



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 06:49 PM EST

PDB ID : 5B5E  
Title : Crystal structure analysis of Photosystem II complex  
Authors : Tanaka, A.; Fukushima, Y.; Kamiya, N.  
Deposited on : 2016-05-02  
Resolution : 1.87 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

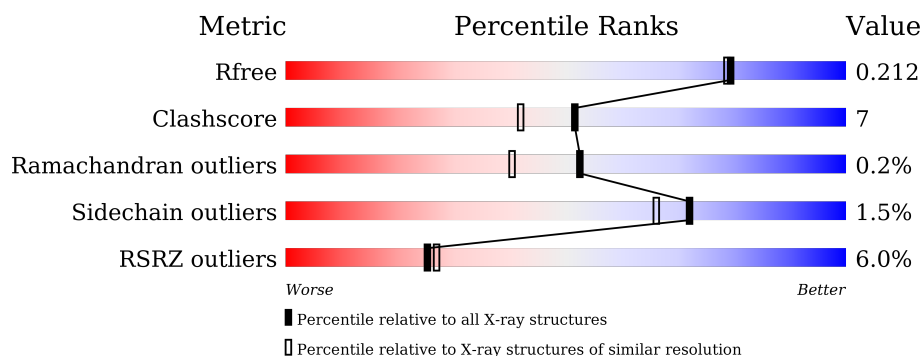
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.87 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




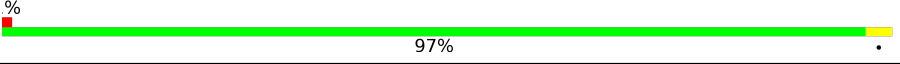

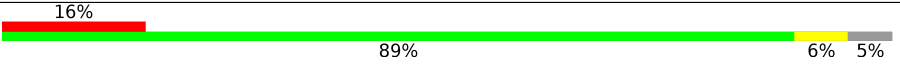
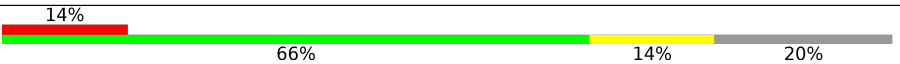

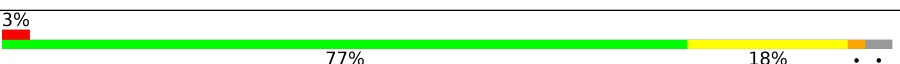
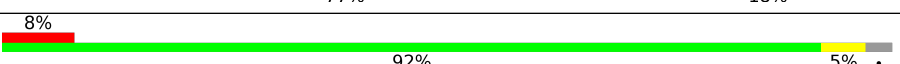
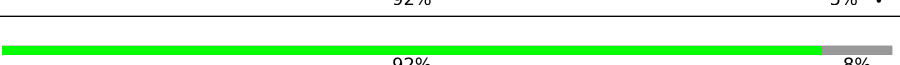
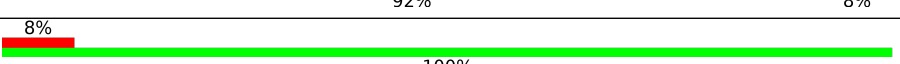
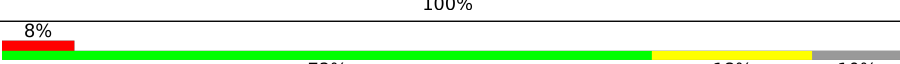
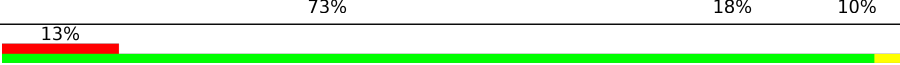
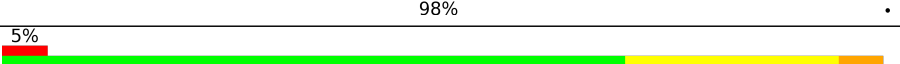
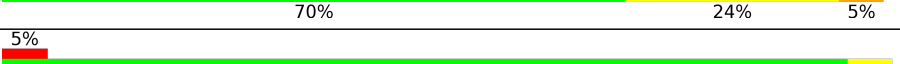
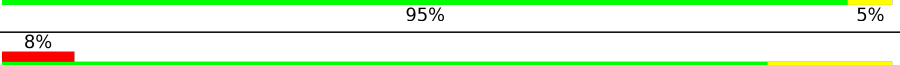

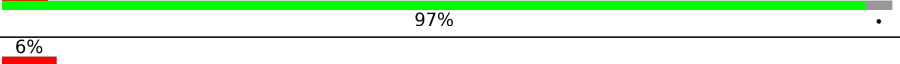
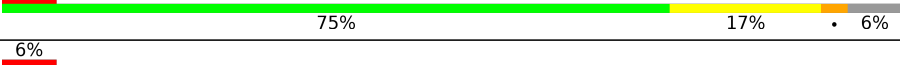
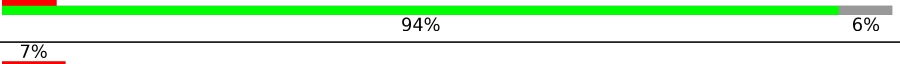
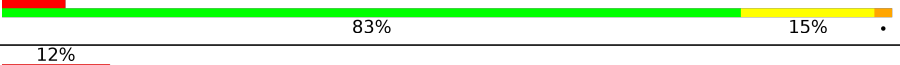
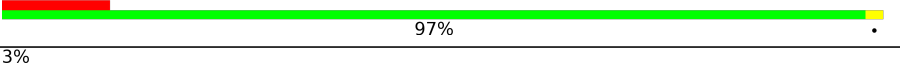

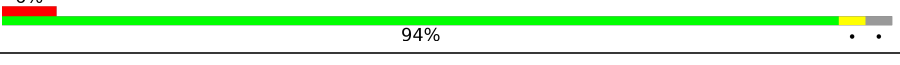
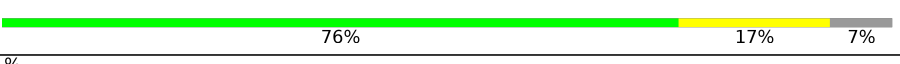
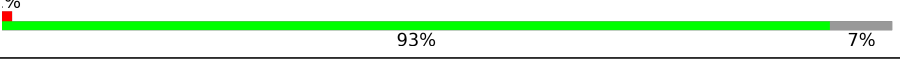
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	6965 (1.90-1.86)
Clashscore	102246	7778 (1.90-1.86)
Ramachandran outliers	100387	7691 (1.90-1.86)
Sidechain outliers	100360	7692 (1.90-1.86)
RSRZ outliers	91569	6979 (1.90-1.86)

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

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 86%, yellow 86%, yellow 96%, green 96%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>86%</span> <span>10%</span> <span>.</span> </div> </div>
1	a	344	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 95%, yellow 95%, yellow 98%, green 98%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>95%</span> <span>.</span> <span>.</span> </div> </div>
2	B	505	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 6%, orange 6%, orange 86%, yellow 86%, yellow 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>6%</span> <span>86%</span> <span>14%</span> </div> </div>
2	b	505	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 6%, orange 6%, orange 96%, yellow 96%, yellow 98%, green 98%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>6%</span> <span>96%</span> <span>.</span> <span>.</span> </div> </div>
3	C	455	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 84%, yellow 84%, yellow 99%, green 99%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>84%</span> <span>15%</span> <span>.</span> </div> </div>
3	c	455	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 97%, yellow 97%, yellow 99%, green 99%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>97%</span> <span>.</span> </div> </div>

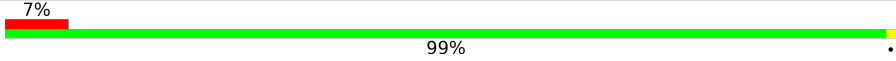

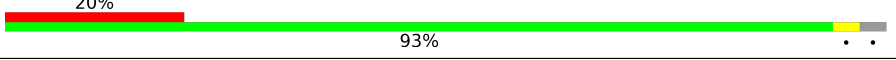

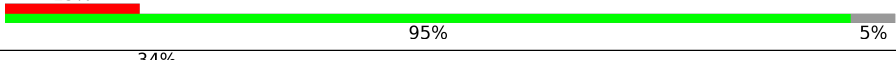
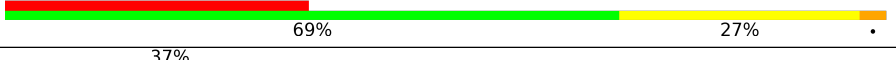

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Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	

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

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	401	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	407	X	-	-	-
23	CLA	a	410	X	-	-	-
23	CLA	b	602	X	-	-	X
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	c	902	X	-	-	-
23	CLA	c	903	X	-	-	-
23	CLA	c	904	X	-	-	-
23	CLA	c	905	X	-	-	-
23	CLA	c	906	X	-	-	-
23	CLA	c	907	X	-	-	-
23	CLA	c	908	X	-	-	-
23	CLA	c	909	X	-	-	-
23	CLA	c	910	X	-	-	-
23	CLA	c	911	X	-	-	-
23	CLA	c	912	X	-	-	-
23	CLA	c	913	X	-	-	-
23	CLA	c	914	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	401	X	-	-	-
23	CLA	d	403	X	-	-	-
23	CLA	d	404	X	-	-	-
25	BCR	B	619	-	-	-	X
25	BCR	D	405	-	-	-	X
25	BCR	T	101	-	-	-	X
25	BCR	d	405	-	-	-	X
26	SQD	A	415	-	-	-	X
26	SQD	B	621	-	-	-	X
26	SQD	L	102	-	-	-	X
26	SQD	a	417	-	-	-	X
27	PL9	A	411	-	-	-	X
27	PL9	a	414	-	-	-	X
28	LHG	A	412	-	-	-	X
28	LHG	E	101	-	-	-	X
28	LHG	K	101	-	-	-	X
28	LHG	d	402	-	-	-	X
28	LHG	d	408	-	-	-	X
28	LHG	e	101	-	-	-	X
29	UNL	A	414	-	-	-	X
29	UNL	A	417	-	-	-	X
29	UNL	B	629	-	-	-	X
29	UNL	B	632	-	-	-	X
29	UNL	D	413	-	-	-	X
29	UNL	E	102	-	-	-	X
29	UNL	E	103	-	-	-	X
29	UNL	I	103	-	-	-	X
29	UNL	J	103	-	-	-	X
29	UNL	J	104	-	-	-	X
29	UNL	J	105	-	-	-	X
29	UNL	T	102	-	-	-	X
29	UNL	U	201	-	-	-	X
29	UNL	X	101	-	-	-	X
29	UNL	Z	102	-	-	-	X
29	UNL	a	419	-	-	-	X
29	UNL	b	626	-	-	-	X
29	UNL	d	412	-	-	-	X
29	UNL	e	102	-	-	-	X
29	UNL	i	103	-	-	-	X
29	UNL	j	103	-	-	-	X
29	UNL	k	101	-	-	-	X
29	UNL	t	102	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	UNL	u	201	-	-	-	X
29	UNL	u	202	-	-	-	X
29	UNL	x	103	-	-	-	X
29	UNL	z	102	-	-	-	X
30	LMT	A	416	-	-	-	X
30	LMT	B	643	-	-	-	X
30	LMT	B	644	-	-	-	X
30	LMT	F	101	-	-	-	X
30	LMT	I	101	-	-	-	X
30	LMT	T	103	-	-	-	X
30	LMT	a	418	-	-	-	X
30	LMT	e	103	-	-	-	X
30	LMT	z	101	-	-	-	X
31	DMS	A	419	-	-	-	X
31	DMS	A	421	-	-	-	X
31	DMS	B	636	-	-	X	X
31	DMS	B	638	-	-	-	X
31	DMS	B	639	-	-	X	-
31	DMS	B	641	-	-	-	X
31	DMS	B	645	-	-	X	X
31	DMS	C	525	-	-	-	X
31	DMS	C	526	-	-	-	X
31	DMS	C	527	-	-	-	X
31	DMS	C	529	-	-	-	X
31	DMS	D	416	-	-	X	X
31	DMS	D	417	-	-	-	X
31	DMS	F	102	-	-	X	X
31	DMS	O	303	-	-	-	X
31	DMS	O	304	-	-	-	X
31	DMS	O	305	-	-	X	X
31	DMS	O	308	-	-	X	X
31	DMS	O	311	-	-	-	X
31	DMS	U	202	-	-	-	X
31	DMS	V	202	-	-	-	X
31	DMS	V	207	-	-	X	-
31	DMS	V	209	-	-	X	-
31	DMS	V	210	-	-	-	X
31	DMS	V	211	-	-	-	X
31	DMS	b	635	-	-	-	X
31	DMS	b	637	-	-	-	X
31	DMS	b	638	-	-	-	X
31	DMS	b	640	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	DMS	b	644	-	-	-	X
31	DMS	b	645	-	-	-	X
31	DMS	b	646	-	-	-	X
31	DMS	b	647	-	-	-	X
31	DMS	c	925	-	-	-	X
31	DMS	c	929	-	-	-	X
31	DMS	c	932	-	-	-	X
31	DMS	c	933	-	-	-	X
31	DMS	d	415	-	-	-	X
31	DMS	k	103	-	-	-	X
31	DMS	o	303	-	-	-	X
31	DMS	o	304	-	-	-	X
31	DMS	u	203	-	-	-	X
31	DMS	u	206	-	-	-	X
31	DMS	v	201	-	-	-	X
31	DMS	v	202	-	-	-	X
31	DMS	v	209	-	-	-	X
34	LMG	C	531	-	-	-	X
34	LMG	J	101	-	-	-	X
34	LMG	c	930	-	-	-	X
34	LMG	d	411	-	-	-	X
35	HTG	B	625	-	-	-	X
35	HTG	C	522	-	-	-	X
35	HTG	C	523	-	-	-	X
35	HTG	D	414	-	-	-	X
35	HTG	O	302	-	-	-	X
35	HTG	V	204	-	-	-	X
35	HTG	b	622	-	-	-	X
35	HTG	c	922	-	-	-	X
35	HTG	c	923	-	-	-	X
35	HTG	d	413	-	-	-	X
35	HTG	v	204	-	-	-	X
36	DGD	C	519	-	-	-	X
36	DGD	D	407	-	-	-	X
36	DGD	d	407	-	-	-	X
39	MG	j	102	-	-	-	X



## 2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 55401 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	1	0
			2622	1718	431	458	15			
1	a	334	Total	C	N	O	S	0	4	0
			2633	1727	431	460	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	see sequence details	UNP P51765
a	279	PRO	ARG	see sequence details	UNP P51765

- 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	4	0
			3992	2619	668	692	13			
2	b	501	Total	C	N	O	S	0	3	0
			3929	2582	653	681	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	4	0
			3511	2297	591	610	13			
3	c	455	Total	C	N	O	S	0	1	0
			3521	2305	589	614	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	see sequence details	UNP D0VWR7
C	20	SER	-	see sequence details	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	see sequence details	UNP D0VWR7
C	22	PHE	-	see sequence details	UNP D0VWR7
c	19	ASN	-	see sequence details	UNP D0VWR7
c	20	SER	-	see sequence details	UNP D0VWR7
c	21	ILE	-	see sequence details	UNP D0VWR7
c	22	PHE	-	see sequence details	UNP D0VWR7

- 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	2	0
			2733	1813	446	462	12			
4	d	342	Total	C	N	O	S	0	2	0
			2733	1813	446	462	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			651	426	103	122			
5	e	79	Total	C	N	O	0	0	0
			637	419	101	117			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			280	190	46	43	1			
6	f	32	Total	C	N	O	S	0	0	0
			255	173	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total	C	N	O	S	0	2	0
			511	341	83	85	2			
7	h	63	Total	C	N	O	S	0	1	0
			506	338	83	83	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
			285	195	45	44	1			
8	i	38	Total	C	N	O	S	0	0	0
			303	205	48	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	40	Total	C	N	O	S	0	0	0
			285	190	44	49	2			

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	see sequence details	UNP P19054
K	39	TRP	VAL	see sequence details	UNP P19054
k	33	LEU	PHE	see sequence details	UNP P19054
k	39	TRP	VAL	see sequence details	UNP P19054

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	0	1	0
			306	205	48	53			
11	l	36	Total	C	N	O	0	1	0
			297	200	47	50			

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			264	178	38	47	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	1	0
			264	178	38	47	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	see sequence details	UNP P12312
m	8	LEU	PHE	see sequence details	UNP P12312

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	2	0
			1861	1164	311	382	4			
13	o	243	Total	C	N	O	S	0	1	0
			1852	1159	310	379	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			
14	t	31	Total	C	N	O	S	0	0	0
			261	183	37	39	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O		0	0	0
			766	486	128	152				
15	u	97	Total	C	N	O		0	1	0
			776	493	129	154				

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	4			
16	v	137	Total	C	N	O	S	0	1	0
			1060	671	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	0	0
			210	137	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			207	134	37	33	3			

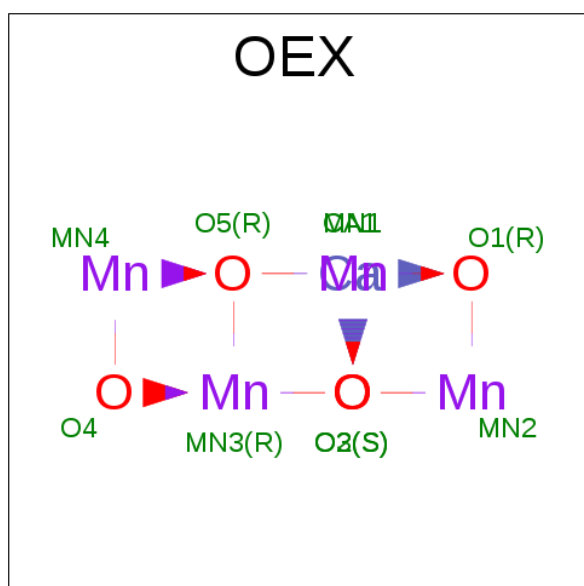
- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O		0	1	0
			280	190	44	46				
18	x	38	Total	C	N	O		0	0	0
			275	185	44	46				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			468	320	71	75	2			
19	z	61	Total	C	N	O	S	0	0	0
			457	312	70	73	2			

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



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

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

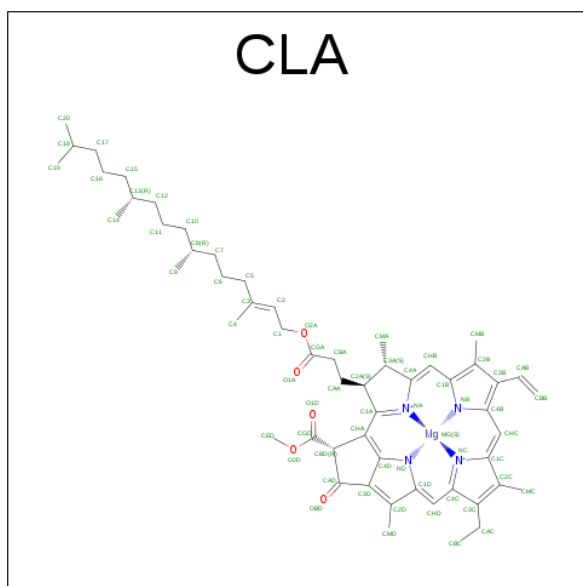
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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

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

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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

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

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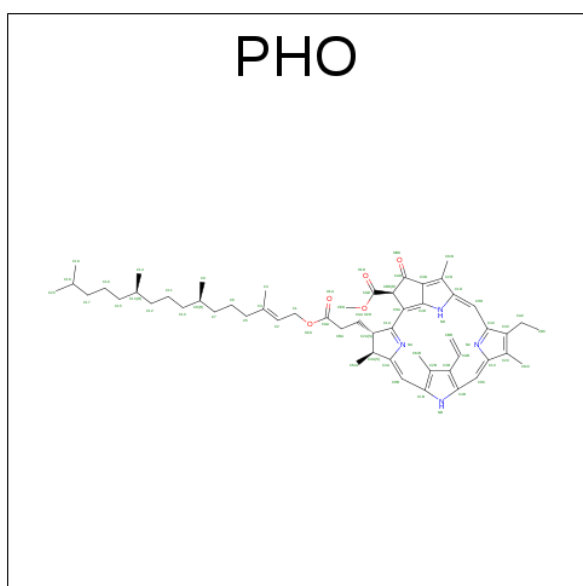
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N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

