



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:28 PM GMT

PDB ID : 3WU2  
Title : Crystal structure analysis of Photosystem II complex  
Authors : Umena, Y.; Kawakami, K.; Shen, J.R.; Kamiya, N.  
Deposited on : 2014-04-21  
Resolution : 1.90 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

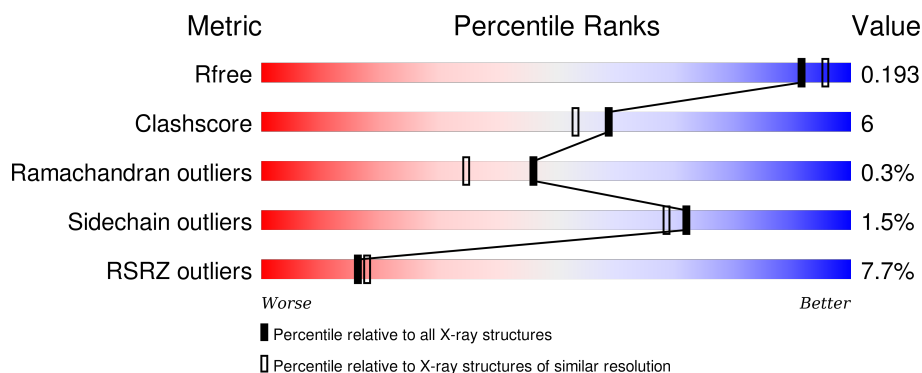
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div>85%</div> <div>10% ..</div> </div>
1	a	344	<div> <div>4%</div> <div>93%</div> <div>..</div> </div>
2	B	504	<div> <div>8%</div> <div>87%</div> <div>13%</div> </div>
2	b	504	<div> <div>9%</div> <div>97%</div> <div>..</div> </div>
3	C	455	<div> <div>3%</div> <div>87%</div> <div>11% ..</div> </div>

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Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	63	
7	h	63	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	

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

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
12	FME	M	1	-	-	X	-
23	CLA	A	405	X	-	-	-
23	CLA	A	406	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	A	410	X	-	-	-
23	CLA	B	602	X	-	-	X
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	B	617	X	-	-	-
23	CLA	C	501	X	-	-	-
23	CLA	C	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	402	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	a	410	X	-	-	-
23	CLA	a	411	X	-	-	-
23	CLA	a	414	X	-	-	-
23	CLA	b	604	X	-	-	X
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	-
23	CLA	c	902	X	-	-	-
23	CLA	c	903	X	-	-	-
23	CLA	c	904	X	-	-	-
23	CLA	c	905	X	-	-	-
23	CLA	c	906	X	-	-	-
23	CLA	c	907	X	-	-	-
23	CLA	c	908	X	-	-	-
23	CLA	c	909	X	-	-	-
23	CLA	c	910	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	911	X	-	-	-
23	CLA	c	912	X	-	-	-
23	CLA	c	913	X	-	-	-
23	CLA	c	914	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
25	BCR	B	618	-	-	-	X
25	BCR	B	619	-	-	-	X
25	BCR	D	404	-	-	-	X
25	BCR	T	101	-	-	-	X
26	SQD	A	418	-	-	-	X
26	SQD	B	621	-	-	-	X
26	SQD	L	103	-	-	-	X
26	SQD	a	401	-	-	-	X
27	LMG	A	413	-	-	-	X
27	LMG	D	411	-	-	-	X
27	LMG	c	921	-	-	-	X
27	LMG	d	410	-	-	-	X
28	PL9	A	414	-	-	-	X
28	PL9	a	419	-	-	-	X
29	UNL	A	417	-	-	-	X
29	UNL	A	420	-	-	-	X
29	UNL	B	627	-	-	X	-
29	UNL	B	629	-	-	-	X
29	UNL	B	632	-	-	-	X
29	UNL	C	523	-	-	-	X
29	UNL	D	412	-	-	X	X
29	UNL	D	413	-	-	-	X
29	UNL	E	102	-	-	-	X
29	UNL	E	103	-	-	-	X
29	UNL	T	102	-	-	-	X
29	UNL	X	101	-	-	-	X
29	UNL	a	403	-	-	-	X
29	UNL	b	628	-	-	-	X
29	UNL	b	630	-	-	-	X
29	UNL	b	631	-	-	-	X
29	UNL	d	411	-	-	-	X
29	UNL	i	103	-	-	-	X
29	UNL	j	102	-	-	-	X
29	UNL	t	103	-	-	-	X
29	UNL	x	101	-	-	-	X
29	UNL	z	102	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	LMT	A	419	-	-	-	X
30	LMT	C	520	-	-	-	X
30	LMT	F	102	-	-	-	X
30	LMT	J	102	-	-	-	X
30	LMT	M	101	-	-	-	X
30	LMT	b	625	-	-	-	X
30	LMT	c	922	-	-	-	X
30	LMT	m	102	-	-	-	X
30	LMT	t	102	-	-	-	X
31	GOL	A	421	-	-	-	X
31	GOL	A	422	-	-	-	X
31	GOL	A	423	-	-	-	X
31	GOL	B	633	-	-	-	X
31	GOL	C	524	-	-	X	X
31	GOL	C	526	-	-	-	X
31	GOL	D	415	-	-	-	X
31	GOL	L	104	-	-	-	X
31	GOL	V	204	-	-	-	X
31	GOL	V	205	-	-	-	X
31	GOL	a	422	-	-	-	X
31	GOL	a	423	-	-	-	X
31	GOL	a	424	-	-	-	X
31	GOL	b	632	-	-	-	X
31	GOL	b	633	-	-	-	X
31	GOL	c	928	-	-	-	X
31	GOL	c	930	-	-	-	X
31	GOL	f	104	-	-	-	X
31	GOL	l	102	-	-	-	X
33	HTG	C	522	-	-	-	X
33	HTG	D	414	-	-	-	X
33	HTG	U	201	-	-	-	X
33	HTG	V	202	-	-	-	X
33	HTG	b	602	-	-	-	X
33	HTG	b	626	-	-	-	X
33	HTG	c	924	-	-	-	X
33	HTG	d	401	-	-	-	X
33	HTG	u	201	-	-	-	X
34	DGD	C	518	-	-	-	X
34	DGD	D	406	-	-	-	X
34	DGD	d	406	-	-	-	X
36	LHG	D	408	-	-	-	X
36	LHG	D	410	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	LHG	d	407	-	-	-	X
39	MG	j	101	-	-	-	X
40	SO4	O	302	-	-	-	X



