
31	DMS	o	303	-	3,3,3	2.68	1 (33%)	3,3,3	0.79	0
31	DMS	o	304	-	3,3,3	2.80	1 (33%)	3,3,3	1.11	0
31	DMS	o	305	-	3,3,3	2.59	1 (33%)	3,3,3	0.64	0
31	DMS	o	306	-	3,3,3	2.63	1 (33%)	3,3,3	0.58	0
31	DMS	o	307	-	3,3,3	2.59	1 (33%)	3,3,3	0.56	0
31	DMS	o	308	-	3,3,3	2.77	1 (33%)	3,3,3	0.81	0
29	LMT	t	101	-	24,24,36	0.45	0	29,29,47	1.38	3 (10%)
31	DMS	t	103	-	3,3,3	2.69	1 (33%)	3,3,3	0.62	0
31	DMS	t	104	-	3,3,3	2.70	1 (33%)	3,3,3	0.58	0
31	DMS	t	105	-	3,3,3	2.69	1 (33%)	3,3,3	0.60	0
31	DMS	u	202	-	3,3,3	2.60	1 (33%)	3,3,3	1.02	0
31	DMS	u	203	-	3,3,3	2.71	1 (33%)	3,3,3	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	u	204	-	3,3,3	2.78	1 (33%)	3,3,3	0.79	0
31	DMS	u	205	-	3,3,3	3.05	1 (33%)	3,3,3	1.16	0
31	DMS	v	201	-	3,3,3	2.57	1 (33%)	3,3,3	0.83	0
36	HEM	v	202	15	28,50,50	2.38	10 (35%)	17,82,82	1.82	4 (23%)
34	HTG	v	203	-	16,16,19	1.03	1 (6%)	20,21,24	3.20	7 (35%)
31	DMS	v	204	-	3,3,3	2.65	1 (33%)	3,3,3	0.67	0
31	DMS	v	205	-	3,3,3	2.64	1 (33%)	3,3,3	0.81	0
31	DMS	v	206	-	3,3,3	2.67	1 (33%)	3,3,3	0.71	0
31	DMS	v	207	-	3,3,3	2.70	1 (33%)	3,3,3	0.63	0
31	DMS	v	208	-	3,3,3	2.62	1 (33%)	3,3,3	0.52	0
31	DMS	v	209	-	3,3,3	2.62	1 (33%)	3,3,3	0.61	0
31	DMS	v	210	-	3,3,3	2.82	1 (33%)	3,3,3	0.76	0
31	DMS	v	211	-	3,3,3	2.74	1 (33%)	3,3,3	0.74	0
24	BCR	y	101	-	41,41,41	0.88	0	56,56,56	1.59	14 (25%)

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
19	OEX	A	401	1,3,39	-	0/0/68/68	0/0/6/6
22	CLA	A	405	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	A	406	39	2/2/18/25	0/25/123/135	0/0/9/9
23	PHO	A	407	-	-	0/53/103/103	0/1/6/6
22	CLA	A	408	-	2/2/20/25	0/37/135/135	0/0/9/9
24	BCR	A	409	-	-	0/29/63/63	0/2/2/2
25	LMG	A	410	-	-	0/46/66/70	0/1/1/1
26	PL9	A	411	-	-	0/53/73/73	0/1/1/1
27	LHG	A	412	-	-	0/33/33/53	0/0/0/0
28	SQD	A	413	-	-	0/44/64/69	0/1/1/1
29	LMT	A	414	-	-	0/21/61/61	0/2/2/2
31	DMS	A	416	-	-	0/0/0/0	0/0/0/0
31	DMS	A	417	-	-	0/0/0/0	0/0/0/0
31	DMS	A	418	-	-	0/0/0/0	0/0/0/0
31	DMS	A	419	-	-	0/0/0/0	0/0/0/0
31	DMS	A	420	-	-	0/0/0/0	0/0/0/0
32	BCT	A	421[A]	20	-	0/0/0/0	0/0/0/0
32	BCT	A	421[B]	20	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	602	39	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	606	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	B	607	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	608	39	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	609	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	B	610	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	611	39	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	614	-	3/3/19/25	0/33/131/135	0/0/9/9
22	CLA	B	615	-	3/3/17/25	0/23/121/135	0/0/9/9
22	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	617	-	3/3/18/25	0/25/123/135	0/0/9/9
24	BCR	B	618	-	-	0/11/28/63	0/1/1/2
24	BCR	B	619	-	-	0/24/41/63	0/1/1/2
24	BCR	B	620	-	-	0/29/63/63	0/2/2/2
25	LMG	B	621	-	-	0/35/55/70	0/1/1/1
29	LMT	B	622	-	-	0/15/35/61	0/1/1/2
34	HTG	B	623	-	-	0/10/30/30	0/1/1/1
34	HTG	B	626	-	-	0/10/30/30	0/1/1/1
34	HTG	B	627	-	-	0/10/30/30	0/1/1/1
31	DMS	B	628	-	-	0/0/0/0	0/0/0/0
31	DMS	B	629	-	-	0/0/0/0	0/0/0/0
31	DMS	B	630	-	-	0/0/0/0	0/0/0/0
31	DMS	B	631	-	-	0/0/0/0	0/0/0/0
31	DMS	B	632	-	-	0/0/0/0	0/0/0/0
31	DMS	B	633	-	-	0/0/0/0	0/0/0/0
31	DMS	B	634	-	-	0/0/0/0	0/0/0/0
31	DMS	B	635	-	-	0/0/0/0	0/0/0/0
31	DMS	B	636	-	-	0/0/0/0	0/0/0/0
31	DMS	B	637	-	-	0/0/0/0	0/0/0/0
31	DMS	B	638	-	-	0/0/0/0	0/0/0/0
31	DMS	B	639	-	-	0/0/0/0	0/0/0/0
31	DMS	B	640	-	-	0/0/0/0	0/0/0/0
31	DMS	B	641	-	-	0/0/0/0	0/0/0/0
31	DMS	B	642	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SQD	C	501	-	-	0/49/69/69	0/1/1/1
22	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	504	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	C	505	39	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	C	506	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	508	39	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	511	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	512	3	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	C	513	-	3/3/18/25	0/27/125/135	0/0/9/9
22	CLA	C	514	-	2/2/20/25	0/37/135/135	0/0/9/9
24	BCR	C	515	-	-	0/29/63/63	0/2/2/2
24	BCR	C	516	-	-	0/29/63/63	0/2/2/2
35	DGD	C	517	-	-	0/51/91/95	0/2/2/2
35	DGD	C	518	-	-	0/51/91/95	0/2/2/2
35	DGD	C	519	-	-	0/51/91/95	0/2/2/2
25	LMG	C	520	-	-	0/46/66/70	0/1/1/1
34	HTG	C	521	-	-	0/10/30/30	0/1/1/1
27	LHG	C	522	-	-	0/31/31/53	0/0/0/0
34	HTG	C	523	-	-	0/6/6/30	0/0/0/1
31	DMS	C	524	-	-	0/0/0/0	0/0/0/0
31	DMS	C	525	-	-	0/0/0/0	0/0/0/0
31	DMS	C	526	-	-	0/0/0/0	0/0/0/0
31	DMS	C	527	-	-	0/0/0/0	0/0/0/0
31	DMS	C	528	-	-	0/0/0/0	0/0/0/0
31	DMS	C	529	-	-	0/0/0/0	0/0/0/0
31	DMS	C	530	-	-	0/0/0/0	0/0/0/0
25	LMG	C	531	-	-	0/35/55/70	0/1/1/1