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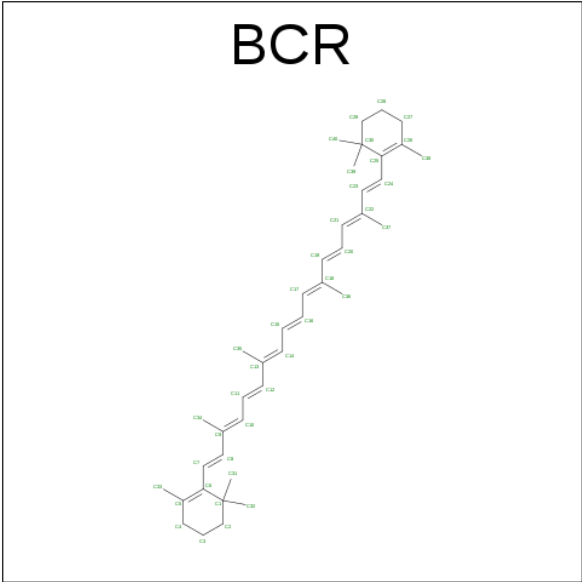
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



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

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



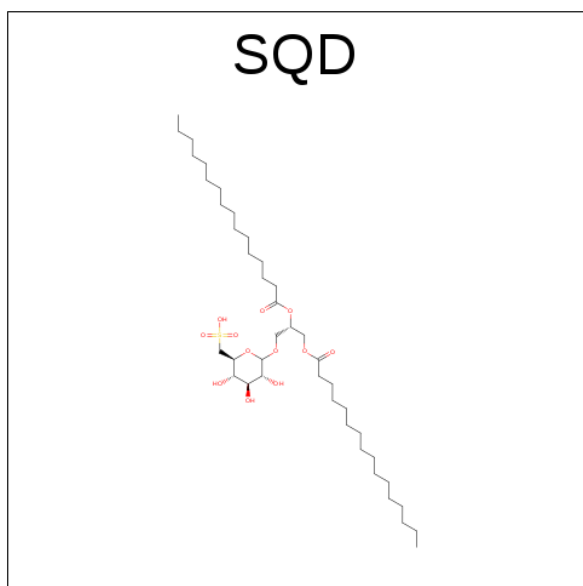
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total C 40 40	0	0
25	a	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	d	1	Total C 40 40	0	0
25	j	1	Total C 40 40	0	0
25	k	1	Total C 40 40	0	0
25	t	1	Total C 40 40	0	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



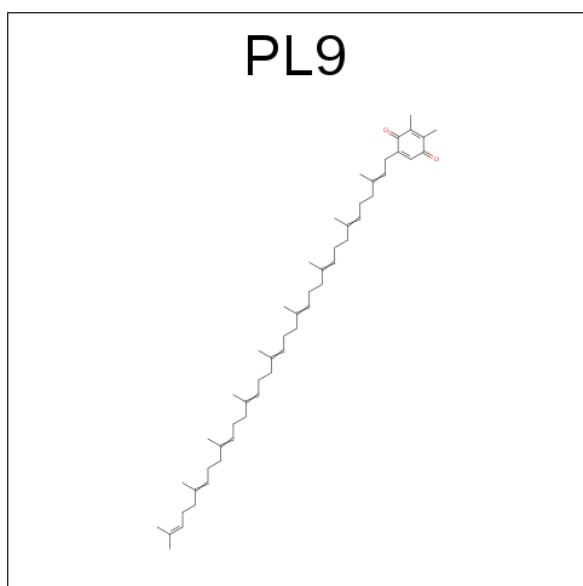
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0
26	D	1	Total C O S 45 32 12 1	0	0
26	L	1	Total C O S 54 41 12 1	0	0

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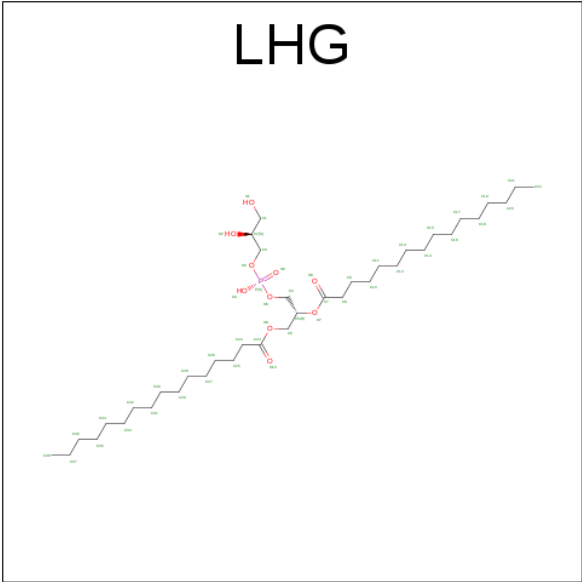
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	x	1	Total	C	O	S	0	0
			41	28	12	1		

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



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

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	P	0	0
			49	38	10	1		
28	D	1	Total	C	O	P	0	0
			49	38	10	1		
28	D	1	Total	C	O	P	0	0
			49	38	10	1		
28	D	1	Total	C	O	P	0	0
			46	35	10	1		
28	E	1	Total	C	O	P	0	0
			49	38	10	1		
28	K	1	Total	C	O	P	0	0
			44	35	8	1		
28	L	1	Total	C	O	P	0	0
			49	38	10	1		
28	a	1	Total	C	O	P	0	0
			49	38	10	1		
28	d	1	Total	C	O	P	0	0
			44	33	10	1		
28	d	1	Total	C	O	P	0	0
			49	38	10	1		
28	d	1	Total	C	O	P	0	0
			49	38	10	1		
28	d	1	Total	C	O	P	0	0
			46	35	10	1		
28	e	1	Total	C	O	P	0	0
			40	29	10	1		
28	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 29 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

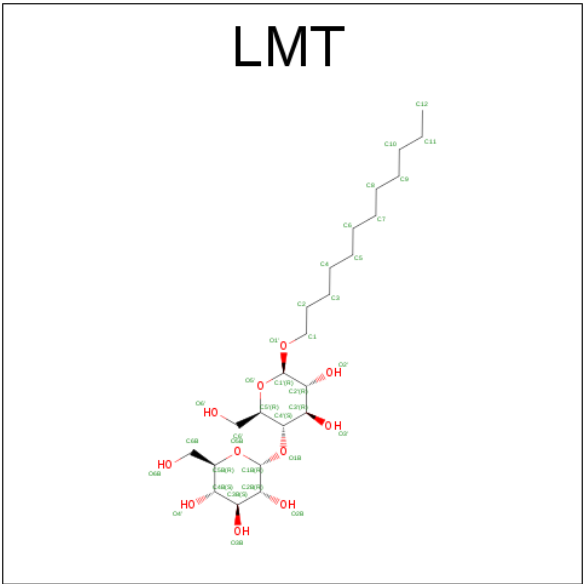
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	B	7	Total C 97 97	0	0
29	c	1	Total C 10 10	0	0
29	t	1	Total C 16 16	0	0
29	X	1	Total C 16 16	0	0
29	J	3	Total C 43 43	0	0
29	k	1	Total C 8 8	0	0
29	E	3	Total C 45 45	0	0
29	b	7	Total C 102 102	0	0
29	A	3	Total C 33 33	0	0
29	x	1	Total C 15 15	0	0
29	M	1	Total C 11 11	0	0
29	j	1	Total C 16 16	0	0
29	D	1	Total C 16 16	0	0
29	e	1	Total C 16 16	0	0
29	I	3	Total C 45 45	0	0
29	Z	2	Total C 23 23	0	0
29	a	2	Total C 16 16	0	0
29	U	1	Total C 14 14	0	0
29	m	1	Total C 11 11	0	0
29	d	2	Total C 27 27	0	0
29	H	1	Total C 14 14	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	i	4	Total	C	0	0
			64	64		
29	C	1	Total	C	0	0
			11	11		
29	z	1	Total	C	0	0
			13	13		
29	T	1	Total	C	0	0
			13	13		
29	u	2	Total	C	0	0
			27	27		

- Molecule 30 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			35	24	11		
30	B	1	Total	C	O	0	0
			35	24	11		
30	B	1	Total	C	O	0	0
			24	18	6		
30	B	1	Total	C	O	0	0
			24	18	6		
30	F	1	Total	C	O	0	0
			35	24	11		
30	I	1	Total	C	O	0	0
			35	24	11		

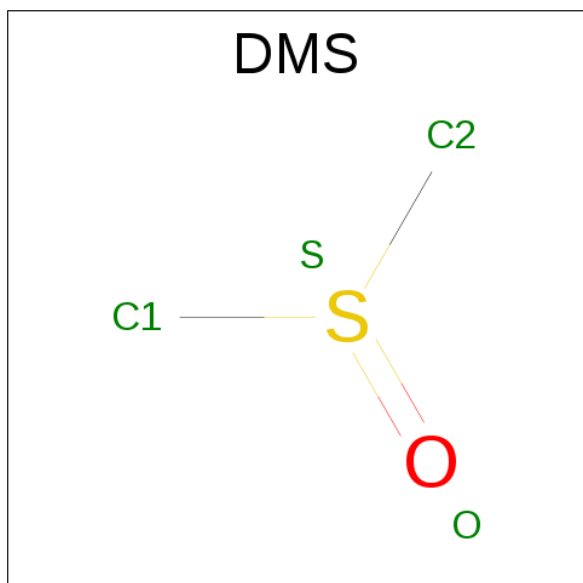
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	M	1	Total	C	O	0	0
			35	24	11		
30	T	1	Total	C	O	0	0
			24	18	6		
30	Z	1	Total	C	O	0	0
			35	24	11		
30	a	1	Total	C	O	0	0
			35	24	11		
30	a	1	Total	C	O	0	0
			35	24	11		
30	b	1	Total	C	O	0	0
			25	19	6		
30	e	1	Total	C	O	0	0
			25	19	6		
30	m	1	Total	C	O	0	0
			35	24	11		
30	m	1	Total	C	O	0	0
			35	24	11		
30	z	1	Total	C	O	0	0
			32	21	11		

- Molecule 31 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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
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	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

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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	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	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	H	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
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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	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	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	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	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

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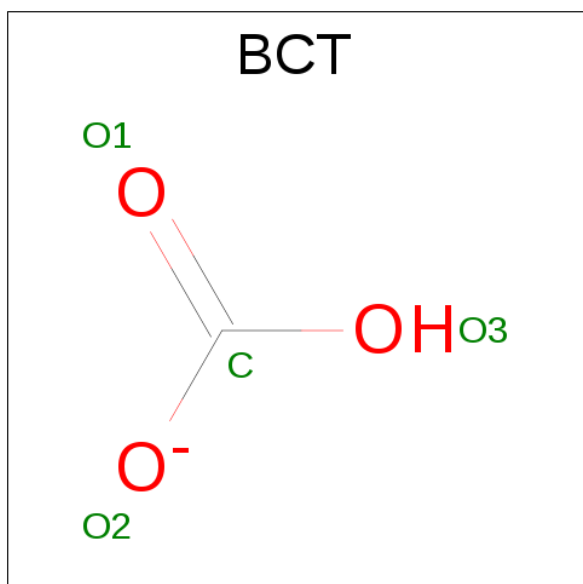
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	e	1	Total 4	C 2	O 1	S 1	0	0
31	h	1	Total 4	C 2	O 1	S 1	0	0
31	h	1	Total 4	C 2	O 1	S 1	0	0
31	h	1	Total 4	C 2	O 1	S 1	0	0
31	h	1	Total 4	C 2	O 1	S 1	0	0
31	i	1	Total 4	C 2	O 1	S 1	0	0
31	i	1	Total 4	C 2	O 1	S 1	0	0
31	k	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	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

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

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



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

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

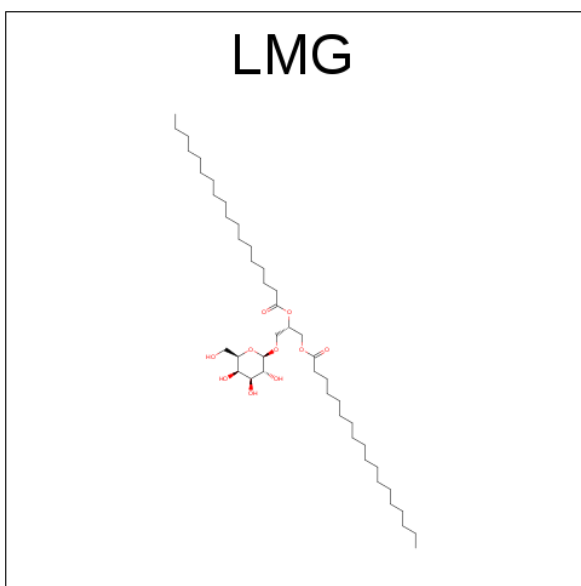
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	o	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	D	1	Total	C	O	0	0
			51	41	10		
34	J	1	Total	C	O	0	0
			51	41	10		
34	a	1	Total	C	O	0	0
			51	41	10		

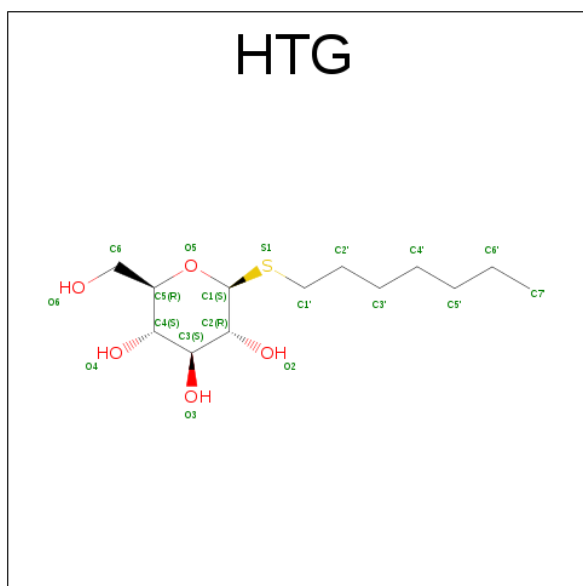
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	c	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	d	1	Total	C	O	0	0
			51	41	10		
34	j	1	Total	C	O	0	0
			51	41	10		
34	m	1	Total	C	O	0	0
			51	41	10		

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



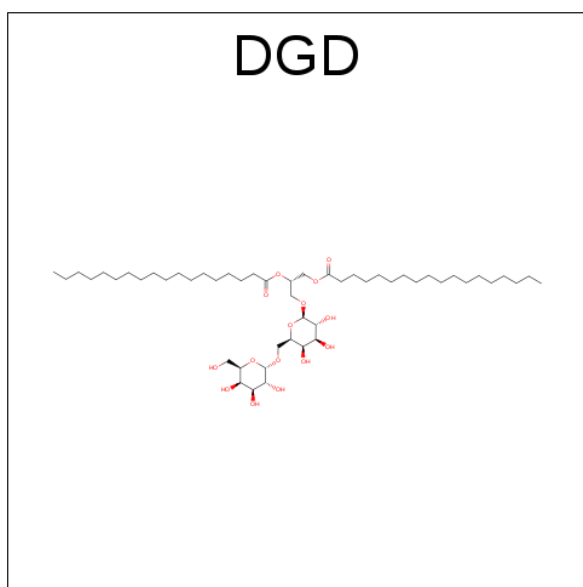
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			19	13	5	1		
35	O	1	Total	C	O	S	0	0
			19	13	5	1		
35	V	1	Total	C	O	S	0	0
			14	8	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			13	10	2	1		
35	d	1	Total	C	O	S	0	0
			19	13	5	1		
35	v	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>).



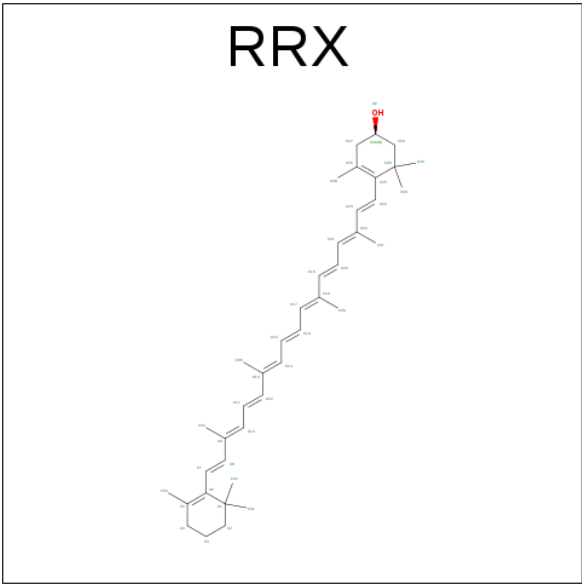
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			62	47	15		
36	D	1	Total	C	O	0	0
			50	41	9		
36	H	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C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

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: C<sub>40</sub>H<sub>56</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
38	H	1	Total	C	O	0	0
			41	40	1		
38	x	1	Total	C	O	0	0
			41	40	1		

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

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

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	A	176	Total	O	0	11
			187	187		
40	B	420	Total	O	0	17
			437	437		
40	C	286	Total	O	0	8
			294	294		
40	D	159	Total	O	0	7
			166	166		
40	E	44	Total	O	0	3
			47	47		
40	F	9	Total	O	0	0
			9	9		
40	H	54	Total	O	0	0
			54	54		
40	I	11	Total	O	0	2
			13	13		
40	J	16	Total	O	0	1
			17	17		
40	K	13	Total	O	0	1
			14	14		
40	L	23	Total	O	0	3
			26	26		
40	M	15	Total	O	0	2
			17	17		
40	O	251	Total	O	0	14
			265	265		
40	T	15	Total	O	0	1
			16	16		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	U	123	Total 128	O 128	0	5
40	V	165	Total 169	O 169	0	4
40	Y	8	Total 8	O 8	0	0
40	X	14	Total 14	O 14	0	0
40	Z	8	Total 10	O 10	0	2
40	a	172	Total 175	O 175	0	3
40	b	405	Total 423	O 423	0	18
40	c	300	Total 320	O 320	0	20
40	d	177	Total 185	O 185	0	8
40	e	52	Total 56	O 56	0	4
40	f	9	Total 9	O 9	0	0
40	h	56	Total 57	O 57	0	1
40	i	12	Total 13	O 13	0	1
40	j	13	Total 13	O 13	0	0
40	k	14	Total 14	O 14	0	0
40	l	16	Total 19	O 19	0	3
40	m	14	Total 15	O 15	0	1
40	o	223	Total 240	O 240	0	17
40	t	19	Total 21	O 21	0	2
40	u	146	Total 157	O 157	0	11
40	v	147	Total 154	O 154	0	7

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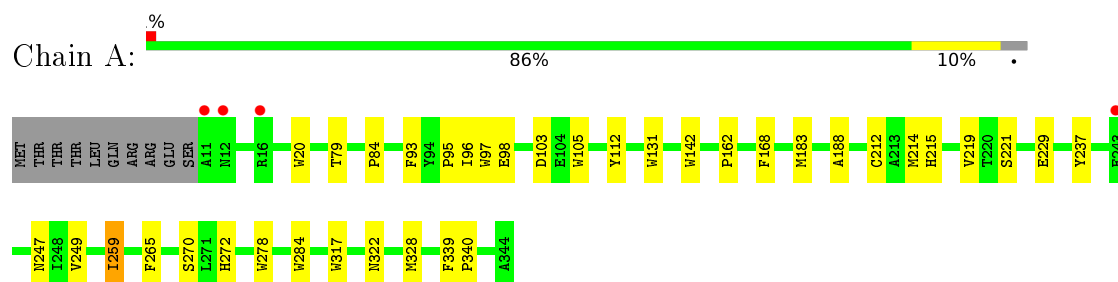
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	y	16	Total 16	O 16	0	0
40	x	18	Total 19	O 19	0	1
40	z	5	Total 5	O 5	0	0

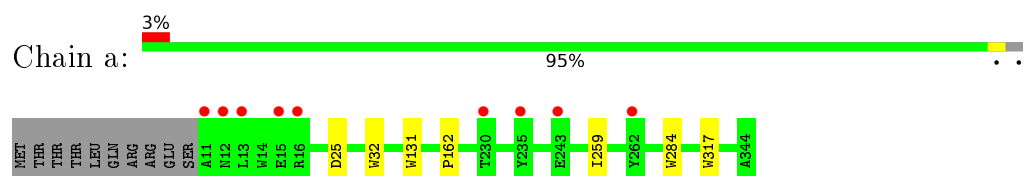
### 3 Residue-property plots [i](#)