## 2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 54036 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	4	0
			2633	1729	429	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2625	1722	431	457	15			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Photosystem II CP47 chlorophyll apoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4009	2633	668	695	13			
2	b	501	Total	C	N	O	S	0	11	0
			3964	2605	658	688	13			

- Molecule 3 is a protein called Photosystem II 44 kDa reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	3	0
			3502	2291	588	610	13			
3	c	455	Total	C	N	O	S	0	4	0
			3536	2315	593	615	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	SEE REMARK 999	UNP D0VWR7
C	20	SER	-	SEE REMARK 999	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	SEE REMARK 999	UNP D0VWR7
C	22	PHE	-	SEE REMARK 999	UNP D0VWR7
c	19	ASN	-	SEE REMARK 999	UNP D0VWR7
c	20	SER	-	SEE REMARK 999	UNP D0VWR7
c	21	ILE	-	SEE REMARK 999	UNP D0VWR7
c	22	PHE	-	SEE REMARK 999	UNP D0VWR7

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	2	0
			2726	1809	443	462	12			
4	d	341	Total	C	N	O	S	0	4	0
			2741	1817	449	463	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O		0	0	0
			657	429	106	122				
5	e	79	Total	C	N	O		0	0	0
			639	419	103	117				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			274	187	45	41	1			
6	f	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	N	O	S	0	0	0
			294	199	45	49	1			
8	i	38	Total	C	N	O	S	0	0	0
			311	210	48	52	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	39	Total	C	N	O	S	0	0	0
			271	182	40	48	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	1	0
			290	202	42	46			
10	k	37	Total	C	N	O	0	0	0
			286	198	42	46			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	SEE REMARK 999	UNP P19054
K	39	TRP	VAL	SEE REMARK 999	UNP P19054
k	33	LEU	PHE	SEE REMARK 999	UNP P19054
k	39	TRP	VAL	SEE REMARK 999	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	2	0
			300	204	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
			261	176	37	47	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	2	0
			271	184	38	48	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	SEE REMARK 999	UNP P12312
m	8	LEU	PHE	SEE REMARK 999	UNP P12312

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	5	0
			1878	1177	314	382	5			
13	o	241	Total	C	N	O	S	0	5	0
			1855	1163	305	381	6			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O		0	0	0
			770	489	129	152				
15	u	97	Total	C	N	O		0	1	0
			772	490	129	153				

- 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	2	0
			1066	677	180	205	4			
16	v	137	Total	C	N	O	S	0	1	0
			1060	671	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0	0
			196	130	32	31	3			
17	y	28	Total	C	N	O	S	0	0	0
			196	128	33	32	3			

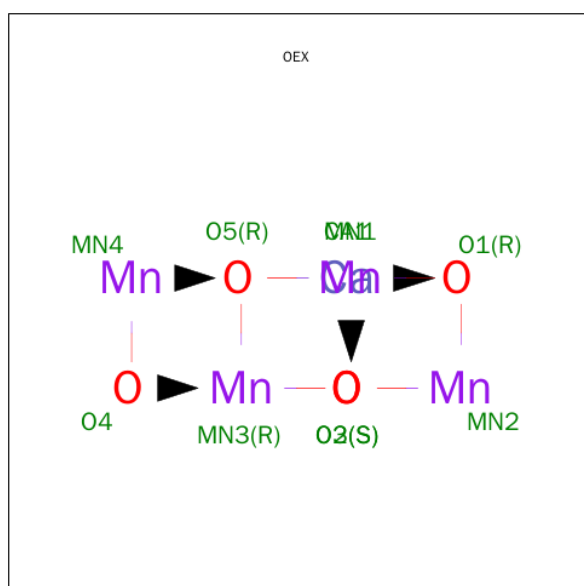
- Molecule 18 is a protein called Photosystem II reaction center protein X.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			459	318	67	73	1			
19	z	60	Total	C	N	O	S	0	0	0
			431	301	64	65	1			

