wwPDB X-ray Structure Validation Summary Report (i)

Feb 13, 2017 – 12:22 PM EST

PDB ID	:	5B66
Title	:	Crystal structure analysis of Photosystem II complex
Authors	:	Tanaka, A.; Fukushima, Y.; Kamiya, N.
Deposited on	:	2016-05-25
Resolution	:	1.85 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

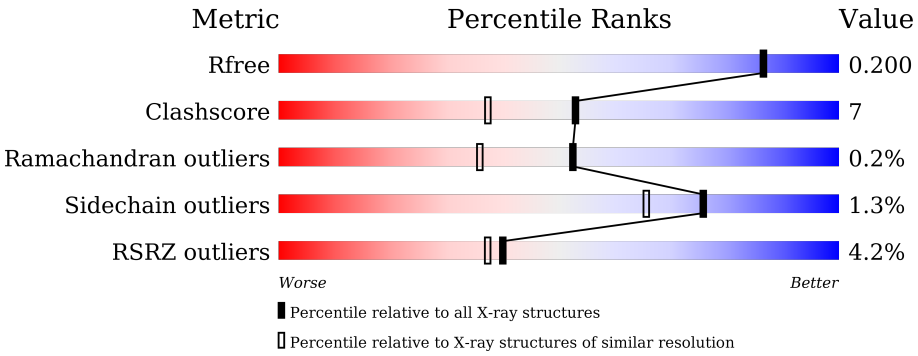
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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 >=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 <=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	87% 10%
1	a	344	2% 95%
2	B	505	4% 87% 13%
2	b	505	4% 95%
3	C	455	2% 87% 12%
3	c	455	97%

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Mol	Chain	Length	Quality of chain
4	D	342	87% 13%
4	d	342	96%
5	E	83	23% 75% 18% 6%
5	e	83	19% 88% 6% 6%
6	F	44	9% 52% 23% 25%
6	f	44	7% 70% 27%
7	H	65	5% 85% 12%
7	h	65	91% 5% 5%
8	I	38	8% 76% 16% 8%
8	i	38	5% 89% 5% 5%
9	J	40	5% 78% 13% 10%
9	j	40	8% 98%
10	K	37	5% 78% 22%
10	k	37	3% 95% 5%
11	L	37	8% 100%
11	l	37	8% 100%
12	M	36	3% 78% 11% 8%
12	m	36	8% 94% 6%
13	O	244	3% 84% 15%
13	o	244	8% 97%
14	T	32	3% 81% 6% 9%
14	t	32	6% 91% 6%
15	U	104	2% 82% 12% 7%
15	u	104	91% 7%
16	V	137	91% 9%

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Mol	Chain	Length	Quality of chain
16	v	137	4% 99%
17	Y	30	20% 70% 27%
17	y	30	17% 97%
18	X	40	13% 90% 5% 5%
18	x	40	5% 88% 13%
19	Z	62	23% 77% 18% 5%
19	z	62	19% 90% 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	401	X	-	-	-
20	CLA	A	402	X	-	-	-
20	CLA	A	404	X	-	-	-
20	CLA	B	601	X	-	-	-
20	CLA	B	602	X	-	-	X
20	CLA	B	603	X	-	-	-
20	CLA	B	604	X	-	-	-
20	CLA	B	605	X	-	-	-
20	CLA	B	606	X	-	-	-
20	CLA	B	607	X	-	-	-
20	CLA	B	608	X	-	-	-
20	CLA	B	609	X	-	-	-
20	CLA	B	610	X	-	-	-
20	CLA	B	611	X	-	-	-
20	CLA	B	612	X	-	-	-
20	CLA	B	613	X	-	-	-
20	CLA	B	614	X	-	-	-
20	CLA	B	615	X	-	-	-
20	CLA	B	616	X	-	-	-
20	CLA	C	501	X	-	-	-
20	CLA	C	502	X	-	-	-
20	CLA	C	503	X	-	-	-
20	CLA	C	504	X	-	-	-
20	CLA	C	505	X	-	-	-
20	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	C	507	X	-	-	-
20	CLA	C	508	X	-	-	-
20	CLA	C	509	X	-	-	-
20	CLA	C	510	X	-	-	-
20	CLA	C	511	X	-	-	-
20	CLA	C	512	X	-	-	-
20	CLA	C	513	X	-	-	-
20	CLA	D	401	X	-	-	-
20	CLA	D	402	X	-	-	-
20	CLA	D	404	X	-	-	X
20	CLA	a	403	X	-	-	-
20	CLA	a	404	X	-	-	X
20	CLA	a	407	X	-	-	-
20	CLA	b	603	X	-	-	X
20	CLA	b	604	X	-	-	-
20	CLA	b	605	X	-	-	-
20	CLA	b	606	X	-	-	-
20	CLA	b	607	X	-	-	-
20	CLA	b	608	X	-	-	-
20	CLA	b	609	X	-	-	-
20	CLA	b	610	X	-	-	-
20	CLA	b	611	X	-	-	-
20	CLA	b	612	X	-	-	-
20	CLA	b	613	X	-	-	-
20	CLA	b	614	X	-	-	-
20	CLA	b	615	X	-	-	-
20	CLA	b	616	X	-	-	-
20	CLA	b	617	X	-	-	-
20	CLA	b	618	X	-	-	-
20	CLA	c	501	X	-	-	-
20	CLA	c	502	X	-	-	-
20	CLA	c	503	X	-	-	-
20	CLA	c	504	X	-	-	-
20	CLA	c	505	X	-	-	-
20	CLA	c	506	X	-	-	-
20	CLA	c	507	X	-	-	-
20	CLA	c	508	X	-	-	-
20	CLA	c	509	X	-	-	-
20	CLA	c	510	X	-	-	-
20	CLA	c	511	X	-	-	-
20	CLA	c	512	X	-	-	-
20	CLA	c	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	d	402	X	-	-	-
20	CLA	d	403	X	-	-	-
20	CLA	d	404	X	-	-	-
22	BCR	K	102	-	-	-	X
23	SQD	a	401	-	-	-	X
23	SQD	b	622	-	-	-	X
23	SQD	f	101	-	-	-	X
23	SQD	l	101	-	-	-	X
24	LMG	A	407	-	-	-	X
24	LMG	B	620	-	-	-	X
24	LMG	C	524	-	-	-	X
24	LMG	a	410	-	-	-	X
24	LMG	b	623	-	-	-	X
24	LMG	c	518	-	-	-	X
26	UNL	A	410	-	-	-	X
26	UNL	B	630	-	-	-	X
26	UNL	B	633	-	-	-	X
26	UNL	C	523	-	-	-	X
26	UNL	D	410	-	-	-	X
26	UNL	D	411	-	-	-	X
26	UNL	E	102	-	-	-	X
26	UNL	J	105	-	-	-	X
26	UNL	T	103	-	-	-	X
26	UNL	U	901	-	-	X	X
26	UNL	X	101	-	-	-	X
26	UNL	b	630	-	-	-	X
26	UNL	d	409	-	-	-	X
26	UNL	d	410	-	-	-	X
26	UNL	d	411	-	-	-	X
26	UNL	h	103	-	-	-	X
26	UNL	j	106	-	-	-	X
26	UNL	t	102	-	-	-	X
27	PL9	A	411	-	-	-	X
27	PL9	a	415	-	-	-	X
28	DMS	A	416	-	-	-	X
28	DMS	A	417	-	-	-	X
28	DMS	A	418	-	-	-	X
28	DMS	B	634	-	-	-	X
28	DMS	B	637	-	-	-	X
28	DMS	B	638	-	-	-	X
28	DMS	B	639	-	-	X	X
28	DMS	B	641	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	DMS	B	642	-	-	X	X
28	DMS	B	644	-	-	X	-
28	DMS	C	525[A]	-	-	-	X
28	DMS	C	525[B]	-	-	-	X
28	DMS	C	526	-	-	-	X
28	DMS	C	527	-	-	-	X
28	DMS	C	530	-	-	X	X
28	DMS	C	531	-	-	X	X
28	DMS	C	532	-	-	X	X
28	DMS	D	413	-	-	-	X
28	DMS	D	414	-	-	X	-
28	DMS	D	415	-	-	-	X
28	DMS	O	304	-	-	-	X
28	DMS	O	305	-	-	-	X
28	DMS	O	306	-	-	-	X
28	DMS	O	307	-	-	X	-
28	DMS	O	309	-	-	-	X
28	DMS	O	310	-	-	-	X
28	DMS	U	902	-	-	-	X
28	DMS	U	903[A]	-	-	-	X
28	DMS	U	903[B]	-	-	X	X
28	DMS	V	205	-	-	-	X
28	DMS	V	206	-	-	X	-
28	DMS	b	631	-	-	-	X
28	DMS	b	633	-	-	-	X
28	DMS	b	636	-	-	-	X
28	DMS	c	528	-	-	-	X
28	DMS	c	530	-	-	-	X
28	DMS	c	535	-	-	-	X
28	DMS	c	536	-	-	-	X
28	DMS	d	413	-	-	-	X
28	DMS	d	414	-	-	-	X
28	DMS	o	304	-	-	-	X
28	DMS	o	306	-	-	-	X
28	DMS	o	307	-	-	-	X
28	DMS	u	202	-	-	-	X
28	DMS	v	202	-	-	-	X
28	DMS	v	206	-	-	-	X
31	BCT	A	421	-	-	X	-
32	HTG	B	621	-	-	-	X
32	HTG	B	622	-	-	-	X
32	HTG	C	521	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	HTG	C	522	-	-	-	X
32	HTG	D	417	-	-	-	X
32	HTG	O	302	-	-	-	X
32	HTG	V	202	-	-	-	X
32	HTG	b	625	-	-	-	X
32	HTG	c	521	-	-	-	X
32	HTG	d	401	-	-	-	X
32	HTG	v	210	-	-	-	X
34	LMT	B	626	-	-	-	X
34	LMT	B	627	-	-	-	X
34	LMT	E	101	-	-	-	X
34	LMT	J	103	-	-	-	X
34	LMT	T	102	-	-	-	X
34	LMT	a	418	-	-	-	X
34	LMT	b	627	-	-	-	X
34	LMT	b	628	-	-	-	X
34	LMT	f	102	-	-	-	X
34	LMT	m	101	-	-	-	X
35	DGD	D	406	-	-	-	X
35	DGD	H	102	-	-	-	X
35	DGD	d	416	-	-	-	X
35	DGD	h	101	-	-	-	X
36	LHG	D	409	-	-	-	X
36	LHG	E	103	-	-	-	X
36	LHG	d	407	-	-	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 54996 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	3	0
			2626	1721	430	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2622	1719	431	457	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	11	0
			4012	2632	668	699	13			
2	b	495	Total	C	N	O	S	0	4	0
			3884	2550	650	671	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	1	0
			3483	2280	582	608	13			
3	c	455	Total	C	N	O	S	0	1	0
			3523	2305	591	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	1	0
			2728	1808	446	462	12			
4	d	342	Total	C	N	O	S	0	0	0
			2722	1803	445	462	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	78	Total	C	N	O	0	1	0
			632	413	101	118			
5	e	78	Total	C	N	O	0	2	0
			636	419	99	118			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			
6	f	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	1	0
			508	339	81	86	2			
7	h	62	Total	C	N	O	S	0	1	0
			501	335	82	82	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			284	194	45	44	1			
8	i	36	Total	C	N	O	S	0	1	0
			300	203	49	47	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	40	Total	C	N	O	S	0	0	0
			272	183	41	47	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			
10	k	37	Total	C	N	O	0	0	0
			285	199	42	44			

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
			302	203	48	51			
11	l	37	Total	C	N	O	0	1	0
			296	200	45	51			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			259	175	37	46	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	6	0
			1870	1172	309	384	5			
13	o	243	Total	C	N	O	S	0	2	0
			1838	1153	305	376	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	29	Total	C	N	O	S	0	1	0
			257	181	35	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	0	0
			766	486	128	152			
15	u	97	Total	C	N	O	0	0	0
			770	489	129	152			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	3	0
			1080	685	181	210	4			
16	v	137	Total	C	N	O	S	0	0	0
			1052	666	174	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
			212	139	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			213	140	37	33	3			

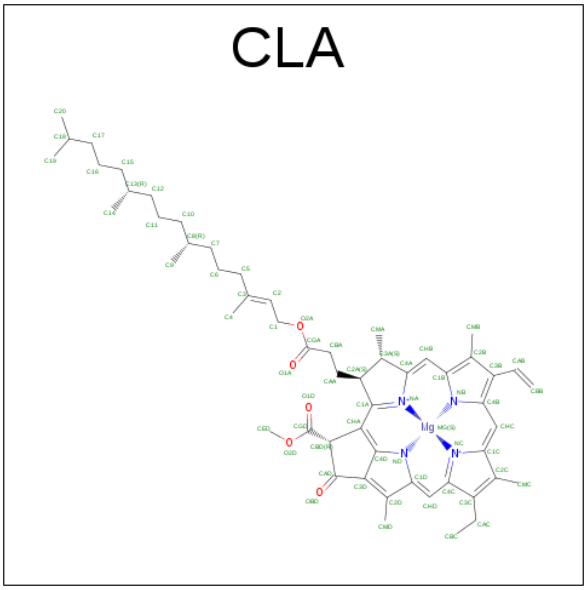
- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	0	0	0
			274	183	44	47			
18	x	35	Total	C	N	O	0	0	0
			252	171	38	43			

- 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
			450	308	67	73	2			
19	z	61	Total	C	N	O	S	0	0	0
			433	297	66	69	1			

- Molecule 20 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C Mg N O 59 49 1 4 5	0	0
20	A	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 60 50 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 55 45 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	D	1	Total C Mg N O 65 55 1 4 5	0	0
20	D	1	Total C Mg N O 65 55 1 4 5	0	0
20	D	1	Total C Mg N O 65 55 1 4 5	0	0
20	a	1	Total C Mg N O 65 55 1 4 5	0	0
20	a	1	Total C Mg N O 60 50 1 4 5	0	0
20	a	1	Total C Mg N O 47 37 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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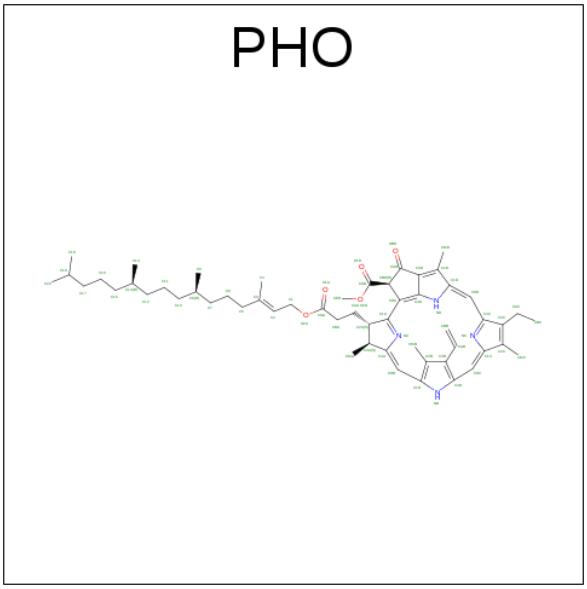
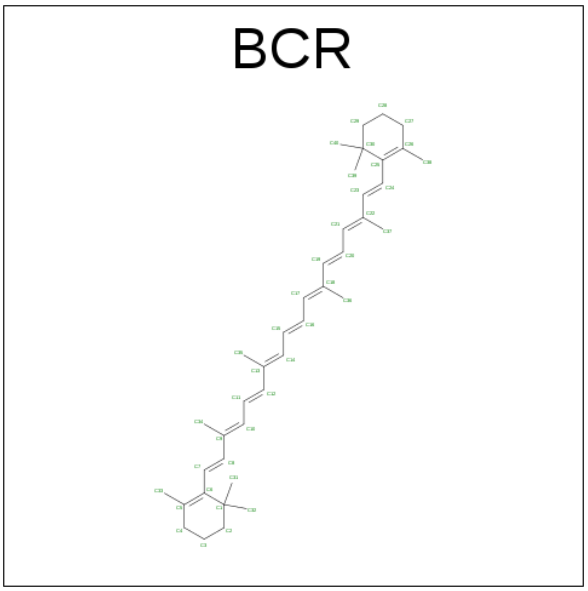
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 21 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

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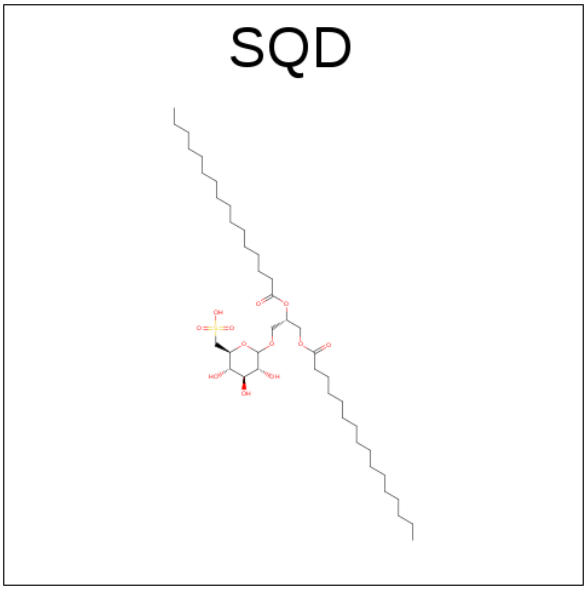
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	c	1	Total C 40 40	0	0
22	d	1	Total C 40 40	0	0
22	j	1	Total C 40 40	0	0
22	k	1	Total C 40 40	0	0
22	k	1	Total C 40 40	0	0
22	t	1	Total C 40 40	0	0

- Molecule 23 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O S 54 41 12 1	0	0
23	A	1	Total C O S 54 41 12 1	0	0
23	F	1	Total C O S 35 23 11 1	0	0
23	a	1	Total C O S 54 41 12 1	0	0
23	a	1	Total C O S 54 41 12 1	0	0

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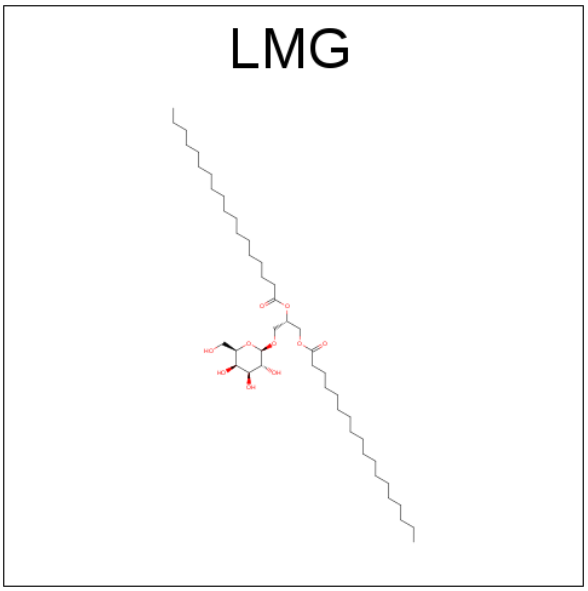
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	b	1	Total C O S 54 41 12 1	0	0
23	f	1	Total C O S 40 27 12 1	0	0
23	l	1	Total C O S 54 41 12 1	0	0

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C O 51 41 10	0	0
24	B	1	Total C O 51 41 10	0	0
24	C	1	Total C O 51 41 10	0	0
24	C	1	Total C O 45 35 10	0	0
24	J	1	Total C O 45 35 10	0	0
24	a	1	Total C O 51 41 10	0	0
24	b	1	Total C O 49 39 10	0	0
24	c	1	Total C O 51 41 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	c	1	Total C O 51 41 10	0	0
24	j	1	Total C O 45 35 10	0	0

- Molecule 25 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 26 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	h	1	Total C 16 16	0	0
26	B	6	Total C 84 84	0	0
26	c	3	Total C O 48 43 5	0	0
26	t	1	Total C 16 16	0	0
26	X	1	Total C 16 16	0	0
26	J	4	Total C 33 33	0	0
26	E	1	Total C 15 15	0	0
26	b	7	Total C 68 68	0	0
26	A	2	Total C O 40 35 5	0	0
26	x	1	Total C 9 9	0	0
26	M	1	Total C 12 12	0	0
26	j	2	Total C 22 22	0	0
26	D	2	Total C O 53 48 5	0	0