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

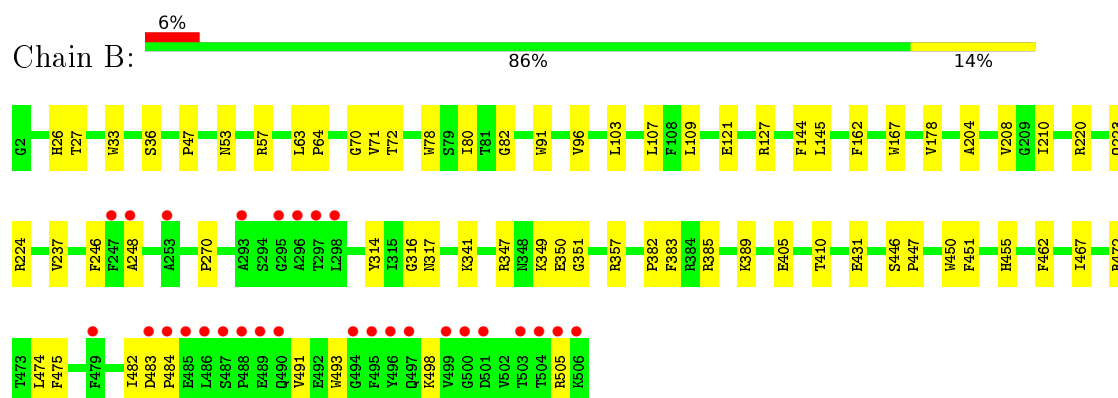
- Molecule 1: Photosystem II protein D1



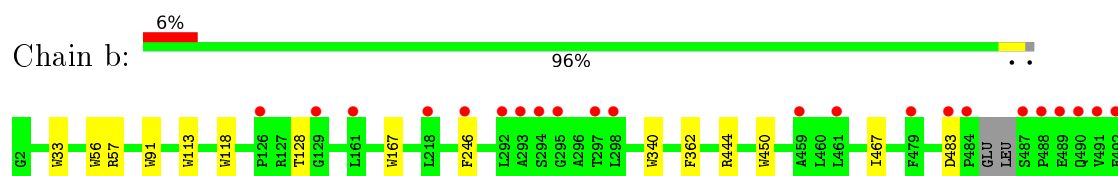
- Molecule 1: Photosystem II protein D1



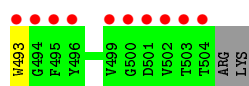
- Molecule 2: Photosystem II CP47 reaction center protein



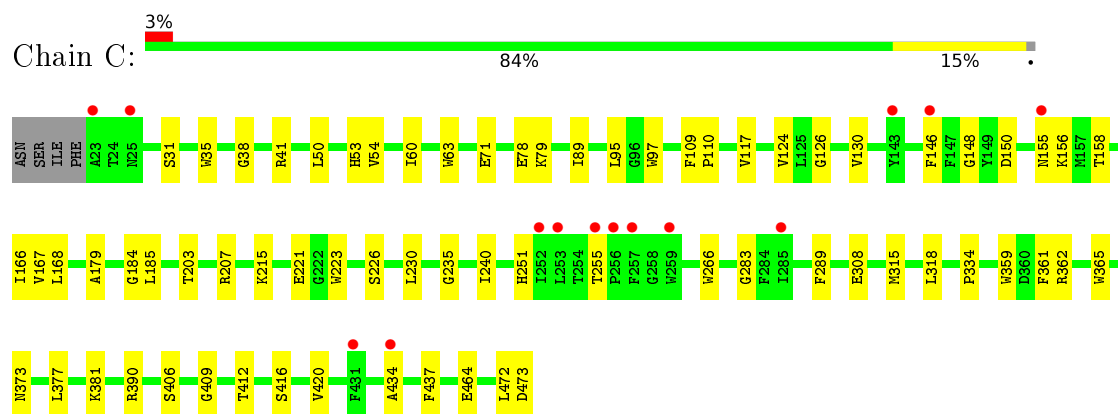
- Molecule 2: Photosystem II CP47 reaction center protein



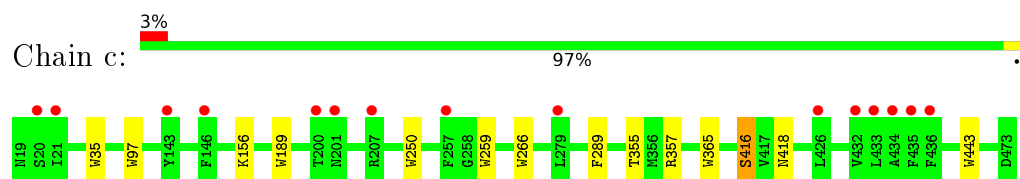




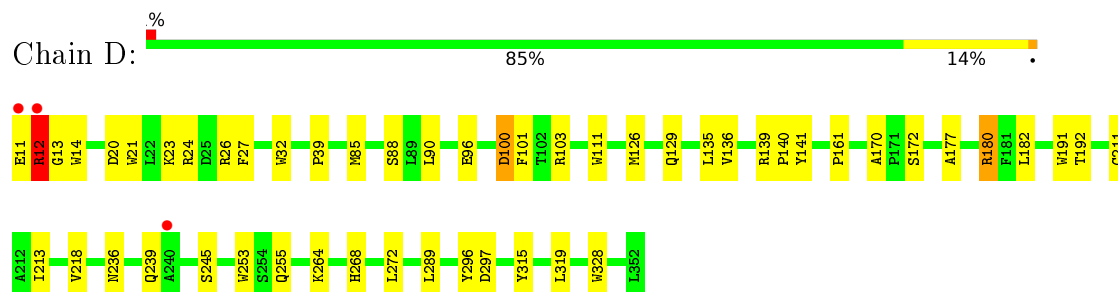
- Molecule 3: Photosystem II CP43 reaction center protein



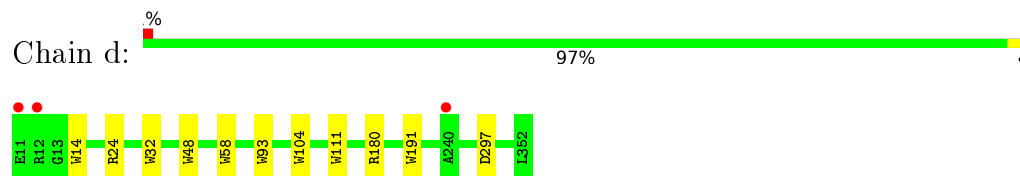
- Molecule 3: Photosystem II CP43 reaction center protein



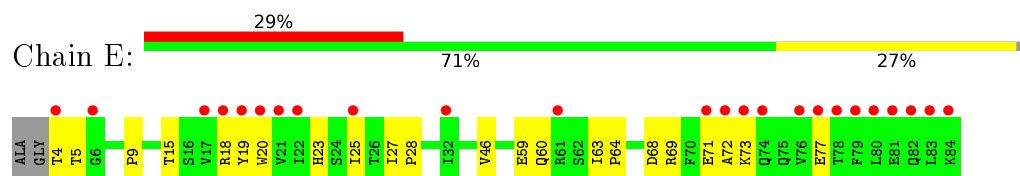
- Molecule 4: Photosystem II D2 protein



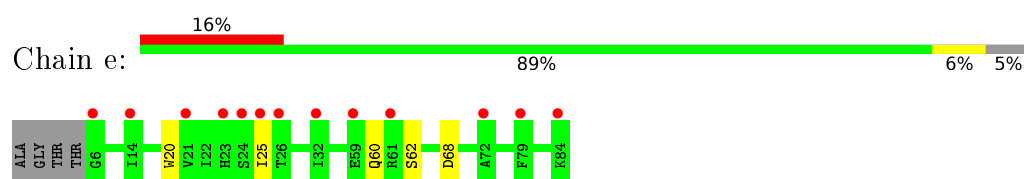
- Molecule 4: Photosystem II D2 protein



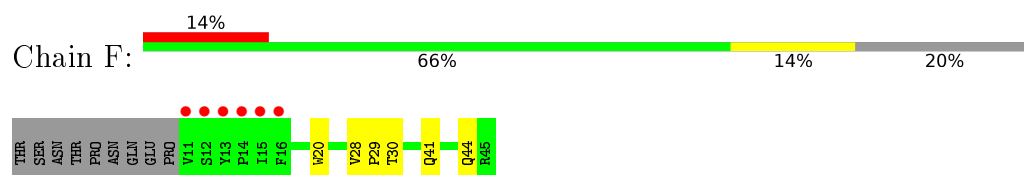
- Molecule 5: Cytochrome b559 subunit alpha



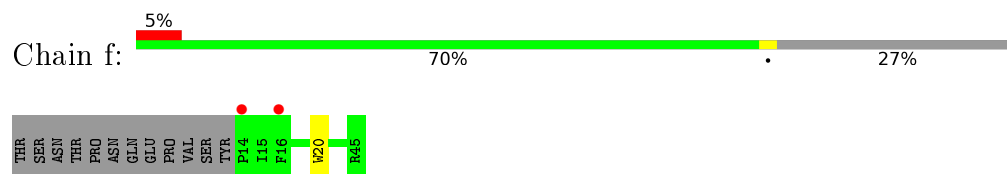
- Molecule 5: Cytochrome b559 subunit alpha



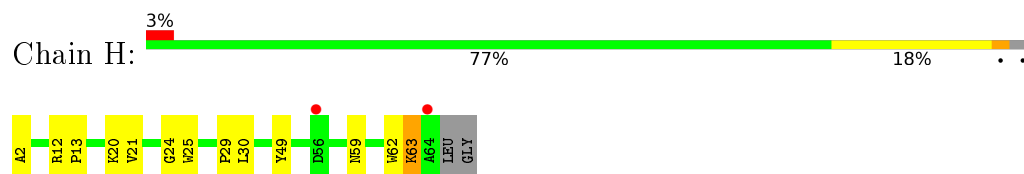
- Molecule 6: Cytochrome b559 subunit beta



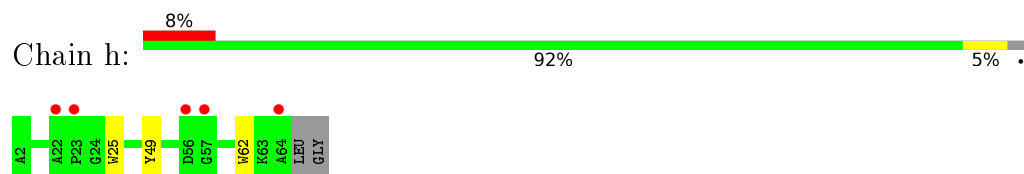
- Molecule 6: Cytochrome b559 subunit beta



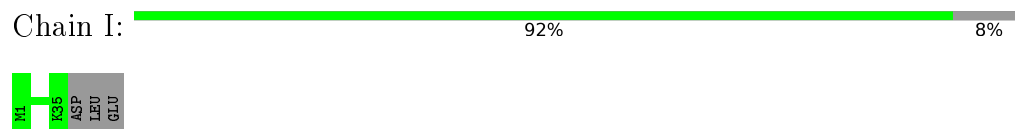
- Molecule 7: Photosystem II reaction center protein H



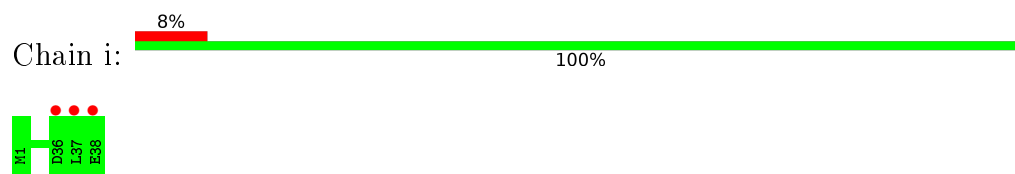
- Molecule 7: Photosystem II reaction center protein H



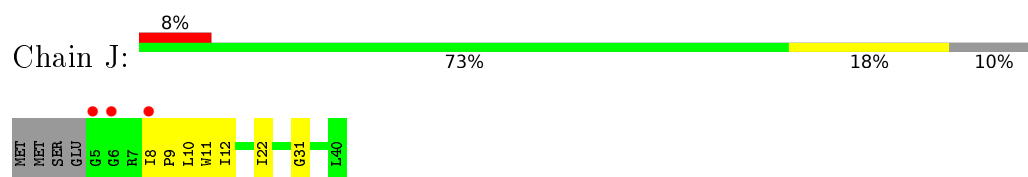
- Molecule 8: Photosystem II reaction center protein I



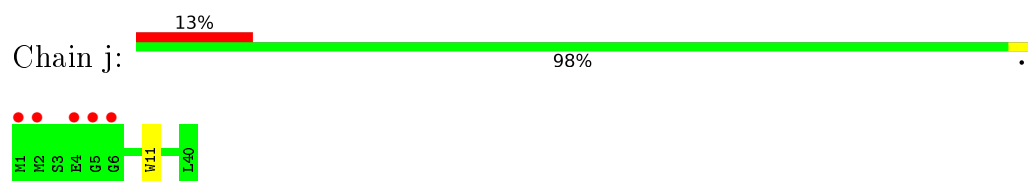
- Molecule 8: Photosystem II reaction center protein I



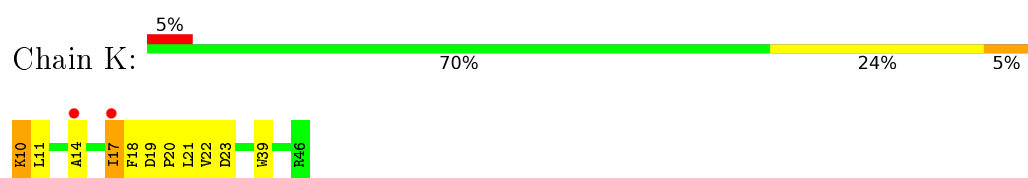
- Molecule 9: Photosystem II reaction center protein J



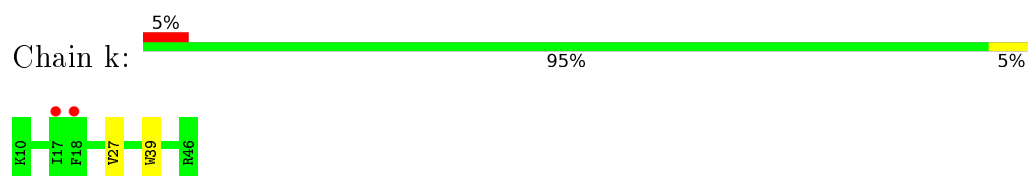
- Molecule 9: Photosystem II reaction center protein J



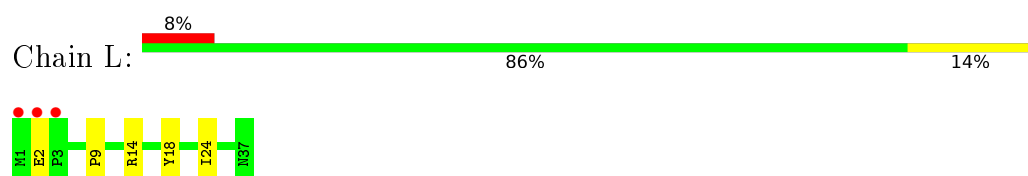
- Molecule 10: Photosystem II reaction center protein K



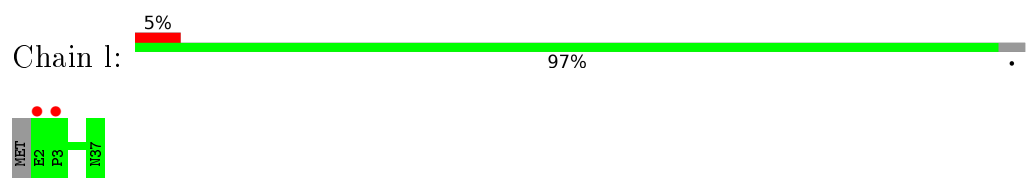
- Molecule 10: Photosystem II reaction center protein K



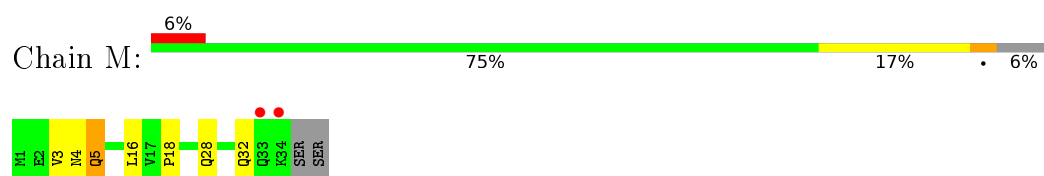
- Molecule 11: Photosystem II reaction center protein L



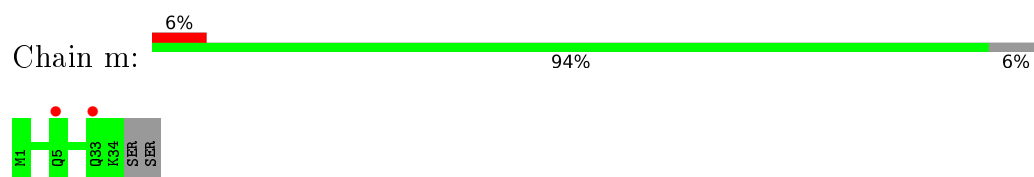
- Molecule 11: Photosystem II reaction center protein L



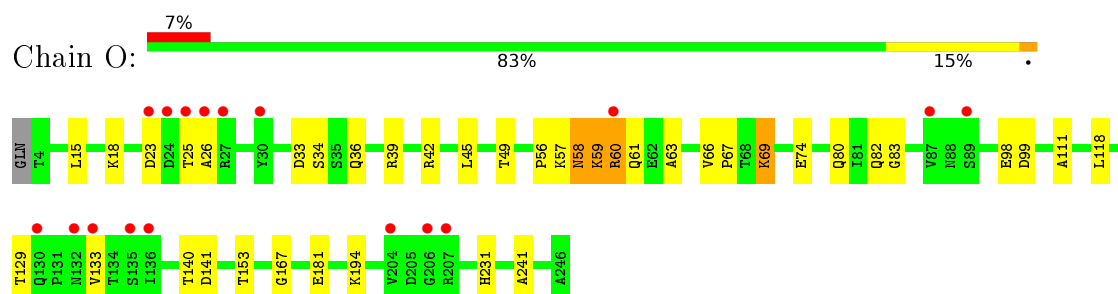
- Molecule 12: Photosystem II reaction center protein M



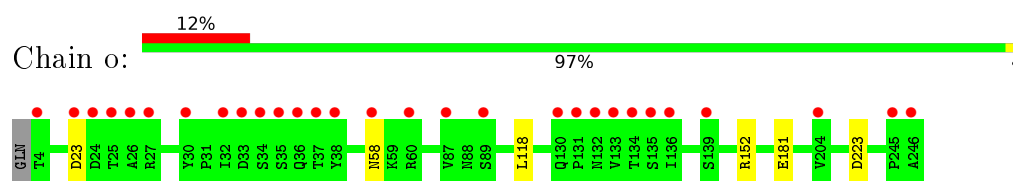
- Molecule 12: Photosystem II reaction center protein M



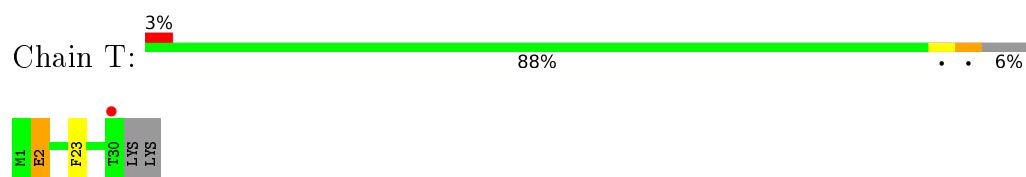
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



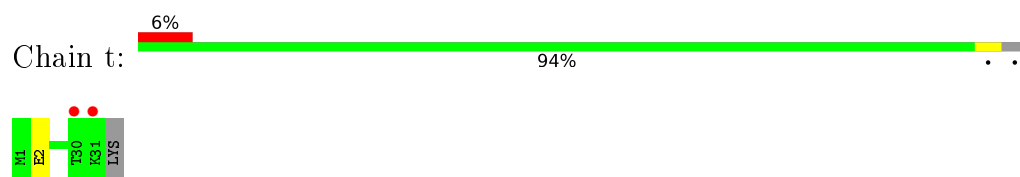
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



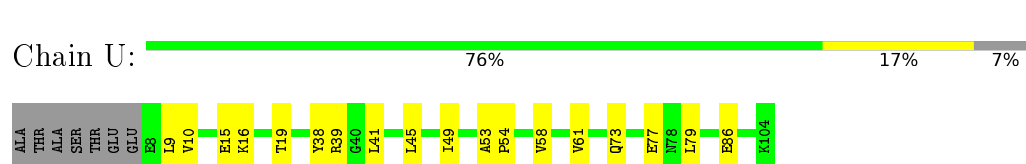
- Molecule 14: Photosystem II reaction center protein T