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



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

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

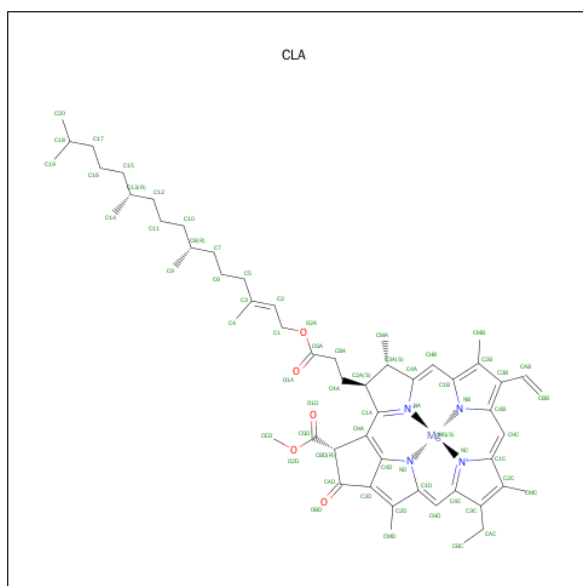
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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

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

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



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

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

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

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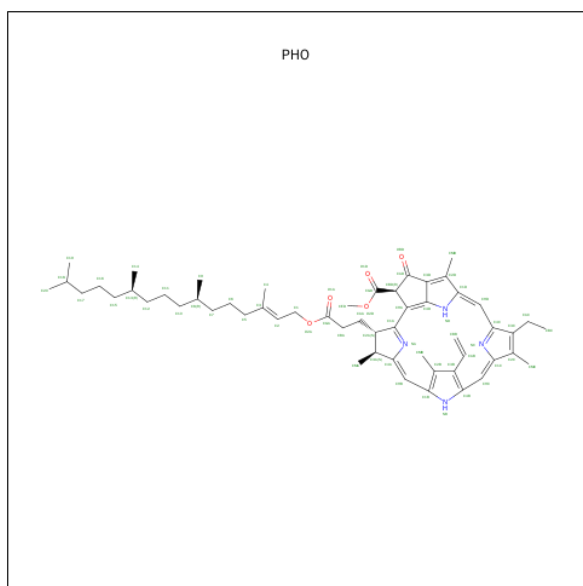
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N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

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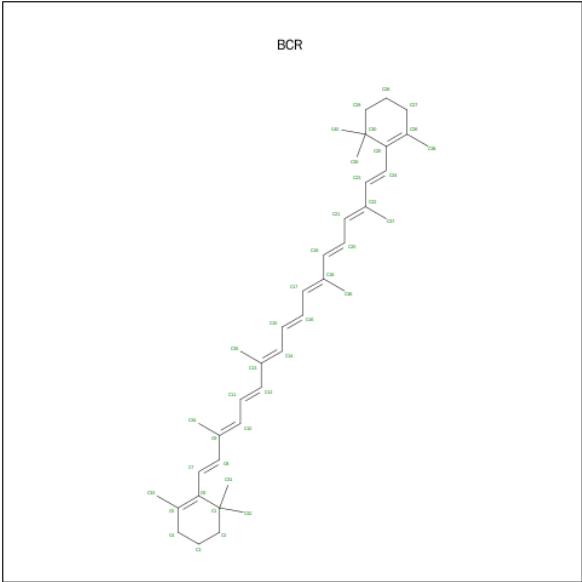
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

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



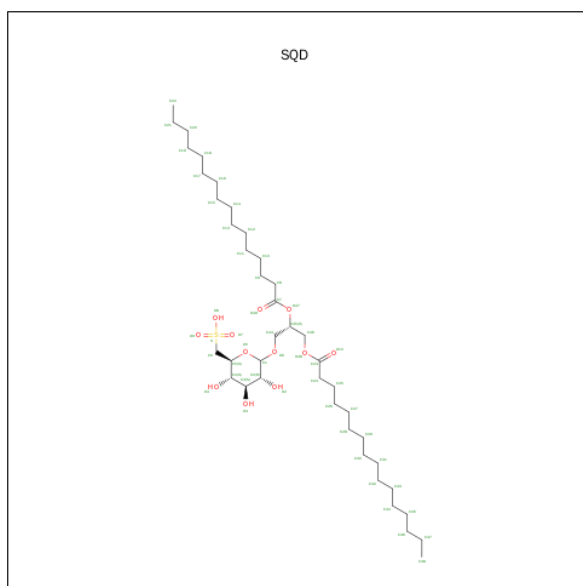
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	a	1	Total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

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

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



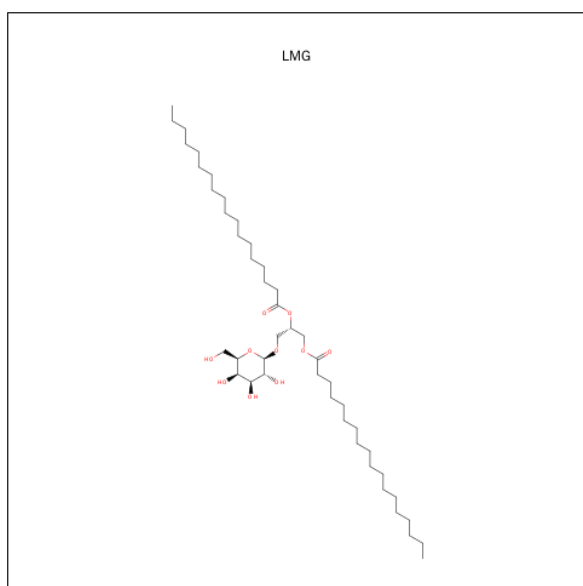
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0
26	D	1	Total C O S 45 32 12 1	0	0
26	L	1	Total C O S 54 41 12 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			33	23	9	1		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