34	HTG	C	532	-	-	1/10/30/30	0/1/1/1
31	DMS	C	533	-	-	0/0/0/0	0/0/0/0
31	DMS	C	534	-	-	0/0/0/0	0/0/0/0
31	DMS	C	535	-	-	0/0/0/0	0/0/0/0
31	DMS	C	536	-	-	0/0/0/0	0/0/0/0
31	DMS	C	537	-	-	0/0/0/0	0/0/0/0
31	DMS	C	538	-	-	0/0/0/0	0/0/0/0
31	DMS	C	539	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DMS	C	540	-	-	0/0/0/0	0/0/0/0
22	CLA	D	401	39	1/1/20/25	0/37/135/135	0/0/9/9
23	PHO	D	402	-	-	0/53/103/103	0/1/6/6
22	CLA	D	403	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	D	404	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	D	405	-	-	0/29/63/63	0/2/2/2
26	PL9	D	406	-	-	0/53/73/73	0/1/1/1
35	DGD	D	407	-	-	0/44/64/95	0/1/1/2
28	SQD	D	408	-	-	0/12/32/69	0/1/1/1
27	LHG	D	409	-	-	0/53/53/53	0/0/0/0
27	LHG	D	410	-	-	0/53/53/53	0/0/0/0
27	LHG	D	411	-	-	0/49/49/53	0/0/0/0
25	LMG	D	412	-	-	0/41/61/70	0/1/1/1
34	HTG	D	414	-	-	0/10/30/30	0/1/1/1
34	HTG	D	415	-	-	0/10/30/30	0/1/1/1
31	DMS	D	416	-	-	0/0/0/0	0/0/0/0
31	DMS	D	417	-	-	0/0/0/0	0/0/0/0
31	DMS	D	418	-	-	0/0/0/0	0/0/0/0
29	LMT	E	101	-	-	0/15/35/61	0/1/1/2
36	HEM	E	102	5,6	-	0/6/54/54	0/0/8/8
31	DMS	F	101	-	-	0/0/0/0	0/0/0/0
37	RRX	H	101	-	-	0/29/65/65	0/2/2/2
35	DGD	H	102	-	-	0/51/91/95	0/2/2/2
31	DMS	H	103	-	-	0/0/0/0	0/0/0/0
31	DMS	I	101	-	-	0/0/0/0	0/0/0/0
29	LMT	I	102	-	-	0/21/61/61	0/2/2/2
31	DMS	I	106	-	-	0/0/0/0	0/0/0/0
25	LMG	J	101	38	-	0/40/60/70	0/1/1/1
24	BCR	K	101	-	-	0/29/63/63	0/2/2/2
27	LHG	L	101	-	-	0/44/44/53	0/0/0/0
31	DMS	L	102	-	-	0/0/0/0	0/0/0/0
31	DMS	O	303	-	-	0/0/0/0	0/0/0/0
31	DMS	O	304	-	-	0/0/0/0	0/0/0/0
31	DMS	O	305	-	-	0/0/0/0	0/0/0/0
31	DMS	O	306	-	-	0/0/0/0	0/0/0/0
31	DMS	O	307	-	-	0/0/0/0	0/0/0/0
31	DMS	O	308	-	-	0/0/0/0	0/0/0/0
31	DMS	O	309	-	-	0/0/0/0	0/0/0/0
31	DMS	O	310	-	-	0/0/0/0	0/0/0/0
31	DMS	O	311	-	-	0/0/0/0	0/0/0/0
31	DMS	O	312	-	-	0/0/0/0	0/0/0/0
31	DMS	O	313	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DMS	O	314	-	-	0/0/0/0	0/0/0/0
29	LMT	T	102	-	-	0/15/35/61	0/1/1/2
31	DMS	U	202	-	-	0/0/0/0	0/0/0/0
31	DMS	U	203	-	-	0/0/0/0	0/0/0/0
31	DMS	V	201	-	-	0/0/0/0	0/0/0/0
36	HEM	V	202	15	-	0/6/54/54	0/0/8/8
34	HTG	V	203	-	-	0/5/25/30	0/1/1/1
31	DMS	V	204	-	-	0/0/0/0	0/0/0/0
31	DMS	V	205	-	-	0/0/0/0	0/0/0/0
31	DMS	V	206	-	-	0/0/0/0	0/0/0/0
31	DMS	V	207	-	-	0/0/0/0	0/0/0/0
31	DMS	V	208	-	-	0/0/0/0	0/0/0/0
31	DMS	V	209	-	-	0/0/0/0	0/0/0/0
31	DMS	V	210	-	-	0/0/0/0	0/0/0/0
31	DMS	V	211	-	-	0/0/0/0	0/0/0/0
31	DMS	V	212	-	-	0/0/0/0	0/0/0/0
24	BCR	Y	101	-	-	0/29/60/63	0/2/2/2
29	LMT	Z	101	-	-	0/21/61/61	0/2/2/2
31	DMS	a	401	-	-	0/0/0/0	0/0/0/0
31	DMS	a	402	-	-	0/0/0/0	0/0/0/0
19	OEX	a	403	1,3,39	-	0/0/68/68	0/0/6/6
22	CLA	a	407	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	a	408	39	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	a	409	39	2/2/19/25	0/33/131/135	0/0/9/9
23	PHO	a	410	-	-	0/53/103/103	0/1/6/6
23	PHO	a	411	-	-	0/53/103/103	0/1/6/6
22	CLA	a	412	-	-	0/37/135/135	0/0/9/9
24	BCR	a	413	-	-	0/29/63/63	0/2/2/2
28	SQD	a	414	-	-	0/49/69/69	0/1/1/1
26	PL9	a	415	-	-	0/53/73/73	0/1/1/1
27	LHG	a	416	-	-	0/53/53/53	0/0/0/0
28	SQD	a	418	-	-	0/46/66/69	0/1/1/1
29	LMT	a	419	-	-	0/21/61/61	0/2/2/2
31	DMS	a	421	-	-	0/0/0/0	0/0/0/0
32	BCT	a	422	20	-	0/0/0/0	0/0/0/0
27	LHG	a	423	-	-	0/49/49/53	0/0/0/0
31	DMS	a	424	-	-	0/0/0/0	0/0/0/0
31	DMS	a	425	-	-	0/0/0/0	0/0/0/0
22	CLA	b	602	39	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	b	603	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	b	604	-	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	608	39	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	609	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	b	610	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	b	611	39	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	612	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	614	-	3/3/18/25	0/30/128/135	0/0/9/9
22	CLA	b	615	-	3/3/17/25	0/22/120/135	0/0/9/9
22	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	617	-	3/3/19/25	0/31/129/135	0/0/9/9
24	BCR	b	618	-	-	0/13/30/63	0/1/1/2
24	BCR	b	619	-	-	2/26/43/63	0/1/1/2
24	BCR	b	620	-	-	0/29/63/63	0/2/2/2
28	SQD	b	621	-	-	0/32/52/69	0/1/1/1
25	LMG	b	622	-	-	0/38/58/70	0/1/1/1
34	HTG	b	623	-	-	0/10/30/30	0/1/1/1
34	HTG	b	624	-	-	0/10/30/30	0/1/1/1
34	HTG	b	626	-	-	0/10/30/30	0/1/1/1
34	HTG	b	627	-	-	0/10/30/30	0/1/1/1
31	DMS	b	629	-	-	0/0/0/0	0/0/0/0
31	DMS	b	630	-	-	0/0/0/0	0/0/0/0
31	DMS	b	631	-	-	0/0/0/0	0/0/0/0
34	HTG	b	632	-	-	0/10/30/30	0/1/1/1
31	DMS	b	633	-	-	0/0/0/0	0/0/0/0
31	DMS	b	634	-	-	0/0/0/0	0/0/0/0
31	DMS	b	635	-	-	0/0/0/0	0/0/0/0
31	DMS	b	636	-	-	0/0/0/0	0/0/0/0
31	DMS	b	637	-	-	0/0/0/0	0/0/0/0
31	DMS	b	638	-	-	0/0/0/0	0/0/0/0