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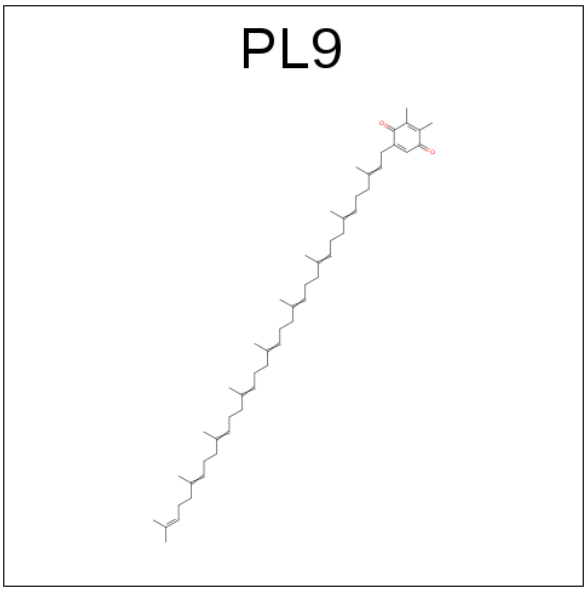
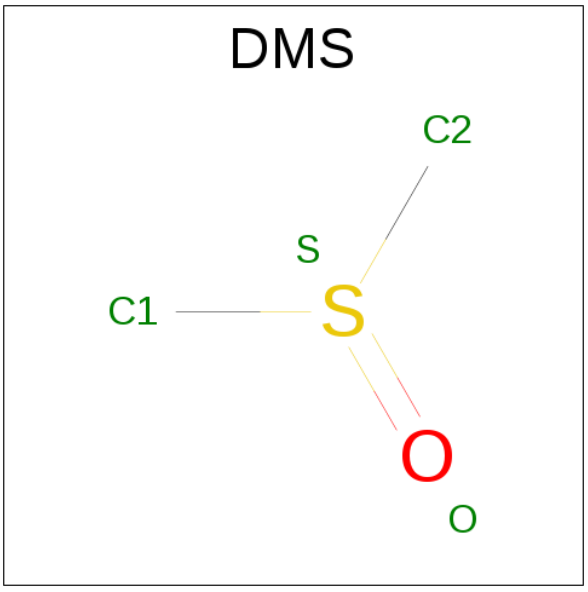
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	e	1	Total C 7 7	0	0
26	I	5	Total C 61 61	0	0
26	Z	1	Total C 4 4	0	0
26	a	3	Total C O 45 40 5	0	0
26	U	1	Total C 14 14	0	0
26	L	1	Total C 14 14	0	0
26	d	3	Total C O 68 63 5	0	0
26	H	2	Total C 10 10	0	0
26	i	3	Total C 38 38	0	0
26	C	1	Total C O 34 29 5	0	0
26	z	1	Total C 6 6	0	0
26	T	1	Total C 13 13	0	0

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



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

- Molecule 28 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O S 4 2 1 1	0	0
28	A	1	Total C O S 4 2 1 1	0	0
28	A	1	Total C O S 4 2 1 1	0	0
28	A	1	Total C O S 4 2 1 1	0	0
28	A	1	Total C O S 4 2 1 1	0	0
28	B	1	Total C O S 4 2 1 1	0	0
28	B	1	Total C O S 4 2 1 1	0	0
28	B	1	Total C O S 4 2 1 1	0	0
28	B	1	Total C O S 4 2 1 1	0	0
28	B	1	Total C O S 4 2 1 1	0	0
28	B	1	Total C O S 4 2 1 1	0	0
28	B	1	Total C O S 4 2 1 1	0	0
28	B	1	Total C O S 4 2 1 1	0	0
28	B	1	Total C O S 4 2 1 1	0	0
28	B	1	Total C O S 4 2 1 1	0	0
28	B	1	Total C O S 4 2 1 1	0	0
28	B	1	Total C O S 4 2 1 1	0	0
28	C	1	Total C O S 8 4 2 2	0	1
28	C	1	Total C O S 4 2 1 1	0	0
28	C	1	Total C O S 4 2 1 1	0	0
28	C	1	Total C O S 4 2 1 1	0	0
28	C	1	Total C O S 4 2 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	C	1	Total C O S 4 2 1 1	0	0
28	C	1	Total C O S 4 2 1 1	0	0
28	C	1	Total C O S 4 2 1 1	0	0
28	C	1	Total C O S 4 2 1 1	0	0
28	D	1	Total C O S 4 2 1 1	0	0
28	D	1	Total C O S 4 2 1 1	0	0
28	D	1	Total C O S 4 2 1 1	0	0
28	D	1	Total C O S 4 2 1 1	0	0
28	F	1	Total C O S 4 2 1 1	0	0
28	H	1	Total C O S 4 2 1 1	0	0
28	O	1	Total C O S 4 2 1 1	0	0
28	O	1	Total C O S 4 2 1 1	0	0
28	O	1	Total C O S 4 2 1 1	0	0
28	O	1	Total C O S 4 2 1 1	0	0
28	O	1	Total C O S 4 2 1 1	0	0
28	O	1	Total C O S 4 2 1 1	0	0
28	O	1	Total C O S 4 2 1 1	0	0
28	O	1	Total C O S 4 2 1 1	0	0
28	O	1	Total C O S 4 2 1 1	0	0
28	U	1	Total C O S 4 2 1 1	0	0
28	U	1	Total C O S 8 4 2 2	0	1

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	c	1	Total C O S 4 2 1 1	0	0
28	c	1	Total C O S 4 2 1 1	0	0
28	c	1	Total C O S 4 2 1 1	0	0
28	c	1	Total C O S 4 2 1 1	0	0
28	c	1	Total C O S 4 2 1 1	0	0
28	c	1	Total C O S 4 2 1 1	0	0
28	c	1	Total C O S 4 2 1 1	0	0
28	d	1	Total C O S 4 2 1 1	0	0
28	d	1	Total C O S 4 2 1 1	0	0
28	d	1	Total C O S 4 2 1 1	0	0
28	h	1	Total C O S 4 2 1 1	0	0
28	i	1	Total C O S 4 2 1 1	0	0
28	j	1	Total C O S 4 2 1 1	0	0
28	o	1	Total C O S 4 2 1 1	0	0
28	o	1	Total C O S 4 2 1 1	0	0
28	o	1	Total C O S 4 2 1 1	0	0
28	o	1	Total C O S 4 2 1 1	0	0
28	o	1	Total C O S 4 2 1 1	0	0
28	o	1	Total C O S 4 2 1 1	0	0
28	o	1	Total C O S 4 2 1 1	0	0
28	u	1	Total C O S 4 2 1 1	0	0

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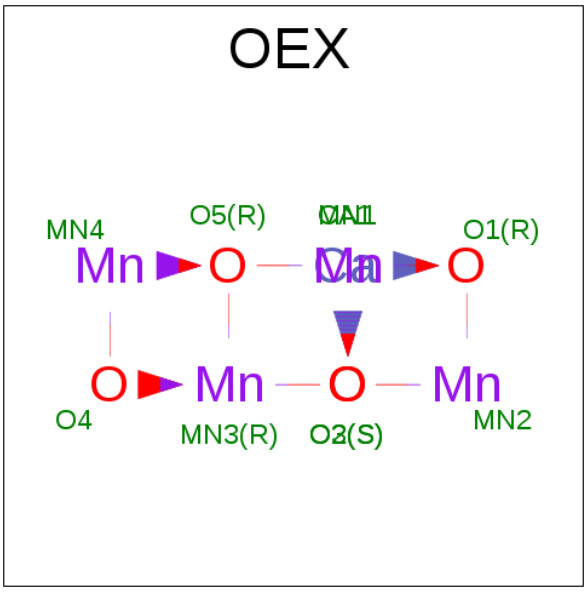
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	u	1	Total C O S 4 2 1 1	0	0
28	u	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total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

- Molecule 29 is FE (II) ION (three-letter code: FE2) (formula: Fe).

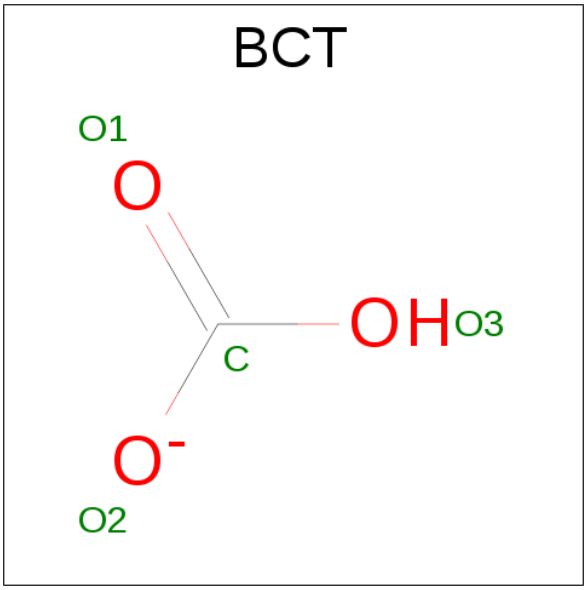
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total Fe 1 1	0	0
29	a	1	Total Fe 1 1	0	0

- Molecule 30 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



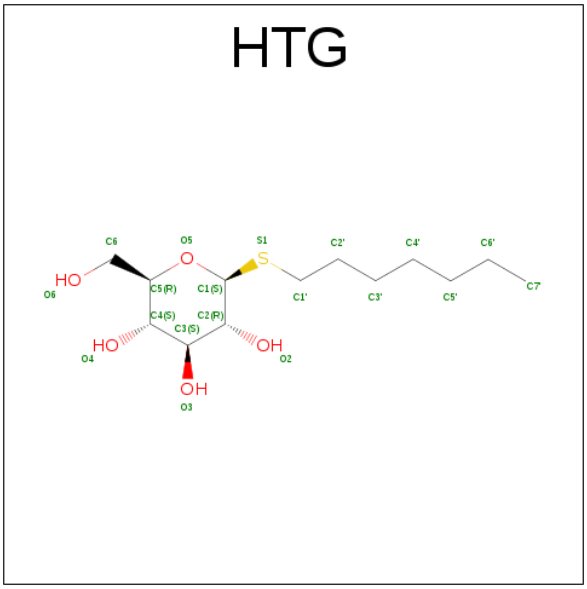
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
30	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

- Molecule 32 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	1	Total C O S 19 13 5 1	0	0
32	B	1	Total C O S 19 13 5 1	0	0
32	B	1	Total C O S 19 13 5 1	0	0
32	B	1	Total C O S 19 13 5 1	0	0
32	B	1	Total C O S 19 13 5 1	0	0
32	C	1	Total C O S 19 13 5 1	0	0
32	C	1	Total C O S 19 13 5 1	0	0
32	C	1	Total C O S 19 13 5 1	0	0
32	C	1	Total C O S 19 13 5 1	0	0
32	D	1	Total C O S 19 13 5 1	0	0
32	O	1	Total C O S 19 13 5 1	0	0
32	V	1	Total C O S 13 7 5 1	0	0

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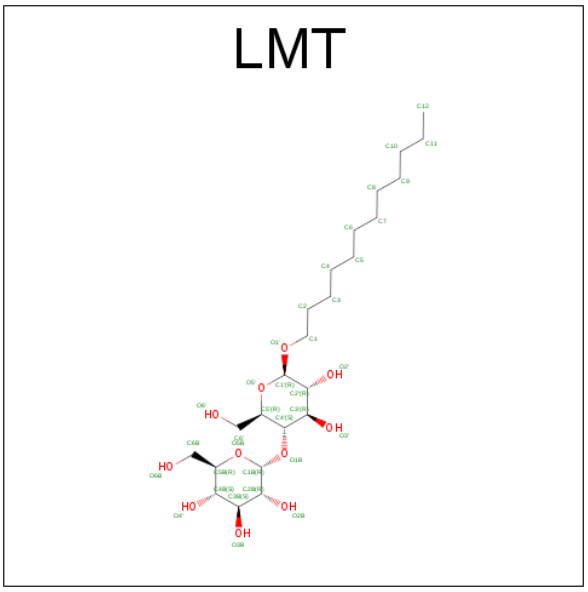
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	b	1	Total C O S 19 13 5 1	0	0
32	b	1	Total C O S 19 13 5 1	0	0
32	b	1	Total C O S 19 13 5 1	0	0
32	b	1	Total C O S 19 13 5 1	0	0
32	c	1	Total C O S 19 13 5 1	0	0
32	c	1	Total C O S 19 13 5 1	0	0
32	d	1	Total C O S 19 13 5 1	0	0
32	u	1	Total C S 8 7 1	0	0
32	v	1	Total C O S 14 8 5 1	0	0

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

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

- Molecule 34 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	B	1	Total C O 24 18 6	0	0
34	B	1	Total C O 24 18 6	0	0
34	B	1	Total C O 16 14 2	0	0
34	E	1	Total C O 24 18 6	0	0
34	I	1	Total C O 35 24 11	0	0
34	J	1	Total C O 24 18 6	0	0
34	M	1	Total C O 35 24 11	0	0
34	T	1	Total C O 24 18 6	0	0
34	Z	1	Total C O 35 24 11	0	0
34	a	1	Total C O 35 24 11	0	0
34	b	1	Total C O 32 21 11	0	0
34	b	1	Total C O 25 19 6	0	0
34	c	1	Total C O 35 24 11	0	0
34	f	1	Total C O 24 18 6	0	0

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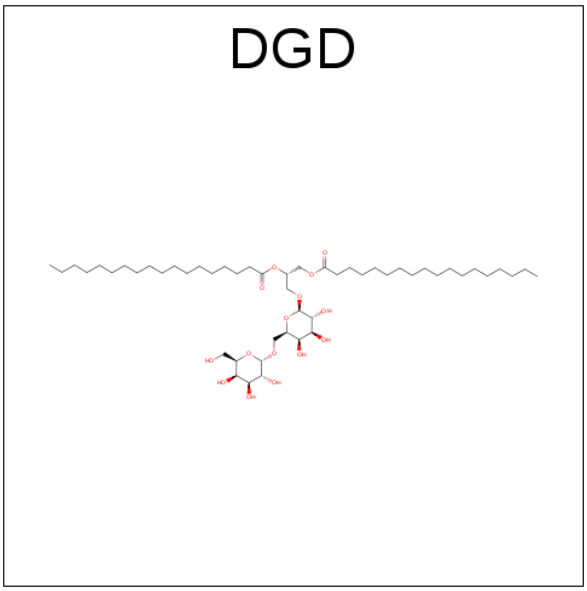
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	m	1	Total C O 35 24 11	0	0
34	m	1	Total C O 35 24 11	0	0
34	z	1	Total C O 35 24 11	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total C O 62 47 15	0	0
35	C	1	Total C O 55 40 15	0	0
35	C	1	Total C O 62 47 15	0	0
35	D	1	Total C O 51 41 10	0	0
35	H	1	Total C O 62 47 15	0	0
35	c	1	Total C O 62 47 15	0	0
35	c	1	Total C O 57 42 15	0	0
35	c	1	Total C O 62 47 15	0	0

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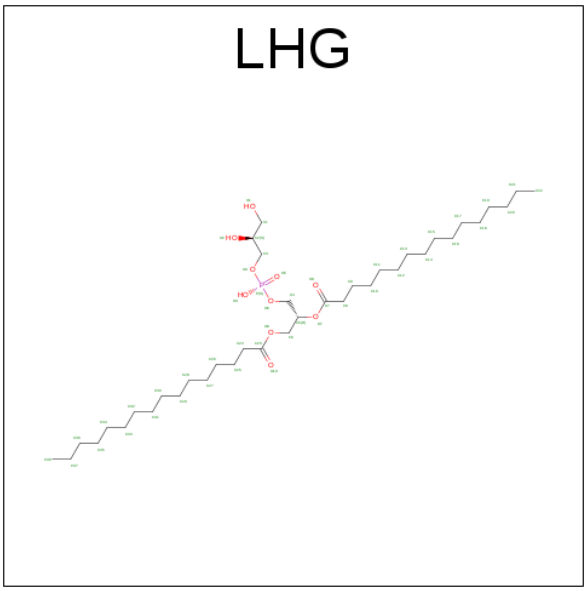
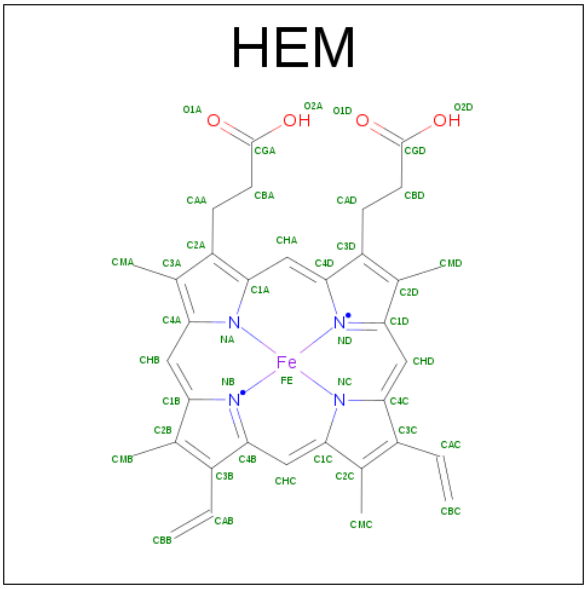
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	d	1	Total C O 51 41 10	0	0
35	h	1	Total C O 62 47 15	0	0

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



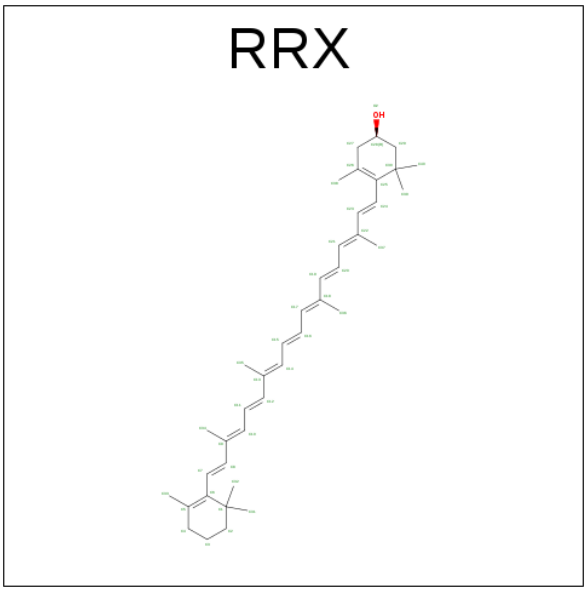
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	D	1	Total C O P 49 38 10 1	0	0
36	D	1	Total C O P 49 38 10 1	0	0
36	D	1	Total C O P 49 38 10 1	0	0
36	E	1	Total C O P 48 37 10 1	0	0
36	L	1	Total C O P 49 38 10 1	0	0
36	d	1	Total C O P 49 38 10 1	0	0
36	d	1	Total C O P 49 38 10 1	0	0
36	d	1	Total C O P 49 38 10 1	0	0
36	l	1	Total C O P 49 38 10 1	0	0

- 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	C	Fe	N	O	0	0
			43	34	1	4	4		
37	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
37	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
37	v	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: $C_{40}H_{56}O$).