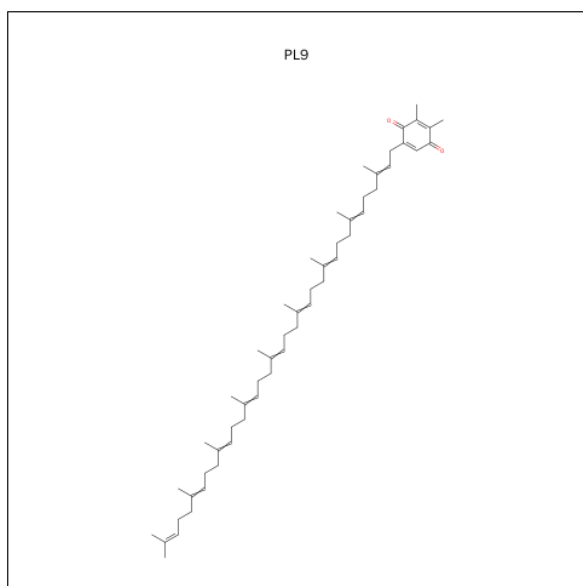
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O		0	0
			51	41	10			
27	B	1	Total	C	O		0	0
			51	41	10			
27	C	1	Total	C	O		0	0
			51	41	10			
27	D	1	Total	C	O		0	0
			51	41	10			
27	Z	1	Total	C	O		0	0
			51	41	10			
27	a	1	Total	C	O		0	0
			51	41	10			
27	b	1	Total	C	O		0	0
			51	41	10	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

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

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:  $C_{53}H_{80}O_2$ ).



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

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

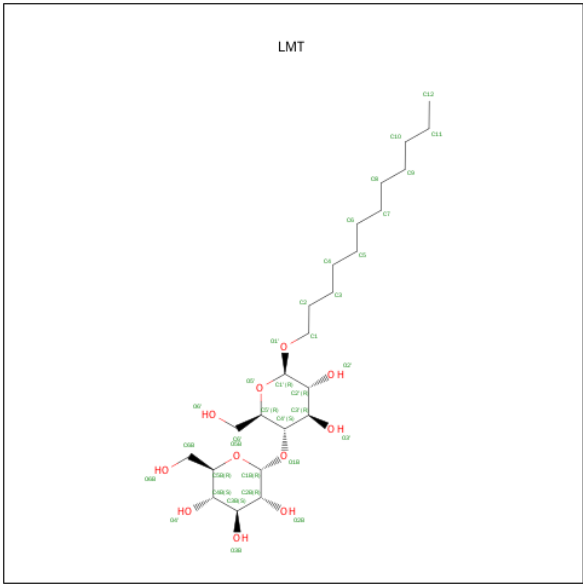
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	B	4	Total	C		0	0
			56	56			
29	c	2	Total	C	O	0	0
			40	35	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	t	1	Total C 16 16	0	0
29	X	1	Total C 16 16	0	0
29	J	2	Total C 26 26	0	0
29	E	2	Total C 27 27	0	0
29	b	4	Total C O 84 79 5	0	0
29	A	4	Total C O 69 64 5	0	0
29	x	1	Total C 16 16	0	0
29	M	1	Total C 16 16	0	0
29	j	2	Total C 28 28	0	0
29	D	2	Total C O 56 51 5	0	0
29	e	1	Total C 11 11	0	0
29	I	2	Total C 24 24	0	0
29	Z	1	Total C 16 16	0	0
29	a	3	Total C O 56 51 5	0	0
29	L	1	Total C 14 14	0	0
29	d	1	Total C 16 16	0	0
29	H	1	Total C 10 10	0	0
29	i	4	Total C 55 55	0	0
29	C	1	Total C O 34 29 5	0	0
29	z	1	Total C 16 16	0	0
29	T	1	Total C 13 13	0	0

- Molecule 30 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			35	24	11		
30	B	1	Total	C	O	0	0
			35	24	11		
30	C	1	Total	C	O	0	0
			35	24	11		
30	F	1	Total	C	O	0	0
			35	24	11		
30	J	1	Total	C	O	0	0
			24	18	6		
30	M	1	Total	C	O	0	0
			35	24	11		
30	M	1	Total	C	O	0	0
			35	24	11		
30	Z	1	Total	C	O	0	0
			35	24	11		
30	a	1	Total	C	O	0	0
			35	24	11		
30	b	1	Total	C	O	0	0
			25	19	6		
30	b	1	Total	C	O	0	0
			24	18	6		
30	c	1	Total	C	O	0	0
			35	24	11		