22	CLA	c	902	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	903	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	904	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	c	905	39	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	c	906	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	c	907	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	908	39	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	909	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	c	910	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	911	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	912	3	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	c	913	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	c	914	-	2/2/20/25	0/37/135/135	0/0/9/9
24	BCR	c	915	-	-	0/29/63/63	0/2/2/2
24	BCR	c	916	-	-	0/29/63/63	0/2/2/2
35	DGD	c	917	-	-	0/51/91/95	0/2/2/2
35	DGD	c	918	-	-	0/51/91/95	0/2/2/2
35	DGD	c	919	-	-	0/51/91/95	0/2/2/2
25	LMG	c	920	-	-	0/46/66/70	0/1/1/1
29	LMT	c	921	-	-	0/21/61/61	0/2/2/2
34	HTG	c	922	-	-	0/10/30/30	0/1/1/1
31	DMS	c	923	-	-	0/0/0/0	0/0/0/0
31	DMS	c	924	-	-	0/0/0/0	0/0/0/0
31	DMS	c	925	-	-	0/0/0/0	0/0/0/0
31	DMS	c	926	-	-	0/0/0/0	0/0/0/0
31	DMS	c	927	-	-	0/0/0/0	0/0/0/0
31	DMS	c	928	-	-	0/0/0/0	0/0/0/0
31	DMS	c	929	-	-	0/0/0/0	0/0/0/0
25	LMG	c	930	-	-	0/44/64/70	0/1/1/1
29	LMT	c	931	-	-	0/15/35/61	0/1/1/2
31	DMS	c	933	-	-	0/0/0/0	0/0/0/0
31	DMS	c	934	-	-	0/0/0/0	0/0/0/0
31	DMS	c	935	-	-	0/0/0/0	0/0/0/0
31	DMS	c	936	-	-	0/0/0/0	0/0/0/0
31	DMS	c	937	-	-	0/0/0/0	0/0/0/0
31	DMS	c	938	-	-	0/0/0/0	0/0/0/0
31	DMS	c	939	-	-	0/0/0/0	0/0/0/0
31	DMS	c	940	-	-	0/0/0/0	0/0/0/0
31	DMS	c	941	-	-	0/0/0/0	0/0/0/0
31	DMS	c	942	-	-	0/0/0/0	0/0/0/0
31	DMS	c	943	-	-	0/0/0/0	0/0/0/0
31	DMS	c	944	-	-	0/0/0/0	0/0/0/0
27	LHG	d	401	-	-	0/34/34/53	0/0/0/0
22	CLA	d	402	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	d	403	-	2/2/20/25	0/37/135/135	0/0/9/9
24	BCR	d	404	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PL9	d	405	-	-	0/53/73/73	0/1/1/1
35	DGD	d	406	-	-	0/44/44/95	0/0/0/2
27	LHG	d	407	-	-	0/53/53/53	0/0/0/0
27	LHG	d	408	-	-	0/50/50/53	0/0/0/0
25	LMG	d	409	-	-	0/42/62/70	0/1/1/1
31	DMS	d	411	-	-	0/0/0/0	0/0/0/0
31	DMS	d	412	-	-	0/0/0/0	0/0/0/0
31	DMS	d	413	-	-	0/0/0/0	0/0/0/0
31	DMS	d	414	-	-	0/0/0/0	0/0/0/0
31	DMS	d	415	-	-	0/0/0/0	0/0/0/0
36	HEM	e	101	5,6	-	0/6/54/54	0/0/8/8
28	SQD	f	101	-	-	0/12/12/69	0/0/0/1
29	LMT	f	102	-	-	0/17/37/61	0/1/1/2
31	DMS	f	103	-	-	0/0/0/0	0/0/0/0
37	RRX	h	101	-	-	0/29/65/65	0/2/2/2
35	DGD	h	102	-	-	0/51/91/95	0/2/2/2
25	LMG	i	101	-	-	0/46/66/70	0/1/1/1
31	DMS	i	106	-	-	0/0/0/0	0/0/0/0
25	LMG	j	101	38	-	0/42/62/70	0/1/1/1
24	BCR	k	101	-	-	0/29/63/63	0/2/2/2
28	SQD	l	101	-	-	0/49/69/69	0/1/1/1
27	LHG	l	102	-	-	0/53/53/53	0/0/0/0
31	DMS	l	103	-	-	0/0/0/0	0/0/0/0
31	DMS	l	104	-	-	0/0/0/0	0/0/0/0
31	DMS	l	105	-	-	0/0/0/0	0/0/0/0
34	HTG	l	106	-	-	0/10/30/30	0/1/1/1
31	DMS	o	302	-	-	0/0/0/0	0/0/0/0
31	DMS	o	303	-	-	0/0/0/0	0/0/0/0
31	DMS	o	304	-	-	0/0/0/0	0/0/0/0
31	DMS	o	305	-	-	0/0/0/0	0/0/0/0
31	DMS	o	306	-	-	0/0/0/0	0/0/0/0
31	DMS	o	307	-	-	0/0/0/0	0/0/0/0
31	DMS	o	308	-	-	0/0/0/0	0/0/0/0
29	LMT	t	101	-	-	0/15/35/61	0/1/1/2
31	DMS	t	103	-	-	0/0/0/0	0/0/0/0
31	DMS	t	104	-	-	0/0/0/0	0/0/0/0
31	DMS	t	105	-	-	0/0/0/0	0/0/0/0
31	DMS	u	202	-	-	0/0/0/0	0/0/0/0
31	DMS	u	203	-	-	0/0/0/0	0/0/0/0
31	DMS	u	204	-	-	0/0/0/0	0/0/0/0
31	DMS	u	205	-	-	0/0/0/0	0/0/0/0
31	DMS	v	201	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	HEM	v	202	15	-	0/6/54/54	0/0/8/8
34	HTG	v	203	-	-	0/7/27/30	0/1/1/1
31	DMS	v	204	-	-	0/0/0/0	0/0/0/0
31	DMS	v	205	-	-	0/0/0/0	0/0/0/0
31	DMS	v	206	-	-	0/0/0/0	0/0/0/0
31	DMS	v	207	-	-	0/0/0/0	0/0/0/0
31	DMS	v	208	-	-	0/0/0/0	0/0/0/0
31	DMS	v	209	-	-	0/0/0/0	0/0/0/0
31	DMS	v	210	-	-	0/0/0/0	0/0/0/0
31	DMS	v	211	-	-	0/0/0/0	0/0/0/0
24	BCR	y	101	-	-	0/29/63/63	0/2/2/2

The worst 5 of 1215 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	f	101	SQD	C6-S	-6.78	1.67	1.77
23	A	407	PHO	C1A-NA	-5.51	1.25	1.37
36	V	202	HEM	C3B-C2B	-4.66	1.34	1.40
36	v	202	HEM	C3B-C2B	-4.47	1.34	1.40
34	B	623	HTG	C1'-S1	-4.29	1.75	1.81

The worst 5 of 1885 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	V	203	HTG	O5-C1-C2	-8.24	98.98	110.28
36	E	102	HEM	CBD-CAD-C3D	-7.63	97.91	112.47
22	b	606	CLA	CHD-C4C-C3C	-7.41	113.75	124.92
34	v	203	HTG	O5-C1-C2	-7.08	100.58	110.28
23	a	411	PHO	C1-C2-C3	-6.80	113.43	125.96

5 of 172 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	C	503	CLA	NC
22	C	503	CLA	ND
22	C	503	CLA	NA
22	C	510	CLA	NC
22	C	510	CLA	NA

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	C	532	HTG	O5-C1-S1-C1'
24	b	619	BCR	C7-C8-C9-C34
24	b	619	BCR	C7-C8-C9-C10

There are no ring outliers.