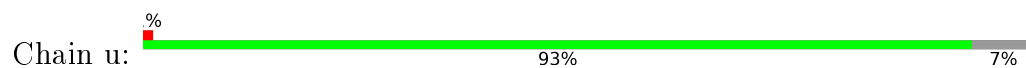
- Molecule 14: Photosystem II reaction center protein T

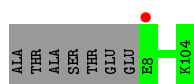


- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein





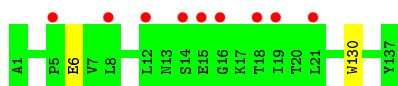
- Molecule 16: Cytochrome c-550

Chain V: 84% 15%



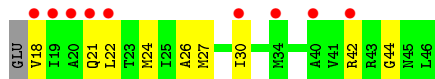
- Molecule 16: Cytochrome c-550

Chain v: 7% 99%



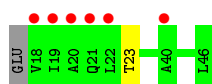
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 30% 67% 30%



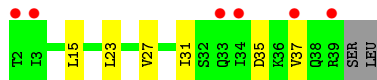
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 20% 93%



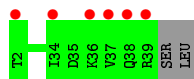
- Molecule 18: Photosystem II reaction center protein X

Chain X: 15% 80% 15% 5%



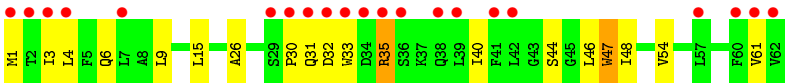
- Molecule 18: Photosystem II reaction center protein X

Chain x: 15% 95%

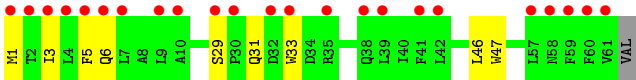
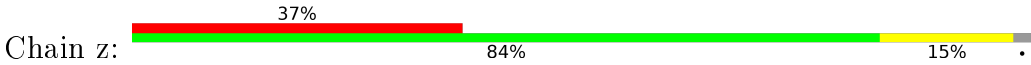


- Molecule 19: Photosystem II reaction center protein Z

Chain Z: 34% 69% 27%



● Molecule 19: Photosystem II reaction center protein Z



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.40Å 228.22Å 286.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 1.87 48.98 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.98-1.87) 99.8 (48.98-1.87)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.171 , 0.212 0.171 , 0.212	Depositor DCC
$R_{free}$ test set	32518 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 70.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	55401	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	1.02	5/2710 (0.2%)	0.81	1/3696 (0.0%)
1	a	0.99	4/2730 (0.1%)	0.81	1/3723 (0.0%)
2	B	0.94	4/4144 (0.1%)	0.82	4/5647 (0.1%)
2	b	0.98	9/4076 (0.2%)	0.83	3/5558 (0.1%)
3	C	0.91	6/3633 (0.2%)	0.78	1/4945 (0.0%)
3	c	0.91	9/3638 (0.2%)	0.78	1/4953 (0.0%)
4	D	1.01	4/2834 (0.1%)	0.83	2/3861 (0.1%)
4	d	1.02	8/2834 (0.3%)	0.82	1/3861 (0.0%)
5	E	0.74	1/670 (0.1%)	0.71	0/917
5	e	0.71	1/656 (0.2%)	0.73	0/896
6	F	0.83	1/289 (0.3%)	0.64	0/394
6	f	0.83	1/262 (0.4%)	0.65	0/356
7	H	0.85	1/530 (0.2%)	0.78	0/722
7	h	0.89	2/522 (0.4%)	0.79	0/711
8	I	0.66	0/282	0.67	0/381
8	i	0.68	0/300	0.67	0/406
9	J	0.80	1/257 (0.4%)	0.63	0/349
9	j	0.84	1/291 (0.3%)	0.69	0/393
10	K	0.73	1/303 (0.3%)	0.70	0/416
10	k	0.77	1/303 (0.3%)	0.71	0/416
11	L	0.94	0/316	0.80	0/430
11	l	0.98	0/307	0.80	0/418
12	M	0.78	0/270	0.75	0/369
12	m	0.72	0/270	0.74	0/369
13	O	0.78	0/1898	0.83	0/2577
13	o	0.74	0/1886	0.83	2/2562 (0.1%)
14	T	0.83	0/255	0.79	0/346
14	t	0.82	0/260	0.74	0/353
15	U	0.82	0/777	0.84	2/1055 (0.2%)
15	u	0.80	0/790	0.82	0/1071
16	V	0.88	0/1096	0.83	1/1487 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.78	1/1084 (0.1%)	0.76	0/1475
17	Y	0.54	0/211	0.71	0/282
17	y	0.51	0/208	0.63	0/278
18	X	0.61	0/286	0.73	0/387
18	x	0.60	0/278	0.71	0/376
19	Z	0.67	1/479 (0.2%)	0.67	0/656
19	z	0.63	2/468 (0.4%)	0.61	0/640
All	All	0.90	64/42403 (0.2%)	0.80	19/57732 (0.0%)

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	365	TRP	CD2-CE2	7.28	1.50	1.41
1	a	131	TRP	CD2-CE2	6.83	1.49	1.41
3	c	35	TRP	CD2-CE2	6.66	1.49	1.41
2	b	56	TRP	CD2-CE2	6.63	1.49	1.41
10	k	39	TRP	CD2-CE2	6.56	1.49	1.41

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	152	ARG	NE-CZ-NH2	-7.84	116.38	120.30
4	d	297	ASP	CB-CG-OD1	7.14	124.73	118.30
2	B	357	ARG	NE-CZ-NH2	-6.52	117.04	120.30
15	U	39	ARG	NE-CZ-NH2	-6.50	117.05	120.30
4	D	100	ASP	CB-CG-OD1	6.18	123.86	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	2622	0	2519	33	0
1	a	2633	0	2540	0	0
2	B	3992	0	3848	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	3929	0	3774	0	0
3	C	3511	0	3440	51	0
3	c	3521	0	3439	0	0
4	D	2733	0	2647	54	0
4	d	2733	0	2647	0	0
5	E	651	0	626	17	0
5	e	637	0	617	0	0
6	F	280	0	284	3	0
6	f	255	0	263	0	0
7	H	511	0	535	10	0
7	h	506	0	531	0	0
8	I	285	0	305	0	0
8	i	303	0	313	0	0
9	J	251	0	257	4	0
9	j	285	0	293	0	0
10	K	293	0	305	9	0
10	k	293	0	305	0	0
11	L	306	0	320	5	0
11	l	297	0	311	0	0
12	M	264	0	283	7	0
12	m	264	0	283	0	0
13	O	1861	0	1825	40	0
13	o	1852	0	1812	0	0
14	T	256	0	256	2	0
14	t	261	0	258	0	0
15	U	766	0	758	15	0
15	u	776	0	775	0	0
16	V	1072	0	1086	26	0
16	v	1060	0	1053	0	0
17	Y	210	0	230	6	0
17	y	207	0	221	0	0
18	X	280	0	312	9	0
18	x	275	0	301	0	0
19	Z	468	0	492	20	0
19	z	457	0	471	0	0
20	A	10	0	0	0	0
20	a	10	0	0	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	195	0	216	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	B	1040	0	1152	55	0
23	C	845	0	936	38	0
23	D	195	0	216	12	0
23	a	195	0	216	0	0
23	b	1040	0	1152	0	0
23	c	845	0	936	0	0
23	d	195	0	216	0	0
24	A	64	0	74	2	0
24	D	64	0	74	3	0
24	a	128	0	148	0	0
25	A	40	0	56	3	0
25	B	120	0	168	15	0
25	C	120	0	168	8	0
25	D	40	0	56	6	0
25	T	40	0	56	9	0
25	Y	40	0	56	1	0
25	a	40	0	56	0	0
25	b	120	0	168	0	0
25	c	80	0	112	0	0
25	d	40	0	56	0	0
25	j	40	0	56	0	0
25	k	40	0	56	0	0
25	t	40	0	56	0	0
26	A	108	0	155	11	0
26	B	54	0	78	4	0
26	D	45	0	57	2	0
26	L	54	0	78	3	0
26	a	108	0	156	0	0
26	x	41	0	49	0	0
27	A	55	0	80	12	0
27	D	55	0	80	0	0
27	a	55	0	80	0	0
27	d	55	0	80	0	0
28	A	49	0	74	1	0
28	D	144	0	213	8	0
28	E	49	0	74	7	0
28	K	44	0	67	0	0
28	L	49	0	74	1	0
28	a	49	0	74	0	0
28	d	188	0	274	0	0
28	e	40	0	53	0	0
28	l	49	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	A	33	0	0	1	0
29	B	97	0	0	1	0
29	C	11	0	0	0	0
29	D	16	0	0	0	0
29	E	45	0	0	0	0
29	H	14	0	0	0	0
29	I	45	0	0	0	0
29	J	43	0	0	1	0
29	M	11	0	0	0	0
29	T	13	0	0	0	0
29	U	14	0	0	3	0
29	X	16	0	0	0	0
29	Z	23	0	0	0	0
29	a	16	0	0	0	0
29	b	102	0	0	0	0
29	c	10	0	0	0	0
29	d	27	0	0	0	0
29	e	16	0	0	0	0
29	i	64	0	0	0	0
29	j	16	0	0	0	0
29	k	8	0	0	0	0
29	m	11	0	0	0	0
29	t	16	0	0	0	0
29	u	27	0	0	0	0
29	x	15	0	0	0	0
29	z	13	0	0	0	0
30	A	35	0	46	2	0
30	B	83	0	116	3	0
30	F	35	0	46	0	0
30	I	35	0	46	2	0
30	M	35	0	46	1	0
30	T	24	0	35	0	0
30	Z	35	0	46	7	0
30	a	70	0	92	0	0
30	b	25	0	35	0	0
30	e	25	0	35	0	0
30	m	70	0	92	0	0
30	z	32	0	33	0	0
31	A	24	0	36	4	0
31	B	48	0	72	26	0
31	C	28	0	42	3	0
31	D	12	0	18	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	F	4	0	6	6	0
31	H	8	0	12	6	0
31	O	36	0	54	20	0
31	U	12	0	18	4	0
31	V	36	0	54	14	0
31	a	16	0	24	0	0
31	b	60	0	90	0	0
31	c	48	0	72	0	0
31	d	20	0	30	0	0
31	e	4	0	6	0	0
31	h	16	0	24	0	0
31	i	8	0	12	0	0
31	k	4	0	6	0	0
31	l	4	0	6	0	0
31	o	12	0	18	0	0
31	u	16	0	24	0	0
31	v	32	0	48	0	0
32	A	4	0	0	0	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	51	0	72	2	0
34	C	153	0	216	4	0
34	D	51	0	72	5	0
34	J	51	0	72	3	0
34	a	51	0	72	0	0
34	c	102	0	144	0	0
34	d	51	0	72	0	0
34	j	51	0	72	0	0
34	m	51	0	72	0	0
35	B	95	0	130	1	0
35	C	57	0	78	1	0
35	D	19	0	26	3	0
35	O	19	0	26	2	0
35	V	14	0	13	2	0
35	b	76	0	104	0	0
35	c	51	0	70	0	0
35	d	19	0	26	0	0
35	v	19	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	C	186	0	246	2	0
36	D	50	0	69	10	0
36	H	62	0	82	0	0
36	c	186	0	246	0	0
36	d	50	0	69	0	0
36	h	62	0	82	0	0
37	E	43	0	30	1	0
37	V	43	0	30	0	0
37	e	43	0	30	0	0
37	v	43	0	30	0	0
38	H	41	0	56	0	0
38	x	41	0	56	0	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	A	187	0	0	6	0
40	B	437	0	0	15	0
40	C	294	0	0	4	0
40	D	166	0	0	5	0
40	E	47	0	0	0	0
40	F	9	0	0	0	0
40	H	54	0	0	2	0
40	I	13	0	0	0	0
40	J	17	0	0	3	0
40	K	14	0	0	1	0
40	L	26	0	0	1	0
40	M	17	0	0	1	0
40	O	265	0	0	17	0
40	T	16	0	0	0	0
40	U	128	0	0	5	0
40	V	169	0	0	9	0
40	X	14	0	0	0	0
40	Y	8	0	0	0	0
40	Z	10	0	0	2	0
40	a	175	0	0	0	0
40	b	423	0	0	0	0
40	c	320	0	0	0	0
40	d	185	0	0	0	0
40	e	56	0	0	0	0
40	f	9	0	0	0	0
40	h	57	0	0	0	0
40	i	13	0	0	0	0
40	j	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	k	14	0	0	0	0
40	l	19	0	0	0	0
40	m	15	0	0	0	0
40	o	240	0	0	0	0
40	t	21	0	0	0	0
40	u	157	0	0	0	0
40	v	154	0	0	0	0
40	x	19	0	0	0	0
40	y	16	0	0	0	0
40	z	5	0	0	0	0
All	All	55401	0	52590	528	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 7.

The worst 5 of 528 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:347[B]:ARG:NH2	40:B:1034[B]:HOH:O	1.80	1.13
1:A:214:MET:HG2	27:A:411:PL9:H102	1.20	1.12
19:Z:35:ARG:HH11	19:Z:35:ARG:HG2	1.18	1.04
2:B:350:GLU:HG3	31:B:639:DMS:H11	1.38	1.04
16:V:90:GLU:HB2	31:V:209:DMS:H13	21.51	1.01

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	333/344 (97%)	325 (98%)	7 (2%)	1 (0%)	46 33
1	a	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	46 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	507/505 (100%)	497 (98%)	10 (2%)	0	100	100
2	b	500/505 (99%)	490 (98%)	10 (2%)	0	100	100
3	C	453/455 (100%)	440 (97%)	12 (3%)	1 (0%)	52	40
3	c	454/455 (100%)	441 (97%)	12 (3%)	1 (0%)	52	40
4	D	342/342 (100%)	333 (97%)	8 (2%)	1 (0%)	46	33
4	d	342/342 (100%)	333 (97%)	9 (3%)	0	100	100
5	E	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
5	e	77/83 (93%)	76 (99%)	1 (1%)	0	100	100
6	F	33/44 (75%)	33 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
7	h	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	38/40 (95%)	38 (100%)	0	0	100	100
10	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
12	m	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
13	O	243/244 (100%)	229 (94%)	11 (4%)	3 (1%)	16	5
13	o	242/244 (99%)	230 (95%)	12 (5%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	29/32 (91%)	28 (97%)	1 (3%)	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	56 (93%)	3 (5%)	1 (2%)	11	2
19	z	59/62 (95%)	54 (92%)	3 (5%)	2 (3%)	5	0
All	All	5210/5350 (97%)	5059 (97%)	140 (3%)	11 (0%)	52	40

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	12	ARG
19	Z	31	GLN
3	c	416	SER
19	z	31	GLN
3	C	416	SER

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/279 (96%)	268 (100%)	1 (0%)	93	93
1	a	272/279 (98%)	271 (100%)	1 (0%)	93	93
2	B	403/403 (100%)	399 (99%)	4 (1%)	82	79
2	b	394/403 (98%)	389 (99%)	5 (1%)	76	71
3	C	355/356 (100%)	351 (99%)	4 (1%)	80	77
3	c	356/356 (100%)	351 (99%)	5 (1%)	74	69
4	D	278/277 (100%)	274 (99%)	4 (1%)	74	69
4	d	278/277 (100%)	276 (99%)	2 (1%)	88	87
5	E	70/72 (97%)	68 (97%)	2 (3%)	50	37
5	e	68/72 (94%)	64 (94%)	4 (6%)	24	11
6	F	28/38 (74%)	27 (96%)	1 (4%)	42	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	f	25/38 (66%)	25 (100%)	0	100	100
7	H	55/54 (102%)	53 (96%)	2 (4%)	42	28
7	h	54/54 (100%)	53 (98%)	1 (2%)	65	56
8	I	30/34 (88%)	30 (100%)	0	100	100
8	i	31/34 (91%)	31 (100%)	0	100	100
9	J	23/28 (82%)	22 (96%)	1 (4%)	35	21
9	j	27/28 (96%)	27 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	20	8
10	k	30/30 (100%)	29 (97%)	1 (3%)	45	31
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	30/33 (91%)	29 (97%)	1 (3%)	45	31
12	m	30/33 (91%)	30 (100%)	0	100	100
13	O	205/207 (99%)	200 (98%)	5 (2%)	57	46
13	o	203/207 (98%)	199 (98%)	4 (2%)	63	54
14	T	25/28 (89%)	24 (96%)	1 (4%)	38	24
14	t	25/28 (89%)	24 (96%)	1 (4%)	38	24
15	U	82/89 (92%)	82 (100%)	0	100	100
15	u	84/89 (94%)	84 (100%)	0	100	100
16	V	118/117 (101%)	115 (98%)	3 (2%)	55	44
16	v	115/117 (98%)	114 (99%)	1 (1%)	84	82
17	Y	20/23 (87%)	18 (90%)	2 (10%)	9	3
17	y	19/23 (83%)	18 (95%)	1 (5%)	28	14
18	X	30/33 (91%)	30 (100%)	0	100	100
18	x	29/33 (88%)	29 (100%)	0	100	100
19	Z	49/52 (94%)	47 (96%)	2 (4%)	37	23
19	z	46/52 (88%)	41 (89%)	5 (11%)	8	2
All	All	4255/4376 (97%)	4189 (98%)	66 (2%)	72	63

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

Mol	Chain	Res	Type
16	V	86	GLN

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Mol	Chain	Res	Type
2	b	128	THR
17	y	23	THR
16	V	122	GLU
19	Z	4	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	331	ASN
3	c	201	ASN
13	o	82	GLN
2	b	179	GLN
13	o	231	HIS

### 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	8,9,10	0.73	0	5,9,11	1.32	1 (20%)
14	FME	T	1	14	8,9,10	0.48	0	5,9,11	2.00	2 (40%)
8	FME	i	1	8	8,9,10	0.68	0	5,9,11	1.95	2 (40%)
14	FME	t	1	14	8,9,10	0.63	0	5,9,11	1.82	2 (40%)

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
14	FME	T	1	14	-	0/6/9/11	0/0/0/0
8	FME	i	1	8	-	0/6/9/11	0/0/0/0
14	FME	t	1	14	-	0/6/9/11	0/0/0/0

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	O1-CN-N	-3.56	119.36	124.80
14	T	1	FME	O-C-CA	-2.72	118.27	125.69
14	t	1	FME	O-C-CA	-2.59	118.60	125.69
8	i	1	FME	O-C-CA	-2.26	119.50	125.69
8	I	1	FME	O1-CN-N	-2.13	121.54	124.80