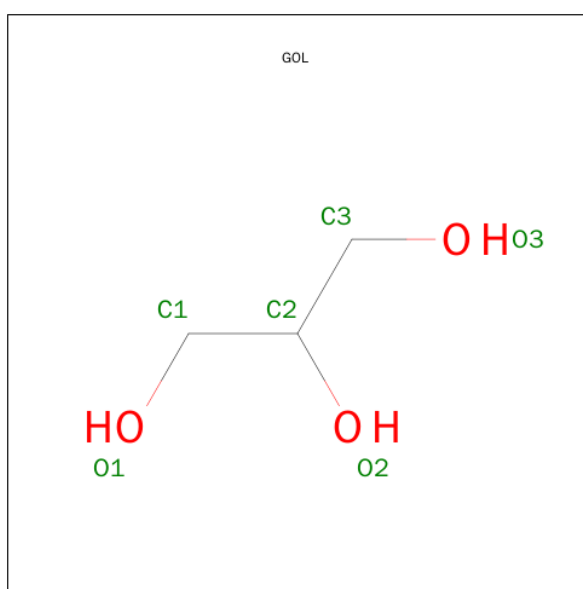
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	m	1	Total	C	O	0	0
			35	24	11		
30	m	1	Total	C	O	0	0
			35	24	11		
30	t	1	Total	C	O	0	0
			24	18	6		
30	z	1	Total	C	O	0	0
			32	21	11		

- Molecule 31 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			6	3	3		
31	A	1	Total	C	O	0	0
			6	3	3		
31	A	1	Total	C	O	0	0
			6	3	3		
31	B	1	Total	C	O	0	0
			6	3	3		
31	B	1	Total	C	O	0	0
			6	3	3		
31	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total 6	C 3	O 3	0	0
31	B	1	Total 6	C 3	O 3	0	0
31	C	1	Total 6	C 3	O 3	0	0
31	C	1	Total 6	C 3	O 3	0	0
31	C	1	Total 6	C 3	O 3	0	0
31	D	1	Total 6	C 3	O 3	0	0
31	L	1	Total 6	C 3	O 3	0	0
31	O	1	Total 6	C 3	O 3	0	0
31	V	1	Total 6	C 3	O 3	0	0
31	V	1	Total 6	C 3	O 3	0	0
31	V	1	Total 6	C 3	O 3	0	0
31	a	1	Total 6	C 3	O 3	0	0
31	a	1	Total 6	C 3	O 3	0	0
31	a	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	b	1	Total 6	C 3	O 3	0	0
31	c	1	Total 6	C 3	O 3	0	0
31	c	1	Total 6	C 3	O 3	0	0

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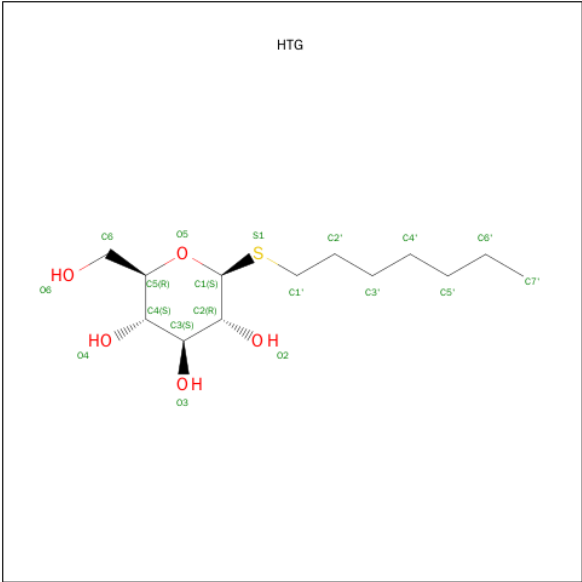
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	c	1	Total C O 6 3 3	0	0
31	c	1	Total C O 6 3 3	0	0
31	f	1	Total C O 6 3 3	0	0
31	h	1	Total C O 6 3 3	0	0
31	l	1	Total C O 6 3 3	0	0
31	v	1	Total C O 6 3 3	0	0
31	v	1	Total C O 6 3 3	0	0
31	v	1	Total C O 6 3 3	0	0

- Molecule 32 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 33 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula: C<sub>13</sub>H<sub>26</sub>O<sub>5</sub>S).



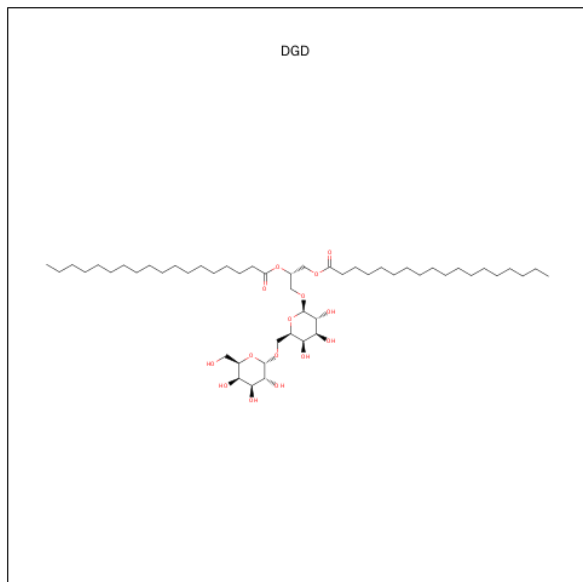
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	C	1	Total	C	O	S	0	0
			19	13	5	1		
33	C	1	Total	C	O	S	0	0
			19	13	5	1		
33	D	1	Total	C	O	S	0	0
			19	13	5	1		
33	O	1	Total	C	O	S	0	0
			19	13	5	1		
33	U	1	Total	C	S		0	0
			9	8	1			
33	V	1	Total	C	O	S	0	0
			13	7	5	1		
33	b	1	Total	C	O	S	0	0
			19	13	5	1		
33	b	1	Total	C	O	S	0	0
			19	13	5	1		
33	b	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	b	1	Total	C	O	S	0	0
			19	13	5	1		
33	c	1	Total	C	O	S	0	0
			19	13	5	1		
33	c	1	Total	C	O	S	0	0
			19	13	5	1		
33	d	1	Total	C	O	S	0	0
			19	13	5	1		
33	u	1	Total	C	O	S	0	0
			14	10	3	1		