103 monomers are involved in 305 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	405	CLA	3	0
22	A	406	CLA	3	0
23	A	407	PHO	1	0
22	A	408	CLA	9	0
25	A	410	LMG	2	0
26	A	411	PL9	11	0
27	A	412	LHG	1	0
28	A	413	SQD	2	0
29	A	414	LMT	6	0
31	A	419	DMS	2	0
32	A	421[B]	BCT	1	0
22	B	602	CLA	6	0
22	B	603	CLA	3	0
22	B	604	CLA	2	0
22	B	605	CLA	5	0
22	B	606	CLA	11	0
22	B	607	CLA	4	0
22	B	608	CLA	9	0
22	B	609	CLA	6	0
22	B	610	CLA	8	0
22	B	611	CLA	9	0
22	B	612	CLA	2	0
22	B	613	CLA	4	0
22	B	614	CLA	6	0
22	B	615	CLA	5	0
22	B	616	CLA	3	0
22	B	617	CLA	2	0
24	B	618	BCR	4	0
24	B	619	BCR	1	0
24	B	620	BCR	3	0
25	B	621	LMG	3	0
29	B	622	LMT	3	0
34	B	623	HTG	3	0
34	B	626	HTG	1	0
31	B	628	DMS	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	B	629	DMS	1	0
31	B	631	DMS	3	0
31	B	638	DMS	7	0
31	B	641	DMS	1	0
31	B	642	DMS	1	0
28	C	501	SQD	6	0
22	C	502	CLA	2	0
22	C	503	CLA	6	0
22	C	504	CLA	3	0
22	C	505	CLA	4	0
22	C	506	CLA	1	0
22	C	507	CLA	5	0
22	C	508	CLA	3	0
22	C	509	CLA	3	0
22	C	510	CLA	3	0
22	C	511	CLA	5	0
22	C	512	CLA	1	0
22	C	513	CLA	5	0
22	C	514	CLA	5	0
24	C	515	BCR	4	0
24	C	516	BCR	1	0
35	C	518	DGD	1	0
35	C	519	DGD	2	0
25	C	520	LMG	1	0
34	C	521	HTG	1	0
27	C	522	LHG	1	0
31	C	530	DMS	1	0
25	C	531	LMG	2	0
34	C	532	HTG	1	0
31	C	536	DMS	1	0
31	C	540	DMS	1	0
22	D	401	CLA	4	0
23	D	402	PHO	5	0
22	D	403	CLA	2	0
22	D	404	CLA	1	0
24	D	405	BCR	1	0
26	D	406	PL9	5	0
27	D	409	LHG	7	0
27	D	410	LHG	3	0
27	D	411	LHG	8	0
25	D	412	LMG	5	0
34	D	414	HTG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	D	415	HTG	8	0
29	E	101	LMT	1	0
36	E	102	HEM	1	0
37	H	101	RRX	12	0
35	H	102	DGD	4	0
25	J	101	LMG	2	0
24	K	101	BCR	2	0
27	L	101	LHG	7	0
31	O	303	DMS	3	0
31	O	304	DMS	9	0
31	O	305	DMS	3	0
31	O	306	DMS	1	0
31	O	307	DMS	1	0
31	O	310	DMS	4	0
31	O	312	DMS	3	0
29	T	102	LMT	1	0
31	U	203	DMS	1	0
31	V	201	DMS	1	0
36	V	202	HEM	1	0
31	V	205	DMS	1	0
31	V	206	DMS	3	0
31	V	207	DMS	2	0
31	V	210	DMS	2	0
31	V	212	DMS	10	0
24	Y	101	BCR	4	0
29	Z	101	LMT	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.33	15 (4%) 34 32	21, 28, 66, 87	0
1	a	334/334 (100%)	-0.02	34 (10%) 7 7	22, 30, 96, 135	0
2	B	505/505 (100%)	-0.21	36 (7%) 17 16	22, 33, 67, 109	0
2	b	483/505 (95%)	-0.35	21 (4%) 36 34	24, 35, 57, 124	0
3	C	451/455 (99%)	-0.32	12 (2%) 55 52	24, 37, 55, 106	0
3	c	455/455 (100%)	-0.34	2 (0%) 92 91	27, 41, 57, 89	0
4	D	342/342 (100%)	-0.52	5 (1%) 74 72	21, 29, 51, 86	0
4	d	341/342 (99%)	-0.25	14 (4%) 38 36	22, 32, 59, 85	0
5	E	79/80 (98%)	0.53	10 (12%) 4 4	30, 53, 77, 89	0
5	e	79/80 (98%)	0.80	12 (15%) 2 2	35, 54, 91, 96	0
6	F	33/33 (100%)	-0.39	4 (12%) 5 4	32, 38, 68, 87	0
6	f	31/33 (93%)	-0.19	1 (3%) 48 46	34, 42, 62, 95	0
7	H	63/63 (100%)	-0.33	1 (1%) 72 70	32, 42, 52, 104	0
7	h	62/63 (98%)	0.27	8 (12%) 4 3	34, 48, 62, 74	0
8	I	34/36 (94%)	-0.50	1 (2%) 52 50	33, 42, 60, 78	0
8	i	35/36 (97%)	-0.64	0 100 100	34, 43, 71, 95	0
9	J	36/40 (90%)	-0.52	2 (5%) 25 24	29, 46, 73, 82	0
9	j	40/40 (100%)	0.08	6 (15%) 3 2	34, 47, 81, 92	0
10	K	37/37 (100%)	-0.42	0 100 100	36, 44, 55, 70	0
10	k	37/37 (100%)	-0.19	1 (2%) 55 52	39, 47, 68, 81	0
11	L	35/35 (100%)	-0.14	7 (20%) 1 1	23, 32, 66, 78	0
11	l	35/35 (100%)	-0.15	4 (11%) 6 5	25, 35, 75, 92	0
12	O	243/243 (100%)	-0.28	8 (3%) 47 44	23, 39, 69, 104	0
12	o	243/243 (100%)	-0.29	15 (6%) 21 20	24, 42, 71, 102	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	T	29/30 (96%)	-0.59	0 100 100	26, 32, 59, 89	0
13	t	29/30 (96%)	-0.51	2 (6%) 18 16	27, 34, 66, 98	0
14	U	97/97 (100%)	-0.19	0 100 100	26, 36, 58, 89	0
14	u	97/97 (100%)	-0.66	0 100 100	28, 37, 51, 76	0
15	V	137/137 (100%)	-0.62	0 100 100	25, 34, 50, 70	0
15	v	137/137 (100%)	-0.22	3 (2%) 62 60	29, 44, 61, 84	0
16	Y	29/29 (100%)	0.46	4 (13%) 3 3	40, 54, 69, 81	0
16	y	29/29 (100%)	0.52	4 (13%) 3 3	51, 62, 70, 74	0
17	X	37/37 (100%)	0.21	4 (10%) 6 6	41, 50, 72, 83	0
17	x	36/37 (97%)	0.94	9 (25%) 1 1	41, 54, 88, 89	0
18	Z	62/62 (100%)	0.40	13 (20%) 1 1	42, 54, 88, 106	0
18	z	61/62 (98%)	0.90	13 (21%) 1 1	49, 64, 98, 102	0
All	All	5147/5190 (99%)	-0.23	271 (5%) 27 26	21, 37, 70, 135	0

The worst 5 of 271 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	z	3	ILE	7.2
2	B	486	LEU	6.5
1	a	235	TYR	6.4
1	a	228	THR	6.2
2	B	488	PRO	6.2

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(Å ²)	Q<0.9
13	FME	T	1	10/11	0.95	0.19	-	38,42,72,75	0
8	FME	I	1	10/11	0.95	0.14	-	33,37,40,41	0