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

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

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

- Molecule 40 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	A	177	Total O 182 182	0	5
40	B	447	Total O 473 473	0	25
40	C	317	Total O 324 324	0	7
40	D	175	Total O 180 180	0	5
40	E	62	Total O 66 66	0	4

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	F	8	Total O 8 8	0	0
40	H	62	Total O 65 65	0	3
40	I	16	Total O 16 16	0	0
40	J	23	Total O 23 23	0	0
40	K	12	Total O 12 12	0	0
40	L	19	Total O 21 21	0	2
40	M	12	Total O 12 12	0	0
40	O	263	Total O 273 273	0	10
40	T	19	Total O 20 20	0	1
40	U	133	Total O 136 136	0	3
40	V	177	Total O 183 183	0	6
40	Y	7	Total O 7 7	0	0
40	X	22	Total O 22 22	0	0
40	Z	5	Total O 5 5	0	0
40	a	182	Total O 185 185	0	3
40	b	451	Total O 465 465	0	14
40	c	362	Total O 374 374	0	12
40	d	176	Total O 182 182	0	6
40	e	48	Total O 49 49	0	1
40	f	15	Total O 16 16	0	1
40	h	68	Total O 70 70	0	2

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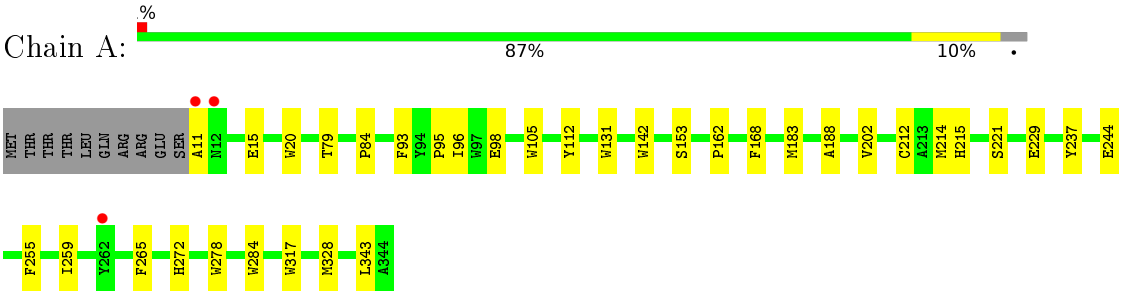
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	i	19	Total O 21 21	0	2
40	j	23	Total O 24 24	0	1
40	k	11	Total O 12 12	0	1
40	l	22	Total O 24 24	0	2
40	m	23	Total O 24 24	0	1
40	o	214	Total O 230 230	0	15
40	t	19	Total O 20 20	0	1
40	u	146	Total O 150 150	0	4
40	v	144	Total O 147 147	0	3
40	y	7	Total O 7 7	0	0
40	x	25	Total O 26 26	0	1
40	z	12	Total O 12 12	0	0

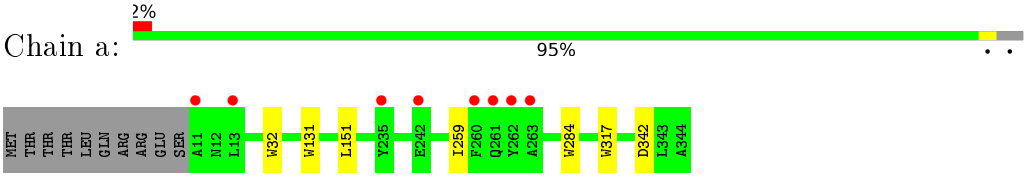
3 Residue-property plots

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

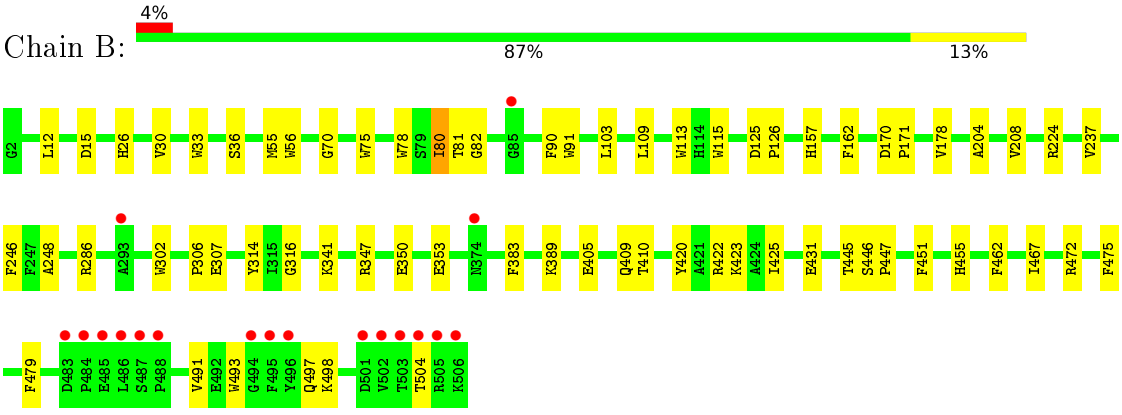
- Molecule 1: Photosystem II protein D1



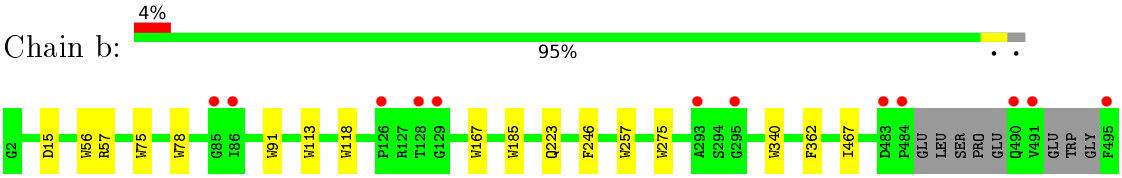
- Molecule 1: Photosystem II protein D1

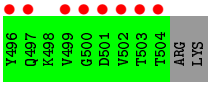


- Molecule 2: Photosystem II CP47 reaction center protein



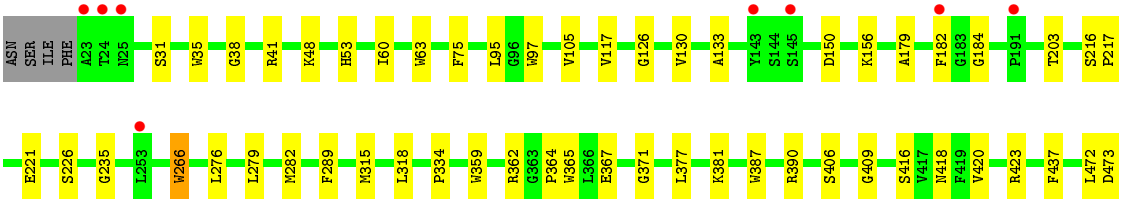
- Molecule 2: Photosystem II CP47 reaction center protein





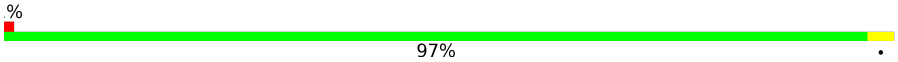
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



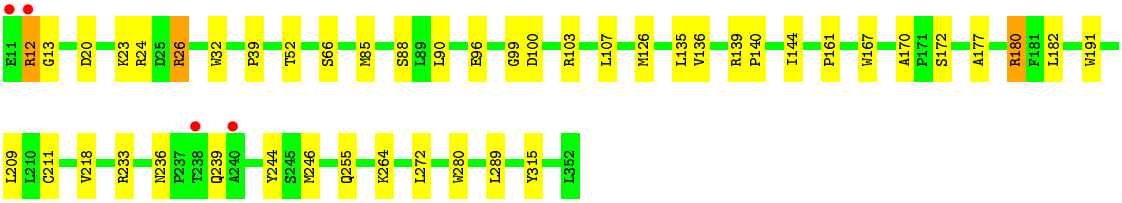
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



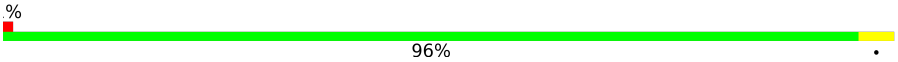
• Molecule 4: Photosystem II D2 protein

Chain D:



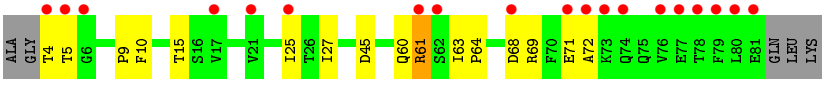
• Molecule 4: Photosystem II D2 protein

Chain d:



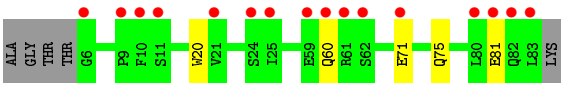
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:

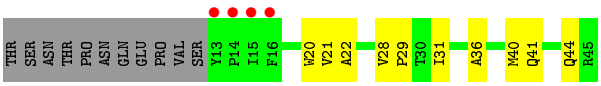


• Molecule 5: Cytochrome b559 subunit alpha

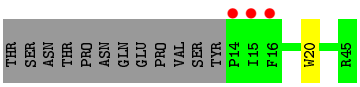
Chain e:



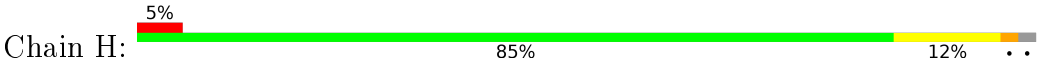
• Molecule 6: Cytochrome b559 subunit beta



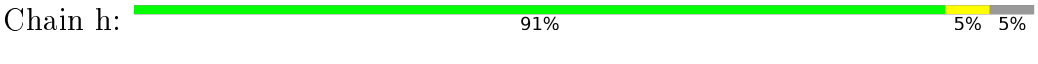
• Molecule 6: Cytochrome b559 subunit beta

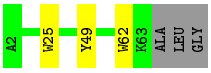


• Molecule 7: Photosystem II reaction center protein H

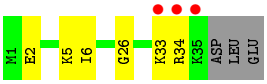


• Molecule 7: Photosystem II reaction center protein H

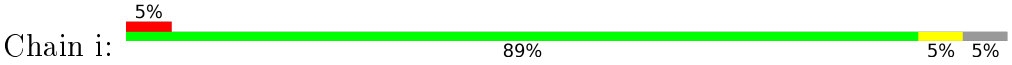


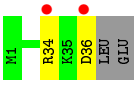


• Molecule 8: Photosystem II reaction center protein I

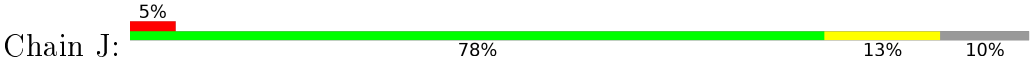


• Molecule 8: Photosystem II reaction center protein I



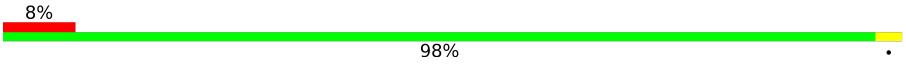


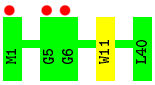
• Molecule 9: Photosystem II reaction center protein J



• Molecule 9: Photosystem II reaction center protein J

Chain j:



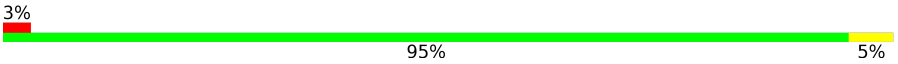


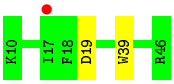
• Molecule 10: Photosystem II reaction center protein K

Chain K:

• Molecule 10: Photosystem II reaction center protein K

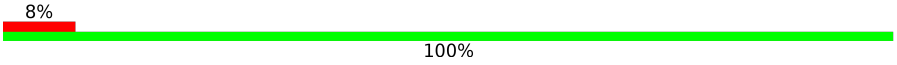
Chain k:





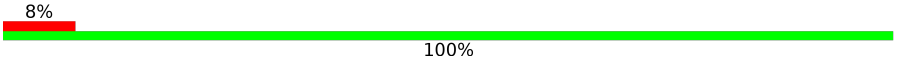
• Molecule 11: Photosystem II reaction center protein L

Chain L:



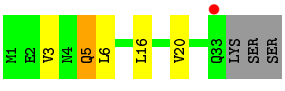
• Molecule 11: Photosystem II reaction center protein L

Chain l:



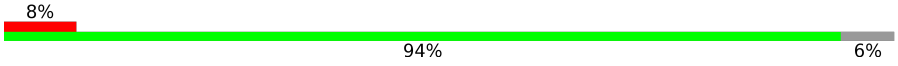
• Molecule 12: Photosystem II reaction center protein M

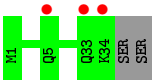
Chain M:



• Molecule 12: Photosystem II reaction center protein M

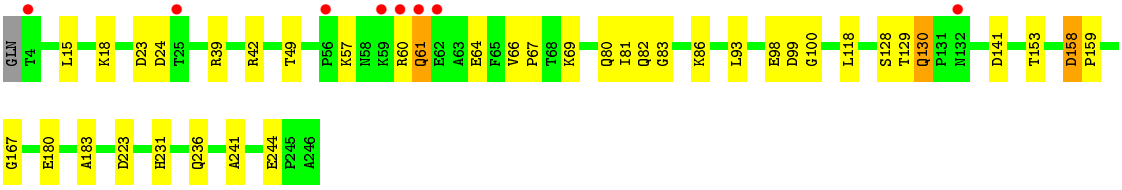
Chain m:





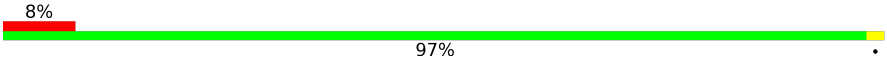
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

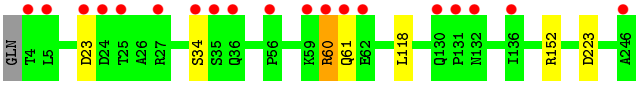
Chain O:



• Molecule 13: Photosystem II manganese-stabilizing polypeptide

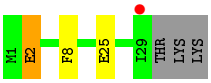
Chain o:





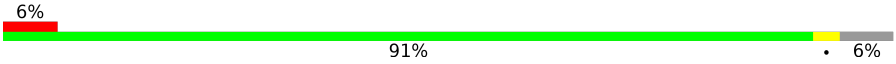
• Molecule 14: Photosystem II reaction center protein T

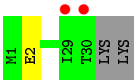
Chain T:



• Molecule 14: Photosystem II reaction center protein T

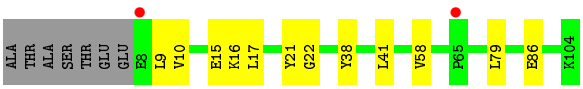
Chain t:





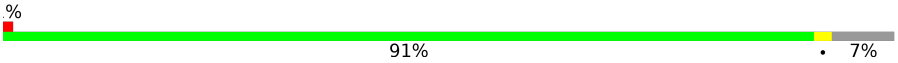
• Molecule 15: Photosystem II 12 kDa extrinsic protein

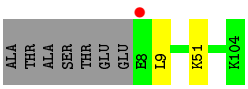
Chain U:



• Molecule 15: Photosystem II 12 kDa extrinsic protein

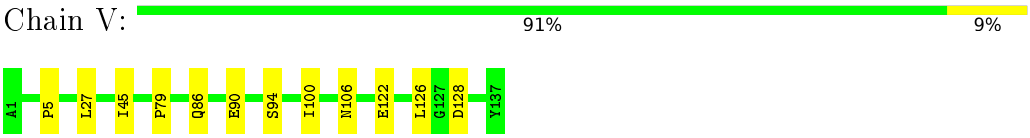
Chain u:





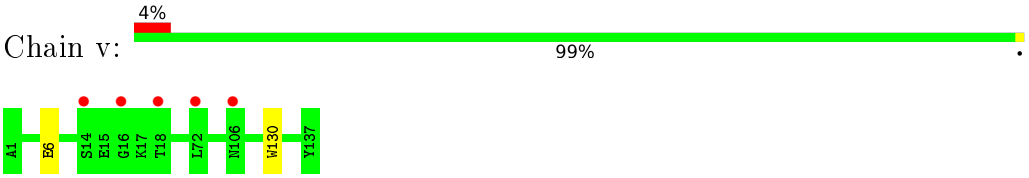
• Molecule 16: Cytochrome c-550

Chain V:



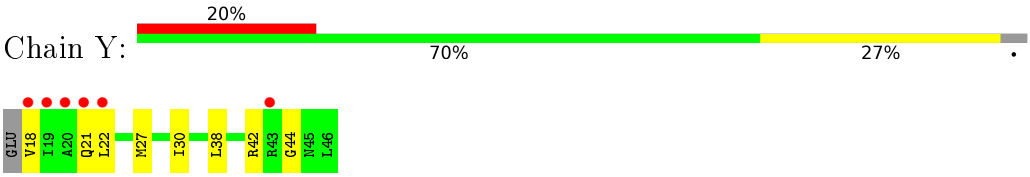
• Molecule 16: Cytochrome c-550

Chain v:



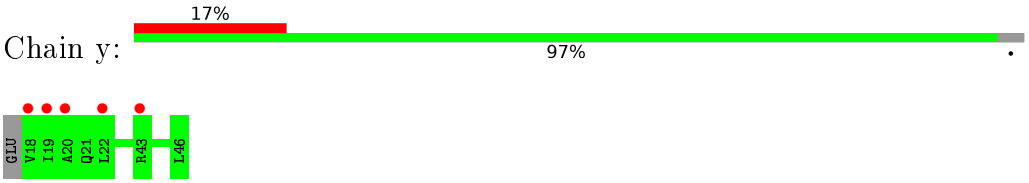
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



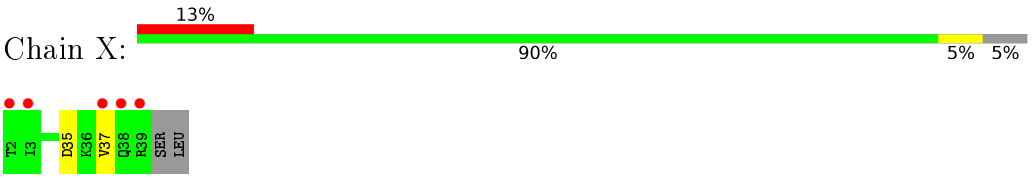
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



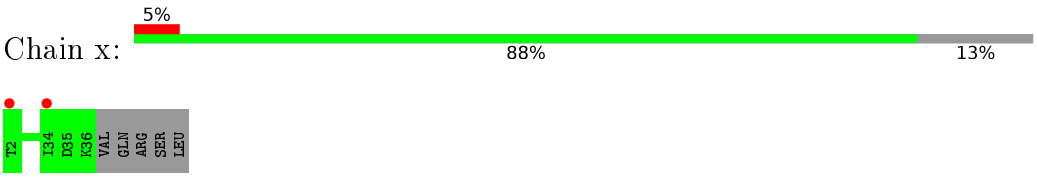
• Molecule 18: Photosystem II reaction center protein X

Chain X:



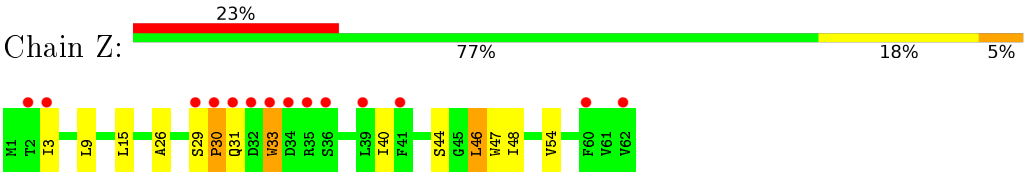
• Molecule 18: Photosystem II reaction center protein X

Chain x:



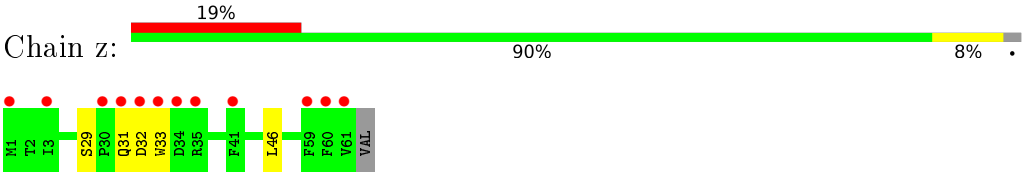
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



• Molecule 19: Photosystem II reaction center protein Z

Chain z:


19%
90%
8%
M1
T2
I3
S29
P30
Q31
D32
W33
D34
R35
F41
L46
F59
F60
V61
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	121.47Å 228.18Å 286.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 1.85 19.99 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.99-1.85) 100.0 (19.99-1.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.162 , 0.201 0.162 , 0.200	Depositor DCC
R_{free} test set	33616 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	29.1	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 70.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	54996	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.95	5/2717 (0.2%)	0.77	1/3707 (0.0%)
1	a	0.93	4/2718 (0.1%)	0.79	2/3707 (0.1%)
2	B	0.90	9/4181 (0.2%)	0.77	1/5700 (0.0%)
2	b	0.91	11/4029 (0.3%)	0.78	2/5490 (0.0%)
3	C	0.87	7/3599 (0.2%)	0.74	2/4901 (0.0%)
3	c	0.86	8/3640 (0.2%)	0.72	2/4956 (0.0%)
4	D	0.95	3/2826 (0.1%)	0.78	1/3850 (0.0%)
4	d	0.95	8/2817 (0.3%)	0.78	1/3839 (0.0%)
5	E	0.71	0/654	0.68	0/896
5	e	0.69	1/661 (0.2%)	0.72	0/904
6	F	0.79	1/278 (0.4%)	0.60	0/379
6	f	0.81	1/265 (0.4%)	0.62	0/360
7	H	0.84	2/524 (0.4%)	0.75	0/715
7	h	0.86	2/517 (0.4%)	0.71	0/704
8	I	0.63	0/281	0.69	0/380
8	i	0.61	0/300	0.62	0/405
9	J	0.82	1/257 (0.4%)	0.61	0/349
9	j	0.81	1/278 (0.4%)	0.62	0/378
10	K	0.70	1/303 (0.3%)	0.65	0/416
10	k	0.72	1/295 (0.3%)	0.64	0/407
11	L	0.88	0/312	0.76	0/425
11	l	0.91	0/306	0.76	0/418
12	M	0.70	0/265	0.74	0/362
12	m	0.70	0/270	0.76	0/369
13	O	0.72	0/1919	0.80	1/2607 (0.0%)
13	o	0.69	0/1875	0.77	2/2548 (0.1%)
14	T	0.78	0/259	0.77	0/352
14	t	0.79	0/257	0.73	0/349
15	U	0.77	0/777	0.78	0/1055
15	u	0.76	0/781	0.77	0/1059
16	V	0.80	0/1110	0.80	1/1506 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.71	1/1073 (0.1%)	0.75	0/1461
17	Y	0.50	0/213	0.63	0/285
17	y	0.45	0/214	0.60	0/286
18	X	0.54	0/277	0.69	0/375
18	x	0.57	0/255	0.66	0/345
19	Z	0.70	2/461 (0.4%)	0.56	0/632
19	z	0.61	1/444 (0.2%)	0.57	0/611
All	All	0.85	70/42208 (0.2%)	0.75	16/57488 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	o	0	1