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



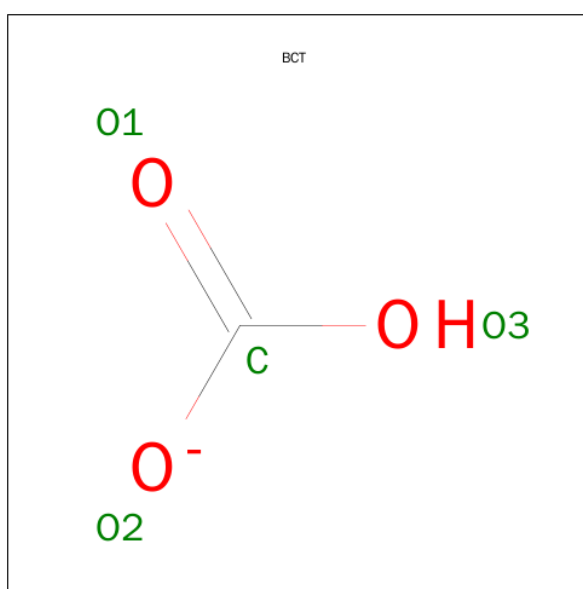
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	C	1	Total	C	O		0	0
			62	47	15			
34	C	1	Total	C	O		0	0
			62	47	15			
34	C	1	Total	C	O		0	0
			62	47	15			
34	D	1	Total	C	O		0	0
			53	42	11			
34	H	1	Total	C	O		0	0
			62	47	15			
34	c	1	Total	C	O		0	0
			62	47	15			

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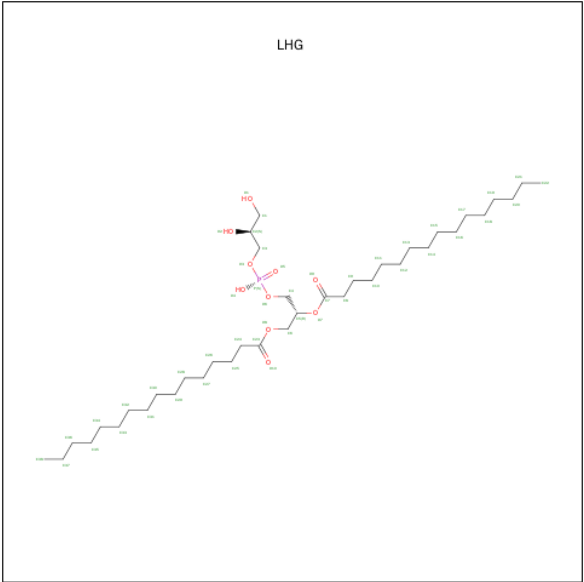
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	c	1	Total	C	O	0	0
			62	47	15		
34	c	1	Total	C	O	0	0
			62	47	15		
34	d	1	Total	C	O	0	0
			50	41	9		
34	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 35 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



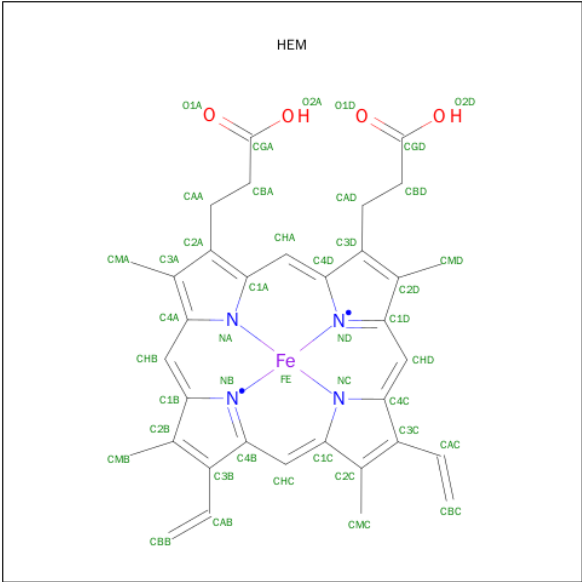
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	D	1	Total	C	O	0	0
			4	1	3		
35	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$ ).



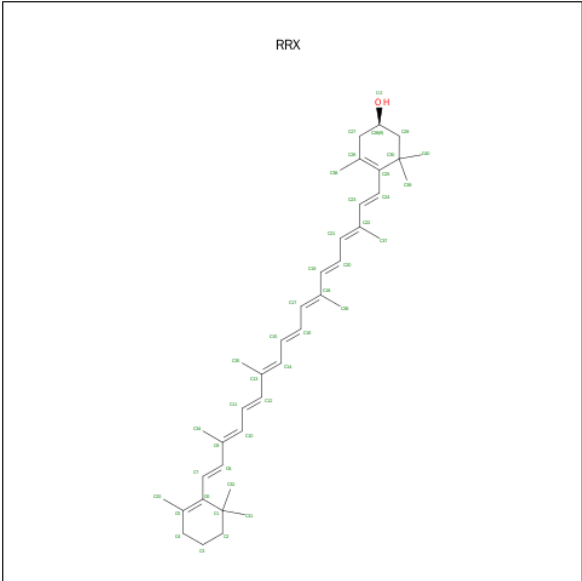
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			46	35	10	1		
36	E	1	Total	C	O	P	0	0
			49	38	10	1		
36	L	1	Total	C	O	P	0	0
			49	38	10	1		
36	a	1	Total	C	O	P	0	0
			40	29	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	l	1	Total	C	O	P	0	0
			49	38	10	1		