8	FME	i	1	10/11	0.97	0.11	-	36,41,45,48	0
13	FME	t	1	10/11	0.97	0.09	-	33,38,80,91	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
30	UNL	a	420	6/-	0.73	0.35	62.60	56,59,60,60	0
30	UNL	t	102	16/-	0.68	0.32	24.65	59,71,78,80	0
29	LMT	A	414	35/35	0.71	0.35	23.58	59,86,109,114	0
30	UNL	A	415	5/-	0.88	0.35	12.87	68,72,73,75	0
31	DMS	o	303	4/4	0.90	0.21	11.25	60,77,80,83	0
24	BCR	b	618	20/40	0.86	0.25	10.06	57,65,70,71	0
29	LMT	T	102	24/35	0.70	0.23	9.55	42,80,98,101	0
30	UNL	T	101	13/-	0.74	0.34	9.00	63,71,77,79	0
31	DMS	O	313	4/4	0.90	0.25	8.78	89,100,100,107	0
31	DMS	C	540	4/4	0.85	0.33	8.55	82,83,91,97	0
30	UNL	i	104	16/-	0.69	0.34	8.36	67,76,87,89	0
31	DMS	u	205	4/4	0.88	0.32	8.30	64,67,73,83	0
35	DGD	d	406	43/66	0.66	0.32	7.91	58,85,139,146	0
30	UNL	B	624	7/-	0.86	0.17	7.78	30,45,51,56	0
31	DMS	C	536	4/4	0.83	0.22	7.35	77,80,94,95	0
35	DGD	D	407	50/66	0.71	0.29	7.10	60,87,120,123	0
29	LMT	a	419	35/35	0.73	0.27	6.92	46,69,93,100	0
31	DMS	c	934	4/4	0.98	0.24	6.91	64,73,74,77	0
31	DMS	L	102	4/4	0.79	0.23	6.59	79,80,91,100	0
31	DMS	b	630	4/4	0.96	0.15	6.55	56,63,63,64	0
31	DMS	c	935	4/4	0.90	0.33	6.49	71,78,81,84	0
34	HTG	b	632	19/19	0.61	0.27	6.39	56,74,91,92	0
29	LMT	E	101	24/35	0.80	0.27	6.19	61,82,97,113	0
31	DMS	C	530	4/4	0.95	0.31	6.09	71,79,82,83	0
29	LMT	f	102	25/35	0.57	0.44	5.91	61,93,105,108	0
31	DMS	b	638	4/4	0.88	0.24	5.91	49,52,54,70	0
31	DMS	U	203	4/4	0.87	0.24	5.79	62,73,74,76	0
31	DMS	c	925	4/4	0.97	0.14	5.32	51,58,60,61	0
31	DMS	C	535	4/4	0.91	0.38	5.16	70,79,83,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	DMS	c	927	4/4	0.89	0.22	5.02	87,89,91,97	0
31	DMS	C	528	4/4	0.95	0.28	5.00	88,89,90,90	0
24	BCR	B	618	19/40	0.82	0.18	4.91	50,59,74,77	0
31	DMS	O	307	4/4	0.86	0.26	4.89	84,97,98,104	0
25	LMG	C	531	40/55	0.72	0.24	4.74	37,81,103,107	0
34	HTG	D	414	19/19	0.66	0.32	4.70	63,103,114,115	0
31	DMS	O	310	4/4	0.97	0.14	4.50	66,68,68,73	0
22	CLA	b	602	65/65	0.81	0.31	4.46	49,67,89,98	0
31	DMS	a	424	4/4	0.96	0.15	4.39	38,47,50,65	0
31	DMS	o	307	4/4	0.99	0.30	4.34	48,56,62,64	0
30	UNL	D	413	16/-	0.88	0.23	4.33	38,46,52,58	0
31	DMS	O	312	4/4	0.97	0.18	4.30	37,51,56,59	0
31	DMS	o	305	4/4	0.92	0.36	4.24	78,82,86,87	0
31	DMS	V	209	4/4	0.95	0.32	4.21	76,87,89,93	0
31	DMS	v	211	4/4	0.92	0.18	4.12	65,77,82,90	0
31	DMS	o	302	4/4	0.95	0.17	4.00	59,64,71,75	0
31	DMS	B	631	4/4	0.90	0.27	3.94	78,80,84,87	0
30	UNL	a	417	10/-	0.66	0.41	3.89	75,80,84,87	0
30	UNL	j	103	16/-	0.81	0.17	3.87	59,67,71,74	0
29	LMT	t	101	24/35	0.76	0.20	3.76	50,71,109,119	0
31	DMS	i	106	4/4	0.95	0.22	3.59	72,76,79,89	0
31	DMS	V	211	4/4	0.83	0.23	3.51	77,84,85,85	0
31	DMS	c	926	4/4	0.97	0.17	3.51	63,64,67,68	0
34	HTG	V	203	14/19	0.91	0.23	3.43	48,52,79,84	0
31	DMS	f	103	4/4	0.88	0.28	3.32	87,89,90,100	0
29	LMT	c	921	35/35	0.84	0.36	3.21	74,90,99,103	0
25	LMG	J	101	45/55	0.95	0.13	3.19	28,36,71,79	0
31	DMS	c	929	4/4	0.89	0.31	3.14	69,73,76,78	0
30	UNL	U	201	14/-	0.82	0.25	3.04	44,57,65,66	0
22	CLA	B	602	65/65	0.92	0.17	3.00	39,56,101,107	0
31	DMS	D	417	4/4	0.91	0.19	2.98	72,72,77,86	0
31	DMS	B	628	4/4	0.99	0.14	2.85	27,29,32,38	0
34	HTG	B	626	19/19	0.83	0.20	2.80	42,69,81,87	0
27	LHG	A	412	31/49	0.74	0.27	2.74	66,83,107,117	0
31	DMS	c	939	4/4	0.95	0.31	2.72	88,92,95,102	0
31	DMS	F	101	4/4	0.93	0.20	2.68	69,70,74,77	0
29	LMT	c	931	24/35	0.69	0.26	2.64	50,84,95,98	0
31	DMS	c	924	4/4	0.98	0.14	2.63	37,42,47,49	0
25	LMG	b	622	43/55	0.63	0.28	2.63	48,78,88,98	0
31	DMS	O	304	4/4	0.94	0.38	2.60	74,80,84,88	0
29	LMT	Z	101	35/35	0.71	0.36	2.59	40,105,123,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	HTG	D	415	19/19	0.68	0.28	2.51	39,69,80,87	0
30	UNL	I	104	16/-	0.86	0.27	2.51	60,71,84,86	0
30	UNL	J	103	16/-	0.89	0.20	2.49	44,57,77,77	0
24	BCR	b	619	31/40	0.92	0.15	2.49	47,54,63,67	0
24	BCR	D	405	40/40	0.95	0.12	2.43	26,35,62,66	0
25	LMG	B	621	40/55	0.67	0.24	2.43	47,82,108,112	0
31	DMS	a	425	4/4	0.88	0.15	2.38	39,47,51,62	0
31	DMS	v	210	4/4	0.87	0.24	2.29	63,71,80,91	0
31	DMS	V	204	4/4	0.88	0.24	2.27	66,73,76,76	0
31	DMS	b	629	4/4	0.97	0.14	2.14	29,31,36,45	0
30	UNL	u	201	11/-	0.65	0.27	2.14	47,53,69,69	0
35	DGD	C	519	62/66	0.95	0.15	2.12	23,36,76,85	0
29	LMT	I	102	35/35	0.81	0.30	2.09	76,88,100,102	0
31	DMS	B	640	4/4	0.96	0.30	2.05	47,53,57,63	0
28	SQD	A	413	49/54	0.84	0.20	2.00	46,65,91,95	0