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 366 ligands modelled in this entry, 53 are unknown and 13 are monoatomic - leaving 300 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
20	OEX	A	401	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	A	405	-	57,73,73	1.69	12 (21%)	61,113,113	2.26	21 (34%)
23	CLA	A	406	40	57,73,73	1.47	9 (15%)	61,113,113	2.26	19 (31%)
24	PHO	A	407	-	67,69,69	1.72	11 (16%)	86,99,99	2.03	24 (27%)
23	CLA	A	408	-	57,73,73	1.67	11 (19%)	61,113,113	2.15	20 (32%)
25	BCR	A	409	-	41,41,41	1.05	3 (7%)	56,56,56	1.44	10 (17%)
26	SQD	A	410	-	53,54,54	1.37	3 (5%)	62,65,65	2.32	17 (27%)
27	PL9	A	411	-	54,55,55	0.75	2 (3%)	68,69,69	1.68	15 (22%)
28	LHG	A	412	-	48,48,48	1.03	2 (4%)	49,54,54	1.00	4 (8%)
26	SQD	A	415	-	53,54,54	1.56	3 (5%)	62,65,65	2.32	12 (19%)
30	LMT	A	416	-	36,36,36	0.82	1 (2%)	47,47,47	1.26	6 (12%)
31	DMS	A	418	-	3,3,3	2.74	1 (33%)	3,3,3	0.59	0
31	DMS	A	419	-	3,3,3	2.75	1 (33%)	3,3,3	0.65	0
32	BCT	A	420	21	0,3,3	0.00	-	0,3,3	0.00	-
31	DMS	A	421	-	3,3,3	2.72	1 (33%)	3,3,3	0.74	0
31	DMS	A	422	-	3,3,3	2.68	1 (33%)	3,3,3	0.77	0
31	DMS	A	423	-	3,3,3	1.92	1 (33%)	3,3,3	0.61	0
31	DMS	A	424	-	3,3,3	2.76	1 (33%)	3,3,3	0.97	0
23	CLA	B	602	40	57,73,73	1.84	11 (19%)	61,113,113	2.22	15 (24%)
23	CLA	B	603	-	57,73,73	1.89	13 (22%)	61,113,113	2.02	19 (31%)
23	CLA	B	604	-	57,73,73	1.66	10 (17%)	61,113,113	2.70	21 (34%)
23	CLA	B	605	-	57,73,73	1.56	11 (19%)	61,113,113	2.03	18 (29%)
23	CLA	B	606	-	57,73,73	1.64	12 (21%)	61,113,113	2.04	17 (27%)
23	CLA	B	607	-	57,73,73	1.83	12 (21%)	61,113,113	2.13	18 (29%)
23	CLA	B	608	40	57,73,73	1.70	10 (17%)	61,113,113	2.14	18 (29%)
23	CLA	B	609	-	57,73,73	1.67	11 (19%)	61,113,113	2.02	16 (26%)
23	CLA	B	610	-	57,73,73	1.67	10 (17%)	61,113,113	2.22	16 (26%)
23	CLA	B	611	40	57,73,73	1.80	13 (22%)	61,113,113	2.13	16 (26%)
23	CLA	B	612	-	57,73,73	1.61	12 (21%)	61,113,113	2.05	15 (24%)
23	CLA	B	613	-	57,73,73	1.64	11 (19%)	61,113,113	2.20	23 (37%)
23	CLA	B	614	-	57,73,73	1.58	13 (22%)	61,113,113	1.95	16 (26%)
23	CLA	B	615	-	57,73,73	1.78	12 (21%)	61,113,113	2.09	17 (27%)
23	CLA	B	616	-	57,73,73	1.77	13 (22%)	61,113,113	1.91	15 (24%)
23	CLA	B	617	-	57,73,73	1.76	12 (21%)	61,113,113	2.13	18 (29%)
25	BCR	B	618	-	41,41,41	1.05	2 (4%)	56,56,56	1.47	10 (17%)
25	BCR	B	619	-	41,41,41	1.06	2 (4%)	56,56,56	1.18	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	B	620	-	41,41,41	0.99	1 (2%)	56,56,56	1.59	12 (21%)
26	SQD	B	621	-	53,54,54	1.30	4 (7%)	62,65,65	2.05	7 (11%)
34	LMG	B	622	-	51,51,55	0.96	3 (5%)	59,59,63	1.30	9 (15%)
30	LMT	B	623	-	36,36,36	0.57	0	47,47,47	1.08	3 (6%)
35	HTG	B	624	-	19,19,19	1.41	3 (15%)	22,24,24	1.80	4 (18%)
35	HTG	B	625	-	19,19,19	1.35	2 (10%)	22,24,24	2.16	8 (36%)
35	HTG	B	626	-	19,19,19	0.88	1 (5%)	22,24,24	2.08	1 (4%)
35	HTG	B	630	-	19,19,19	0.92	2 (10%)	22,24,24	1.60	2 (9%)
35	HTG	B	631	-	19,19,19	1.03	1 (5%)	22,24,24	1.44	2 (9%)
31	DMS	B	636	-	3,3,3	3.10	1 (33%)	3,3,3	0.72	0
31	DMS	B	637	-	3,3,3	2.27	1 (33%)	3,3,3	0.89	0
31	DMS	B	638	-	3,3,3	2.78	1 (33%)	3,3,3	0.92	0
31	DMS	B	639	-	3,3,3	2.77	1 (33%)	3,3,3	0.81	0
31	DMS	B	640	-	3,3,3	2.64	1 (33%)	3,3,3	0.70	0
31	DMS	B	641	-	3,3,3	2.83	1 (33%)	3,3,3	0.74	0
31	DMS	B	642	-	3,3,3	2.93	1 (33%)	3,3,3	1.17	0
30	LMT	B	643	-	24,24,36	0.38	0	29,29,47	0.93	2 (6%)
30	LMT	B	644	-	24,24,36	0.33	0	29,29,47	1.28	5 (17%)
31	DMS	B	645	-	3,3,3	2.81	1 (33%)	3,3,3	0.64	0
31	DMS	B	646	-	3,3,3	2.61	1 (33%)	3,3,3	0.65	0
31	DMS	B	647	-	3,3,3	2.73	1 (33%)	3,3,3	0.50	0
31	DMS	B	648	-	3,3,3	2.49	1 (33%)	3,3,3	0.96	0
31	DMS	B	649	-	3,3,3	2.71	1 (33%)	3,3,3	0.50	0
34	LMG	C	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.21	4 (6%)
23	CLA	C	502	-	57,73,73	1.70	11 (19%)	61,113,113	2.12	10 (16%)
23	CLA	C	503	-	57,73,73	1.84	11 (19%)	61,113,113	2.06	16 (26%)
23	CLA	C	504	-	57,73,73	1.97	12 (21%)	61,113,113	1.89	16 (26%)
23	CLA	C	505	40	57,73,73	1.72	11 (19%)	61,113,113	2.17	15 (24%)
23	CLA	C	506	-	57,73,73	1.89	13 (22%)	61,113,113	2.11	16 (26%)
23	CLA	C	507	-	57,73,73	1.87	12 (21%)	61,113,113	2.16	19 (31%)
23	CLA	C	508	40	57,73,73	1.89	12 (21%)	61,113,113	2.21	18 (29%)
23	CLA	C	509	-	57,73,73	1.97	12 (21%)	61,113,113	1.81	14 (22%)
23	CLA	C	510	-	57,73,73	1.82	11 (19%)	61,113,113	2.18	19 (31%)
23	CLA	C	511	-	57,73,73	1.90	12 (21%)	61,113,113	2.08	16 (26%)
23	CLA	C	512	3	57,73,73	1.78	12 (21%)	61,113,113	1.95	16 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	C	513	-	57,73,73	2.08	12 (21%)	61,113,113	1.91	16 (26%)
23	CLA	C	514	-	57,73,73	1.99	13 (22%)	61,113,113	1.90	15 (24%)
25	BCR	C	515	-	41,41,41	0.82	0	56,56,56	1.52	8 (14%)
25	BCR	C	516	-	41,41,41	0.99	0	56,56,56	1.38	7 (12%)
36	DGD	C	517	-	63,63,67	0.80	2 (3%)	77,77,81	1.24	9 (11%)
36	DGD	C	518	-	63,63,67	0.93	3 (4%)	77,77,81	1.11	5 (6%)
36	DGD	C	519	-	63,63,67	0.84	2 (3%)	77,77,81	1.13	6 (7%)
34	LMG	C	520	-	51,51,55	1.12	2 (3%)	59,59,63	1.36	9 (15%)
35	HTG	C	521	-	19,19,19	0.91	2 (10%)	22,24,24	2.26	1 (4%)
35	HTG	C	522	-	19,19,19	0.98	1 (5%)	22,24,24	2.31	3 (13%)
35	HTG	C	523	-	19,19,19	1.03	2 (10%)	22,24,24	2.33	1 (4%)
31	DMS	C	524	-	3,3,3	2.40	1 (33%)	3,3,3	0.88	0
31	DMS	C	525	-	3,3,3	2.63	1 (33%)	3,3,3	0.84	0
31	DMS	C	526	-	3,3,3	2.74	1 (33%)	3,3,3	0.53	0
31	DMS	C	527	-	3,3,3	2.57	1 (33%)	3,3,3	0.58	0
31	DMS	C	528	-	3,3,3	2.65	1 (33%)	3,3,3	0.64	0
31	DMS	C	529	-	3,3,3	2.56	1 (33%)	3,3,3	0.42	0
25	BCR	C	530	-	41,41,41	0.82	0	56,56,56	1.57	9 (16%)
34	LMG	C	531	-	51,51,55	1.00	2 (3%)	59,59,63	1.09	5 (8%)
31	DMS	C	533	-	3,3,3	2.67	1 (33%)	3,3,3	0.47	0
23	CLA	D	401	40	57,73,73	1.86	12 (21%)	61,113,113	2.29	21 (34%)
24	PHO	D	402	-	67,69,69	1.91	14 (20%)	86,99,99	1.86	20 (23%)
23	CLA	D	403	-	57,73,73	1.64	11 (19%)	61,113,113	2.52	20 (32%)
23	CLA	D	404	-	57,73,73	1.75	12 (21%)	61,113,113	1.80	18 (29%)
25	BCR	D	405	-	41,41,41	1.09	3 (7%)	56,56,56	2.00	13 (23%)
27	PL9	D	406	-	54,55,55	0.96	3 (5%)	68,69,69	1.61	13 (19%)
36	DGD	D	407	-	50,50,67	1.25	3 (6%)	58,58,81	1.85	8 (13%)
26	SQD	D	408	-	44,45,54	1.55	4 (9%)	53,56,65	2.59	12 (22%)
28	LHG	D	409	-	48,48,48	0.84	1 (2%)	49,54,54	1.29	6 (12%)
28	LHG	D	410	-	48,48,48	0.81	2 (4%)	49,54,54	1.13	3 (6%)
28	LHG	D	411	-	45,45,48	0.96	2 (4%)	46,51,54	1.03	3 (6%)
34	LMG	D	412	-	51,51,55	1.07	2 (3%)	59,59,63	1.43	8 (13%)
35	HTG	D	414	-	19,19,19	0.88	1 (5%)	22,24,24	1.72	1 (4%)
31	DMS	D	415	-	3,3,3	2.75	1 (33%)	3,3,3	0.64	0
31	DMS	D	416	-	3,3,3	2.50	1 (33%)	3,3,3	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	DMS	D	417	-	3,3,3	3.00	1 (33%)	3,3,3	0.69	0
28	LHG	E	101	-	48,48,48	1.04	2 (4%)	49,54,54	1.21	5 (10%)
37	HEM	E	105	5,6	24,50,50	2.11	10 (41%)	16,82,82	2.49	6 (37%)
30	LMT	F	101	-	36,36,36	0.69	1 (2%)	47,47,47	1.22	5 (10%)
31	DMS	F	102	-	3,3,3	2.62	1 (33%)	3,3,3	0.23	0
31	DMS	H	101	-	3,3,3	2.78	1 (33%)	3,3,3	0.53	0
38	RRX	H	102	-	42,42,42	0.87	1 (2%)	57,58,58	1.57	9 (15%)
36	DGD	H	103	-	63,63,67	1.03	3 (4%)	77,77,81	1.32	7 (9%)
31	DMS	H	105	-	3,3,3	2.75	1 (33%)	3,3,3	0.60	0
30	LMT	I	101	-	36,36,36	0.72	1 (2%)	47,47,47	1.46	5 (10%)
34	LMG	J	101	39	51,51,55	0.91	2 (3%)	59,59,63	0.98	5 (8%)
28	LHG	K	101	-	43,43,48	1.06	2 (4%)	46,48,54	1.14	4 (8%)
28	LHG	L	101	-	48,48,48	0.94	3 (6%)	49,54,54	1.14	3 (6%)
26	SQD	L	102	-	53,54,54	1.46	3 (5%)	62,65,65	2.04	12 (19%)
30	LMT	M	101	-	36,36,36	0.62	0	47,47,47	0.98	2 (4%)
35	HTG	O	302	-	19,19,19	1.37	3 (15%)	22,24,24	1.56	4 (18%)
31	DMS	O	303	-	3,3,3	2.69	1 (33%)	3,3,3	0.52	0
31	DMS	O	304	-	3,3,3	2.80	1 (33%)	3,3,3	0.78	0
31	DMS	O	305	-	3,3,3	2.66	1 (33%)	3,3,3	0.80	0
31	DMS	O	306	-	3,3,3	2.71	1 (33%)	3,3,3	0.50	0
31	DMS	O	307	-	3,3,3	2.75	1 (33%)	3,3,3	0.67	0
31	DMS	O	308	-	3,3,3	2.73	1 (33%)	3,3,3	0.62	0
31	DMS	O	309	-	3,3,3	2.88	1 (33%)	3,3,3	0.85	0
31	DMS	O	310	-	3,3,3	2.62	1 (33%)	3,3,3	0.64	0
31	DMS	O	311	-	3,3,3	2.65	1 (33%)	3,3,3	0.80	0
25	BCR	T	101	-	41,41,41	0.88	0	56,56,56	1.81	17 (30%)
30	LMT	T	103	-	24,24,36	0.49	0	29,29,47	1.35	4 (13%)
31	DMS	U	202	-	3,3,3	2.69	1 (33%)	3,3,3	1.47	1 (33%)
31	DMS	U	203	-	3,3,3	2.71	1 (33%)	3,3,3	0.45	0
31	DMS	U	204	-	3,3,3	2.89	1 (33%)	3,3,3	0.75	0
31	DMS	V	201	-	3,3,3	2.58	1 (33%)	3,3,3	0.68	0
31	DMS	V	202	-	3,3,3	2.66	1 (33%)	3,3,3	0.73	0
37	HEM	V	203	16	24,50,50	2.15	7 (29%)	16,82,82	1.98	4 (25%)
35	HTG	V	204	-	14,14,19	0.63	0	17,19,24	2.51	5 (29%)
31	DMS	V	205	-	3,3,3	2.64	1 (33%)	3,3,3	0.86	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	DMS	V	206	-	3,3,3	2.66	1 (33%)	3,3,3	0.69	0
31	DMS	V	207	-	3,3,3	2.85	1 (33%)	3,3,3	1.14	0
31	DMS	V	208	-	3,3,3	2.60	1 (33%)	3,3,3	0.37	0
31	DMS	V	209	-	3,3,3	2.53	1 (33%)	3,3,3	0.75	0
31	DMS	V	210	-	3,3,3	2.71	1 (33%)	3,3,3	0.47	0
31	DMS	V	211	-	3,3,3	2.98	1 (33%)	3,3,3	0.96	0
25	BCR	Y	101	-	41,41,41	0.83	0	56,56,56	1.69	14 (25%)
30	LMT	Z	101	-	36,36,36	0.67	1 (2%)	47,47,47	0.91	2 (4%)
31	DMS	a	401	-	3,3,3	2.71	1 (33%)	3,3,3	0.63	0
20	OEX	a	402	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
23	CLA	a	406	-	57,73,73	1.74	12 (21%)	61,113,113	2.32	22 (36%)
23	CLA	a	407	40	57,73,73	1.67	13 (22%)	61,113,113	2.39	16 (26%)
24	PHO	a	408	-	67,69,69	1.76	14 (20%)	86,99,99	1.76	20 (23%)
24	PHO	a	409	-	67,69,69	1.88	15 (22%)	86,99,99	1.98	23 (26%)
23	CLA	a	410	-	57,73,73	1.80	10 (17%)	61,113,113	2.28	22 (36%)
25	BCR	a	411	-	41,41,41	1.17	2 (4%)	56,56,56	1.35	5 (8%)
26	SQD	a	412	-	53,54,54	1.43	3 (5%)	62,65,65	2.64	12 (19%)
34	LMG	a	413	-	51,51,55	0.97	2 (3%)	59,59,63	1.14	4 (6%)
27	PL9	a	414	-	54,55,55	0.78	2 (3%)	68,69,69	1.73	18 (26%)
28	LHG	a	415	-	48,48,48	0.99	2 (4%)	49,54,54	1.09	3 (6%)
26	SQD	a	417	-	53,54,54	1.60	4 (7%)	62,65,65	1.45	7 (11%)
30	LMT	a	418	-	36,36,36	0.69	1 (2%)	47,47,47	1.30	5 (10%)
31	DMS	a	420	-	3,3,3	2.66	1 (33%)	3,3,3	0.32	0
31	DMS	a	421	-	3,3,3	2.68	1 (33%)	3,3,3	0.57	0
30	LMT	a	422	-	36,36,36	0.63	1 (2%)	47,47,47	1.02	3 (6%)
31	DMS	a	423	-	3,3,3	2.81	1 (33%)	3,3,3	0.74	0
32	BCT	a	424	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	b	602	40	57,73,73	1.94	13 (22%)	61,113,113	2.21	21 (34%)
23	CLA	b	603	-	57,73,73	1.72	13 (22%)	61,113,113	2.37	21 (34%)
23	CLA	b	604	-	57,73,73	1.65	11 (19%)	61,113,113	2.36	19 (31%)
23	CLA	b	605	-	57,73,73	1.68	11 (19%)	61,113,113	2.16	21 (34%)
23	CLA	b	606	-	57,73,73	1.52	11 (19%)	61,113,113	2.23	17 (27%)
23	CLA	b	607	-	57,73,73	1.82	12 (21%)	61,113,113	1.91	13 (21%)
23	CLA	b	608	40	57,73,73	1.72	11 (19%)	61,113,113	2.07	18 (29%)
23	CLA	b	609	-	57,73,73	1.73	10 (17%)	61,113,113	2.23	22 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	b	610	-	57,73,73	1.86	13 (22%)	61,113,113	1.91	16 (26%)
23	CLA	b	611	40	57,73,73	1.81	13 (22%)	61,113,113	1.79	16 (26%)
23	CLA	b	612	-	57,73,73	1.68	7 (12%)	61,113,113	1.89	16 (26%)
23	CLA	b	613	-	57,73,73	1.63	11 (19%)	61,113,113	2.25	16 (26%)
23	CLA	b	614	-	57,73,73	1.82	11 (19%)	61,113,113	1.97	15 (24%)
23	CLA	b	615	-	57,73,73	1.75	15 (26%)	61,113,113	1.80	17 (27%)
23	CLA	b	616	-	57,73,73	1.94	12 (21%)	61,113,113	2.18	19 (31%)
23	CLA	b	617	-	57,73,73	1.84	12 (21%)	61,113,113	2.11	22 (36%)
25	BCR	b	618	-	41,41,41	0.93	0	56,56,56	1.74	14 (25%)
25	BCR	b	619	-	41,41,41	1.01	1 (2%)	56,56,56	1.33	7 (12%)
25	BCR	b	620	-	41,41,41	0.89	2 (4%)	56,56,56	1.23	4 (7%)
30	LMT	b	621	-	25,25,36	0.60	1 (4%)	30,30,47	1.32	4 (13%)
35	HTG	b	622	-	19,19,19	1.26	2 (10%)	22,24,24	1.48	5 (22%)
35	HTG	b	623	-	19,19,19	1.05	1 (5%)	22,24,24	2.32	4 (18%)
35	HTG	b	627	-	19,19,19	1.15	2 (10%)	22,24,24	1.65	1 (4%)
35	HTG	b	628	-	19,19,19	0.84	1 (5%)	22,24,24	2.00	1 (4%)
31	DMS	b	633	-	3,3,3	1.83	1 (33%)	3,3,3	0.55	0
31	DMS	b	634	-	3,3,3	2.46	1 (33%)	3,3,3	0.88	0
31	DMS	b	635	-	3,3,3	2.72	1 (33%)	3,3,3	0.54	0
31	DMS	b	636	-	3,3,3	2.75	1 (33%)	3,3,3	0.48	0
31	DMS	b	637	-	3,3,3	2.68	1 (33%)	3,3,3	0.94	0
31	DMS	b	638	-	3,3,3	2.93	1 (33%)	3,3,3	0.98	0
31	DMS	b	639	-	3,3,3	2.77	1 (33%)	3,3,3	1.29	1 (33%)
31	DMS	b	640	-	3,3,3	2.70	1 (33%)	3,3,3	0.79	0
31	DMS	b	641	-	3,3,3	2.65	1 (33%)	3,3,3	0.70	0
31	DMS	b	642	-	3,3,3	2.71	1 (33%)	3,3,3	0.52	0
31	DMS	b	643	-	3,3,3	2.68	1 (33%)	3,3,3	0.55	0
31	DMS	b	644	-	3,3,3	2.79	1 (33%)	3,3,3	0.90	0
31	DMS	b	645	-	3,3,3	2.70	1 (33%)	3,3,3	0.44	0
31	DMS	b	646	-	3,3,3	2.75	1 (33%)	3,3,3	0.63	0
31	DMS	b	647	-	3,3,3	2.75	1 (33%)	3,3,3	0.64	0
23	CLA	c	902	-	57,73,73	1.72	12 (21%)	61,113,113	2.15	15 (24%)
23	CLA	c	903	-	57,73,73	1.70	11 (19%)	61,113,113	2.14	22 (36%)
23	CLA	c	904	-	57,73,73	1.87	12 (21%)	61,113,113	1.91	17 (27%)
23	CLA	c	905	40	57,73,73	1.83	12 (21%)	61,113,113	1.91	16 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	c	906	-	57,73,73	1.71	12 (21%)	61,113,113	2.00	17 (27%)
23	CLA	c	907	-	57,73,73	1.77	12 (21%)	61,113,113	1.94	16 (26%)
23	CLA	c	908	40	57,73,73	1.71	12 (21%)	61,113,113	1.98	15 (24%)
23	CLA	c	909	-	57,73,73	1.88	14 (24%)	61,113,113	1.63	11 (18%)
23	CLA	c	910	-	57,73,73	1.96	14 (24%)	61,113,113	2.14	18 (29%)
23	CLA	c	911	-	57,73,73	1.79	10 (17%)	61,113,113	2.03	15 (24%)
23	CLA	c	912	3	57,73,73	1.97	13 (22%)	61,113,113	1.89	14 (22%)
23	CLA	c	913	-	57,73,73	1.95	12 (21%)	61,113,113	2.05	15 (24%)
23	CLA	c	914	-	57,73,73	1.94	12 (21%)	61,113,113	2.01	17 (27%)
25	BCR	c	915	-	41,41,41	0.77	0	56,56,56	1.30	6 (10%)
25	BCR	c	916	-	41,41,41	0.81	0	56,56,56	1.57	11 (19%)
36	DGD	c	917	-	63,63,67	0.82	3 (4%)	77,77,81	1.26	8 (10%)
36	DGD	c	918	-	63,63,67	0.88	2 (3%)	77,77,81	1.18	9 (11%)
36	DGD	c	919	-	63,63,67	0.91	3 (4%)	77,77,81	1.25	10 (12%)
34	LMG	c	920	-	51,51,55	0.93	2 (3%)	59,59,63	1.32	7 (11%)
35	HTG	c	921	-	19,19,19	0.90	2 (10%)	22,24,24	1.72	2 (9%)
35	HTG	c	922	-	19,19,19	0.96	2 (10%)	22,24,24	2.16	3 (13%)