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	365	TRP	CD2-CE2	7.13	1.50	1.41
1	A	343	LEU	C-N	6.74	1.49	1.34
1	a	131	TRP	CD2-CE2	6.46	1.49	1.41
3	C	266	TRP	CD2-CE2	6.43	1.49	1.41
2	B	33	TRP	CD2-CE2	6.27	1.48	1.41

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	342	ASP	CB-CG-OD1	6.34	124.01	118.30
16	V	128	ASP	CB-CG-OD1	6.14	123.82	118.30
3	C	473	ASP	CB-CG-OD2	5.92	123.63	118.30
13	o	152	ARG	NE-CZ-NH1	-5.84	117.38	120.30
3	c	423	ARG	NE-CZ-NH2	-5.79	117.41	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	o	60	ARG	Peptide

5.2 Too-close contacts (i)

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	2626	0	2515	27	0
1	a	2622	0	2529	0	0
2	B	4012	0	3860	82	0
2	b	3884	0	3743	0	0
3	C	3483	0	3397	50	0
3	c	3523	0	3439	0	0
4	D	2728	0	2636	52	0
4	d	2722	0	2623	0	0
5	E	632	0	605	14	0
5	e	636	0	612	0	0
6	F	269	0	277	6	0
6	f	257	0	269	0	0
7	H	508	0	524	7	0
7	h	501	0	526	0	0
8	I	284	0	303	6	0
8	i	300	0	320	0	0
9	J	251	0	257	3	0
9	j	272	0	271	0	0
10	K	293	0	305	6	0
10	k	285	0	290	0	0
11	L	302	0	316	0	0
11	l	296	0	305	0	0
12	M	259	0	281	22	0
12	m	264	0	283	0	0
13	O	1870	0	1836	41	0
13	o	1838	0	1789	0	0
14	T	257	0	260	2	0
14	t	258	0	261	0	0
15	U	766	0	758	21	0
15	u	770	0	769	0	0
16	V	1080	0	1097	15	0
16	v	1052	0	1040	0	0
17	Y	212	0	237	6	0
17	y	213	0	239	0	0
18	X	274	0	297	2	0
18	x	252	0	277	0	0
19	Z	450	0	455	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	z	433	0	422	0	0
20	A	189	0	202	11	0
20	B	1040	0	1152	54	0
20	C	830	0	900	51	0
20	D	195	0	216	7	0
20	a	172	0	166	0	0
20	b	1040	0	1152	0	0
20	c	840	0	923	0	0
20	d	195	0	216	0	0
21	A	64	0	74	2	0
21	D	64	0	74	2	0
21	a	128	0	148	0	0
22	A	40	0	56	4	0
22	B	120	0	168	6	0
22	C	80	0	112	5	0
22	D	40	0	56	3	0
22	K	80	0	112	8	0
22	T	40	0	56	7	0
22	a	40	0	56	0	0
22	b	120	0	168	0	0
22	c	40	0	56	0	0
22	d	40	0	56	0	0
22	j	40	0	56	0	0
22	k	80	0	112	0	0
22	t	40	0	56	0	0
23	A	108	0	156	5	0
23	F	35	0	40	3	0
23	a	108	0	156	0	0
23	b	54	0	78	0	0
23	f	40	0	47	0	0
23	l	54	0	78	0	0
24	A	51	0	72	4	0
24	B	51	0	72	0	0
24	C	96	0	132	5	0
24	J	45	0	60	0	0
24	a	51	0	72	0	0
24	b	49	0	68	0	0
24	c	102	0	144	0	0
24	j	45	0	60	0	0
25	A	2	0	0	0	0
25	a	2	0	0	0	0
26	A	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	B	84	0	0	2	0
26	C	34	0	0	0	0
26	D	53	0	0	0	0
26	E	15	0	0	0	0
26	H	10	0	0	0	0
26	I	61	0	0	0	0
26	J	33	0	0	1	0
26	L	14	0	0	0	0
26	M	12	0	0	0	0
26	T	13	0	0	0	0
26	U	14	0	0	3	0
26	X	16	0	0	0	0
26	Z	4	0	0	0	0
26	a	45	0	0	0	0
26	b	68	0	0	0	0
26	c	48	0	0	0	0
26	d	68	0	0	0	0
26	e	7	0	0	0	0
26	h	16	0	0	0	0
26	i	38	0	0	0	0
26	j	22	0	0	0	0
26	t	16	0	0	0	0
26	x	9	0	0	0	0
26	z	6	0	0	0	0
27	A	55	0	80	11	0
27	D	55	0	80	0	0
27	a	55	0	80	0	0
27	d	55	0	80	0	0
28	A	20	0	30	1	0
28	B	48	0	72	29	0
28	C	40	0	60	20	0
28	D	16	0	24	16	0
28	F	4	0	6	3	0
28	H	4	0	6	0	0
28	O	36	0	54	17	0
28	U	16	0	24	16	0
28	V	24	0	36	7	0
28	b	44	0	66	0	0
28	c	40	0	60	0	0
28	d	12	0	18	0	0
28	h	4	0	6	0	0
28	i	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	j	4	0	6	0	0
28	o	28	0	42	0	0
28	u	12	0	18	0	0
28	v	32	0	48	0	0
29	A	1	0	0	0	0
29	a	1	0	0	0	0
30	A	10	0	0	0	0
30	a	10	0	0	0	0
31	A	4	0	0	5	0
31	a	4	0	0	0	0
32	B	95	0	130	11	0
32	C	76	0	104	3	0
32	D	19	0	26	3	0
32	O	19	0	26	0	0
32	V	13	0	11	0	0
32	b	76	0	104	0	0
32	c	38	0	52	0	0
32	d	19	0	26	0	0
32	u	8	0	15	0	0
32	v	14	0	13	0	0
33	B	1	0	0	0	0
33	O	1	0	0	0	0
33	V	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	64	0	95	3	0
34	E	24	0	35	0	0
34	I	35	0	46	2	0
34	J	24	0	35	1	0
34	M	35	0	46	0	0
34	T	24	0	35	0	0
34	Z	35	0	46	0	0
34	a	35	0	46	0	0
34	b	57	0	72	0	0
34	c	35	0	46	0	0
34	f	24	0	35	0	0
34	m	70	0	92	0	0
34	z	35	0	46	0	0
35	C	179	0	232	3	0
35	D	51	0	71	5	0
35	H	62	0	82	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	c	181	0	236	0	0
35	d	51	0	71	0	0
35	h	62	0	82	0	0
36	D	147	0	222	37	0
36	E	48	0	71	6	0
36	L	49	0	74	0	0
36	d	147	0	222	0	0
36	l	49	0	74	0	0
37	E	43	0	30	2	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	182	0	0	5	0
40	B	473	0	0	25	0
40	C	324	0	0	10	0
40	D	180	0	0	1	0
40	E	66	0	0	1	0
40	F	8	0	0	0	0
40	H	65	0	0	3	0
40	I	16	0	0	1	0
40	J	23	0	0	0	0
40	K	12	0	0	0	0
40	L	21	0	0	0	0
40	M	12	0	0	1	0
40	O	273	0	0	20	0
40	T	20	0	0	0	0
40	U	136	0	0	3	0
40	V	183	0	0	3	0
40	X	22	0	0	1	0
40	Y	7	0	0	1	0
40	Z	5	0	0	1	0
40	a	185	0	0	0	0
40	b	465	0	0	0	0
40	c	374	0	0	0	0
40	d	182	0	0	0	0
40	e	49	0	0	0	0
40	f	16	0	0	0	0
40	h	70	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	i	21	0	0	0	0
40	j	24	0	0	0	0
40	k	12	0	0	0	0
40	l	24	0	0	0	0
40	m	24	0	0	0	0
40	o	230	0	0	0	0
40	t	20	0	0	0	0
40	u	150	0	0	0	0
40	v	147	0	0	0	0
40	x	26	0	0	0	0
40	y	7	0	0	0	0
40	z	12	0	0	0	0
All	All	54996	0	51554	535	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 535 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)
12:M:16[B]:LEU:CD2	12:M:16[B]:LEU:HD11	2.58	1.58
12:M:16[B]:LEU:HD22	12:M:16[B]:LEU:CD1	2.65	1.45
12:M:16[B]:LEU:CD2	12:M:16[B]:LEU:CD1	2.45	1.19
15:U:22:GLY:HA2	28:U:903[B]:DMS:H12	1.24	1.19
2:B:347[B]:ARG:NH1	40:B:1031[B]:HOH:O	1.81	1.14

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	335/344 (97%)	329 (98%)	5 (2%)	1 (0%)	46 29
1	a	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	46 29
2	B	514/505 (102%)	503 (98%)	11 (2%)	0	100 100
2	b	493/505 (98%)	485 (98%)	8 (2%)	0	100 100
3	C	450/455 (99%)	436 (97%)	13 (3%)	1 (0%)	52 36
3	c	454/455 (100%)	442 (97%)	11 (2%)	1 (0%)	52 36
4	D	341/342 (100%)	334 (98%)	6 (2%)	1 (0%)	46 29
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100 100
5	E	77/83 (93%)	75 (97%)	2 (3%)	0	100 100
5	e	78/83 (94%)	78 (100%)	0	0	100 100
6	F	31/44 (70%)	31 (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	61/65 (94%)	59 (97%)	2 (3%)	0	100 100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100 100
8	i	35/38 (92%)	34 (97%)	1 (3%)	0	100 100
9	J	34/40 (85%)	34 (100%)	0	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%)	34 (97%)	1 (3%)	0	100 100
11	L	36/37 (97%)	36 (100%)	0	0	100 100
11	l	36/37 (97%)	36 (100%)	0	0	100 100
12	M	32/36 (89%)	32 (100%)	0	0	100 100
12	m	33/36 (92%)	32 (97%)	1 (3%)	0	100 100
13	O	247/244 (101%)	235 (95%)	11 (4%)	1 (0%)	39 22
13	o	243/244 (100%)	231 (95%)	9 (4%)	3 (1%)	16 4
14	T	28/32 (88%)	28 (100%)	0	0	100 100
14	t	28/32 (88%)	28 (100%)	0	0	100 100
15	U	95/104 (91%)	93 (98%)	2 (2%)	0	100 100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100 100
16	V	138/137 (101%)	133 (96%)	5 (4%)	0	100 100
16	v	135/137 (98%)	131 (97%)	4 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	Y	27/30 (90%)	27 (100%)	0	0	100 100
17	y	27/30 (90%)	27 (100%)	0	0	100 100
18	X	36/40 (90%)	35 (97%)	1 (3%)	0	100 100
18	x	33/40 (82%)	32 (97%)	1 (3%)	0	100 100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	11 2
19	z	59/62 (95%)	54 (92%)	3 (5%)	2 (3%)	5 0
All	All	5201/5350 (97%)	5069 (98%)	120 (2%)	12 (0%)	52 36

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	o	60	ARG
19	z	32	ASP
3	C	416	SER
4	D	12	ARG
13	O	61	GLN

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	269/279 (96%)	268 (100%)	1 (0%)	93 92
1	a	270/279 (97%)	270 (100%)	0	100 100
2	B	405/403 (100%)	401 (99%)	4 (1%)	82 76
2	b	390/403 (97%)	386 (99%)	4 (1%)	82 76
3	C	351/356 (99%)	349 (99%)	2 (1%)	90 87
3	c	356/356 (100%)	351 (99%)	5 (1%)	74 63
4	D	277/277 (100%)	274 (99%)	3 (1%)	80 72
4	d	276/277 (100%)	272 (99%)	4 (1%)	74 63
5	E	68/72 (94%)	65 (96%)	3 (4%)	35 15
5	e	68/72 (94%)	63 (93%)	5 (7%)	17 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	F	27/38 (71%)	26 (96%)	1 (4%)	41 20
6	f	26/38 (68%)	26 (100%)	0	100 100
7	H	54/54 (100%)	52 (96%)	2 (4%)	41 20
7	h	54/54 (100%)	53 (98%)	1 (2%)	65 49
8	I	30/34 (88%)	30 (100%)	0	100 100
8	i	32/34 (94%)	29 (91%)	3 (9%)	11 1
9	J	23/28 (82%)	22 (96%)	1 (4%)	35 16
9	j	24/28 (86%)	24 (100%)	0	100 100
10	K	30/30 (100%)	30 (100%)	0	100 100
10	k	28/30 (93%)	27 (96%)	1 (4%)	42 21
11	L	34/35 (97%)	34 (100%)	0	100 100
11	l	33/35 (94%)	33 (100%)	0	100 100
12	M	30/33 (91%)	29 (97%)	1 (3%)	45 25
12	m	30/33 (91%)	30 (100%)	0	100 100
13	O	207/207 (100%)	202 (98%)	5 (2%)	57 39
13	o	199/207 (96%)	197 (99%)	2 (1%)	82 76
14	T	26/28 (93%)	23 (88%)	3 (12%)	7 1
14	t	26/28 (93%)	25 (96%)	1 (4%)	40 19
15	U	82/89 (92%)	82 (100%)	0	100 100
15	u	83/89 (93%)	81 (98%)	2 (2%)	57 39
16	V	120/117 (103%)	119 (99%)	1 (1%)	86 82
16	v	114/117 (97%)	113 (99%)	1 (1%)	84 79
17	Y	21/23 (91%)	19 (90%)	2 (10%)	11 1
17	y	21/23 (91%)	21 (100%)	0	100 100
18	X	29/33 (88%)	29 (100%)	0	100 100
18	x	27/33 (82%)	27 (100%)	0	100 100
19	Z	44/52 (85%)	43 (98%)	1 (2%)	58 41
19	z	39/52 (75%)	37 (95%)	2 (5%)	29 11
All	All	4223/4376 (96%)	4162 (99%)	61 (1%)	76 63

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Y	27	MET
3	c	156	LYS
15	u	9	LEU
17	Y	30	ILE
2	b	223	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
13	O	82	GLN
1	a	315	ASN
13	o	231	HIS
11	L	6	ASN
12	M	5	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	0.68	0	5,9,11	1.31	1 (20%)
14	FME	T	1	14	8,9,10	0.40	0	5,9,11	1.95	2 (40%)
8	FME	i	1	8	8,9,10	0.47	0	5,9,11	1.77	2 (40%)
14	FME	t	1	14	8,9,10	0.48	0	5,9,11	1.93	3 (60%)

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 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	T	1	FME	O-C-CA	-2.69	118.34	125.69
14	t	1	FME	O-C-CA	-2.48	118.90	125.69
8	i	1	FME	O1-CN-N	-2.43	121.08	124.80
8	i	1	FME	O-C-CA	-2.17	119.76	125.69
8	I	1	FME	O-C-CA	-2.12	119.91	125.69