31	DMS	V	201	4/4	0.96	0.20	1.99	46,48,54,58	0
26	PL9	A	411	55/55	0.78	0.23	1.99	61,73,87,92	0
27	LHG	a	416	49/49	0.71	0.28	1.98	60,84,100,108	0
31	DMS	C	527	4/4	0.96	0.17	1.97	74,80,80,81	0
31	DMS	u	202	4/4	0.96	0.15	1.97	47,53,55,68	0
25	LMG	d	409	47/55	0.85	0.18	1.94	49,76,113,114	0
31	DMS	O	306	4/4	0.98	0.19	1.94	69,69,70,81	0
31	DMS	I	106	4/4	0.95	0.28	1.93	64,74,78,80	0
31	DMS	O	311	4/4	0.95	0.13	1.85	48,56,59,61	0
28	SQD	l	101	54/54	0.70	0.25	1.83	53,82,119,123	0
31	DMS	C	539	4/4	0.94	0.23	1.72	88,90,93,95	0
31	DMS	d	415	4/4	0.90	0.15	1.71	60,63,67,79	0
31	DMS	b	631	4/4	0.94	0.17	1.65	68,72,79,80	0
28	SQD	a	418	51/54	0.87	0.15	1.64	47,70,91,97	0
31	DMS	A	420	4/4	0.91	0.15	1.61	37,39,39,57	0
31	DMS	A	416	4/4	0.95	0.12	1.60	60,67,69,72	0
31	DMS	d	413	4/4	0.98	0.19	1.59	67,69,73,80	0
26	PL9	D	406	55/55	0.94	0.12	1.57	21,30,37,51	0
30	UNL	d	410	16/-	0.94	0.16	1.57	40,49,57,60	0
26	PL9	a	415	55/55	0.76	0.27	1.57	64,84,106,111	0
34	HTG	C	523	9/19	0.91	0.22	1.56	63,69,81,86	0
31	DMS	U	202	4/4	0.93	0.15	1.55	42,49,58,67	0
31	DMS	o	304	4/4	0.94	0.17	1.54	70,70,70,74	0
24	BCR	B	619	30/40	0.92	0.14	1.52	44,51,61,63	0
25	LMG	c	930	49/55	0.74	0.20	1.49	44,78,96,106	0
31	DMS	o	306	4/4	0.96	0.21	1.48	66,71,74,83	0
34	HTG	b	623	19/19	0.95	0.10	1.47	42,46,54,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	DMS	B	630	4/4	0.94	0.16	1.44	63,67,68,75	0
28	SQD	D	408	20/54	0.89	0.30	1.39	65,97,105,108	0
25	LMG	D	412	46/55	0.69	0.25	1.38	41,68,138,142	0
34	HTG	b	626	19/19	0.90	0.13	1.38	47,69,86,90	0
30	UNL	O	301	16/-	0.93	0.13	1.34	39,47,73,74	0
35	DGD	C	518	62/66	0.92	0.17	1.34	29,40,89,109	0
27	LHG	d	408	46/49	0.94	0.15	1.27	29,41,93,97	0
31	DMS	B	629	4/4	0.96	0.15	1.26	48,52,58,65	0
27	LHG	d	401	33/49	0.81	0.16	1.22	62,94,138,142	0
34	HTG	b	624	19/19	0.78	0.28	1.19	69,97,109,110	0
22	CLA	c	904	65/65	0.94	0.22	1.18	32,44,50,54	0
27	LHG	D	411	45/49	0.96	0.13	1.16	31,39,90,94	0
26	PL9	d	405	55/55	0.96	0.11	1.13	23,32,39,43	0
22	CLA	b	606	65/65	0.97	0.14	1.12	24,28,40,40	0
31	DMS	O	303	4/4	0.93	0.17	1.11	68,71,78,79	0
25	LMG	A	410	51/55	0.84	0.19	1.10	47,62,83,91	0
31	DMS	d	412	4/4	0.94	0.18	1.09	58,59,66,66	0
22	CLA	c	903	65/65	0.94	0.21	1.08	27,34,54,65	0
31	DMS	V	212	4/4	0.91	0.18	1.07	51,54,55,72	0
22	CLA	B	611	65/65	0.96	0.17	1.07	26,33,41,46	0
31	DMS	b	633	4/4	0.97	0.09	1.05	68,68,70,78	0
23	PHO	a	410	64/64	0.97	0.13	1.03	21,28,32,36	0
28	SQD	b	621	38/54	0.84	0.17	1.01	58,90,110,112	0
29	LMT	B	622	24/35	0.84	0.16	0.97	57,67,73,78	0
22	CLA	c	909	65/65	0.96	0.14	0.95	31,37,80,97	0
25	LMG	i	101	51/55	0.88	0.16	0.93	45,57,80,81	0
27	LHG	D	409	49/49	0.91	0.19	0.90	38,56,85,97	0
31	DMS	d	411	4/4	0.98	0.13	0.89	60,62,64,64	0
31	DMS	O	314	4/4	0.89	0.26	0.88	78,80,86,91	0
35	DGD	c	917	62/66	0.96	0.14	0.84	26,42,81,94	0
25	LMG	c	920	51/55	0.85	0.18	0.84	37,61,87,91	0
34	HTG	B	623	19/19	0.95	0.11	0.83	41,47,64,66	0
25	LMG	j	101	47/55	0.94	0.11	0.83	33,43,69,74	0
22	CLA	C	510	65/65	0.95	0.16	0.82	31,36,59,64	0
30	UNL	x	101	15/-	0.89	0.13	0.80	43,50,56,58	0
27	LHG	D	410	49/49	0.97	0.12	0.79	29,36,51,61	0
22	CLA	c	910	65/65	0.96	0.16	0.79	28,38,58,64	0
30	UNL	X	101	16/-	0.89	0.13	0.78	35,53,62,64	0
28	SQD	a	414	54/54	0.91	0.14	0.77	36,69,81,87	0
35	DGD	c	919	62/66	0.96	0.12	0.76	29,40,73,79	0
22	CLA	C	514	65/65	0.92	0.15	0.75	44,55,83,86	0
25	LMG	C	520	51/55	0.87	0.19	0.75	34,60,90,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	DMS	c	928	4/4	0.94	0.17	0.75	73,74,74,80	0
31	DMS	V	210	4/4	0.90	0.13	0.74	70,73,78,88	0
27	LHG	C	522	30/49	0.82	0.16	0.73	55,79,127,134	0
28	SQD	C	501	54/54	0.94	0.13	0.73	32,64,83,89	0
37	RRX	H	101	41/41	0.85	0.16	0.71	32,42,58,62	0
22	CLA	B	606	65/65	0.97	0.14	0.70	24,30,42,46	0
24	BCR	d	404	40/40	0.95	0.10	0.67	27,38,63,66	0
27	LHG	l	102	49/49	0.89	0.18	0.65	38,61,91,95	0
24	BCR	A	409	40/40	0.97	0.12	0.65	25,30,37,38	0
31	DMS	v	206	4/4	0.97	0.20	0.63	69,72,72,77	0
22	CLA	c	913	65/65	0.92	0.14	0.63	42,54,96,98	0
35	DGD	H	102	62/66	0.90	0.19	0.61	28,37,46,50	0
22	CLA	C	511	65/65	0.97	0.20	0.58	31,36,41,46	0
22	CLA	B	616	65/65	0.97	0.11	0.56	30,36,50,57	0
22	CLA	C	502	65/65	0.95	0.13	0.55	33,39,52,62	0
35	DGD	h	102	62/66	0.86	0.20	0.54	28,42,53,58	0
22	CLA	a	409	61/65	0.97	0.15	0.53	25,29,80,87	0
23	PHO	D	402	64/64	0.97	0.14	0.53	25,29,35,39	0
23	PHO	A	407	64/64	0.97	0.13	0.52	20,25,30,32	0