35	HTG	c	923	-	11,12,19	0.54	0	10,11,24	1.17	1 (10%)
31	DMS	c	924	-	3,3,3	2.37	1 (33%)	3,3,3	0.40	0
31	DMS	c	925	-	3,3,3	2.82	1 (33%)	3,3,3	0.77	0
31	DMS	c	926	-	3,3,3	2.62	1 (33%)	3,3,3	0.26	0
31	DMS	c	927	-	3,3,3	2.71	1 (33%)	3,3,3	1.16	0
31	DMS	c	928	-	3,3,3	2.65	1 (33%)	3,3,3	0.45	0
31	DMS	c	929	-	3,3,3	2.84	1 (33%)	3,3,3	0.63	0
34	LMG	c	930	-	51,51,55	1.05	3 (5%)	59,59,63	1.34	4 (6%)
31	DMS	c	932	-	3,3,3	2.65	1 (33%)	3,3,3	0.69	0
31	DMS	c	933	-	3,3,3	2.68	1 (33%)	3,3,3	0.85	0
31	DMS	c	934	-	3,3,3	2.70	1 (33%)	3,3,3	0.67	0
31	DMS	c	935	-	3,3,3	2.68	1 (33%)	3,3,3	0.69	0
31	DMS	c	936	-	3,3,3	2.74	1 (33%)	3,3,3	0.76	0
31	DMS	c	937	-	3,3,3	2.66	1 (33%)	3,3,3	0.56	0
23	CLA	d	401	40	57,73,73	1.59	10 (17%)	61,113,113	2.07	18 (29%)
28	LHG	d	402	-	43,43,48	1.04	2 (4%)	44,49,54	1.00	4 (9%)
23	CLA	d	403	-	57,73,73	1.69	10 (17%)	61,113,113	2.18	19 (31%)
23	CLA	d	404	-	57,73,73	1.71	13 (22%)	61,113,113	2.20	18 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	d	405	-	41,41,41	0.97	1 (2%)	56,56,56	1.93	19 (33%)
27	PL9	d	406	-	54,55,55	0.96	2 (3%)	68,69,69	1.65	12 (17%)
36	DGD	d	407	-	50,50,67	1.09	2 (4%)	58,58,81	1.26	6 (10%)
28	LHG	d	408	-	48,48,48	0.89	2 (4%)	49,54,54	1.29	3 (6%)
28	LHG	d	409	-	48,48,48	0.78	2 (4%)	49,54,54	1.27	9 (18%)
28	LHG	d	410	-	45,45,48	0.99	2 (4%)	46,51,54	1.02	3 (6%)
34	LMG	d	411	-	51,51,55	1.10	3 (5%)	59,59,63	1.34	8 (13%)
35	HTG	d	413	-	19,19,19	1.10	1 (5%)	22,24,24	2.60	3 (13%)
31	DMS	d	414	-	3,3,3	2.70	1 (33%)	3,3,3	0.70	0
31	DMS	d	415	-	3,3,3	2.66	1 (33%)	3,3,3	0.80	0
31	DMS	d	416	-	3,3,3	2.69	1 (33%)	3,3,3	0.52	0
31	DMS	d	418	-	3,3,3	2.75	1 (33%)	3,3,3	0.55	0
31	DMS	d	419	-	3,3,3	2.69	1 (33%)	3,3,3	0.65	0
28	LHG	e	101	-	39,39,48	1.13	2 (5%)	40,45,54	1.06	2 (5%)
30	LMT	e	103	-	25,25,36	0.68	1 (4%)	30,30,47	1.07	3 (10%)
31	DMS	e	104	-	3,3,3	2.68	1 (33%)	3,3,3	0.52	0
37	HEM	e	105	5,6	24,50,50	2.37	11 (45%)	16,82,82	2.49	9 (56%)
31	DMS	h	101	-	3,3,3	2.69	1 (33%)	3,3,3	1.24	0
36	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	1.28	10 (12%)
31	DMS	h	103	-	3,3,3	2.65	1 (33%)	3,3,3	0.54	0
31	DMS	h	104	-	3,3,3	2.70	1 (33%)	3,3,3	0.52	0
31	DMS	h	105	-	3,3,3	2.75	1 (33%)	3,3,3	0.61	0
31	DMS	i	105	-	3,3,3	2.70	1 (33%)	3,3,3	0.83	0
31	DMS	i	106	-	3,3,3	2.74	1 (33%)	3,3,3	0.60	0
34	LMG	j	101	39	51,51,55	0.96	3 (5%)	59,59,63	1.17	7 (11%)
25	BCR	j	104	-	41,41,41	0.80	0	56,56,56	1.47	11 (19%)
25	BCR	k	102	-	41,41,41	1.00	1 (2%)	56,56,56	1.21	8 (14%)
31	DMS	k	103	-	3,3,3	2.66	1 (33%)	3,3,3	0.74	0
28	LHG	l	101	-	48,48,48	0.81	2 (4%)	49,54,54	1.04	2 (4%)
31	DMS	l	102	-	3,3,3	2.64	1 (33%)	3,3,3	0.43	0
34	LMG	m	102	-	51,51,55	0.93	2 (3%)	59,59,63	1.34	7 (11%)
30	LMT	m	103	-	36,36,36	0.60	1 (2%)	47,47,47	1.04	3 (6%)
30	LMT	m	104	-	36,36,36	0.54	0	47,47,47	1.28	3 (6%)
31	DMS	o	301	-	3,3,3	2.14	1 (33%)	3,3,3	0.37	0
31	DMS	o	303	-	3,3,3	2.69	1 (33%)	3,3,3	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	DMS	o	304	-	3,3,3	2.76	1 (33%)	3,3,3	0.74	0
25	BCR	t	101	-	41,41,41	1.03	0	56,56,56	1.52	14 (25%)
31	DMS	u	203	-	3,3,3	2.58	1 (33%)	3,3,3	0.85	0
31	DMS	u	204	-	3,3,3	2.77	1 (33%)	3,3,3	0.78	0
31	DMS	u	205	-	3,3,3	2.63	1 (33%)	3,3,3	0.96	0
31	DMS	u	206	-	3,3,3	2.79	1 (33%)	3,3,3	0.57	0
31	DMS	v	201	-	3,3,3	2.43	1 (33%)	3,3,3	0.42	0
31	DMS	v	202	-	3,3,3	2.61	1 (33%)	3,3,3	0.29	0
37	HEM	v	203	16	24,50,50	2.40	7 (29%)	16,82,82	2.20	4 (25%)
35	HTG	v	204	-	19,19,19	0.85	1 (5%)	22,24,24	3.38	7 (31%)
31	DMS	v	205	-	3,3,3	2.65	1 (33%)	3,3,3	0.51	0
31	DMS	v	206	-	3,3,3	2.61	1 (33%)	3,3,3	0.73	0
31	DMS	v	207	-	3,3,3	2.73	1 (33%)	3,3,3	0.67	0
31	DMS	v	208	-	3,3,3	2.73	1 (33%)	3,3,3	0.67	0
31	DMS	v	209	-	3,3,3	2.72	1 (33%)	3,3,3	0.64	0
31	DMS	v	210	-	3,3,3	2.68	1 (33%)	3,3,3	0.51	0
26	SQD	x	101	-	40,41,54	1.69	3 (7%)	49,52,65	1.56	9 (18%)
38	RRX	x	102	-	42,42,42	0.89	0	57,58,58	1.37	7 (12%)
30	LMT	z	101	-	32,32,36	0.62	1 (3%)	42,42,47	1.19	5 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	OEX	A	401	1,3,40	-	0/0/68/68	0/0/6/6
23	CLA	A	405	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	A	406	40	2/2/20/25	0/37/135/135	0/0/9/9
24	PHO	A	407	-	-	0/53/103/103	0/1/6/6
23	CLA	A	408	-	2/2/20/25	0/37/135/135	0/0/9/9
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
26	SQD	A	410	-	-	0/49/69/69	0/1/1/1
27	PL9	A	411	-	-	0/53/73/73	0/1/1/1
28	LHG	A	412	-	-	0/53/53/53	0/0/0/0
26	SQD	A	415	-	-	0/49/69/69	0/1/1/1
30	LMT	A	416	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DMS	A	418	-	-	0/0/0/0	0/0/0/0
31	DMS	A	419	-	-	0/0/0/0	0/0/0/0
32	BCT	A	420	21	-	0/0/0/0	0/0/0/0
31	DMS	A	421	-	-	0/0/0/0	0/0/0/0
31	DMS	A	422	-	-	0/0/0/0	0/0/0/0
31	DMS	A	423	-	-	0/0/0/0	0/0/0/0
31	DMS	A	424	-	-	0/0/0/0	0/0/0/0
23	CLA	B	602	40	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	607	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	608	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	609	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	B	610	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	B	611	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	617	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
26	SQD	B	621	-	-	0/49/69/69	0/1/1/1
34	LMG	B	622	-	-	0/46/66/70	0/1/1/1
30	LMT	B	623	-	-	0/21/61/61	0/2/2/2
35	HTG	B	624	-	-	0/10/30/30	0/1/1/1
35	HTG	B	625	-	-	0/10/30/30	0/1/1/1
35	HTG	B	626	-	-	0/10/30/30	0/1/1/1
35	HTG	B	630	-	-	0/10/30/30	0/1/1/1
35	HTG	B	631	-	-	0/10/30/30	0/1/1/1
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DMS	B	641	-	-	0/0/0/0	0/0/0/0
31	DMS	B	642	-	-	0/0/0/0	0/0/0/0
30	LMT	B	643	-	-	0/15/35/61	0/1/1/2
30	LMT	B	644	-	-	0/15/35/61	0/1/1/2
31	DMS	B	645	-	-	0/0/0/0	0/0/0/0
31	DMS	B	646	-	-	0/0/0/0	0/0/0/0
31	DMS	B	647	-	-	0/0/0/0	0/0/0/0
31	DMS	B	648	-	-	0/0/0/0	0/0/0/0
31	DMS	B	649	-	-	0/0/0/0	0/0/0/0
34	LMG	C	501	-	-	0/46/66/70	0/1/1/1
23	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	503	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	C	504	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	C	505	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	506	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	508	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	511	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	512	3	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	C	513	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	514	-	1/1/20/25	0/37/135/135	0/0/9/9
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
36	DGD	C	517	-	-	0/51/91/95	0/2/2/2
36	DGD	C	518	-	-	0/51/91/95	0/2/2/2
36	DGD	C	519	-	-	0/51/91/95	0/2/2/2
34	LMG	C	520	-	-	0/46/66/70	0/1/1/1
35	HTG	C	521	-	-	0/10/30/30	0/1/1/1
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1
35	HTG	C	523	-	-	0/10/30/30	0/1/1/1
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
25	BCR	C	530	-	-	0/29/63/63	0/2/2/2
34	LMG	C	531	-	-	0/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DMS	C	533	-	-	0/0/0/0	0/0/0/0
23	CLA	D	401	40	1/1/20/25	0/37/135/135	0/0/9/9
24	PHO	D	402	-	-	0/53/103/103	0/1/6/6
23	CLA	D	403	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	D	404	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	D	405	-	-	0/29/63/63	0/2/2/2
27	PL9	D	406	-	-	0/53/73/73	0/1/1/1
36	DGD	D	407	-	-	0/44/64/95	0/1/1/2
26	SQD	D	408	-	-	0/40/60/69	0/1/1/1
28	LHG	D	409	-	-	0/53/53/53	0/0/0/0
28	LHG	D	410	-	-	0/53/53/53	0/0/0/0
28	LHG	D	411	-	-	0/50/50/53	0/0/0/0
34	LMG	D	412	-	-	0/46/66/70	0/1/1/1
35	HTG	D	414	-	-	0/10/30/30	0/1/1/1
31	DMS	D	415	-	-	0/0/0/0	0/0/0/0
31	DMS	D	416	-	-	0/0/0/0	0/0/0/0
31	DMS	D	417	-	-	0/0/0/0	0/0/0/0
28	LHG	E	101	-	-	0/53/53/53	0/0/0/0
37	HEM	E	105	5,6	-	0/6/54/54	0/0/8/8
30	LMT	F	101	-	-	0/21/61/61	0/2/2/2
31	DMS	F	102	-	-	0/0/0/0	0/0/0/0
31	DMS	H	101	-	-	0/0/0/0	0/0/0/0
38	RRX	H	102	-	-	0/29/65/65	0/2/2/2
36	DGD	H	103	-	-	0/51/91/95	0/2/2/2
31	DMS	H	105	-	-	0/0/0/0	0/0/0/0
30	LMT	I	101	-	-	0/21/61/61	0/2/2/2
34	LMG	J	101	39	-	0/46/66/70	0/1/1/1
28	LHG	K	101	-	-	0/45/45/53	0/0/0/0
28	LHG	L	101	-	-	0/53/53/53	0/0/0/0
26	SQD	L	102	-	-	1/49/69/69	0/1/1/1
30	LMT	M	101	-	-	0/21/61/61	0/2/2/2
35	HTG	O	302	-	-	0/10/30/30	0/1/1/1
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
25	BCR	T	101	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMT	T	103	-	-	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	U	204	-	-	0/0/0/0	0/0/0/0
31	DMS	V	201	-	-	0/0/0/0	0/0/0/0
31	DMS	V	202	-	-	0/0/0/0	0/0/0/0
37	HEM	V	203	16	-	0/6/54/54	0/0/8/8
35	HTG	V	204	-	-	0/5/25/30	0/1/1/1
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
25	BCR	Y	101	-	-	0/29/63/63	0/2/2/2
30	LMT	Z	101	-	-	0/21/61/61	0/2/2/2
31	DMS	a	401	-	-	0/0/0/0	0/0/0/0
20	OEX	a	402	1,3,40	-	0/0/68/68	0/0/6/6
23	CLA	a	406	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	a	407	40	2/2/20/25	0/37/135/135	0/0/9/9
24	PHO	a	408	-	-	0/53/103/103	0/1/6/6
24	PHO	a	409	-	-	0/53/103/103	0/1/6/6
23	CLA	a	410	-	1/1/20/25	0/37/135/135	0/0/9/9
25	BCR	a	411	-	-	0/29/63/63	0/2/2/2
26	SQD	a	412	-	-	0/49/69/69	0/1/1/1
34	LMG	a	413	-	-	0/46/66/70	0/1/1/1
27	PL9	a	414	-	-	0/53/73/73	0/1/1/1
28	LHG	a	415	-	-	0/53/53/53	0/0/0/0
26	SQD	a	417	-	-	0/49/69/69	0/1/1/1
30	LMT	a	418	-	-	0/21/61/61	0/2/2/2
31	DMS	a	420	-	-	0/0/0/0	0/0/0/0
31	DMS	a	421	-	-	0/0/0/0	0/0/0/0
30	LMT	a	422	-	-	0/21/61/61	0/2/2/2
31	DMS	a	423	-	-	0/0/0/0	0/0/0/0
32	BCT	a	424	21	-	0/0/0/0	0/0/0/0
23	CLA	b	602	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	603	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	604	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	608	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	609	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	b	610	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	611	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	612	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
25	BCR	b	619	-	-	0/29/63/63	0/2/2/2
25	BCR	b	620	-	-	0/29/63/63	0/2/2/2
30	LMT	b	621	-	-	0/17/37/61	0/1/1/2
35	HTG	b	622	-	-	0/10/30/30	0/1/1/1
35	HTG	b	623	-	-	0/10/30/30	0/1/1/1
35	HTG	b	627	-	-	0/10/30/30	0/1/1/1
35	HTG	b	628	-	-	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
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
31	DMS	b	643	-	-	0/0/0/0	0/0/0/0
31	DMS	b	644	-	-	0/0/0/0	0/0/0/0
31	DMS	b	645	-	-	0/0/0/0	0/0/0/0
31	DMS	b	646	-	-	0/0/0/0	0/0/0/0
31	DMS	b	647	-	-	0/0/0/0	0/0/0/0
23	CLA	c	902	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	903	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	c	904	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	c	905	40	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	c	906	-	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	907	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	c	908	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	909	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	c	910	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	911	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	912	3	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	c	913	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	914	-	1/1/20/25	0/37/135/135	0/0/9/9
25	BCR	c	915	-	-	0/29/63/63	0/2/2/2
25	BCR	c	916	-	-	0/29/63/63	0/2/2/2
36	DGD	c	917	-	-	0/51/91/95	0/2/2/2
36	DGD	c	918	-	-	0/51/91/95	0/2/2/2
36	DGD	c	919	-	-	0/51/91/95	0/2/2/2
34	LMG	c	920	-	-	0/46/66/70	0/1/1/1
35	HTG	c	921	-	-	0/10/30/30	0/1/1/1
35	HTG	c	922	-	-	0/10/30/30	0/1/1/1
35	HTG	c	923	-	-	0/8/10/30	0/0/0/1
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
34	LMG	c	930	-	-	0/46/66/70	0/1/1/1
31	DMS	c	932	-	-	0/0/0/0	0/0/0/0
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
23	CLA	d	401	40	1/1/20/25	0/37/135/135	0/0/9/9
28	LHG	d	402	-	-	0/48/48/53	0/0/0/0
23	CLA	d	403	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	d	404	-	1/1/20/25	0/37/135/135	0/0/9/9
25	BCR	d	405	-	-	0/29/63/63	0/2/2/2
27	PL9	d	406	-	-	0/53/73/73	0/1/1/1
36	DGD	d	407	-	-	0/44/64/95	0/1/1/2
28	LHG	d	408	-	-	0/53/53/53	0/0/0/0
28	LHG	d	409	-	-	0/53/53/53	0/0/0/0
28	LHG	d	410	-	-	0/50/50/53	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	d	411	-	-	0/46/66/70	0/1/1/1
35	HTG	d	413	-	-	1/10/30/30	0/1/1/1
31	DMS	d	414	-	-	0/0/0/0	0/0/0/0
31	DMS	d	415	-	-	0/0/0/0	0/0/0/0
31	DMS	d	416	-	-	0/0/0/0	0/0/0/0
31	DMS	d	418	-	-	0/0/0/0	0/0/0/0
31	DMS	d	419	-	-	0/0/0/0	0/0/0/0
28	LHG	e	101	-	-	0/44/44/53	0/0/0/0
30	LMT	e	103	-	-	0/17/37/61	0/1/1/2
31	DMS	e	104	-	-	0/0/0/0	0/0/0/0
37	HEM	e	105	5,6	-	0/6/54/54	0/0/8/8
31	DMS	h	101	-	-	0/0/0/0	0/0/0/0
36	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	h	104	-	-	0/0/0/0	0/0/0/0
31	DMS	h	105	-	-	0/0/0/0	0/0/0/0
31	DMS	i	105	-	-	0/0/0/0	0/0/0/0
31	DMS	i	106	-	-	0/0/0/0	0/0/0/0
34	LMG	j	101	39	-	0/46/66/70	0/1/1/1
25	BCR	j	104	-	-	0/29/63/63	0/2/2/2
25	BCR	k	102	-	-	0/29/63/63	0/2/2/2
31	DMS	k	103	-	-	0/0/0/0	0/0/0/0
28	LHG	l	101	-	-	0/53/53/53	0/0/0/0
31	DMS	l	102	-	-	0/0/0/0	0/0/0/0
34	LMG	m	102	-	-	0/46/66/70	0/1/1/1
30	LMT	m	103	-	-	0/21/61/61	0/2/2/2
30	LMT	m	104	-	-	0/21/61/61	0/2/2/2
31	DMS	o	301	-	-	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
25	BCR	t	101	-	-	0/29/63/63	0/2/2/2
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	u	206	-	-	0/0/0/0	0/0/0/0
31	DMS	v	201	-	-	0/0/0/0	0/0/0/0
31	DMS	v	202	-	-	0/0/0/0	0/0/0/0
37	HEM	v	203	16	-	0/6/54/54	0/0/8/8
35	HTG	v	204	-	-	0/10/30/30	0/1/1/1
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
26	SQD	x	101	-	-	0/36/56/69	0/1/1/1
38	RRX	x	102	-	-	0/29/65/65	0/2/2/2
30	LMT	z	101	-	-	0/15/55/61	0/2/2/2