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 349 ligands modelled in this entry, 55 are unknown and 14 are monoatomic - leaving 280 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	CLA	A	401	-	57,73,73	1.68	11 (19%)	61,113,113	2.06	19 (31%)
20	CLA	A	402	40	51,67,73	1.50	10 (19%)	53,105,113	2.37	14 (26%)
21	PHO	A	403	-	67,69,69	1.66	11 (16%)	86,99,99	2.08	23 (26%)
20	CLA	A	404	-	57,73,73	1.78	12 (21%)	61,113,113	1.80	16 (26%)
22	BCR	A	405	-	41,41,41	0.94	3 (7%)	56,56,56	1.27	6 (10%)
23	SQD	A	406	-	53,54,54	1.45	3 (5%)	62,65,65	2.01	15 (24%)
24	LMG	A	407	-	51,51,55	0.93	2 (3%)	59,59,63	1.11	3 (5%)
27	PL9	A	411	-	54,55,55	0.71	2 (3%)	68,69,69	1.74	17 (25%)
23	SQD	A	412	-	53,54,54	1.52	3 (5%)	62,65,65	2.08	10 (16%)
28	DMS	A	414	-	3,3,3	1.98	1 (33%)	3,3,3	0.51	0
28	DMS	A	415	-	3,3,3	2.76	1 (33%)	3,3,3	0.92	0
28	DMS	A	416	-	3,3,3	2.69	1 (33%)	3,3,3	0.70	0
28	DMS	A	417	-	3,3,3	2.63	1 (33%)	3,3,3	0.41	0
28	DMS	A	418	-	3,3,3	2.80	1 (33%)	3,3,3	0.68	0
30	OEX	A	420	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
31	BCT	A	421	29	0,3,3	0.00	-	0,3,3	0.00	-
20	CLA	B	601	-	57,73,73	1.72	12 (21%)	61,113,113	2.02	17 (27%)
20	CLA	B	602	40	57,73,73	1.92	13 (22%)	61,113,113	2.27	17 (27%)
20	CLA	B	603	-	57,73,73	1.84	12 (21%)	61,113,113	2.05	17 (27%)
20	CLA	B	604	-	57,73,73	1.73	12 (21%)	61,113,113	2.40	18 (29%)
20	CLA	B	605	-	57,73,73	1.59	12 (21%)	61,113,113	2.07	15 (24%)
20	CLA	B	606	-	57,73,73	1.67	9 (15%)	61,113,113	2.21	20 (32%)
20	CLA	B	607	-	57,73,73	1.93	12 (21%)	61,113,113	1.98	16 (26%)
20	CLA	B	608	40	57,73,73	1.61	11 (19%)	61,113,113	2.09	15 (24%)
20	CLA	B	609	-	57,73,73	1.67	10 (17%)	61,113,113	2.17	21 (34%)
20	CLA	B	610	-	57,73,73	1.69	10 (17%)	61,113,113	2.08	17 (27%)
20	CLA	B	611	40	57,73,73	1.83	13 (22%)	61,113,113	2.03	15 (24%)
20	CLA	B	612	-	57,73,73	1.53	10 (17%)	61,113,113	2.06	19 (31%)
20	CLA	B	613	-	57,73,73	1.65	11 (19%)	61,113,113	2.23	17 (27%)
20	CLA	B	614	-	57,73,73	1.69	14 (24%)	61,113,113	2.07	15 (24%)
20	CLA	B	615	-	57,73,73	1.68	11 (19%)	61,113,113	1.92	16 (26%)
20	CLA	B	616	-	57,73,73	1.75	12 (21%)	61,113,113	1.96	15 (24%)
22	BCR	B	617	-	41,41,41	0.96	0	56,56,56	1.61	10 (17%)
22	BCR	B	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.26	7 (12%)
22	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.60	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	LMG	B	620	-	51,51,55	0.99	2 (3%)	59,59,63	1.30	5 (8%)
32	HTG	B	621	-	19,19,19	1.35	3 (15%)	22,24,24	1.93	6 (27%)
32	HTG	B	622	-	19,19,19	1.26	3 (15%)	22,24,24	2.19	5 (22%)
32	HTG	B	623	-	19,19,19	0.90	1 (5%)	22,24,24	2.01	2 (9%)
34	LMT	B	625	-	24,24,36	0.51	0	29,29,47	1.24	4 (13%)
34	LMT	B	626	-	24,24,36	0.52	0	29,29,47	1.23	3 (10%)
34	LMT	B	627	-	15,15,36	0.50	0	14,14,47	1.16	1 (7%)
32	HTG	B	631	-	19,19,19	0.88	1 (5%)	22,24,24	2.52	4 (18%)
32	HTG	B	632	-	19,19,19	0.95	1 (5%)	22,24,24	1.44	2 (9%)
28	DMS	B	634	-	3,3,3	1.94	1 (33%)	3,3,3	0.29	0
28	DMS	B	635	-	3,3,3	2.64	1 (33%)	3,3,3	0.41	0
28	DMS	B	636	-	3,3,3	2.77	1 (33%)	3,3,3	0.71	0
28	DMS	B	637	-	3,3,3	2.56	1 (33%)	3,3,3	0.68	0
28	DMS	B	638	-	3,3,3	2.76	1 (33%)	3,3,3	0.75	0
28	DMS	B	639	-	3,3,3	2.74	1 (33%)	3,3,3	0.57	0
28	DMS	B	640	-	3,3,3	2.55	1 (33%)	3,3,3	0.87	0
28	DMS	B	641	-	3,3,3	2.66	1 (33%)	3,3,3	0.61	0
28	DMS	B	642	-	3,3,3	2.80	1 (33%)	3,3,3	0.69	0
28	DMS	B	643	-	3,3,3	2.78	1 (33%)	3,3,3	0.67	0
28	DMS	B	644	-	3,3,3	2.88	1 (33%)	3,3,3	1.15	0
28	DMS	B	645	-	3,3,3	2.73	1 (33%)	3,3,3	0.85	0
20	CLA	C	501	-	57,73,73	1.73	11 (19%)	61,113,113	2.11	13 (21%)
20	CLA	C	502	-	57,73,73	1.78	12 (21%)	61,113,113	1.98	16 (26%)
20	CLA	C	503	-	57,73,73	1.89	11 (19%)	61,113,113	1.97	17 (27%)
20	CLA	C	504	40	57,73,73	1.76	9 (15%)	61,113,113	2.15	17 (27%)
20	CLA	C	505	-	57,73,73	1.85	13 (22%)	61,113,113	1.97	17 (27%)
20	CLA	C	506	-	57,73,73	1.95	13 (22%)	61,113,113	1.98	18 (29%)
20	CLA	C	507	40	57,73,73	1.88	13 (22%)	61,113,113	2.03	16 (26%)
20	CLA	C	508	-	52,68,73	2.03	13 (25%)	55,107,113	1.91	14 (25%)
20	CLA	C	509	-	57,73,73	1.81	11 (19%)	61,113,113	2.12	17 (27%)
20	CLA	C	510	-	57,73,73	1.80	12 (21%)	61,113,113	2.20	17 (27%)
20	CLA	C	511	3	57,73,73	1.85	13 (22%)	61,113,113	1.93	14 (22%)
20	CLA	C	512	-	47,63,73	2.21	12 (25%)	49,101,113	2.15	16 (32%)
20	CLA	C	513	-	57,73,73	1.98	12 (21%)	61,113,113	1.97	15 (24%)
22	BCR	C	514	-	41,41,41	0.84	0	56,56,56	1.31	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	BCR	C	515	-	41,41,41	0.96	0	56,56,56	1.21	6 (10%)
35	DGD	C	516	-	63,63,67	0.87	2 (3%)	77,77,81	1.21	6 (7%)
35	DGD	C	517	-	56,56,67	0.95	2 (3%)	70,70,81	0.94	4 (5%)
35	DGD	C	518	-	63,63,67	0.83	2 (3%)	77,77,81	1.04	4 (5%)
24	LMG	C	519	-	51,51,55	1.00	2 (3%)	59,59,63	1.23	7 (11%)
32	HTG	C	520	-	19,19,19	0.83	1 (5%)	22,24,24	1.92	1 (4%)
32	HTG	C	521	-	19,19,19	0.92	1 (5%)	22,24,24	2.34	4 (18%)
32	HTG	C	522	-	19,19,19	0.99	2 (10%)	22,24,24	2.10	1 (4%)
24	LMG	C	524	-	45,45,55	1.07	3 (6%)	53,53,63	1.41	6 (11%)
28	DMS	C	525[A]	-	3,3,3	2.80	1 (33%)	3,3,3	0.77	0
28	DMS	C	525[B]	-	3,3,3	2.59	1 (33%)	3,3,3	0.73	0
28	DMS	C	526	-	3,3,3	2.56	1 (33%)	3,3,3	0.77	0
28	DMS	C	527	-	3,3,3	2.57	1 (33%)	3,3,3	0.45	0
28	DMS	C	528	-	3,3,3	2.32	1 (33%)	3,3,3	0.55	0
28	DMS	C	529	-	3,3,3	2.69	1 (33%)	3,3,3	0.73	0
28	DMS	C	530	-	3,3,3	2.62	1 (33%)	3,3,3	0.94	0
28	DMS	C	531	-	3,3,3	2.66	1 (33%)	3,3,3	0.89	0
28	DMS	C	532	-	3,3,3	3.29	1 (33%)	3,3,3	1.19	0
28	DMS	C	533	-	3,3,3	2.64	1 (33%)	3,3,3	0.44	0
32	HTG	C	534	-	19,19,19	1.01	1 (5%)	22,24,24	1.58	5 (22%)
20	CLA	D	401	-	57,73,73	1.58	11 (19%)	61,113,113	2.33	20 (32%)
20	CLA	D	402	40	57,73,73	1.69	13 (22%)	61,113,113	2.25	19 (31%)
21	PHO	D	403	-	67,69,69	1.88	14 (20%)	86,99,99	1.90	22 (25%)
20	CLA	D	404	-	57,73,73	1.77	14 (24%)	61,113,113	1.85	20 (32%)
22	BCR	D	405	-	41,41,41	1.01	3 (7%)	56,56,56	1.74	13 (23%)
35	DGD	D	406	-	51,51,67	1.09	2 (3%)	59,59,81	1.23	6 (10%)
36	LHG	D	407	-	48,48,48	0.85	1 (2%)	49,54,54	1.28	5 (10%)
36	LHG	D	408	-	48,48,48	0.80	2 (4%)	49,54,54	1.04	1 (2%)
36	LHG	D	409	-	48,48,48	0.93	2 (4%)	49,54,54	1.05	3 (6%)
27	PL9	D	412	-	54,55,55	1.00	2 (3%)	68,69,69	1.62	11 (16%)
28	DMS	D	413	-	3,3,3	2.74	1 (33%)	3,3,3	0.62	0
28	DMS	D	414	-	3,3,3	2.53	1 (33%)	3,3,3	0.21	0
28	DMS	D	415	-	3,3,3	2.93	1 (33%)	3,3,3	0.66	0
28	DMS	D	416	-	3,3,3	2.68	1 (33%)	3,3,3	0.51	0
32	HTG	D	417	-	19,19,19	0.99	1 (5%)	22,24,24	1.79	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	LMT	E	101	-	24,24,36	0.60	1 (4%)	29,29,47	1.01	3 (10%)
36	LHG	E	103	-	46,46,48	1.03	3 (6%)	48,50,54	1.16	5 (10%)
37	HEM	E	104	5,6	24,50,50	2.16	8 (33%)	16,82,82	2.47	6 (37%)
23	SQD	F	101	-	34,35,54	1.55	2 (5%)	42,45,65	1.92	8 (19%)
28	DMS	F	102	-	3,3,3	2.64	1 (33%)	3,3,3	0.57	0
38	RRX	H	101	-	42,42,42	0.75	0	57,58,58	1.49	7 (12%)
35	DGD	H	102	-	63,63,67	1.01	3 (4%)	77,77,81	1.27	8 (10%)
28	DMS	H	103	-	3,3,3	2.75	1 (33%)	3,3,3	0.57	0
34	LMT	I	101	-	36,36,36	0.64	1 (2%)	47,47,47	1.31	5 (10%)
24	LMG	J	101	39	45,45,55	0.98	2 (4%)	53,53,63	0.98	2 (3%)
34	LMT	J	103	-	24,24,36	0.63	1 (4%)	29,29,47	1.17	2 (6%)
22	BCR	K	101	-	41,41,41	0.81	1 (2%)	56,56,56	1.50	11 (19%)
22	BCR	K	102	-	41,41,41	0.90	0	56,56,56	1.48	7 (12%)
36	LHG	L	101	-	48,48,48	0.88	3 (6%)	49,54,54	0.90	1 (2%)
34	LMT	M	101	-	36,36,36	0.62	0	47,47,47	0.98	4 (8%)
32	HTG	O	302	-	19,19,19	1.22	2 (10%)	22,24,24	1.21	2 (9%)
28	DMS	O	303	-	3,3,3	2.62	1 (33%)	3,3,3	0.58	0
28	DMS	O	304	-	3,3,3	2.62	1 (33%)	3,3,3	0.56	0
28	DMS	O	305	-	3,3,3	2.64	1 (33%)	3,3,3	0.74	0
28	DMS	O	306	-	3,3,3	2.54	1 (33%)	3,3,3	0.59	0
28	DMS	O	307	-	3,3,3	2.69	1 (33%)	3,3,3	0.38	0
28	DMS	O	308	-	3,3,3	2.76	1 (33%)	3,3,3	0.73	0
28	DMS	O	309	-	3,3,3	2.68	1 (33%)	3,3,3	1.12	0
28	DMS	O	310	-	3,3,3	2.71	1 (33%)	3,3,3	0.63	0
28	DMS	O	311	-	3,3,3	2.88	1 (33%)	3,3,3	0.83	0
22	BCR	T	101	-	41,41,41	0.80	0	56,56,56	1.50	11 (19%)
34	LMT	T	102	-	24,24,36	0.44	0	29,29,47	1.19	2 (6%)
28	DMS	U	902	-	3,3,3	2.66	1 (33%)	3,3,3	1.53	0
28	DMS	U	903[A]	-	3,3,3	2.57	1 (33%)	3,3,3	0.71	0
28	DMS	U	903[B]	-	3,3,3	2.45	1 (33%)	3,3,3	0.16	0
28	DMS	U	904	-	3,3,3	2.86	1 (33%)	3,3,3	0.64	0
37	HEM	V	201	16	24,50,50	2.07	10 (41%)	16,82,82	2.07	5 (31%)
32	HTG	V	202	-	13,13,19	0.69	0	16,18,24	2.31	6 (37%)
28	DMS	V	204	-	3,3,3	2.66	1 (33%)	3,3,3	0.71	0
28	DMS	V	205	-	3,3,3	2.72	1 (33%)	3,3,3	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	DMS	V	206	-	3,3,3	2.68	1 (33%)	3,3,3	0.62	0
28	DMS	V	207	-	3,3,3	2.59	1 (33%)	3,3,3	0.42	0
28	DMS	V	208	-	3,3,3	2.65	1 (33%)	3,3,3	0.69	0
28	DMS	V	209	-	3,3,3	2.61	1 (33%)	3,3,3	0.58	0
34	LMT	Z	101	-	36,36,36	0.66	1 (2%)	47,47,47	1.03	5 (10%)
23	SQD	a	401	-	53,54,54	1.57	3 (5%)	62,65,65	1.55	9 (14%)
20	CLA	a	403	-	57,73,73	1.66	13 (22%)	61,113,113	1.98	18 (29%)
20	CLA	a	404	40	52,68,73	1.71	11 (21%)	55,107,113	2.38	17 (30%)
21	PHO	a	405	-	67,69,69	1.77	12 (17%)	86,99,99	1.84	19 (22%)
21	PHO	a	406	-	67,69,69	1.86	14 (20%)	86,99,99	1.90	24 (27%)
20	CLA	a	407	-	39,55,73	2.22	11 (28%)	42,91,113	2.69	19 (45%)
22	BCR	a	408	-	41,41,41	1.18	3 (7%)	56,56,56	1.45	10 (17%)
23	SQD	a	409	-	53,54,54	1.62	3 (5%)	62,65,65	2.69	11 (17%)
24	LMG	a	410	-	51,51,55	0.87	2 (3%)	59,59,63	1.11	3 (5%)
31	BCT	a	413	29	0,3,3	0.00	-	0,3,3	0.00	-
27	PL9	a	415	-	54,55,55	0.70	2 (3%)	68,69,69	1.75	19 (27%)
34	LMT	a	418	-	36,36,36	0.66	1 (2%)	47,47,47	1.59	6 (12%)
30	OEX	a	419	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
32	HTG	b	601	-	19,19,19	0.98	2 (10%)	22,24,24	1.46	1 (4%)
32	HTG	b	602	-	19,19,19	0.94	2 (10%)	22,24,24	1.45	1 (4%)
20	CLA	b	603	40	57,73,73	2.02	14 (24%)	61,113,113	1.99	16 (26%)
20	CLA	b	604	-	57,73,73	1.68	13 (22%)	61,113,113	2.24	21 (34%)
20	CLA	b	605	-	57,73,73	1.69	10 (17%)	61,113,113	2.41	20 (32%)
20	CLA	b	606	-	57,73,73	1.62	10 (17%)	61,113,113	2.25	18 (29%)
20	CLA	b	607	-	57,73,73	1.52	9 (15%)	61,113,113	2.33	15 (24%)
20	CLA	b	608	-	57,73,73	1.85	12 (21%)	61,113,113	1.97	13 (21%)
20	CLA	b	609	40	57,73,73	1.65	12 (21%)	61,113,113	2.09	20 (32%)
20	CLA	b	610	-	57,73,73	1.79	11 (19%)	61,113,113	2.21	17 (27%)
20	CLA	b	611	-	57,73,73	1.96	12 (21%)	61,113,113	1.79	14 (22%)
20	CLA	b	612	40	57,73,73	1.73	12 (21%)	61,113,113	1.92	16 (26%)
20	CLA	b	613	-	57,73,73	1.61	8 (14%)	61,113,113	2.04	15 (24%)
20	CLA	b	614	-	57,73,73	1.55	11 (19%)	61,113,113	2.34	18 (29%)
20	CLA	b	615	-	57,73,73	1.66	12 (21%)	61,113,113	1.97	17 (27%)
20	CLA	b	616	-	57,73,73	1.70	11 (19%)	61,113,113	1.99	19 (31%)
20	CLA	b	617	-	57,73,73	1.84	12 (21%)	61,113,113	2.10	20 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	b	618	-	57,73,73	1.80	11 (19%)	61,113,113	2.29	19 (31%)
22	BCR	b	619	-	41,41,41	0.93	0	56,56,56	1.76	8 (14%)
22	BCR	b	620	-	41,41,41	1.05	1 (2%)	56,56,56	1.23	4 (7%)
22	BCR	b	621	-	41,41,41	0.79	1 (2%)	56,56,56	1.48	7 (12%)
23	SQD	b	622	-	53,54,54	1.49	3 (5%)	62,65,65	1.85	11 (17%)
24	LMG	b	623	-	49,49,55	0.93	2 (4%)	57,57,63	1.31	5 (8%)
32	HTG	b	624	-	19,19,19	1.08	2 (10%)	22,24,24	1.96	2 (9%)
32	HTG	b	625	-	19,19,19	1.16	2 (10%)	22,24,24	1.27	4 (18%)
34	LMT	b	627	-	33,33,36	0.85	1 (3%)	44,44,47	1.82	10 (22%)
34	LMT	b	628	-	25,25,36	0.53	0	30,30,47	1.21	2 (6%)
28	DMS	b	631	-	3,3,3	2.89	1 (33%)	3,3,3	1.18	0
28	DMS	b	632	-	3,3,3	2.72	1 (33%)	3,3,3	0.50	0
28	DMS	b	633	-	3,3,3	2.55	1 (33%)	3,3,3	0.97	0
28	DMS	b	634	-	3,3,3	2.68	1 (33%)	3,3,3	0.61	0
28	DMS	b	635	-	3,3,3	2.69	1 (33%)	3,3,3	0.70	0
28	DMS	b	636	-	3,3,3	2.72	1 (33%)	3,3,3	0.71	0
28	DMS	b	637	-	3,3,3	2.67	1 (33%)	3,3,3	0.53	0
28	DMS	b	638	-	3,3,3	2.79	1 (33%)	3,3,3	0.87	0
28	DMS	b	639	-	3,3,3	2.82	1 (33%)	3,3,3	0.52	0
28	DMS	b	640	-	3,3,3	2.77	1 (33%)	3,3,3	1.33	1 (33%)
28	DMS	b	641	-	3,3,3	2.79	1 (33%)	3,3,3	1.01	0
20	CLA	c	501	-	57,73,73	1.84	12 (21%)	61,113,113	2.27	16 (26%)
20	CLA	c	502	-	57,73,73	1.75	12 (21%)	61,113,113	2.10	20 (32%)
20	CLA	c	503	-	57,73,73	1.86	13 (22%)	61,113,113	1.94	13 (21%)
20	CLA	c	504	40	57,73,73	1.77	11 (19%)	61,113,113	1.91	14 (22%)
20	CLA	c	505	-	57,73,73	1.72	11 (19%)	61,113,113	1.99	17 (27%)
20	CLA	c	506	-	57,73,73	1.72	12 (21%)	61,113,113	1.90	18 (29%)
20	CLA	c	507	40	57,73,73	1.75	11 (19%)	61,113,113	2.21	17 (27%)
20	CLA	c	508	-	52,68,73	1.95	12 (23%)	55,107,113	1.87	13 (23%)
20	CLA	c	509	-	57,73,73	1.94	13 (22%)	61,113,113	1.90	17 (27%)
20	CLA	c	510	-	57,73,73	1.73	11 (19%)	61,113,113	1.94	17 (27%)
20	CLA	c	511	3	57,73,73	1.98	14 (24%)	61,113,113	1.95	15 (24%)
20	CLA	c	512	-	57,73,73	1.99	12 (21%)	61,113,113	1.97	16 (26%)
20	CLA	c	513	-	57,73,73	1.84	11 (19%)	61,113,113	2.03	16 (26%)
22	BCR	c	514	-	41,41,41	0.84	0	56,56,56	1.49	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	DGD	c	515	-	63,63,67	0.83	3 (4%)	77,77,81	1.21	8 (10%)
35	DGD	c	516	-	58,58,67	0.84	2 (3%)	72,72,81	1.12	6 (8%)
35	DGD	c	517	-	63,63,67	1.02	4 (6%)	77,77,81	1.20	8 (10%)
24	LMG	c	518	-	51,51,55	1.08	3 (5%)	59,59,63	1.37	6 (10%)
24	LMG	c	519	-	51,51,55	0.98	3 (5%)	59,59,63	1.20	8 (13%)
32	HTG	c	520	-	19,19,19	0.84	2 (10%)	22,24,24	1.58	2 (9%)
32	HTG	c	521	-	19,19,19	0.90	1 (5%)	22,24,24	2.56	3 (13%)
34	LMT	c	523	-	36,36,36	0.78	1 (2%)	47,47,47	1.63	6 (12%)
28	DMS	c	527	-	3,3,3	2.32	1 (33%)	3,3,3	0.46	0
28	DMS	c	528	-	3,3,3	2.58	1 (33%)	3,3,3	0.39	0
28	DMS	c	529	-	3,3,3	2.67	1 (33%)	3,3,3	0.50	0
28	DMS	c	530	-	3,3,3	2.80	1 (33%)	3,3,3	0.96	0
28	DMS	c	531	-	3,3,3	2.67	1 (33%)	3,3,3	0.43	0
28	DMS	c	532	-	3,3,3	2.60	1 (33%)	3,3,3	0.44	0
28	DMS	c	533	-	3,3,3	2.74	1 (33%)	3,3,3	0.77	0
28	DMS	c	534	-	3,3,3	2.70	1 (33%)	3,3,3	0.71	0
28	DMS	c	535	-	3,3,3	2.78	1 (33%)	3,3,3	0.72	0
28	DMS	c	536	-	3,3,3	2.85	1 (33%)	3,3,3	1.18	0
32	HTG	d	401	-	19,19,19	1.01	1 (5%)	22,24,24	3.16	2 (9%)
20	CLA	d	402	-	57,73,73	1.73	11 (19%)	61,113,113	2.05	19 (31%)
20	CLA	d	403	40	57,73,73	1.65	9 (15%)	61,113,113	2.22	19 (31%)
20	CLA	d	404	-	57,73,73	1.72	12 (21%)	61,113,113	2.01	15 (24%)
22	BCR	d	405	-	41,41,41	0.94	0	56,56,56	1.85	11 (19%)
36	LHG	d	406	-	48,48,48	0.92	2 (4%)	49,54,54	1.21	4 (8%)
36	LHG	d	407	-	48,48,48	0.72	2 (4%)	49,54,54	0.98	2 (4%)
36	LHG	d	408	-	48,48,48	0.91	3 (6%)	49,54,54	1.00	5 (10%)
27	PL9	d	412	-	54,55,55	0.93	2 (3%)	68,69,69	1.69	18 (26%)
28	DMS	d	413	-	3,3,3	2.58	1 (33%)	3,3,3	0.84	0
28	DMS	d	414	-	3,3,3	2.51	1 (33%)	3,3,3	0.22	0
28	DMS	d	415	-	3,3,3	2.72	1 (33%)	3,3,3	0.49	0
35	DGD	d	416	-	51,51,67	1.08	3 (5%)	59,59,81	1.24	6 (10%)
37	HEM	e	102	5,6	24,50,50	2.22	10 (41%)	16,82,82	2.79	7 (43%)
23	SQD	f	101	-	39,40,54	1.77	3 (7%)	48,51,65	5.16	12 (25%)
34	LMT	f	102	-	24,24,36	0.76	1 (4%)	29,29,47	0.99	2 (6%)
35	DGD	h	101	-	63,63,67	0.95	3 (4%)	77,77,81	1.07	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	DMS	h	102	-	3,3,3	2.76	1 (33%)	3,3,3	0.51	0
28	DMS	i	104	-	3,3,3	2.63	1 (33%)	3,3,3	0.30	0
24	LMG	j	101	39	45,45,55	0.98	2 (4%)	53,53,63	1.05	6 (11%)
22	BCR	j	102	-	41,41,41	0.84	0	56,56,56	1.37	8 (14%)
28	DMS	j	105	-	3,3,3	2.81	1 (33%)	3,3,3	0.77	0
22	BCR	k	101	-	41,41,41	0.92	0	56,56,56	1.11	6 (10%)
22	BCR	k	102	-	41,41,41	0.77	0	56,56,56	1.27	8 (14%)
23	SQD	l	101	-	53,54,54	1.36	4 (7%)	62,65,65	2.11	9 (14%)
36	LHG	l	102	-	48,48,48	0.77	2 (4%)	49,54,54	1.01	2 (4%)
34	LMT	m	101	-	36,36,36	0.60	0	47,47,47	0.99	2 (4%)
34	LMT	m	102	-	36,36,36	0.57	0	47,47,47	1.20	5 (10%)
28	DMS	o	302	-	3,3,3	2.76	1 (33%)	3,3,3	0.83	0
28	DMS	o	303	-	3,3,3	2.68	1 (33%)	3,3,3	0.48	0
28	DMS	o	304	-	3,3,3	2.64	1 (33%)	3,3,3	0.58	0
28	DMS	o	305	-	3,3,3	2.73	1 (33%)	3,3,3	0.72	0
28	DMS	o	306	-	3,3,3	2.79	1 (33%)	3,3,3	0.95	0
28	DMS	o	307	-	3,3,3	2.66	1 (33%)	3,3,3	0.77	0
28	DMS	o	308	-	3,3,3	2.86	1 (33%)	3,3,3	0.74	0
22	BCR	t	101	-	41,41,41	1.03	2 (4%)	56,56,56	1.73	19 (33%)
32	HTG	u	201	-	7,7,19	0.43	0	5,6,24	0.86	0
28	DMS	u	202	-	3,3,3	2.66	1 (33%)	3,3,3	1.21	0
28	DMS	u	203	-	3,3,3	2.57	1 (33%)	3,3,3	0.71	0
28	DMS	u	204	-	3,3,3	2.66	1 (33%)	3,3,3	0.45	0
37	HEM	v	201	16	24,50,50	2.30	9 (37%)	16,82,82	2.14	3 (18%)
28	DMS	v	202	-	3,3,3	2.50	1 (33%)	3,3,3	0.53	0
28	DMS	v	203	-	3,3,3	2.59	1 (33%)	3,3,3	0.81	0
28	DMS	v	204	-	3,3,3	2.65	1 (33%)	3,3,3	0.77	0
28	DMS	v	205	-	3,3,3	2.65	1 (33%)	3,3,3	0.48	0
28	DMS	v	206	-	3,3,3	2.67	1 (33%)	3,3,3	0.60	0
28	DMS	v	207	-	3,3,3	2.76	1 (33%)	3,3,3	0.50	0
28	DMS	v	208	-	3,3,3	2.64	1 (33%)	3,3,3	0.59	0
28	DMS	v	209	-	3,3,3	2.64	1 (33%)	3,3,3	0.51	0
32	HTG	v	210	-	14,14,19	0.59	0	17,19,24	1.70	3 (17%)
38	RRX	x	101	-	42,42,42	0.80	0	57,58,58	1.21	5 (8%)
34	LMT	z	102	-	36,36,36	0.74	1 (2%)	47,47,47	1.53	8 (17%)