22	CLA	a	412	65/65	0.96	0.10	0.52	27,32,102,116	0
22	CLA	b	604	65/65	0.97	0.16	0.51	26,32,45,50	0
37	RRX	h	101	41/41	0.78	0.21	0.49	40,49,75,82	0
22	CLA	A	406	55/65	0.98	0.12	0.48	21,27,49,60	0
31	DMS	c	933	4/4	0.96	0.10	0.47	57,64,66,70	0
22	CLA	B	604	65/65	0.95	0.15	0.46	26,30,40,47	0
22	CLA	D	404	65/65	0.95	0.11	0.46	30,37,94,104	0
22	CLA	C	505	65/65	0.96	0.17	0.45	28,34,58,60	0
22	CLA	B	613	65/65	0.96	0.15	0.43	24,30,37,40	0
22	CLA	c	911	65/65	0.97	0.20	0.41	29,38,46,52	0
22	CLA	B	609	65/65	0.97	0.17	0.41	25,30,38,39	0
24	BCR	b	620	40/40	0.95	0.12	0.41	33,39,48,49	0
22	CLA	b	613	65/65	0.96	0.14	0.40	26,32,37,40	0
22	CLA	c	905	65/65	0.96	0.18	0.39	30,35,62,66	0
35	DGD	c	918	62/66	0.94	0.15	0.39	34,42,98,113	0
31	DMS	v	209	4/4	0.97	0.25	0.39	72,74,76,81	0
22	CLA	C	509	65/65	0.96	0.14	0.37	29,35,81,102	0
22	CLA	c	914	65/65	0.93	0.16	0.35	47,60,95,108	0
22	CLA	B	608	65/65	0.95	0.12	0.33	24,29,64,79	0
22	CLA	C	503	65/65	0.96	0.17	0.33	28,32,47,56	0
28	SQD	f	101	14/54	0.88	0.22	0.33	77,89,96,96	0
22	CLA	c	902	65/65	0.96	0.11	0.32	34,39,50,51	0
24	BCR	a	413	40/40	0.96	0.09	0.30	26,31,38,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	DGD	C	517	62/66	0.95	0.13	0.28	24,35,80,88	0
27	LHG	a	423	45/49	0.90	0.15	0.28	39,58,72,74	0
22	CLA	A	405	65/65	0.97	0.11	0.28	18,23,36,54	0
22	CLA	A	408	65/65	0.97	0.11	0.27	19,29,99,110	0
22	CLA	a	407	65/65	0.98	0.13	0.24	23,26,45,61	0
31	DMS	B	633	4/4	0.98	0.16	0.23	65,71,71,73	0
24	BCR	C	516	40/40	0.95	0.10	0.23	32,39,47,54	0
22	CLA	a	408	65/65	0.98	0.10	0.22	20,26,35,41	0
22	CLA	B	610	65/65	0.93	0.12	0.22	30,37,42,46	0
31	DMS	B	641	4/4	0.95	0.10	0.22	46,49,61,66	0
22	CLA	D	401	65/65	0.98	0.09	0.21	19,23,31,36	0
27	LHG	d	407	49/49	0.96	0.11	0.21	28,36,56,63	0
24	BCR	y	101	40/40	0.91	0.12	0.20	32,41,51,53	0
22	CLA	c	907	65/65	0.95	0.12	0.20	39,47,102,108	0
24	BCR	B	620	40/40	0.95	0.10	0.17	30,37,49,50	0
22	CLA	b	607	65/65	0.93	0.11	0.17	29,37,58,65	0
24	BCR	C	515	40/40	0.94	0.10	0.17	37,50,58,59	0
22	CLA	B	603	65/65	0.93	0.14	0.16	27,36,43,47	0
22	CLA	C	506	65/65	0.96	0.14	0.16	30,37,50,54	0
22	CLA	b	605	65/65	0.97	0.17	0.13	23,29,63,65	0
22	CLA	b	611	65/65	0.96	0.11	0.10	28,35,40,43	0
22	CLA	B	605	65/65	0.97	0.18	0.09	24,28,60,66	0
27	LHG	L	101	40/49	0.94	0.12	0.09	37,53,63,66	0
22	CLA	c	906	65/65	0.95	0.10	0.08	30,40,50,54	0
22	CLA	C	504	65/65	0.96	0.13	0.02	29,37,42,51	0
31	DMS	D	416	4/4	0.98	0.19	0.01	55,59,60,69	0
34	HTG	v	203	16/19	0.84	0.16	-0.02	52,69,81,97	0
22	CLA	b	603	65/65	0.94	0.14	-0.04	29,36,46,49	0
22	CLA	D	403	65/65	0.97	0.12	-0.05	18,24,45,52	0
38	MG	j	102	1/1	0.99	0.11	-0.08	40,40,40,40	0
22	CLA	d	403	65/65	0.95	0.11	-0.11	35,40,85,90	0
24	BCR	c	915	40/40	0.93	0.12	-0.12	43,59,68,69	0
22	CLA	b	612	65/65	0.96	0.12	-0.13	27,31,72,83	0
31	DMS	V	208	4/4	0.97	0.10	-0.13	73,74,77,78	0
23	PHO	a	411	64/64	0.96	0.14	-0.14	26,33,40,48	0
22	CLA	C	507	65/65	0.94	0.12	-0.14	37,45,85,88	0
38	MG	J	102	1/1	0.99	0.07	-0.15	30,30,30,30	0
22	CLA	b	614	59/65	0.97	0.14	-0.16	26,32,76,82	0
22	CLA	d	402	65/65	0.98	0.13	-0.17	21,27,42,50	0
22	CLA	B	607	65/65	0.94	0.10	-0.18	28,34,56,65	0
22	CLA	c	908	65/65	0.95	0.10	-0.18	34,39,53,61	0
22	CLA	B	612	65/65	0.96	0.13	-0.18	23,29,55,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
24	BCR	K	101	40/40	0.96	0.10	-0.19	31,39,43,43	0
36	HEM	V	202	43/43	0.98	0.09	-0.19	23,29,36,40	0
19	OEX	A	401	10/10	0.99	0.12	-0.19	25,27,31,32	0
36	HEM	e	101	43/43	0.98	0.17	-0.20	43,55,85,93	0
22	CLA	B	614	61/65	0.97	0.14	-0.21	25,31,70,83	0
31	DMS	V	206	4/4	0.96	0.09	-0.22	45,48,51,62	0
22	CLA	c	912	65/65	0.93	0.10	-0.24	35,45,50,53	0
22	CLA	b	616	65/65	0.94	0.10	-0.27	30,37,53,57	0
22	CLA	b	608	65/65	0.95	0.10	-0.28	27,31,73,74	0
22	CLA	B	615	53/65	0.93	0.11	-0.29	31,36,71,84	0
22	CLA	b	609	65/65	0.96	0.14	-0.30	27,34,42,45	0
22	CLA	b	610	65/65	0.94	0.10	-0.30	32,41,45,54	0
24	BCR	k	101	40/40	0.93	0.11	-0.31	36,45,51,52	0
34	HTG	l	106	19/19	0.83	0.18	-0.33	63,97,108,109	0
22	CLA	b	615	52/65	0.95	0.10	-0.34	36,42,71,76	0
24	BCR	Y	101	39/40	0.96	0.09	-0.37	34,40,48,50	0
36	HEM	E	102	43/43	0.96	0.14	-0.41	48,56,62,65	0
24	BCR	c	916	40/40	0.96	0.10	-0.42	33,42,48,49	0
22	CLA	C	513	56/65	0.95	0.10	-0.45	37,48,62,65	0
22	CLA	C	512	65/65	0.95	0.09	-0.46	31,39,48,51	0
32	BCT	A	421[A]	4/4	0.98	0.08	-0.46	34,36,39,39	4
32	BCT	A	421[B]	4/4	0.98	0.08	-0.47	27,29,30,34	4