The worst 5 of 1197 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	415	SQD	C6-S	-9.11	1.66	1.77
26	a	417	SQD	C6-S	-9.06	1.66	1.77
26	a	412	SQD	C6-S	-8.43	1.67	1.77
26	x	101	SQD	C6-S	-7.70	1.68	1.77
26	L	102	SQD	C6-S	-7.66	1.68	1.77

The worst 5 of 2025 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	E	105	HEM	CBD-CAD-C3D	-7.65	99.05	112.47
35	V	204	HTG	O5-C1-C2	-7.21	100.39	110.22
25	D	405	BCR	C7-C8-C9	-6.73	116.05	126.21
23	b	603	CLA	C3B-CAB-CBB	-6.62	113.08	126.40
23	C	511	CLA	CHD-C4C-C3C	-6.33	115.15	124.91

5 of 169 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	b	605	CLA	NC
23	b	605	CLA	ND
23	b	605	CLA	NA
23	C	504	CLA	NC
23	C	504	CLA	NA

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	d	413	HTG	O5-C1-S1-C1'
26	L	102	SQD	C45-O47-C7-C8

There are no ring outliers.

107 monomers are involved in 318 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	405	CLA	4	0
23	A	406	CLA	6	0
24	A	407	PHO	2	0
23	A	408	CLA	2	0
25	A	409	BCR	3	0
26	A	410	SQD	9	0
27	A	411	PL9	12	0
28	A	412	LHG	1	0
26	A	415	SQD	2	0
30	A	416	LMT	2	0
31	A	421	DMS	1	0
31	A	422	DMS	1	0
31	A	424	DMS	2	0
23	B	602	CLA	4	0
23	B	603	CLA	4	0
23	B	604	CLA	3	0
23	B	605	CLA	2	0
23	B	606	CLA	7	0
23	B	607	CLA	1	0
23	B	609	CLA	1	0
23	B	610	CLA	1	0
23	B	611	CLA	7	0
23	B	612	CLA	2	0
23	B	613	CLA	4	0
23	B	614	CLA	6	0
23	B	615	CLA	5	0
23	B	616	CLA	5	0
23	B	617	CLA	13	0
25	B	618	BCR	1	0
25	B	619	BCR	5	0
25	B	620	BCR	9	0
26	B	621	SQD	4	0
34	B	622	LMG	2	0
30	B	623	LMT	2	0
35	B	625	HTG	1	0
31	B	636	DMS	5	0
31	B	639	DMS	10	0
31	B	641	DMS	3	0
30	B	644	LMT	1	0
31	B	645	DMS	4	0
31	B	646	DMS	3	0
31	B	648	DMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	C	501	LMG	1	0
23	C	502	CLA	2	0
23	C	503	CLA	3	0
23	C	504	CLA	5	0
23	C	505	CLA	1	0
23	C	506	CLA	1	0
23	C	507	CLA	5	0
23	C	508	CLA	2	0
23	C	509	CLA	3	0
23	C	510	CLA	3	0
23	C	511	CLA	5	0
23	C	512	CLA	3	0
23	C	513	CLA	6	0
23	C	514	CLA	5	0
25	C	515	BCR	4	0
25	C	516	BCR	2	0
36	C	517	DGD	1	0
36	C	518	DGD	1	0
35	C	521	HTG	1	0
31	C	525	DMS	1	0
31	C	526	DMS	1	0
31	C	529	DMS	1	0
25	C	530	BCR	2	0
34	C	531	LMG	3	0
23	D	401	CLA	6	0
24	D	402	PHO	3	0
23	D	403	CLA	3	0
23	D	404	CLA	3	0
25	D	405	BCR	6	0
36	D	407	DGD	10	0
26	D	408	SQD	2	0
28	D	409	LHG	2	0
28	D	410	LHG	1	0
28	D	411	LHG	5	0
34	D	412	LMG	5	0
35	D	414	HTG	3	0
31	D	415	DMS	1	0
31	D	416	DMS	6	0
28	E	101	LHG	7	0
37	E	105	HEM	1	0
31	F	102	DMS	6	0
31	H	101	DMS	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	H	105	DMS	3	0
30	I	101	LMT	2	0
34	J	101	LMG	3	0
28	L	101	LHG	1	0
26	L	102	SQD	3	0
30	M	101	LMT	1	0
35	O	302	HTG	2	0
31	O	303	DMS	3	0
31	O	304	DMS	3	0
31	O	305	DMS	6	0
31	O	308	DMS	5	0
31	O	311	DMS	3	0
25	T	101	BCR	9	0
31	U	202	DMS	1	0
31	U	204	DMS	3	0
31	V	202	DMS	1	0
35	V	204	HTG	2	0
31	V	206	DMS	3	0
31	V	207	DMS	4	0
31	V	209	DMS	5	0
31	V	210	DMS	1	0
25	Y	101	BCR	1	0
30	Z	101	LMT	7	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	334/344 (97%)	-0.26	4 (1%) 81 83	14, 21, 43, 67	0
1	a	334/344 (97%)	-0.09	9 (2%) 58 60	14, 21, 44, 91	0
2	B	505/505 (100%)	0.00	28 (5%) 29 30	17, 26, 50, 81	0
2	b	501/505 (99%)	0.01	32 (6%) 23 24	16, 25, 53, 109	0
3	C	451/455 (99%)	-0.03	14 (3%) 52 54	18, 30, 46, 73	0
3	c	455/455 (100%)	-0.00	15 (3%) 50 52	20, 31, 43, 68	0
4	D	342/342 (100%)	-0.24	3 (0%) 85 87	15, 22, 41, 88	0
4	d	342/342 (100%)	-0.30	3 (0%) 85 87	15, 22, 40, 73	0
5	E	81/83 (97%)	1.43	24 (29%) 1 0	25, 45, 75, 97	0
5	e	79/83 (95%)	0.86	13 (16%) 2 2	28, 42, 67, 87	0
6	F	35/44 (79%)	0.43	6 (17%) 2 2	24, 35, 59, 96	0
6	f	32/44 (72%)	0.03	2 (6%) 23 25	26, 31, 70, 82	0
7	H	63/65 (96%)	-0.00	2 (3%) 51 53	24, 34, 44, 77	0
7	h	63/65 (96%)	0.35	5 (7%) 15 16	23, 34, 46, 72	0
8	I	34/38 (89%)	-0.19	0 100 100	27, 35, 58, 77	0
8	i	37/38 (97%)	0.23	3 (8%) 15 16	26, 32, 84, 89	0
9	J	36/40 (90%)	0.21	3 (8%) 14 15	24, 38, 65, 81	0
9	j	40/40 (100%)	0.22	5 (12%) 5 5	24, 36, 69, 76	0
10	K	37/37 (100%)	0.05	2 (5%) 29 31	31, 37, 47, 56	0
10	k	37/37 (100%)	0.24	2 (5%) 29 31	29, 37, 55, 66	0
11	L	37/37 (100%)	-0.10	3 (8%) 15 16	15, 20, 62, 80	0
11	l	36/37 (97%)	-0.04	2 (5%) 28 30	17, 20, 68, 76	0
12	M	34/36 (94%)	-0.16	2 (5%) 26 27	19, 23, 52, 75	0
12	m	34/36 (94%)	0.11	2 (5%) 26 27	19, 24, 53, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/244 (99%)	0.08	17 (6%) 19 20	16, 30, 55, 86	0
13	o	243/244 (99%)	0.17	29 (11%) 6 6	16, 32, 65, 86	0
14	T	29/32 (90%)	0.26	1 (3%) 49 50	17, 21, 45, 81	0
14	t	30/32 (93%)	0.29	2 (6%) 21 22	18, 22, 55, 85	0
15	U	97/104 (93%)	-0.22	0 100 100	20, 28, 46, 59	0
15	u	97/104 (93%)	-0.37	1 (1%) 84 85	22, 27, 40, 63	0
16	V	137/137 (100%)	-0.35	0 100 100	20, 26, 41, 59	0
16	v	137/137 (100%)	0.23	9 (6%) 22 23	23, 33, 51, 71	0
17	Y	29/30 (96%)	1.27	9 (31%) 1 0	38, 46, 69, 72	0
17	y	29/30 (96%)	0.85	6 (20%) 1 1	38, 47, 59, 69	0
18	X	38/40 (95%)	0.58	6 (15%) 3 3	29, 39, 58, 62	0
18	x	38/40 (95%)	0.82	6 (15%) 3 3	31, 38, 83, 98	0
19	Z	62/62 (100%)	1.61	21 (33%) 0 0	36, 45, 83, 96	0
19	z	61/62 (98%)	1.64	23 (37%) 0 0	42, 52, 83, 103	0
All	All	5249/5350 (98%)	0.05	314 (5%) 25 27	14, 28, 55, 109	0

The worst 5 of 314 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	487	SER	9.5
6	F	11	VAL	8.0
2	b	496	TYR	7.7
19	z	3	ILE	7.4
18	x	37	VAL	7.3