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

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



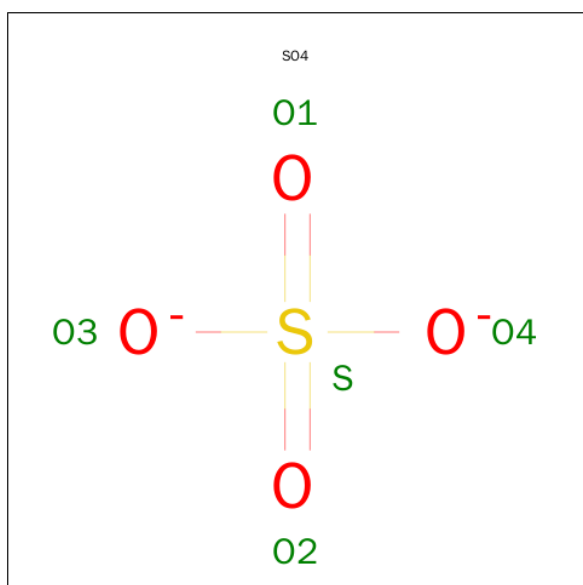


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
38	H	1	Total	C	O	0	0
			41	40	1		
38	h	1	Total	C	O	0	0
			41	40	1		

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

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

- Molecule 40 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
40	O	1	Total	O	S	0	0
			5	4	1		

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	168	Total	O	0	2
			170	170		
41	B	311	Total	O	0	8
			319	319		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	C	253	Total 263	O 263	0	10
41	D	156	Total 161	O 161	0	5
41	E	32	Total 35	O 35	0	3
41	F	12	Total 12	O 12	0	0
41	H	50	Total 52	O 52	0	2
41	I	8	Total 8	O 8	0	0
41	J	9	Total 9	O 9	0	0
41	K	8	Total 8	O 8	0	0
41	L	23	Total 24	O 24	0	1
41	M	15	Total 16	O 16	0	1
41	O	193	Total 202	O 202	0	9
41	T	10	Total 10	O 10	0	0
41	U	98	Total 100	O 100	0	2
41	V	140	Total 144	O 144	0	4
41	Y	6	Total 6	O 6	0	0
41	X	13	Total 14	O 14	0	1
41	Z	1	Total 1	O 1	0	0
41	a	153	Total 155	O 155	0	2
41	b	295	Total 306	O 306	0	11
41	c	238	Total 245	O 245	0	7
41	d	156	Total 160	O 160	0	4

*Continued on next page...*

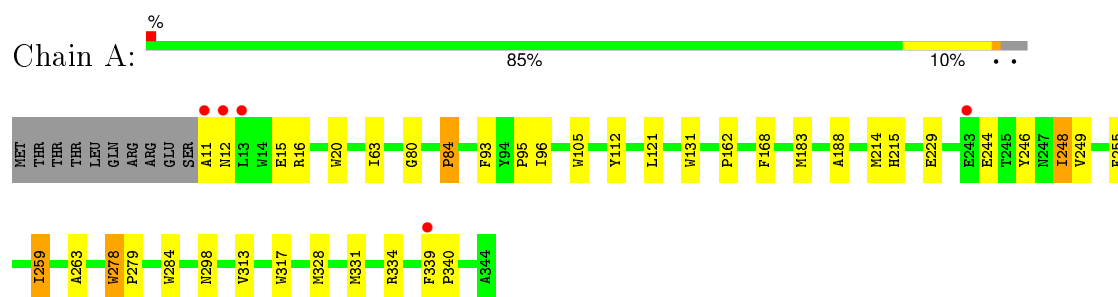
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	e	22	Total 22	O 22	0	0
41	f	13	Total 14	O 14	0	1
41	h	48	Total 53	O 53	0	5
41	i	13	Total 14	O 14	0	1
41	j	9	Total 9	O 9	0	0
41	k	5	Total 5	O 5	0	0
41	l	17	Total 18	O 18	0	1
41	m	15	Total 16	O 16	0	1
41	o	167	Total 175	O 175	0	8
41	t	12	Total 12	O 12	0	0
41	u	102	Total 106	O 106	0	4
41	v	98	Total 104	O 104	0	6
41	y	7	Total 7	O 7	0	0
41	x	6	Total 6	O 6	0	0
41	z	2	Total 2	O 2	0	0

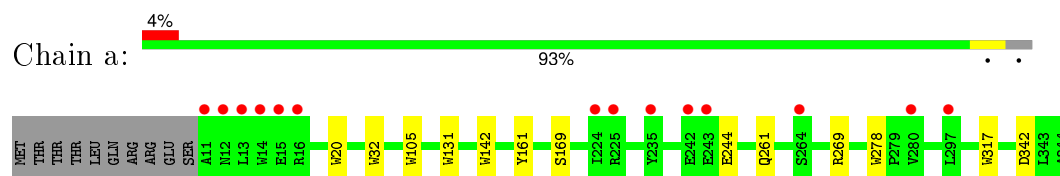
### 3 Residue-property plots

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.