22	CLA	C	508	65/65	0.96	0.10	-0.47	32,42,55,59	0
31	DMS	v	208	4/4	0.94	0.13	-0.48	88,90,91,94	0
31	DMS	v	204	4/4	0.94	0.13	-0.49	87,88,90,91	0
31	DMS	v	201	4/4	0.97	0.13	-0.54	42,48,50,51	0
22	CLA	b	617	60/65	0.94	0.11	-0.62	32,41,75,80	0
22	CLA	B	617	55/65	0.96	0.08	-0.64	28,35,72,76	0
21	CL	a	406	1/1	0.99	0.13	-0.64	32,32,32,32	0
36	HEM	v	202	43/43	0.98	0.08	-0.67	33,37,42,46	0
21	CL	A	403	1/1	0.99	0.09	-0.67	29,29,29,29	0
31	DMS	C	526	4/4	0.99	0.08	-0.70	48,48,50,51	0
32	BCT	a	422	4/4	0.96	0.07	-0.77	51,52,56,57	0
20	FE2	A	402	1/1	1.00	0.07	-0.98	39,39,39,39	0
20	FE2	a	404	1/1	0.99	0.07	-1.11	42,42,42,42	0
19	OEX	a	403	10/10	1.00	0.09	-1.40	29,31,32,33	0
31	DMS	C	525	4/4	0.99	0.06	-1.47	34,35,38,40	0
21	CL	A	404	1/1	0.99	0.12	-1.47	28,28,28,28	0
21	CL	a	405	1/1	0.99	0.07	-1.83	31,31,31,31	0
33	CA	O	302	1/1	0.96	0.04	-3.41	59,59,59,59	0
33	CA	c	901	1/1	0.99	0.03	-3.99	48,48,48,48	0
33	CA	o	301	1/1	0.99	0.03	-4.18	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	DMS	b	634	4/4	0.93	0.25	-	68,76,79,86	0
31	DMS	V	207	4/4	0.91	0.15	-	64,71,71,76	0
31	DMS	O	308	4/4	0.90	0.20	-	64,72,73,80	0
31	DMS	l	104	4/4	0.89	0.16	-	79,80,86,87	0
31	DMS	b	636	4/4	0.79	0.25	-	88,95,109,113	0
30	UNL	b	628	11/-	0.84	0.32	-	58,63,78,79	0
34	HTG	c	922	19/19	0.76	0.29	-	70,93,109,112	0
31	DMS	A	419	4/4	0.97	0.21	-	58,60,70,72	0
30	UNL	i	105	10/-	0.59	0.33	-	67,78,86,87	0
31	DMS	A	418	4/4	0.99	0.10	-	29,30,31,31	0
31	DMS	C	537	4/4	0.68	0.37	-	88,103,104,113	0
31	DMS	b	637	4/4	0.80	0.18	-	90,97,101,112	0
30	UNL	B	625	16/-	0.95	0.09	-	40,47,59,59	0
31	DMS	t	103	4/4	0.95	0.13	-	89,102,103,103	0
31	DMS	B	637	4/4	0.93	0.30	-	69,76,80,88	0
30	UNL	b	625	16/-	0.88	0.13	-	43,52,64,67	0
31	DMS	d	414	4/4	0.64	0.38	-	102,112,113,120	0
31	DMS	c	936	4/4	0.70	0.26	-	106,116,116,124	0
31	DMS	B	639	4/4	0.74	0.41	-	72,87,90,102	0
31	DMS	c	923	4/4	0.99	0.15	-	37,40,42,43	0
31	DMS	C	534	4/4	0.76	0.33	-	105,111,112,121	0
31	DMS	D	418	4/4	0.99	0.11	-	35,39,42,43	0
31	DMS	C	524	4/4	0.99	0.07	-	38,42,43,43	0
30	UNL	I	105	16/-	0.56	0.37	-	70,82,88,90	0
31	DMS	v	205	4/4	0.90	0.26	-	70,72,78,80	0
31	DMS	c	938	4/4	0.87	0.32	-	86,91,98,103	0
31	DMS	V	205	4/4	0.95	0.16	-	64,66,67,71	0
31	DMS	c	940	4/4	0.93	0.30	-	74,74,75,80	0
31	DMS	o	308	4/4	0.91	0.26	-	76,77,82,91	0
38	MG	k	102	1/1	0.97	0.05	-	48,48,48,48	0
31	DMS	c	937	4/4	0.72	0.17	-	80,90,91,100	0
33	CA	b	601	1/1	0.99	0.04	-	59,59,59,59	0
30	UNL	c	932	10/-	0.79	0.23	-	56,74,80,83	0
31	DMS	l	105	4/4	0.80	0.19	-	100,103,110,115	0
31	DMS	H	103	4/4	0.83	0.26	-	63,67,69,74	0
31	DMS	A	417	4/4	0.96	0.14	-	76,82,83,85	0
38	MG	K	102	1/1	0.97	0.05	-	51,51,51,51	0
30	UNL	I	103	13/-	0.73	0.23	-	53,57,77,82	0
31	DMS	I	101	4/4	0.93	0.23	-	64,69,74,76	0
31	DMS	l	103	4/4	0.87	0.21	-	91,95,97,99	0
31	DMS	C	538	4/4	0.94	0.36	-	79,86,86,87	0
34	HTG	B	627	19/19	0.59	0.32	-	51,104,113,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	DMS	c	944	4/4	0.92	0.20	-	79,82,89,92	0
31	DMS	B	642	4/4	0.94	0.20	-	65,66,75,82	0
31	DMS	a	401	4/4	0.66	0.28	-	75,84,85,104	0
31	DMS	C	533	4/4	0.91	0.22	-	79,84,85,89	0
31	DMS	O	305	4/4	0.54	0.23	-	68,70,79,99	0
31	DMS	B	636	4/4	0.94	0.23	-	60,62,67,69	0
31	DMS	B	632	4/4	0.86	0.20	-	49,57,67,69	0
31	DMS	u	204	4/4	0.88	0.34	-	50,68,69,75	0
30	UNL	i	102	16/-	0.92	0.13	-	41,51,80,81	0
31	DMS	B	634	4/4	0.74	0.25	-	57,68,73,95	0
31	DMS	t	105	4/4	0.86	0.18	-	89,93,101,108	0
31	DMS	b	635	4/4	0.90	0.17	-	62,69,76,86	0
31	DMS	u	203	4/4	0.89	0.17	-	56,68,72,84	0
31	DMS	B	635	4/4	0.95	0.18	-	61,63,66,73	0
33	CA	B	601	1/1	0.95	0.04	-	64,64,64,64	0
31	DMS	O	309	4/4	0.95	0.25	-	61,70,70,74	0
31	DMS	c	941	4/4	0.96	0.23	-	73,79,87,88	0
31	DMS	c	942	4/4	0.56	0.23	-	101,103,111,117	0
34	HTG	C	521	19/19	0.88	0.22	-	55,80,93,96	0
34	HTG	C	532	19/19	0.69	0.27	-	69,98,111,112	0
31	DMS	B	638	4/4	0.94	0.16	-	81,82,86,93	0
31	DMS	t	104	4/4	0.87	0.15	-	101,101,104,111	0
30	UNL	i	103	16/-	0.82	0.20	-	53,64,79,82	0
31	DMS	a	402	4/4	0.99	0.10	-	30,32,34,34	0
34	HTG	b	627	19/19	0.59	0.25	-	50,92,108,109	0
31	DMS	C	529	4/4	0.89	0.32	-	72,78,78,86	0
31	DMS	c	943	4/4	0.91	0.15	-	77,82,87,92	0
30	UNL	Z	102	9/-	0.75	0.30	-	57,71,79,81	0
31	DMS	v	207	4/4	0.82	0.17	-	84,93,97,117	0
31	DMS	a	421	4/4	0.90	0.26	-	85,87,87,94	0

6.5 Other polymers ⓘ

There are no such residues in this entry.