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	CLA	A	401	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	A	402	40	2/2/18/25	0/30/128/135	0/0/9/9
21	PHO	A	403	-	-	0/53/103/103	0/1/6/6
20	CLA	A	404	-	1/1/20/25	0/37/135/135	0/0/9/9
22	BCR	A	405	-	-	0/29/63/63	0/2/2/2
23	SQD	A	406	-	-	0/49/69/69	0/1/1/1
24	LMG	A	407	-	-	0/46/66/70	0/1/1/1
27	PL9	A	411	-	-	0/53/73/73	0/1/1/1
23	SQD	A	412	-	-	0/49/69/69	0/1/1/1
28	DMS	A	414	-	-	0/0/0/0	0/0/0/0
28	DMS	A	415	-	-	0/0/0/0	0/0/0/0
28	DMS	A	416	-	-	0/0/0/0	0/0/0/0
28	DMS	A	417	-	-	0/0/0/0	0/0/0/0
28	DMS	A	418	-	-	0/0/0/0	0/0/0/0
30	OEX	A	420	1,3,40	-	0/0/68/68	0/0/6/6
31	BCT	A	421	29	-	0/0/0/0	0/0/0/0
20	CLA	B	601	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	602	40	2/2/20/25	0/37/135/135	0/0/9/9
20	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	607	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	608	40	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	609	-	1/1/20/25	0/37/135/135	0/0/9/9
20	CLA	B	610	-	2/2/20/25	0/37/135/135	0/0/9/9
20	CLA	B	611	40	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
22	BCR	B	617	-	-	0/29/63/63	0/2/2/2
22	BCR	B	618	-	-	0/29/63/63	0/2/2/2
22	BCR	B	619	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LMG	B	620	-	-	0/46/66/70	0/1/1/1
32	HTG	B	621	-	-	0/10/30/30	0/1/1/1
32	HTG	B	622	-	-	0/10/30/30	0/1/1/1
32	HTG	B	623	-	-	0/10/30/30	0/1/1/1
34	LMT	B	625	-	-	0/15/35/61	0/1/1/2
34	LMT	B	626	-	-	0/15/35/61	0/1/1/2
34	LMT	B	627	-	-	0/13/13/61	0/0/0/2
32	HTG	B	631	-	-	0/10/30/30	0/1/1/1
32	HTG	B	632	-	-	0/10/30/30	0/1/1/1
28	DMS	B	634	-	-	0/0/0/0	0/0/0/0
28	DMS	B	635	-	-	0/0/0/0	0/0/0/0
28	DMS	B	636	-	-	0/0/0/0	0/0/0/0
28	DMS	B	637	-	-	0/0/0/0	0/0/0/0
28	DMS	B	638	-	-	0/0/0/0	0/0/0/0
28	DMS	B	639	-	-	0/0/0/0	0/0/0/0
28	DMS	B	640	-	-	0/0/0/0	0/0/0/0
28	DMS	B	641	-	-	0/0/0/0	0/0/0/0
28	DMS	B	642	-	-	0/0/0/0	0/0/0/0
28	DMS	B	643	-	-	0/0/0/0	0/0/0/0
28	DMS	B	644	-	-	0/0/0/0	0/0/0/0
28	DMS	B	645	-	-	0/0/0/0	0/0/0/0
20	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	502	-	1/1/20/25	0/37/135/135	0/0/9/9
20	CLA	C	503	-	2/2/20/25	0/37/135/135	0/0/9/9
20	CLA	C	504	40	2/2/20/25	0/37/135/135	0/0/9/9
20	CLA	C	505	-	2/2/20/25	0/37/135/135	0/0/9/9
20	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	507	40	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	508	-	3/3/19/25	0/31/129/135	0/0/9/9
20	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	511	3	2/2/20/25	0/37/135/135	0/0/9/9
20	CLA	C	512	-	3/3/18/25	0/25/123/135	0/0/9/9
20	CLA	C	513	-	1/1/20/25	0/37/135/135	0/0/9/9
22	BCR	C	514	-	-	0/29/63/63	0/2/2/2
22	BCR	C	515	-	-	0/29/63/63	0/2/2/2
35	DGD	C	516	-	-	0/51/91/95	0/2/2/2
35	DGD	C	517	-	-	0/44/84/95	0/2/2/2
35	DGD	C	518	-	-	0/51/91/95	0/2/2/2
24	LMG	C	519	-	-	0/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	HTG	C	520	-	-	0/10/30/30	0/1/1/1
32	HTG	C	521	-	-	0/10/30/30	0/1/1/1
32	HTG	C	522	-	-	0/10/30/30	0/1/1/1
24	LMG	C	524	-	-	0/40/60/70	0/1/1/1
28	DMS	C	525[A]	-	-	0/0/0/0	0/0/0/0
28	DMS	C	525[B]	-	-	0/0/0/0	0/0/0/0
28	DMS	C	526	-	-	0/0/0/0	0/0/0/0
28	DMS	C	527	-	-	0/0/0/0	0/0/0/0
28	DMS	C	528	-	-	0/0/0/0	0/0/0/0
28	DMS	C	529	-	-	0/0/0/0	0/0/0/0
28	DMS	C	530	-	-	0/0/0/0	0/0/0/0
28	DMS	C	531	-	-	0/0/0/0	0/0/0/0
28	DMS	C	532	-	-	0/0/0/0	0/0/0/0
28	DMS	C	533	-	-	0/0/0/0	0/0/0/0
32	HTG	C	534	-	-	0/10/30/30	0/1/1/1
20	CLA	D	401	-	1/1/20/25	0/37/135/135	0/0/9/9
20	CLA	D	402	40	1/1/20/25	0/37/135/135	0/0/9/9
21	PHO	D	403	-	-	0/53/103/103	0/1/6/6
20	CLA	D	404	-	3/3/20/25	0/37/135/135	0/0/9/9
22	BCR	D	405	-	-	0/29/63/63	0/2/2/2
35	DGD	D	406	-	-	0/46/66/95	0/1/1/2
36	LHG	D	407	-	-	0/53/53/53	0/0/0/0
36	LHG	D	408	-	-	0/53/53/53	0/0/0/0
36	LHG	D	409	-	-	0/53/53/53	0/0/0/0
27	PL9	D	412	-	-	0/53/73/73	0/1/1/1
28	DMS	D	413	-	-	0/0/0/0	0/0/0/0
28	DMS	D	414	-	-	0/0/0/0	0/0/0/0
28	DMS	D	415	-	-	0/0/0/0	0/0/0/0
28	DMS	D	416	-	-	0/0/0/0	0/0/0/0
32	HTG	D	417	-	-	0/10/30/30	0/1/1/1
34	LMT	E	101	-	-	0/15/35/61	0/1/1/2
36	LHG	E	103	-	-	0/45/45/53	0/0/0/0
37	HEM	E	104	5,6	-	0/6/54/54	0/0/8/8
23	SQD	F	101	-	-	0/28/48/69	0/1/1/1
28	DMS	F	102	-	-	0/0/0/0	0/0/0/0
38	RRX	H	101	-	-	0/29/65/65	0/2/2/2
35	DGD	H	102	-	-	0/51/91/95	0/2/2/2
28	DMS	H	103	-	-	0/0/0/0	0/0/0/0
34	LMT	I	101	-	-	0/21/61/61	0/2/2/2
24	LMG	J	101	39	-	0/40/60/70	0/1/1/1
34	LMT	J	103	-	-	0/15/35/61	0/1/1/2
22	BCR	K	101	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	K	102	-	-	0/29/63/63	0/2/2/2
36	LHG	L	101	-	-	0/53/53/53	0/0/0/0
34	LMT	M	101	-	-	0/21/61/61	0/2/2/2
32	HTG	O	302	-	-	0/10/30/30	0/1/1/1
28	DMS	O	303	-	-	0/0/0/0	0/0/0/0
28	DMS	O	304	-	-	0/0/0/0	0/0/0/0
28	DMS	O	305	-	-	0/0/0/0	0/0/0/0
28	DMS	O	306	-	-	0/0/0/0	0/0/0/0
28	DMS	O	307	-	-	0/0/0/0	0/0/0/0
28	DMS	O	308	-	-	0/0/0/0	0/0/0/0
28	DMS	O	309	-	-	0/0/0/0	0/0/0/0
28	DMS	O	310	-	-	0/0/0/0	0/0/0/0
28	DMS	O	311	-	-	0/0/0/0	0/0/0/0
22	BCR	T	101	-	-	0/29/63/63	0/2/2/2
34	LMT	T	102	-	-	0/15/35/61	0/1/1/2
28	DMS	U	902	-	-	0/0/0/0	0/0/0/0
28	DMS	U	903[A]	-	-	0/0/0/0	0/0/0/0
28	DMS	U	903[B]	-	-	0/0/0/0	0/0/0/0
28	DMS	U	904	-	-	0/0/0/0	0/0/0/0
37	HEM	V	201	16	-	0/6/54/54	0/0/8/8
32	HTG	V	202	-	-	0/3/24/30	0/1/1/1
28	DMS	V	204	-	-	0/0/0/0	0/0/0/0
28	DMS	V	205	-	-	0/0/0/0	0/0/0/0
28	DMS	V	206	-	-	0/0/0/0	0/0/0/0
28	DMS	V	207	-	-	0/0/0/0	0/0/0/0
28	DMS	V	208	-	-	0/0/0/0	0/0/0/0
28	DMS	V	209	-	-	0/0/0/0	0/0/0/0
34	LMT	Z	101	-	-	0/21/61/61	0/2/2/2
23	SQD	a	401	-	-	0/49/69/69	0/1/1/1
20	CLA	a	403	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	a	404	40	2/2/19/25	0/31/129/135	0/0/9/9
21	PHO	a	405	-	-	0/53/103/103	0/1/6/6
21	PHO	a	406	-	-	0/53/103/103	0/1/6/6
20	CLA	a	407	-	1/1/16/25	0/16/114/135	0/0/9/9
22	BCR	a	408	-	-	0/29/63/63	0/2/2/2
23	SQD	a	409	-	-	0/49/69/69	0/1/1/1
24	LMG	a	410	-	-	0/46/66/70	0/1/1/1
31	BCT	a	413	29	-	0/0/0/0	0/0/0/0
27	PL9	a	415	-	-	0/53/73/73	0/1/1/1
34	LMT	a	418	-	-	0/21/61/61	0/2/2/2
30	OEX	a	419	1,3,40	-	0/0/68/68	0/0/6/6
32	HTG	b	601	-	-	0/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	HTG	b	602	-	-	0/10/30/30	0/1/1/1
20	CLA	b	603	40	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	604	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	609	40	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	610	-	1/1/20/25	0/37/135/135	0/0/9/9
20	CLA	b	611	-	2/2/20/25	0/37/135/135	0/0/9/9
20	CLA	b	612	40	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	613	-	1/1/20/25	0/37/135/135	0/0/9/9
20	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	618	-	3/3/20/25	0/37/135/135	0/0/9/9
22	BCR	b	619	-	-	0/29/63/63	0/2/2/2
22	BCR	b	620	-	-	0/29/63/63	0/2/2/2
22	BCR	b	621	-	-	0/29/63/63	0/2/2/2
23	SQD	b	622	-	-	0/49/69/69	0/1/1/1
24	LMG	b	623	-	-	0/44/64/70	0/1/1/1
32	HTG	b	624	-	-	0/10/30/30	0/1/1/1
32	HTG	b	625	-	-	0/10/30/30	0/1/1/1
34	LMT	b	627	-	-	0/18/58/61	0/2/2/2
34	LMT	b	628	-	-	0/17/37/61	0/1/1/2
28	DMS	b	631	-	-	0/0/0/0	0/0/0/0
28	DMS	b	632	-	-	0/0/0/0	0/0/0/0
28	DMS	b	633	-	-	0/0/0/0	0/0/0/0
28	DMS	b	634	-	-	0/0/0/0	0/0/0/0
28	DMS	b	635	-	-	0/0/0/0	0/0/0/0
28	DMS	b	636	-	-	0/0/0/0	0/0/0/0
28	DMS	b	637	-	-	0/0/0/0	0/0/0/0
28	DMS	b	638	-	-	0/0/0/0	0/0/0/0
28	DMS	b	639	-	-	0/0/0/0	0/0/0/0
28	DMS	b	640	-	-	0/0/0/0	0/0/0/0
28	DMS	b	641	-	-	0/0/0/0	0/0/0/0
20	CLA	c	501	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	c	502	-	2/2/20/25	0/37/135/135	0/0/9/9
20	CLA	c	503	-	1/1/20/25	0/37/135/135	0/0/9/9
20	CLA	c	504	40	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	505	-	2/2/20/25	0/37/135/135	0/0/9/9
20	CLA	c	506	-	2/2/20/25	0/37/135/135	0/0/9/9
20	CLA	c	507	40	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	508	-	2/2/19/25	0/31/129/135	0/0/9/9
20	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	510	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	511	3	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	512	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	513	-	1/1/20/25	0/37/135/135	0/0/9/9
22	BCR	c	514	-	-	0/29/63/63	0/2/2/2
35	DGD	c	515	-	-	0/51/91/95	0/2/2/2
35	DGD	c	516	-	-	0/46/86/95	0/2/2/2
35	DGD	c	517	-	-	0/51/91/95	0/2/2/2
24	LMG	c	518	-	-	0/46/66/70	0/1/1/1
24	LMG	c	519	-	-	0/46/66/70	0/1/1/1
32	HTG	c	520	-	-	0/10/30/30	0/1/1/1
32	HTG	c	521	-	-	0/10/30/30	0/1/1/1
34	LMT	c	523	-	-	0/21/61/61	0/2/2/2
28	DMS	c	527	-	-	0/0/0/0	0/0/0/0
28	DMS	c	528	-	-	0/0/0/0	0/0/0/0
28	DMS	c	529	-	-	0/0/0/0	0/0/0/0
28	DMS	c	530	-	-	0/0/0/0	0/0/0/0
28	DMS	c	531	-	-	0/0/0/0	0/0/0/0
28	DMS	c	532	-	-	0/0/0/0	0/0/0/0
28	DMS	c	533	-	-	0/0/0/0	0/0/0/0
28	DMS	c	534	-	-	0/0/0/0	0/0/0/0
28	DMS	c	535	-	-	0/0/0/0	0/0/0/0
28	DMS	c	536	-	-	0/0/0/0	0/0/0/0
32	HTG	d	401	-	-	1/10/30/30	0/1/1/1
20	CLA	d	402	-	2/2/20/25	0/37/135/135	0/0/9/9
20	CLA	d	403	40	1/1/20/25	0/37/135/135	0/0/9/9
20	CLA	d	404	-	1/1/20/25	0/37/135/135	0/0/9/9
22	BCR	d	405	-	-	0/29/63/63	0/2/2/2
36	LHG	d	406	-	-	0/53/53/53	0/0/0/0
36	LHG	d	407	-	-	0/53/53/53	0/0/0/0
36	LHG	d	408	-	-	0/53/53/53	0/0/0/0
27	PL9	d	412	-	-	0/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DMS	d	413	-	-	0/0/0/0	0/0/0/0
28	DMS	d	414	-	-	0/0/0/0	0/0/0/0
28	DMS	d	415	-	-	0/0/0/0	0/0/0/0
35	DGD	d	416	-	-	0/46/66/95	0/1/1/2
37	HEM	e	102	5,6	-	0/6/54/54	0/0/8/8
23	SQD	f	101	-	-	0/34/54/69	0/1/1/1
34	LMT	f	102	-	-	0/15/35/61	0/1/1/2
35	DGD	h	101	-	-	0/51/91/95	0/2/2/2
28	DMS	h	102	-	-	0/0/0/0	0/0/0/0
28	DMS	i	104	-	-	0/0/0/0	0/0/0/0
24	LMG	j	101	39	-	0/40/60/70	0/1/1/1
22	BCR	j	102	-	-	0/29/63/63	0/2/2/2
28	DMS	j	105	-	-	0/0/0/0	0/0/0/0
22	BCR	k	101	-	-	0/29/63/63	0/2/2/2
22	BCR	k	102	-	-	0/29/63/63	0/2/2/2
23	SQD	l	101	-	-	0/49/69/69	0/1/1/1
36	LHG	l	102	-	-	0/53/53/53	0/0/0/0
34	LMT	m	101	-	-	0/21/61/61	0/2/2/2
34	LMT	m	102	-	-	0/21/61/61	0/2/2/2
28	DMS	o	302	-	-	0/0/0/0	0/0/0/0
28	DMS	o	303	-	-	0/0/0/0	0/0/0/0
28	DMS	o	304	-	-	0/0/0/0	0/0/0/0
28	DMS	o	305	-	-	0/0/0/0	0/0/0/0
28	DMS	o	306	-	-	0/0/0/0	0/0/0/0
28	DMS	o	307	-	-	0/0/0/0	0/0/0/0
28	DMS	o	308	-	-	0/0/0/0	0/0/0/0
22	BCR	t	101	-	-	0/29/63/63	0/2/2/2
32	HTG	u	201	-	-	0/5/5/30	0/0/0/1
28	DMS	u	202	-	-	0/0/0/0	0/0/0/0
28	DMS	u	203	-	-	0/0/0/0	0/0/0/0
28	DMS	u	204	-	-	0/0/0/0	0/0/0/0
37	HEM	v	201	16	-	0/6/54/54	0/0/8/8
28	DMS	v	202	-	-	0/0/0/0	0/0/0/0
28	DMS	v	203	-	-	0/0/0/0	0/0/0/0
28	DMS	v	204	-	-	0/0/0/0	0/0/0/0
28	DMS	v	205	-	-	0/0/0/0	0/0/0/0
28	DMS	v	206	-	-	0/0/0/0	0/0/0/0
28	DMS	v	207	-	-	0/0/0/0	0/0/0/0
28	DMS	v	208	-	-	0/0/0/0	0/0/0/0
28	DMS	v	209	-	-	0/0/0/0	0/0/0/0
32	HTG	v	210	-	-	0/5/25/30	0/1/1/1
38	RRX	x	101	-	-	0/29/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMT	z	102	-	-	0/21/61/61	0/2/2/2

The worst 5 of 1152 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	409	SQD	C6-S	-9.84	1.65	1.77
23	A	412	SQD	C6-S	-8.74	1.67	1.77
23	a	401	SQD	C6-S	-8.68	1.67	1.77
23	A	406	SQD	C6-S	-8.28	1.67	1.77
23	b	622	SQD	C6-S	-7.92	1.68	1.77

The worst 5 of 1894 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	f	101	SQD	O9-S-C6	-23.68	90.24	106.92
23	f	101	SQD	O9-S-O7	-11.63	81.11	113.96
23	f	101	SQD	O8-S-O9	-11.61	85.57	111.26
37	E	104	HEM	CBD-CAD-C3D	-7.33	99.61	112.47
22	d	405	BCR	C24-C23-C22	-6.78	115.96	126.21

5 of 170 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	c	502	CLA	NC
20	c	502	CLA	NA
20	b	614	CLA	NA
20	b	614	CLA	NC
20	b	614	CLA	ND

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	d	401	HTG	O5-C1-S1-C1'

There are no ring outliers.