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
14	FME	T	1	10/11	0.97	0.07	-	19,26,45,49	0
8	FME	I	1	10/11	0.97	0.09	-	27,32,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	FME	i	1	10/11	0.98	0.08	-	28,29,33,33	0
14	FME	t	1	10/11	0.97	0.08	-	18,24,45,50	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	DMS	b	637	4/4	0.89	0.32	23.67	61,63,68,74	0
29	UNL	T	102	13/-	0.80	0.50	22.60	62,68,75,75	0
29	UNL	A	417	4/-	0.92	0.52	17.13	58,61,63,67	0
31	DMS	b	640	4/4	0.86	0.19	15.87	67,70,78,83	0
31	DMS	b	645	4/4	0.82	0.46	15.86	70,77,83,84	0
29	UNL	J	104	16/-	0.54	0.37	14.81	62,82,99,99	0
31	DMS	O	311	4/4	0.84	0.27	14.36	59,59,71,73	0
29	UNL	t	102	16/-	0.76	0.37	13.77	53,62,74,75	0
29	UNL	a	419	6/-	0.81	0.36	11.31	47,53,53,53	0
31	DMS	b	644	4/4	0.46	0.39	10.59	73,76,78,96	0
31	DMS	U	202	4/4	0.88	0.22	10.53	33,45,50,55	0
31	DMS	C	525	4/4	0.93	0.19	10.40	39,39,43,46	0
30	LMT	F	101	35/35	0.66	0.39	10.39	64,88,93,96	0
36	DGD	D	407	50/66	0.61	0.31	9.92	54,71,97,97	0
31	DMS	O	304	4/4	0.66	0.26	9.78	69,71,78,87	0
31	DMS	u	206	4/4	0.75	0.30	9.70	70,71,76,93	0
31	DMS	V	211	4/4	0.52	0.36	9.49	61,61,68,79	0
31	DMS	A	421	4/4	0.83	0.25	9.36	57,63,74,78	0
31	DMS	b	646	4/4	0.81	0.36	9.27	84,87,89,96	0
31	DMS	c	929	4/4	0.81	0.43	8.93	46,62,67,70	0
35	HTG	d	413	19/19	0.65	0.27	8.47	62,86,104,106	0
31	DMS	o	303	4/4	0.94	0.23	8.34	51,55,67,70	0
35	HTG	D	414	19/19	0.59	0.37	8.09	76,92,111,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
29	UNL	B	629	14/-	0.54	0.28	7.79	62,72,81,82	0
31	DMS	u	203	4/4	0.94	0.21	7.32	38,50,51,52	0
31	DMS	C	529	4/4	0.89	0.29	7.29	54,66,72,74	0
31	DMS	c	932	4/4	0.95	0.32	7.28	54,57,63,64	0
29	UNL	e	102	16/-	0.72	0.38	7.09	54,61,69,72	0
31	DMS	o	304	4/4	0.73	0.28	7.04	63,68,70,84	0
29	UNL	x	103	15/-	0.87	0.17	6.73	31,40,57,58	0
29	UNL	E	102	16/-	0.68	0.39	6.59	58,61,76,77	0
31	DMS	c	925	4/4	0.96	0.16	6.29	35,37,42,49	0
29	UNL	i	103	16/-	0.73	0.33	6.20	58,61,67,70	0
35	HTG	b	622	19/19	0.88	0.23	5.97	28,41,57,64	0
36	DGD	d	407	50/66	0.63	0.27	5.92	58,74,97,98	0
29	UNL	D	413	16/-	0.92	0.21	5.91	36,42,57,58	0
29	UNL	b	626	16/-	0.63	0.28	5.64	59,68,73,73	0
35	HTG	c	922	19/19	0.68	0.41	5.49	53,84,96,100	0
29	UNL	E	103	13/-	0.71	0.34	5.38	63,68,85,87	0
27	PL9	A	411	55/55	0.73	0.25	5.36	45,59,80,84	0
29	UNL	u	202	16/-	0.79	0.28	5.35	41,54,60,62	0
30	LMT	e	103	25/35	0.75	0.32	5.15	60,77,93,95	0
31	DMS	C	527	4/4	0.92	0.19	5.14	58,68,73,83	0
29	UNL	d	412	16/-	0.89	0.25	4.82	31,40,54,57	0
35	HTG	C	522	19/19	0.72	0.35	4.66	41,78,86,87	0
30	LMT	A	416	35/35	0.82	0.20	4.65	42,63,86,98	0
28	LHG	K	101	44/49	0.67	0.32	4.57	63,93,124,137	0
27	PL9	a	414	55/55	0.71	0.24	4.55	46,61,86,88	0
31	DMS	O	305	4/4	0.95	0.41	4.54	65,70,70,77	0
30	LMT	T	103	24/35	0.84	0.20	4.45	34,56,76,83	0
31	DMS	B	636	4/4	0.97	0.12	4.33	18,20,22,28	0
31	DMS	B	638	4/4	0.95	0.17	4.32	55,60,62,71	0
31	DMS	B	645	4/4	0.85	0.24	4.30	50,61,64,69	0
31	DMS	v	209	4/4	0.92	0.15	4.27	49,50,58,64	0
30	LMT	B	644	24/35	0.82	0.21	4.08	34,52,81,87	0
29	UNL	I	103	16/-	0.72	0.28	3.95	51,57,70,74	0
30	LMT	B	643	24/35	0.71	0.23	3.94	50,77,114,118	0
31	DMS	O	308	4/4	0.85	0.27	3.86	54,64,77,81	0
31	DMS	F	102	4/4	0.97	0.14	3.77	48,48,50,64	0
30	LMT	a	418	35/35	0.73	0.23	3.73	44,63,79,80	0
35	HTG	B	625	19/19	0.85	0.17	3.72	28,42,49,51	0
29	UNL	k	101	8/-	0.77	0.18	3.57	59,71,78,80	0
31	DMS	A	419	4/4	0.67	0.37	3.52	75,76,91,97	0
39	MG	j	102	1/1	0.99	0.14	3.49	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
28	LHG	d	402	44/49	0.62	0.23	3.47	59,78,125,135	0
31	DMS	d	415	4/4	0.93	0.20	3.45	45,53,57,73	0
23	CLA	B	602	65/65	0.93	0.19	3.41	28,39,75,85	0
29	UNL	B	632	16/-	0.76	0.25	3.21	44,61,68,70	0
35	HTG	C	523	19/19	0.82	0.29	3.16	60,78,95,97	0
26	SQD	B	621	54/54	0.68	0.24	3.13	43,63,88,93	0
31	DMS	k	103	4/4	0.72	0.33	3.11	90,92,93,104	0
35	HTG	c	923	13/19	0.68	0.34	3.09	59,72,86,87	0
25	BCR	D	405	40/40	0.95	0.16	3.06	22,28,54,57	0
29	UNL	U	201	14/-	0.79	0.26	3.06	38,50,58,61	0
25	BCR	B	619	40/40	0.96	0.19	3.02	20,25,41,45	0
28	LHG	E	101	49/49	0.70	0.28	2.99	39,83,104,109	0
34	LMG	C	531	51/55	0.76	0.22	2.98	38,78,93,98	0
28	LHG	A	412	49/49	0.63	0.35	2.94	59,83,104,111	0
31	DMS	C	526	4/4	0.92	0.16	2.87	49,56,57,62	0
34	LMG	J	101	51/55	0.93	0.17	2.86	25,31,85,93	0
34	LMG	d	411	51/55	0.77	0.23	2.85	39,70,101,108	0
29	UNL	Z	102	14/-	0.76	0.32	2.82	63,67,74,76	0
26	SQD	a	417	54/54	0.81	0.17	2.79	38,53,72,73	0
36	DGD	C	519	62/66	0.95	0.12	2.60	21,28,68,83	0
31	DMS	v	202	4/4	0.93	0.17	2.60	68,74,76,81	0
28	LHG	e	101	40/49	0.61	0.25	2.58	55,93,121,126	0
31	DMS	O	303	4/4	0.94	0.21	2.56	59,66,69,73	0
29	UNL	A	414	13/-	0.62	0.34	2.55	58,71,83,83	0
29	UNL	j	103	16/-	0.81	0.17	2.52	45,56,61,62	0
31	DMS	B	641	4/4	0.83	0.21	2.52	62,63,65,66	0
25	BCR	d	405	40/40	0.95	0.09	2.51	21,27,50,54	0
26	SQD	L	102	54/54	0.75	0.20	2.50	42,58,87,90	0
35	HTG	O	302	19/19	0.93	0.12	2.49	36,39,48,49	0
29	UNL	J	103	16/-	0.82	0.17	2.47	46,54,60,63	0
34	LMG	c	930	51/55	0.77	0.22	2.47	33,69,81,84	0
31	DMS	c	933	4/4	0.80	0.17	2.46	61,64,65,77	0
28	LHG	d	408	49/49	0.94	0.20	2.45	25,33,43,44	0
31	DMS	V	210	4/4	0.90	0.15	2.39	64,65,67,73	0
31	DMS	D	417	4/4	0.86	0.23	2.35	53,54,58,59	0
31	DMS	D	416	4/4	0.97	0.20	2.35	56,57,58,62	0
23	CLA	b	602	65/65	0.92	0.17	2.26	29,42,66,71	0
31	DMS	b	635	4/4	0.89	0.17	2.19	53,63,69,71	0
35	HTG	V	204	14/19	0.90	0.18	2.19	42,45,71,82	0
29	UNL	J	105	11/-	0.54	0.27	2.19	61,67,75,78	0
29	UNL	z	102	13/-	0.72	0.23	2.17	53,62,72,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	DMS	b	638	4/4	0.75	0.20	2.17	54,60,67,74	0
35	HTG	v	204	19/19	0.69	0.33	2.13	62,70,81,91	0
31	DMS	V	202	4/4	0.91	0.16	2.13	31,32,38,48	0
29	UNL	X	101	16/-	0.84	0.17	2.11	33,37,60,61	0
31	DMS	v	201	4/4	0.98	0.12	2.10	46,48,51,51	0
29	UNL	u	201	11/-	0.81	0.28	2.09	39,50,60,61	0
30	LMT	z	101	32/35	0.78	0.23	2.07	43,88,96,99	0
26	SQD	A	415	54/54	0.84	0.18	2.02	39,54,72,76	0
25	BCR	T	101	40/40	0.96	0.16	2.02	22,29,40,41	0
31	DMS	b	647	4/4	0.87	0.28	2.01	67,78,85,86	0
30	LMT	I	101	35/35	0.77	0.30	2.00	63,75,85,91	0
35	HTG	b	627	19/19	0.89	0.14	1.97	39,59,72,82	0
26	SQD	D	408	45/54	0.85	0.29	1.96	45,67,86,93	0
31	DMS	i	105	4/4	0.94	0.24	1.90	61,64,71,73	0
34	LMG	a	413	51/55	0.81	0.19	1.90	41,53,68,74	0
28	LHG	a	415	49/49	0.53	0.34	1.89	56,72,99,108	0
34	LMG	C	501	51/55	0.83	0.20	1.86	37,51,63,70	0
29	UNL	E	104	16/-	0.71	0.23	1.77	67,71,74,76	0
26	SQD	A	410	54/54	0.90	0.17	1.77	31,55,74,80	0
34	LMG	D	412	51/55	0.66	0.25	1.76	37,65,106,119	0
31	DMS	B	639	4/4	0.95	0.15	1.75	44,48,51,54	0
31	DMS	c	926	4/4	0.97	0.15	1.72	66,68,69,77	0
31	DMS	b	633	4/4	0.98	0.10	1.72	21,23,24,25	0
34	LMG	B	622	51/55	0.85	0.17	1.71	31,41,52,67	0
34	LMG	m	102	51/55	0.83	0.19	1.70	33,41,54,61	0
26	SQD	x	101	41/54	0.84	0.24	1.70	54,76,95,101	0
23	CLA	a	407	65/65	0.97	0.13	1.59	17,20,95,102	0
23	CLA	A	406	65/65	0.97	0.14	1.59	18,20,90,96	0
31	DMS	b	636	4/4	0.95	0.17	1.58	44,48,50,52	0
26	SQD	a	412	54/54	0.91	0.15	1.57	31,53,72,76	0
23	CLA	B	611	65/65	0.96	0.13	1.57	20,24,33,39	0
25	BCR	b	619	40/40	0.96	0.18	1.57	20,27,41,43	0
28	LHG	D	411	46/49	0.96	0.12	1.53	25,30,82,85	0
30	LMT	a	422	35/35	0.83	0.35	1.51	61,74,82,85	0
28	LHG	d	409	49/49	0.95	0.13	1.49	18,24,44,47	0
36	DGD	C	518	62/66	0.93	0.13	1.47	24,33,70,80	0
28	LHG	D	409	49/49	0.93	0.15	1.47	27,34,41,47	0
31	DMS	H	101	4/4	0.83	0.28	1.46	54,58,62,65	0
25	BCR	B	618	40/40	0.96	0.12	1.44	19,24,30,33	0
36	DGD	h	102	62/66	0.88	0.18	1.42	24,31,41,47	0
28	LHG	L	101	49/49	0.94	0.12	1.41	22,31,42,48	0
23	CLA	B	606	65/65	0.97	0.16	1.41	18,22,32,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	DGD	H	103	62/66	0.92	0.18	1.38	23,32,38,39	0
31	DMS	c	927	4/4	0.93	0.15	1.38	30,37,37,44	0
36	DGD	C	517	62/66	0.95	0.17	1.37	21,29,69,71	0
24	PHO	a	409	64/64	0.97	0.13	1.35	17,22,27,30	0
31	DMS	a	421	4/4	0.88	0.28	1.34	81,84,85,92	0
23	CLA	b	608	65/65	0.97	0.14	1.30	16,20,28,36	0
35	HTG	B	630	19/19	0.87	0.13	1.29	41,55,62,66	0
28	LHG	d	410	46/49	0.96	0.14	1.29	24,27,73,84	0
31	DMS	d	416	4/4	0.96	0.15	1.25	47,52,59,64	0
23	CLA	B	608	65/65	0.97	0.13	1.24	16,19,32,35	0
25	BCR	C	516	40/40	0.94	0.12	1.23	28,34,40,43	0
34	LMG	j	101	51/55	0.94	0.10	1.20	22,33,80,85	0
30	LMT	m	103	35/35	0.71	0.19	1.20	48,92,102,103	0
30	LMT	Z	101	35/35	0.70	0.25	1.18	41,88,100,102	0
34	LMG	C	520	51/55	0.84	0.20	1.17	31,61,74,79	0
35	HTG	B	624	19/19	0.93	0.12	1.16	35,39,46,47	0
25	BCR	A	409	40/40	0.97	0.12	1.13	19,23,29,32	0
23	CLA	c	909	65/65	0.95	0.16	1.12	22,26,79,92	0
27	PL9	d	406	55/55	0.96	0.12	1.10	16,21,27,34	0
23	CLA	c	910	65/65	0.96	0.17	1.08	23,27,49,60	0
23	CLA	d	401	65/65	0.98	0.12	1.06	15,17,26,31	0
34	LMG	c	920	51/55	0.84	0.19	1.04	27,55,81,84	0
28	LHG	l	101	49/49	0.94	0.15	1.02	20,28,48,52	0
25	BCR	t	101	40/40	0.95	0.14	1.00	19,26,38,40	0
23	CLA	c	911	65/65	0.97	0.21	0.98	20,26,36,40	0
23	CLA	C	506	65/65	0.96	0.13	0.94	25,31,40,44	0
31	DMS	d	414	4/4	0.94	0.11	0.93	62,66,71,78	0
35	HTG	b	623	19/19	0.80	0.25	0.92	47,76,83,84	0
23	CLA	b	612	65/65	0.96	0.16	0.91	18,21,36,42	0
30	LMT	b	621	25/35	0.71	0.19	0.90	45,70,90,91	0
36	DGD	c	917	62/66	0.95	0.15	0.90	20,30,74,77	0
23	CLA	b	606	65/65	0.97	0.12	0.88	18,22,29,33	0
23	CLA	C	509	65/65	0.95	0.13	0.88	24,29,76,85	0
36	DGD	c	919	62/66	0.94	0.11	0.87	22,29,50,56	0
23	CLA	B	610	65/65	0.88	0.13	0.87	21,28,32,34	0
23	CLA	b	614	65/65	0.97	0.18	0.86	17,21,47,54	0
23	CLA	B	605	65/65	0.97	0.17	0.83	18,21,52,53	0
31	DMS	B	648	4/4	0.93	0.31	0.82	43,45,47,48	0
23	CLA	B	617	65/65	0.96	0.11	0.81	20,27,93,106	0
23	CLA	D	404	65/65	0.94	0.13	0.79	23,27,67,73	0
24	PHO	D	402	64/64	0.97	0.13	0.79	16,21,25,29	0
23	CLA	a	410	65/65	0.97	0.10	0.79	17,22,91,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	B	613	65/65	0.96	0.13	0.78	18,23,28,31	0
30	LMT	m	104	35/35	0.74	0.20	0.77	34,51,56,58	0
31	DMS	u	205	4/4	0.91	0.21	0.77	41,50,54,58	0
23	CLA	A	408	65/65	0.97	0.11	0.76	18,22,89,96	0
23	CLA	C	502	65/65	0.95	0.14	0.75	25,31,41,51	0
23	CLA	b	609	65/65	0.97	0.15	0.75	19,23,31,32	0
30	LMT	M	101	35/35	0.71	0.22	0.75	31,50,59,60	0
28	LHG	D	410	49/49	0.96	0.11	0.73	20,27,42,46	0
23	CLA	b	615	65/65	0.96	0.14	0.73	19,24,71,76	0
23	CLA	B	614	65/65	0.98	0.15	0.72	18,20,44,51	0
31	DMS	b	634	4/4	0.97	0.11	0.70	42,45,48,48	0
24	PHO	A	407	64/64	0.97	0.11	0.69	17,19,22,22	0
31	DMS	V	208	4/4	0.93	0.13	0.67	69,70,71,72	0
23	CLA	c	904	65/65	0.93	0.15	0.67	25,32,37,40	0
23	CLA	b	604	65/65	0.96	0.13	0.65	19,23,29,32	0
23	CLA	c	903	65/65	0.95	0.18	0.61	20,24,37,43	0
23	CLA	B	612	65/65	0.97	0.12	0.61	17,20,36,52	0
25	BCR	b	618	40/40	0.96	0.13	0.59	20,25,32,33	0
25	BCR	b	620	40/40	0.96	0.11	0.59	25,29,40,44	0
23	CLA	d	403	65/65	0.97	0.11	0.56	13,18,36,42	0
23	CLA	C	510	65/65	0.95	0.12	0.55	25,31,52,55	0
23	CLA	c	902	65/65	0.96	0.12	0.54	24,27,38,46	0
27	PL9	D	406	55/55	0.96	0.09	0.53	17,22,28,30	0
23	CLA	B	616	65/65	0.95	0.10	0.52	23,27,43,49	0
23	CLA	C	505	65/65	0.96	0.13	0.52	25,28,58,60	0
23	CLA	B	604	65/65	0.96	0.14	0.52	18,21,30,36	0
23	CLA	C	504	65/65	0.95	0.10	0.52	24,31,36,41	0
23	CLA	B	609	65/65	0.97	0.14	0.50	19,23,28,29	0
23	CLA	b	607	65/65	0.93	0.11	0.47	22,27,54,63	0
31	DMS	V	201	4/4	0.98	0.10	0.47	41,46,47,47	0
30	LMT	B	623	35/35	0.74	0.21	0.46	48,72,89,93	0
31	DMS	B	637	4/4	0.97	0.11	0.41	35,38,40,42	0
23	CLA	D	403	65/65	0.96	0.10	0.40	13,17,33,41	0
23	CLA	c	905	65/65	0.95	0.16	0.40	21,27,51,54	0
23	CLA	B	603	65/65	0.92	0.13	0.39	20,26,33,36	0
23	CLA	B	615	65/65	0.96	0.11	0.38	18,23,66,71	0
23	CLA	c	913	65/65	0.92	0.12	0.37	30,39,65,68	0
31	DMS	V	209	4/4	0.94	0.12	0.36	58,59,62,65	0
23	CLA	b	610	65/65	0.91	0.11	0.35	22,27,31,39	0
31	DMS	h	101	4/4	0.94	0.17	0.34	47,51,52,53	0
38	RRX	H	102	41/41	0.89	0.13	0.32	25,29,38,44	0
24	PHO	a	408	64/64	0.97	0.11	0.32	15,18,20,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
21	FE2	a	403	1/1	0.99	0.07	0.31	25,25,25,25	0
22	CL	A	403	1/1	1.00	0.07	0.30	19,19,19,19	0
23	CLA	c	914	65/65	0.92	0.12	0.30	36,44,76,80	0
23	CLA	C	514	65/65	0.89	0.15	0.29	37,47,67,72	0
23	CLA	b	605	65/65	0.96	0.14	0.28	17,22,53,55	0
23	CLA	D	401	65/65	0.98	0.09	0.27	13,17,27,35	0
23	CLA	C	511	65/65	0.96	0.12	0.17	24,30,35,40	0
23	CLA	A	405	65/65	0.97	0.09	0.17	14,17,26,34	0
23	CLA	b	613	65/65	0.97	0.13	0.16	18,24,29,34	0
23	CLA	d	404	65/65	0.96	0.10	0.12	22,27,66,72	0
23	CLA	b	603	65/65	0.93	0.12	0.11	21,24,33,41	0
23	CLA	c	906	65/65	0.95	0.10	0.08	25,29,44,47	0
23	CLA	a	406	65/65	0.97	0.11	0.07	14,17,25,37	0
36	DGD	c	918	62/66	0.95	0.13	0.07	24,30,75,84	0
23	CLA	b	611	65/65	0.96	0.10	0.05	19,24,32,37	0
25	BCR	Y	101	40/40	0.95	0.09	0.05	29,33,40,41	0
23	CLA	B	607	65/65	0.94	0.10	0.05	20,26,53,60	0
38	RRX	x	102	41/41	0.88	0.13	0.04	23,29,46,52	0
23	CLA	C	507	65/65	0.90	0.13	0.02	25,42,79,81	0
23	CLA	c	908	65/65	0.95	0.11	-0.02	23,28,46,54	0
23	CLA	C	503	65/65	0.96	0.12	-0.05	23,27,37,42	0
25	BCR	a	411	40/40	0.95	0.08	-0.07	20,23,27,28	0
25	BCR	k	102	40/40	0.93	0.11	-0.08	27,32,38,40	0
23	CLA	C	513	65/65	0.93	0.11	-0.09	34,42,73,76	0
25	BCR	c	916	40/40	0.94	0.10	-0.13	25,32,38,38	0
37	HEM	e	105	43/43	0.98	0.15	-0.13	35,39,51,63	0
31	DMS	v	207	4/4	0.96	0.14	-0.16	53,54,54,60	0
23	CLA	b	617	65/65	0.94	0.12	-0.18	20,30,81,89	0
25	BCR	B	620	40/40	0.95	0.09	-0.22	21,29,41,42	0
23	CLA	c	907	65/65	0.93	0.10	-0.36	23,36,73,76	0
23	CLA	C	508	65/65	0.94	0.10	-0.36	28,35,49,55	0
37	HEM	V	203	43/43	0.98	0.07	-0.38	19,22,26,29	0
31	DMS	e	104	4/4	0.95	0.11	-0.38	72,73,78,83	0
25	BCR	c	915	40/40	0.94	0.10	-0.40	36,44,48,50	0
37	HEM	E	105	43/43	0.95	0.12	-0.40	36,42,46,47	0
25	BCR	C	515	40/40	0.93	0.09	-0.42	35,43,46,48	0
39	MG	J	102	1/1	0.99	0.09	-0.44	30,30,30,30	0
25	BCR	C	530	40/40	0.95	0.08	-0.47	27,32,36,37	0
37	HEM	v	203	43/43	0.98	0.08	-0.48	22,27,29,32	0
23	CLA	c	912	65/65	0.96	0.09	-0.54	26,31,37,41	0
25	BCR	j	104	40/40	0.95	0.08	-0.59	27,32,39,43	0
20	OEX	a	402	10/10	1.00	0.09	-0.71	21,23,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
20	OEX	A	401	10/10	1.00	0.08	-0.73	19,21,23,24	0
23	CLA	b	616	65/65	0.95	0.09	-0.76	21,26,42,44	0
23	CLA	C	512	65/65	0.94	0.08	-0.77	26,34,39,40	0
32	BCT	A	420	4/4	0.95	0.07	-0.78	31,32,35,40	0
32	BCT	a	424	4/4	0.97	0.06	-0.83	32,35,37,41	0
31	DMS	D	415	4/4	0.98	0.09	-1.16	50,53,56,59	0
22	CL	a	405	1/1	0.99	0.09	-1.53	21,21,21,21	0
21	FE2	A	402	1/1	0.99	0.04	-1.86	28,28,28,28	0
22	CL	a	404	1/1	0.99	0.06	-2.21	19,19,19,19	0
22	CL	A	404	1/1	1.00	0.08	-2.37	20,20,20,20	0
33	CA	o	302	1/1	0.94	0.06	-3.20	43,43,43,43	0
33	CA	c	901	1/1	0.98	0.04	-3.49	39,39,39,39	0
33	CA	O	301	1/1	0.95	0.08	-4.40	42,42,42,42	0
31	DMS	v	210	4/4	0.94	0.21	-	62,65,68,72	0
29	UNL	d	417	11/-	0.83	0.17	-	48,63,69,71	0
31	DMS	A	422	4/4	0.93	0.20	-	65,68,68,71	0
29	UNL	A	413	16/-	0.93	0.14	-	38,43,70,76	0
29	UNL	B	633	16/-	0.59	0.30	-	61,80,87,88	0
31	DMS	d	419	4/4	0.87	0.23	-	63,70,76,82	0
31	DMS	B	649	4/4	0.86	0.28	-	70,71,73,84	0
31	DMS	u	204	4/4	0.92	0.14	-	62,68,68,73	0
31	DMS	C	524	4/4	0.99	0.10	-	32,33,36,36	0
31	DMS	a	420	4/4	0.93	0.32	-	48,61,64,66	0
29	UNL	b	632	16/-	0.59	0.34	-	58,83,101,101	0
29	UNL	B	634	16/-	0.50	0.27	-	73,80,95,97	0
31	DMS	a	423	4/4	0.94	0.17	-	53,56,63,73	0
31	DMS	B	646	4/4	0.85	0.19	-	76,77,77,84	0
33	CA	B	601	1/1	0.96	0.10	-	41,41,41,41	0
31	DMS	c	936	4/4	0.65	0.29	-	80,80,81,90	0
31	DMS	B	647	4/4	0.80	0.37	-	81,85,85,89	0
31	DMS	v	205	4/4	0.95	0.11	-	63,66,68,69	0
31	DMS	h	105	4/4	0.80	0.19	-	76,83,89,90	0
31	DMS	b	641	4/4	0.92	0.21	-	52,59,66,66	0
31	DMS	b	643	4/4	0.83	0.33	-	81,82,85,85	0
29	UNL	b	631	16/-	0.41	0.23	-	61,73,81,82	0
29	UNL	I	104	16/-	0.50	0.29	-	69,76,89,92	0
31	DMS	i	106	4/4	0.17	0.34	-	120,121,124,138	0
31	DMS	U	204	4/4	0.61	0.21	-	53,62,62,80	0
31	DMS	l	102	4/4	0.88	0.14	-	64,65,70,84	0
29	UNL	Z	103	9/-	0.74	0.22	-	50,61,69,70	0
35	HTG	B	631	19/19	0.64	0.21	-	41,88,97,100	0
29	UNL	B	628	10/-	0.73	0.42	-	62,67,70,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
29	UNL	M	102	11/-	0.90	0.21	-	45,50,63,69	0
31	DMS	O	309	4/4	0.85	0.22	-	53,63,64,70	0
31	DMS	V	207	4/4	0.82	0.15	-	51,52,60,62	0
31	DMS	A	424	4/4	0.90	0.21	-	53,54,58,69	0
35	HTG	C	521	19/19	0.90	0.19	-	61,66,74,77	0
35	HTG	b	628	19/19	0.61	0.22	-	52,96,109,112	0
29	UNL	i	104	16/-	0.63	0.35	-	69,76,78,79	0
31	DMS	C	533	4/4	0.94	0.17	-	67,67,68,71	0
31	DMS	B	642	4/4	0.91	0.30	-	46,54,59,67	0
31	DMS	V	205	4/4	0.90	0.23	-	49,60,60,63	0
29	UNL	b	625	10/-	0.86	0.28	-	44,59,68,68	0
29	UNL	a	416	10/-	0.77	0.33	-	54,68,75,76	0
31	DMS	V	206	4/4	0.95	0.25	-	55,55,55,61	0
31	DMS	B	640	4/4	0.89	0.25	-	50,56,60,61	0
29	UNL	c	931	10/-	0.83	0.21	-	55,60,62,64	0
31	DMS	A	418	4/4	0.88	0.29	-	70,79,79,85	0
31	DMS	c	937	4/4	0.95	0.30	-	76,80,84,84	0
31	DMS	A	423	4/4	0.99	0.09	-	23,27,27,28	0
29	UNL	b	624	16/-	0.88	0.13	-	42,51,58,60	0
31	DMS	b	639	4/4	0.84	0.26	-	41,55,63,67	0
31	DMS	c	928	4/4	0.96	0.14	-	57,59,61,61	0
31	DMS	H	105	4/4	0.89	0.26	-	60,74,74,84	0
29	UNL	B	627	16/-	0.82	0.15	-	38,45,55,60	0
31	DMS	h	103	4/4	0.92	0.16	-	82,84,97,101	0
31	DMS	a	401	4/4	0.78	0.27	-	75,81,85,96	0
29	UNL	i	102	16/-	0.73	0.21	-	52,62,75,76	0
31	DMS	v	206	4/4	0.90	0.26	-	66,68,76,78	0
29	UNL	B	635	9/-	0.77	0.20	-	60,67,76,77	0
31	DMS	d	418	4/4	0.90	0.28	-	68,69,71,71	0
35	HTG	B	626	19/19	0.66	0.46	-	52,88,96,96	0
31	DMS	O	307	4/4	0.79	0.21	-	64,69,69,84	0
29	UNL	m	101	11/-	0.92	0.18	-	47,51,56,58	0
29	UNL	H	104	14/-	0.64	0.42	-	64,69,74,76	0
31	DMS	O	306	4/4	0.95	0.28	-	68,68,73,76	0
31	DMS	U	203	4/4	0.60	0.32	-	70,74,80,89	0
31	DMS	o	301	4/4	0.99	0.08	-	22,27,28,31	0
33	CA	b	601	1/1	0.98	0.08	-	41,41,41,41	0
31	DMS	c	935	4/4	0.86	0.28	-	71,72,75,83	0
29	UNL	I	102	13/-	0.83	0.16	-	47,53,65,69	0
29	UNL	b	629	12/-	0.84	0.34	-	49,59,70,71	0
31	DMS	O	310	4/4	0.86	0.25	-	61,67,74,76	0
31	DMS	c	924	4/4	0.99	0.09	-	31,33,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	DMS	C	528	4/4	0.91	0.15	-	60,63,65,66	0
29	UNL	i	101	16/-	0.91	0.13	-	37,43,60,60	0
35	HTG	c	921	19/19	0.84	0.21	-	68,82,88,91	0
31	DMS	b	642	4/4	0.70	0.34	-	90,90,97,101	0
31	DMS	c	934	4/4	0.86	0.27	-	87,87,89,99	0
29	UNL	C	532	11/-	0.88	0.23	-	54,59,66,66	0
31	DMS	h	104	4/4	0.87	0.27	-	97,99,103,103	0
31	DMS	v	208	4/4	0.89	0.22	-	54,67,71,87	0
29	UNL	b	630	16/-	0.38	0.34	-	74,86,106,110	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.