102 monomers are involved in 348 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	401	CLA	5	0
20	A	402	CLA	3	0
21	A	403	PHO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	404	CLA	3	0
22	A	405	BCR	4	0
23	A	406	SQD	3	0
24	A	407	LMG	4	0
27	A	411	PL9	11	0
23	A	412	SQD	2	0
28	A	416	DMS	1	0
31	A	421	BCT	5	0
20	B	601	CLA	5	0
20	B	602	CLA	2	0
20	B	603	CLA	2	0
20	B	604	CLA	6	0
20	B	605	CLA	4	0
20	B	606	CLA	9	0
20	B	607	CLA	6	0
20	B	608	CLA	2	0
20	B	609	CLA	1	0
20	B	610	CLA	2	0
20	B	611	CLA	5	0
20	B	612	CLA	4	0
20	B	613	CLA	4	0
20	B	614	CLA	5	0
20	B	615	CLA	3	0
20	B	616	CLA	2	0
22	B	618	BCR	3	0
22	B	619	BCR	3	0
32	B	622	HTG	8	0
34	B	625	LMT	1	0
34	B	626	LMT	1	0
34	B	627	LMT	1	0
32	B	631	HTG	1	0
32	B	632	HTG	2	0
28	B	634	DMS	1	0
28	B	635	DMS	3	0
28	B	637	DMS	1	0
28	B	639	DMS	6	0
28	B	640	DMS	2	0
28	B	641	DMS	7	0
28	B	642	DMS	5	0
28	B	644	DMS	4	0
20	C	501	CLA	5	0
20	C	502	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	C	503	CLA	2	0
20	C	504	CLA	6	0
20	C	505	CLA	2	0
20	C	506	CLA	5	0
20	C	507	CLA	4	0
20	C	508	CLA	6	0
20	C	509	CLA	5	0
20	C	510	CLA	8	0
20	C	511	CLA	3	0
20	C	512	CLA	4	0
20	C	513	CLA	3	0
22	C	514	BCR	3	0
22	C	515	BCR	2	0
35	C	516	DGD	2	0
35	C	517	DGD	2	0
24	C	519	LMG	3	0
32	C	520	HTG	2	0
24	C	524	LMG	2	0
28	C	527	DMS	2	0
28	C	530	DMS	9	0
28	C	531	DMS	4	0
28	C	532	DMS	4	0
28	C	533	DMS	1	0
32	C	534	HTG	1	0
20	D	401	CLA	1	0
20	D	402	CLA	4	0
21	D	403	PHO	2	0
20	D	404	CLA	2	0
22	D	405	BCR	3	0
35	D	406	DGD	5	0
36	D	408	LHG	18	0
36	D	409	LHG	19	0
28	D	413	DMS	1	0
28	D	414	DMS	13	0
28	D	415	DMS	2	0
32	D	417	HTG	3	0
36	E	103	LHG	6	0
37	E	104	HEM	2	0
23	F	101	SQD	3	0
28	F	102	DMS	3	0
35	H	102	DGD	2	0
34	I	101	LMT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	J	103	LMT	1	0
22	K	101	BCR	5	0
22	K	102	BCR	3	0
28	O	303	DMS	3	0
28	O	305	DMS	1	0
28	O	306	DMS	3	0
28	O	307	DMS	6	0
28	O	308	DMS	2	0
28	O	310	DMS	2	0
22	T	101	BCR	7	0
28	U	902	DMS	1	0
28	U	903[B]	DMS	12	0
28	U	904	DMS	3	0
28	V	205	DMS	1	0
28	V	206	DMS	6	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.70	3 (0%) 85 85	16, 23, 46, 68	0
1	a	334/344 (97%)	-0.63	8 (2%) 62 60	18, 23, 48, 78	0
2	B	505/505 (100%)	-0.47	18 (3%) 46 44	19, 28, 54, 85	0
2	b	495/505 (98%)	-0.40	20 (4%) 42 39	19, 28, 53, 95	0
3	C	451/455 (99%)	-0.45	8 (1%) 71 71	21, 33, 49, 83	0
3	c	455/455 (100%)	-0.47	6 (1%) 79 79	22, 33, 46, 79	0
4	D	342/342 (100%)	-0.67	4 (1%) 81 81	17, 24, 44, 90	0
4	d	342/342 (100%)	-0.73	5 (1%) 76 76	18, 25, 42, 86	0
5	E	78/83 (93%)	0.76	19 (24%) 1 0	28, 47, 75, 87	0
5	e	78/83 (93%)	0.64	16 (20%) 1 1	29, 44, 67, 81	0
6	F	33/44 (75%)	-0.09	4 (12%) 6 6	28, 36, 63, 66	0
6	f	32/44 (72%)	-0.05	3 (9%) 11 10	28, 34, 72, 90	0
7	H	64/65 (98%)	0.07	3 (4%) 35 33	26, 37, 50, 78	0
7	h	62/65 (95%)	-0.24	0 100 100	25, 36, 48, 58	0
8	I	34/38 (89%)	-0.11	3 (8%) 12 12	29, 36, 60, 78	0
8	i	35/38 (92%)	-0.16	2 (5%) 27 26	29, 34, 52, 85	0
9	J	36/40 (90%)	-0.04	2 (5%) 28 26	26, 41, 74, 90	0
9	j	40/40 (100%)	-0.04	3 (7%) 17 16	27, 39, 56, 65	0
10	K	37/37 (100%)	-0.27	2 (5%) 29 28	33, 40, 52, 59	0
10	k	37/37 (100%)	-0.21	1 (2%) 58 55	32, 40, 56, 64	0
11	L	37/37 (100%)	-0.36	3 (8%) 15 14	18, 22, 65, 81	0
11	l	37/37 (100%)	-0.22	3 (8%) 15 14	18, 22, 76, 91	0
12	M	33/36 (91%)	-0.64	1 (3%) 54 51	21, 25, 39, 57	0
12	m	34/36 (94%)	-0.56	3 (8%) 12 12	20, 26, 53, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	-0.23	8 (3%) 50 47	18, 32, 56, 85	0
13	o	243/244 (99%)	-0.09	19 (7%) 16 15	19, 35, 67, 89	0
14	T	28/32 (87%)	-0.70	1 (3%) 46 44	19, 24, 37, 54	0
14	t	29/32 (90%)	-0.36	2 (6%) 20 18	20, 23, 49, 74	0
15	U	97/104 (93%)	-0.34	2 (2%) 67 65	22, 29, 49, 67	0
15	u	97/104 (93%)	-0.36	1 (1%) 84 84	24, 29, 44, 75	0
16	V	137/137 (100%)	-0.62	0 100 100	22, 28, 43, 60	0
16	v	137/137 (100%)	-0.25	5 (3%) 46 44	25, 36, 53, 74	0
17	Y	29/30 (96%)	1.08	6 (20%) 1 1	41, 51, 72, 79	0
17	y	29/30 (96%)	0.76	5 (17%) 2 2	41, 50, 66, 70	0
18	X	38/40 (95%)	0.26	5 (13%) 4 4	32, 42, 68, 72	0
18	x	35/40 (87%)	-0.09	2 (5%) 27 26	33, 40, 63, 67	0
19	Z	62/62 (100%)	0.66	14 (22%) 1 1	38, 48, 86, 98	0
19	z	61/62 (98%)	0.71	12 (19%) 1 1	45, 54, 86, 96	0
All	All	5230/5350 (97%)	-0.37	222 (4%) 40 37	16, 30, 57, 98	0

The worst 5 of 222 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	496	TYR	9.7
2	b	495	PHE	9.2
2	b	503	THR	8.4
13	o	246	ALA	8.3
2	b	502	VAL	7.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	FME	I	1	10/11	0.98	0.07	-	26,32,36,37	0
14	FME	T	1	10/11	0.97	0.07	-	23,29,48,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	FME	i	1	10/11	0.98	0.09	-	30,31,34,35	0
14	FME	t	1	10/11	0.96	0.07	-	23,27,49,50	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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
34	LMT	b	627	32/35	0.71	0.24	21.38	42,67,84,87	0
26	UNL	T	103	13/-	0.69	0.17	19.83	64,68,72,72	0
28	DMS	B	641	4/4	0.95	0.31	17.73	68,69,75,80	0
28	DMS	b	636	4/4	0.90	0.15	16.16	66,71,72,79	0
26	UNL	h	103	16/-	0.75	0.29	15.91	61,69,73,76	0
34	LMT	E	101	24/35	0.81	0.26	13.84	64,78,84,90	0
28	DMS	A	416	4/4	0.91	0.23	12.08	59,60,69,77	0
28	DMS	c	530	4/4	0.97	0.16	11.95	36,43,45,49	0
28	DMS	A	418	4/4	0.90	0.32	11.89	68,74,80,85	0
26	UNL	B	630	14/-	0.70	0.20	11.54	67,74,83,84	0
34	LMT	T	102	24/35	0.80	0.20	11.40	36,53,78,85	0
28	DMS	C	531	4/4	0.92	0.24	10.97	53,54,58,74	0
34	LMT	f	102	24/35	0.59	0.26	10.92	62,77,94,98	0
34	LMT	a	418	35/35	0.73	0.21	10.82	45,69,78,81	0
26	UNL	C	523	34/-	0.75	0.22	10.58	59,80,92,101	0
32	HTG	d	401	19/19	0.58	0.29	10.40	58,99,111,120	0
28	DMS	O	309	4/4	0.81	0.23	10.35	58,65,72,73	0
32	HTG	C	522	19/19	0.81	0.27	10.11	66,83,104,107	0
28	DMS	d	413	4/4	0.95	0.17	10.04	47,53,55,57	0
28	DMS	B	639	4/4	0.90	0.24	9.77	65,70,71,76	0
35	DGD	D	406	51/66	0.60	0.30	9.56	57,74,100,108	0
28	DMS	C	532	4/4	0.87	0.19	9.54	33,40,41,48	0
28	DMS	D	415	4/4	0.85	0.25	9.05	57,58,63,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
26	UNL	t	102	16/-	0.77	0.17	8.66	61,71,80,80	0
28	DMS	B	638	4/4	0.86	0.19	8.64	53,61,63,68	0
34	LMT	B	626	24/35	0.74	0.20	8.62	37,54,86,95	0
28	DMS	B	642	4/4	0.77	0.30	8.15	43,51,68,71	0
34	LMT	B	627	16/35	0.81	0.18	7.80	52,60,78,78	0
35	DGD	d	416	51/66	0.64	0.27	7.75	56,75,96,103	0
28	DMS	o	307	4/4	0.95	0.17	7.60	53,58,63,65	0
28	DMS	O	305	4/4	0.68	0.30	7.38	64,66,77,86	0
26	UNL	J	105	12/-	0.79	0.23	7.31	63,67,71,71	0
28	DMS	C	525[A]	4/4	0.97	0.19	7.29	48,49,51,57	4
28	DMS	c	536	4/4	0.92	0.15	6.76	33,33,45,46	0
28	DMS	C	525[B]	4/4	0.97	0.19	6.54	32,33,35,35	4
26	UNL	E	102	15/-	0.68	0.28	6.49	55,62,76,77	0
28	DMS	A	417	4/4	0.93	0.17	6.34	70,72,77,81	0
28	DMS	b	631	4/4	0.96	0.10	6.24	23,24,27,35	0
28	DMS	V	205	4/4	0.81	0.25	6.09	67,76,77,79	0
23	SQD	a	401	54/54	0.81	0.16	5.57	39,58,82,86	0
26	UNL	d	410	16/-	0.82	0.18	5.54	33,45,63,63	0
26	UNL	d	409	36/-	0.79	0.18	5.48	36,60,91,102	0
28	DMS	O	306	4/4	0.89	0.29	5.39	66,73,73,75	0
28	DMS	v	202	4/4	0.98	0.15	5.09	50,51,53,55	0
28	DMS	O	304	4/4	0.92	0.28	5.04	63,68,72,73	0
28	DMS	U	902	4/4	0.88	0.23	5.03	35,44,49,58	0
24	LMG	C	524	45/55	0.52	0.33	5.03	22,46,51,56	45
32	HTG	c	521	19/19	0.55	0.35	4.97	57,85,102,105	0
24	LMG	B	620	51/55	0.87	0.12	4.89	33,43,55,58	0
28	DMS	O	310	4/4	0.84	0.33	4.87	76,78,82,94	0
28	DMS	c	528	4/4	0.96	0.18	4.73	58,62,63,65	0
27	PL9	A	411	55/55	0.79	0.20	4.69	43,67,89,92	0
26	UNL	B	633	16/-	0.81	0.25	4.46	53,61,69,70	0
32	HTG	O	302	19/19	0.94	0.11	4.39	34,42,50,53	0
28	DMS	C	527	4/4	0.89	0.17	4.27	73,76,79,87	0
32	HTG	C	521	19/19	0.67	0.26	4.27	46,78,89,90	0
26	UNL	d	411	16/-	0.92	0.12	4.25	33,42,55,55	0
32	HTG	b	625	19/19	0.85	0.20	4.05	30,44,66,70	0
32	HTG	B	621	19/19	0.93	0.12	4.01	36,41,48,52	0
26	UNL	A	410	36/-	0.64	0.25	3.93	57,78,84,91	0
28	DMS	o	304	4/4	0.86	0.33	3.93	68,79,82,83	0
26	UNL	D	411	16/-	0.89	0.16	3.93	39,45,58,62	0
36	LHG	E	103	48/49	0.65	0.29	3.92	44,99,108,119	0
26	UNL	j	106	6/-	0.82	0.18	3.81	52,55,58,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	BCR	K	102	40/40	0.92	0.13	3.78	31,36,40,41	0
28	DMS	b	633	4/4	0.97	0.13	3.68	45,48,49,53	0
28	DMS	C	526	4/4	0.97	0.15	3.61	59,60,63,65	0
34	LMT	J	103	24/35	0.60	0.23	3.59	53,61,81,85	0
28	DMS	c	535	4/4	0.91	0.18	3.59	58,59,65,68	0
32	HTG	V	202	13/19	0.86	0.21	3.54	45,49,70,82	0
28	DMS	D	413	4/4	0.96	0.10	3.37	50,56,60,61	0
23	SQD	l	101	54/54	0.75	0.20	3.26	47,68,101,106	0
28	DMS	d	414	4/4	0.95	0.16	3.23	57,62,64,68	0
28	DMS	o	306	4/4	0.84	0.25	3.18	55,58,65,77	0
28	DMS	C	530	4/4	0.96	0.16	3.17	44,44,46,50	0
28	DMS	u	202	4/4	0.91	0.18	3.15	40,46,52,54	0
27	PL9	a	415	55/55	0.77	0.22	3.13	52,67,89,94	0
26	UNL	U	901	14/-	0.74	0.27	3.10	40,49,59,59	0
24	LMG	b	623	49/55	0.89	0.12	3.09	33,42,54,61	0
24	LMG	A	407	51/55	0.87	0.13	3.07	40,55,70,78	0
24	LMG	a	410	51/55	0.88	0.15	3.07	44,55,65,67	0
23	SQD	b	622	54/54	0.80	0.17	3.04	46,63,95,100	0
28	DMS	v	206	4/4	0.93	0.20	3.01	52,53,61,66	0
32	HTG	B	622	19/19	0.84	0.16	2.95	28,46,54,54	0
28	DMS	U	903[B]	4/4	0.97	0.17	2.90	26,28,29,32	4
36	LHG	d	407	49/49	0.97	0.12	2.89	22,27,46,50	0
35	DGD	H	102	62/66	0.93	0.11	2.85	25,33,40,43	0
28	DMS	U	903[A]	4/4	0.97	0.17	2.85	32,34,40,41	4
26	UNL	X	101	16/-	0.81	0.17	2.82	37,40,59,59	0
24	LMG	c	518	51/55	0.72	0.21	2.62	37,72,84,87	0
26	UNL	b	630	11/-	0.82	0.21	2.61	55,60,67,68	0
20	CLA	B	602	65/65	0.88	0.14	2.61	29,42,77,81	0
35	DGD	h	101	62/66	0.93	0.10	2.55	25,34,41,49	0
34	LMT	m	101	35/35	0.63	0.25	2.48	48,94,110,114	0
20	CLA	b	603	65/65	0.89	0.15	2.40	30,45,75,82	0
20	CLA	a	404	60/65	0.96	0.09	2.39	18,22,66,75	0
36	LHG	D	409	49/49	0.95	0.12	2.23	27,33,81,83	0
28	DMS	B	634	4/4	0.98	0.08	2.16	23,24,25,26	0
23	SQD	f	101	40/54	0.83	0.25	2.13	57,86,102,107	0
28	DMS	B	637	4/4	0.96	0.16	2.11	53,53,54,60	0
20	CLA	D	404	65/65	0.95	0.10	2.10	26,29,77,81	0
26	UNL	D	410	37/-	0.83	0.15	2.10	42,57,93,98	0
34	LMT	b	628	25/35	0.64	0.23	2.03	54,79,95,96	0
32	HTG	D	417	19/19	0.53	0.31	2.02	67,105,119,120	0
32	HTG	v	210	14/19	0.69	0.27	2.02	60,80,92,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
20	CLA	d	404	65/65	0.94	0.10	1.93	24,29,78,87	0
28	DMS	b	632	4/4	0.90	0.15	1.92	55,58,66,70	0
34	LMT	c	523	35/35	0.81	0.23	1.88	67,77,83,85	0
23	SQD	A	412	54/54	0.82	0.16	1.86	41,60,78,81	0
28	DMS	b	638	4/4	0.75	0.28	1.85	67,75,77,86	0
22	BCR	d	405	40/40	0.89	0.12	1.85	24,30,56,58	0
35	DGD	C	516	62/66	0.97	0.09	1.84	22,32,74,79	0
34	LMT	I	101	35/35	0.77	0.24	1.81	67,82,91,92	0
35	DGD	c	515	62/66	0.95	0.10	1.80	23,32,71,75	0
34	LMT	Z	101	35/35	0.70	0.23	1.79	44,90,107,109	0
28	DMS	o	308	4/4	0.83	0.21	1.78	60,61,62,63	0
34	LMT	z	102	35/35	0.78	0.19	1.76	46,85,99,101	0
36	LHG	d	406	49/49	0.97	0.10	1.74	29,36,43,48	0
23	SQD	F	101	35/54	0.85	0.23	1.71	51,76,89,90	0
36	LHG	d	408	49/49	0.97	0.10	1.71	24,31,83,88	0
32	HTG	u	201	8/19	0.74	0.21	1.68	45,52,69,89	0
20	CLA	B	605	65/65	0.97	0.08	1.63	19,23,55,58	0
28	DMS	v	204	4/4	0.93	0.15	1.60	48,54,57,69	0
34	LMT	B	625	24/35	0.76	0.17	1.59	48,67,86,89	0
20	CLA	a	403	65/65	0.97	0.09	1.58	17,20,29,38	0
24	LMG	J	101	45/55	0.94	0.10	1.55	27,32,64,70	0
35	DGD	C	518	62/66	0.96	0.09	1.51	24,30,62,73	0
28	DMS	j	105	4/4	0.69	0.19	1.47	70,74,75,88	0
36	LHG	D	408	49/49	0.98	0.09	1.46	23,30,44,49	0
28	DMS	V	209	4/4	0.91	0.20	1.46	57,73,77,81	0
23	SQD	A	406	54/54	0.93	0.13	1.41	34,59,71,76	0
28	DMS	D	414	4/4	0.97	0.14	1.39	55,56,57,58	0
26	UNL	j	104	16/-	0.89	0.10	1.38	49,58,64,66	0
28	DMS	B	640	4/4	0.94	0.33	1.37	45,48,49,50	0
28	DMS	h	102	4/4	0.97	0.16	1.36	50,51,53,62	0
22	BCR	D	405	40/40	0.91	0.11	1.35	26,30,58,60	0
20	CLA	b	606	65/65	0.97	0.07	1.34	20,24,54,59	0
23	SQD	a	409	54/54	0.94	0.12	1.32	33,56,75,78	0
20	CLA	d	402	65/65	0.98	0.08	1.29	16,20,35,41	0
20	CLA	A	404	65/65	0.96	0.10	1.28	20,25,88,90	0
26	UNL	a	416	11/-	0.75	0.16	1.26	66,68,76,78	0
34	LMT	M	101	35/35	0.74	0.20	1.18	34,53,63,64	0
24	LMG	C	519	51/55	0.89	0.15	1.18	31,67,83,84	0
20	CLA	b	611	65/65	0.96	0.09	1.11	24,30,34,41	0
20	CLA	c	512	65/65	0.92	0.11	1.10	28,41,70,72	0
35	DGD	c	517	62/66	0.95	0.09	1.09	23,30,56,71	0
20	CLA	B	606	65/65	0.98	0.09	1.08	19,24,35,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
26	UNL	I	106	11/-	0.75	0.19	1.06	61,73,81,81	0
20	CLA	B	608	65/65	0.97	0.07	1.05	18,21,34,39	0
22	BCR	B	618	40/40	0.96	0.08	1.04	21,28,42,45	0
28	DMS	F	102	4/4	0.97	0.11	1.04	51,52,56,64	0
32	HTG	b	601	19/19	0.87	0.15	1.01	45,61,67,80	0
26	UNL	J	104	14/-	0.60	0.24	1.01	67,77,80,81	0
36	LHG	L	101	49/49	0.97	0.09	1.01	24,31,49,53	0
20	CLA	C	504	65/65	0.95	0.08	1.00	27,30,59,61	0
21	PHO	a	406	64/64	0.98	0.08	0.99	19,24,29,32	0
28	DMS	c	531	4/4	0.94	0.15	0.97	73,78,85,86	0
20	CLA	C	509	65/65	0.96	0.09	0.95	29,34,52,55	0
27	PL9	d	412	55/55	0.96	0.08	0.93	18,23,29,35	0
20	CLA	b	609	65/65	0.97	0.07	0.92	19,22,33,37	0
22	BCR	C	514	40/40	0.90	0.10	0.90	36,45,49,50	0
22	BCR	t	101	40/40	0.95	0.07	0.90	22,29,41,43	0
35	DGD	C	517	55/66	0.95	0.07	0.89	26,34,59,62	0
32	HTG	b	624	19/19	0.81	0.23	0.87	49,74,80,85	0
34	LMT	m	102	35/35	0.74	0.20	0.85	34,53,58,59	0
20	CLA	C	510	65/65	0.96	0.08	0.85	26,31,38,44	0
20	CLA	c	511	65/65	0.95	0.10	0.82	27,33,40,43	0
20	CLA	c	513	65/65	0.92	0.12	0.81	36,46,81,87	0
20	CLA	c	509	65/65	0.96	0.09	0.80	25,30,53,58	0
20	CLA	A	401	65/65	0.98	0.08	0.80	16,19,30,36	0
35	DGD	c	516	57/66	0.96	0.08	0.79	27,32,62,68	0
24	LMG	c	519	51/55	0.89	0.13	0.79	29,59,86,88	0
32	HTG	B	631	19/19	0.88	0.12	0.78	41,57,69,73	0
20	CLA	b	618	65/65	0.91	0.13	0.77	23,33,92,98	0
36	LHG	D	407	49/49	0.96	0.09	0.77	28,37,44,52	0
28	DMS	O	307	4/4	0.94	0.15	0.76	69,76,77,88	0
20	CLA	B	610	65/65	0.96	0.10	0.71	26,31,35,38	0
27	PL9	D	412	55/55	0.97	0.08	0.67	19,23,29,34	0
20	CLA	B	607	65/65	0.95	0.09	0.67	22,29,55,62	0
22	BCR	A	405	40/40	0.97	0.08	0.67	21,26,32,35	0
36	LHG	l	102	49/49	0.97	0.08	0.66	22,30,51,54	0
20	CLA	b	607	65/65	0.98	0.08	0.62	20,24,33,35	0
20	CLA	B	603	65/65	0.96	0.08	0.61	23,28,35,39	0
22	BCR	b	620	40/40	0.96	0.08	0.61	22,27,43,46	0
22	BCR	K	101	40/40	0.92	0.10	0.60	33,37,42,45	0
20	CLA	B	615	65/65	0.97	0.08	0.58	20,24,70,79	0
24	LMG	j	101	45/55	0.94	0.09	0.58	27,32,60,64	0
20	CLA	C	513	65/65	0.87	0.14	0.57	40,48,72,77	0
21	PHO	a	405	64/64	0.97	0.07	0.53	17,20,22,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
28	DMS	B	645	4/4	0.97	0.11	0.51	56,59,64,71	0
22	BCR	j	102	40/40	0.95	0.09	0.49	30,35,42,45	0
20	CLA	B	611	65/65	0.97	0.08	0.47	21,26,34,40	0
20	CLA	d	403	65/65	0.98	0.07	0.47	17,19,27,34	0
20	CLA	b	608	65/65	0.95	0.09	0.46	24,31,59,63	0
22	BCR	B	617	40/40	0.97	0.07	0.44	22,26,32,33	0
20	CLA	C	505	65/65	0.96	0.08	0.41	28,33,44,48	0
20	CLA	b	616	65/65	0.96	0.08	0.41	20,26,73,80	0
20	CLA	D	401	65/65	0.98	0.08	0.41	16,20,35,41	0
20	CLA	A	402	59/65	0.97	0.07	0.38	18,22,52,58	0
20	CLA	D	402	65/65	0.98	0.06	0.37	15,19,30,36	0
20	CLA	c	504	65/65	0.97	0.07	0.31	25,29,55,60	0
22	BCR	k	101	40/40	0.95	0.09	0.30	28,36,41,42	0
22	BCR	B	619	40/40	0.95	0.07	0.29	22,30,42,44	0
20	CLA	C	503	65/65	0.95	0.08	0.29	28,33,37,42	0
20	CLA	C	506	65/65	0.92	0.10	0.26	32,45,86,87	0
20	CLA	b	612	65/65	0.96	0.08	0.26	21,27,36,41	0
22	BCR	T	101	40/40	0.96	0.07	0.23	24,32,43,45	0
20	CLA	b	613	65/65	0.97	0.07	0.23	20,22,38,44	0
21	PHO	A	403	64/64	0.98	0.07	0.22	18,22,24,25	0
20	CLA	c	508	60/65	0.97	0.07	0.22	24,28,52,54	0
28	DMS	i	104	4/4	0.97	0.20	0.20	63,66,67,71	0
28	DMS	D	416	4/4	0.93	0.17	0.18	83,87,89,91	0
22	BCR	a	408	40/40	0.96	0.07	0.18	21,25,30,31	0
20	CLA	c	510	65/65	0.97	0.07	0.17	23,29,39,42	0
20	CLA	a	407	47/65	0.97	0.07	0.16	19,22,41,48	0
20	CLA	b	614	65/65	0.97	0.07	0.16	21,25,31,37	0
37	HEM	V	201	43/43	0.99	0.08	0.14	21,23,27,31	0
22	BCR	C	515	40/40	0.95	0.09	0.14	31,37,43,45	0
20	CLA	B	601	65/65	0.93	0.12	0.13	23,29,82,86	0
20	CLA	c	506	65/65	0.93	0.10	0.11	24,39,71,74	0
31	BCT	A	421	4/4	0.95	0.10	0.10	31,34,40,44	0
39	MG	j	103	1/1	1.00	0.08	0.04	31,31,31,31	0
28	DMS	v	203	4/4	0.93	0.16	0.03	67,69,76,79	0
21	PHO	D	403	64/64	0.97	0.07	0.01	18,24,29,35	0
20	CLA	b	604	65/65	0.96	0.08	-0.02	23,27,33,35	0
37	HEM	v	201	43/43	0.98	0.08	-0.03	25,29,34,37	0
20	CLA	c	503	65/65	0.96	0.08	-0.04	25,35,40,43	0
20	CLA	b	605	65/65	0.97	0.07	-0.05	21,25,34,37	0
38	RRX	x	101	41/41	0.92	0.10	-0.06	26,32,47,58	0
28	DMS	v	208	4/4	0.91	0.27	-0.06	89,92,92,95	0
20	CLA	C	507	65/65	0.95	0.09	-0.07	28,37,52,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
20	CLA	b	610	65/65	0.97	0.07	-0.07	20,26,31,33	0
20	CLA	B	612	65/65	0.98	0.07	-0.07	19,22,36,42	0
28	DMS	V	207	4/4	0.96	0.10	-0.10	62,63,63,70	0
20	CLA	B	613	65/65	0.98	0.07	-0.11	21,25,30,34	0
20	CLA	C	501	65/65	0.96	0.08	-0.11	27,33,45,52	0
22	BCR	k	102	40/40	0.93	0.09	-0.11	41,46,51,51	0
20	CLA	B	604	65/65	0.97	0.07	-0.12	21,24,33,39	0
38	RRX	H	101	41/41	0.94	0.10	-0.15	27,31,41,46	0
20	CLA	C	508	60/65	0.96	0.07	-0.17	23,31,47,51	0
20	CLA	c	501	65/65	0.96	0.08	-0.18	26,30,41,48	0
20	CLA	b	615	65/65	0.98	0.06	-0.19	18,22,53,59	0
20	CLA	c	507	65/65	0.97	0.08	-0.19	25,30,49,57	0
20	CLA	C	502	65/65	0.97	0.07	-0.21	24,29,41,48	0
28	DMS	V	208	4/4	0.95	0.12	-0.22	75,77,82,85	0
20	CLA	c	502	65/65	0.97	0.07	-0.22	22,26,39,48	0
20	CLA	B	614	65/65	0.98	0.06	-0.23	19,22,48,53	0
37	HEM	E	104	43/43	0.96	0.10	-0.25	39,44,52,56	0
20	CLA	c	505	65/65	0.97	0.06	-0.27	25,30,46,50	0
22	BCR	b	619	40/40	0.97	0.07	-0.28	23,26,32,35	0
20	CLA	B	616	65/65	0.97	0.07	-0.33	25,29,48,52	0
37	HEM	e	102	43/43	0.97	0.09	-0.34	34,41,56,68	0
20	CLA	C	512	55/65	0.93	0.09	-0.37	37,44,49,54	0
20	CLA	B	609	65/65	0.98	0.07	-0.38	22,25,31,33	0
20	CLA	C	511	65/65	0.95	0.08	-0.42	30,37,42,45	0
22	BCR	b	621	40/40	0.97	0.07	-0.46	27,32,42,44	0
22	BCR	c	514	40/40	0.96	0.07	-0.51	28,36,39,39	0
31	BCT	a	413	4/4	0.95	0.07	-0.55	32,32,38,42	0
25	CL	a	412	1/1	0.99	0.06	-0.67	24,24,24,24	0
25	CL	A	408	1/1	1.00	0.05	-0.87	22,22,22,22	0
20	CLA	b	617	65/65	0.97	0.07	-0.94	23,30,44,50	0
39	MG	J	102	1/1	0.97	0.05	-1.47	33,33,33,33	0
29	FE2	a	417	1/1	0.99	0.05	-1.56	27,27,27,27	0
29	FE2	A	419	1/1	0.99	0.03	-1.59	29,29,29,29	0
30	OEX	A	420	10/10	1.00	0.04	-1.61	21,23,24,24	0
33	CA	o	301	1/1	0.94	0.07	-1.61	48,48,48,48	0
33	CA	c	522	1/1	0.98	0.04	-1.88	41,41,41,41	0
33	CA	O	301	1/1	0.95	0.06	-2.01	47,47,47,47	0
25	CL	A	409	1/1	0.99	0.03	-2.20	22,22,22,22	0
30	OEX	a	419	10/10	1.00	0.03	-3.10	21,24,26,26	0
25	CL	a	411	1/1	1.00	0.02	-6.01	22,22,22,22	0
26	UNL	Z	102	4/-	0.53	0.17	-	59,61,62,63	0
28	DMS	b	641	4/4	0.83	0.17	-	63,65,75,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
28	DMS	V	206	4/4	0.96	0.20	-	59,61,63,65	0
28	DMS	c	532	4/4	0.94	0.23	-	65,70,76,77	0
28	DMS	O	311	4/4	0.90	0.26	-	57,65,69,72	0
33	CA	V	203	1/1	0.88	0.11	-	63,63,63,63	0
28	DMS	C	529	4/4	0.92	0.19	-	70,73,74,74	0
28	DMS	C	528	4/4	0.99	0.09	-	33,37,39,41	0
26	UNL	B	646	16/-	0.68	0.24	-	85,89,93,94	0
26	UNL	J	106	4/-	0.83	0.15	-	57,60,61,67	0
26	UNL	B	647	13/-	0.77	0.23	-	71,81,90,91	0
28	DMS	O	308	4/4	0.78	0.24	-	66,74,76,87	0
28	DMS	d	415	4/4	0.91	0.25	-	68,71,71,72	0
28	DMS	A	414	4/4	0.99	0.07	-	25,28,28,29	0
26	UNL	B	629	10/-	0.72	0.27	-	54,69,74,74	0
28	DMS	B	644	4/4	0.87	0.32	-	52,53,61,69	0
26	UNL	c	525	10/-	0.84	0.15	-	58,65,66,67	0
26	UNL	b	629	16/-	0.91	0.15	-	41,48,60,60	0
26	UNL	I	105	10/-	0.84	0.15	-	60,66,71,72	0
28	DMS	v	205	4/4	0.96	0.18	-	67,70,72,73	0
26	UNL	H	105	6/-	0.78	0.14	-	51,55,63,65	0
26	UNL	A	413	4/-	0.86	0.19	-	64,64,64,66	0
26	UNL	z	101	6/-	0.90	0.13	-	49,55,55,57	0
26	UNL	c	526	8/-	0.77	0.15	-	54,59,64,65	0
28	DMS	u	203	4/4	0.91	0.29	-	47,55,56,65	0
33	CA	B	624	1/1	0.99	0.16	-	43,43,43,43	0
26	UNL	i	102	11/-	0.80	0.16	-	48,54,64,65	0
26	UNL	H	104	4/-	0.88	0.21	-	60,62,65,67	0
28	DMS	v	207	4/4	0.68	0.20	-	53,66,72,87	0
28	DMS	V	204	4/4	0.91	0.32	-	58,64,64,72	0
28	DMS	C	533	4/4	0.94	0.28	-	72,73,73,74	0
26	UNL	i	103	11/-	0.90	0.27	-	58,61,65,66	0
32	HTG	B	623	19/19	0.59	0.35	-	53,88,93,94	0
26	UNL	M	102	12/-	0.84	0.22	-	49,53,95,98	0
28	DMS	o	303	4/4	0.92	0.39	-	66,69,75,79	0
26	UNL	a	414	28/-	0.67	0.23	-	59,68,84,87	0
32	HTG	C	520	19/19	0.86	0.22	-	64,70,76,79	0
28	DMS	b	634	4/4	0.91	0.29	-	59,67,67,75	0
26	UNL	e	101	7/-	0.82	0.25	-	54,58,64,65	0
26	UNL	b	646	6/-	0.86	0.14	-	54,58,60,62	0
28	DMS	c	529	4/4	0.93	0.23	-	79,82,86,87	0
26	UNL	I	103	13/-	0.88	0.13	-	47,53,84,87	0
26	UNL	b	642	13/-	0.56	0.22	-	71,80,87,90	0
26	UNL	i	101	16/-	0.85	0.17	-	41,45,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
28	DMS	B	636	4/4	0.61	0.40	-	77,86,90,96	0
26	UNL	c	524	30/-	0.71	0.19	-	59,74,86,87	0
28	DMS	b	640	4/4	0.77	0.27	-	49,58,71,73	0
32	HTG	c	520	19/19	0.78	0.22	-	77,88,99,100	0
28	DMS	B	643	4/4	0.94	0.14	-	51,53,62,71	0
26	UNL	b	643	9/-	0.68	0.18	-	67,67,74,74	0
28	DMS	A	415	4/4	0.94	0.20	-	55,58,65,71	0
26	UNL	J	107	3/-	0.74	0.21	-	61,61,63,64	0
28	DMS	B	635	4/4	0.86	0.24	-	90,94,95,96	0
32	HTG	C	534	19/19	0.39	0.38	-	68,110,128,130	0
26	UNL	I	104	11/-	0.84	0.19	-	53,56,59,62	0
28	DMS	u	204	4/4	0.84	0.19	-	71,78,83,86	0
32	HTG	B	632	19/19	0.65	0.23	-	51,97,108,114	0
26	UNL	I	102	16/-	0.85	0.19	-	38,47,63,64	0
26	UNL	L	102	14/-	0.85	0.22	-	56,60,84,84	0
26	UNL	b	644	7/-	0.90	0.18	-	64,65,70,70	0
28	DMS	c	527	4/4	0.99	0.05	-	33,33,34,38	0
33	CA	b	626	1/1	0.95	0.07	-	42,42,42,42	0
28	DMS	b	635	4/4	0.92	0.27	-	58,62,69,73	0
32	HTG	b	602	19/19	0.69	0.20	-	51,103,117,118	0
28	DMS	o	302	4/4	0.98	0.08	-	20,28,31,36	0
28	DMS	b	639	4/4	0.95	0.20	-	46,49,49,50	0
28	DMS	c	534	4/4	0.90	0.24	-	70,71,75,81	0
26	UNL	x	102	9/-	0.84	0.29	-	56,68,72,72	0
28	DMS	H	103	4/4	0.61	0.40	-	84,101,109,112	0
28	DMS	U	904	4/4	0.55	0.22	-	58,66,66,83	0
28	DMS	c	533	4/4	0.85	0.27	-	73,75,77,87	0
28	DMS	O	303	4/4	0.82	0.29	-	63,72,77,78	0
26	UNL	a	402	6/-	0.69	0.17	-	50,57,62,63	0
28	DMS	o	305	4/4	0.92	0.23	-	73,75,77,87	0
26	UNL	b	645	6/-	0.57	0.24	-	57,65,76,76	0
26	UNL	B	628	15/-	0.86	0.15	-	45,50,60,66	0
28	DMS	v	209	4/4	0.86	0.32	-	71,78,79,79	0
28	DMS	b	637	4/4	0.87	0.17	-	77,79,84,93	0

6.5 Other polymers

There are no such residues in this entry.