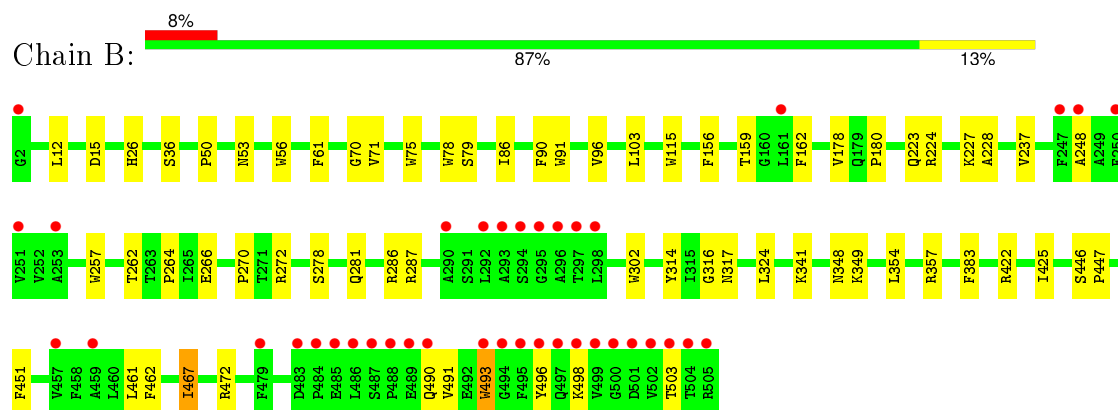
- Molecule 1: Photosystem Q(B) protein



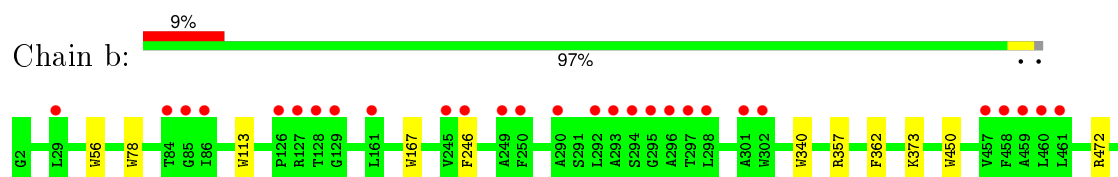
- Molecule 1: Photosystem Q(B) protein



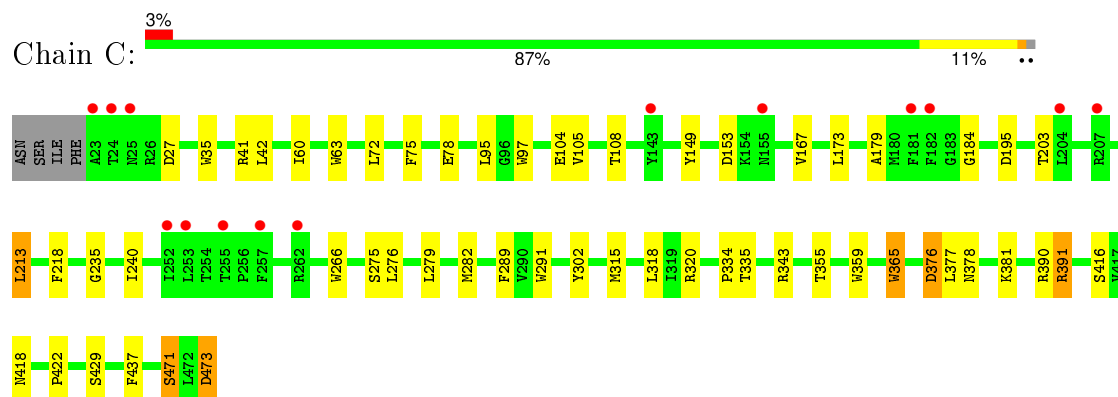
- Molecule 2: Photosystem II CP47 chlorophyll apoprotein



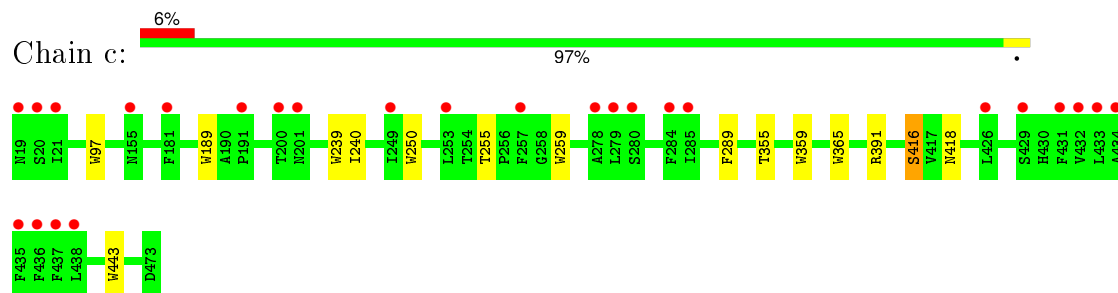
- Molecule 2: Photosystem II CP47 chlorophyll apoprotein



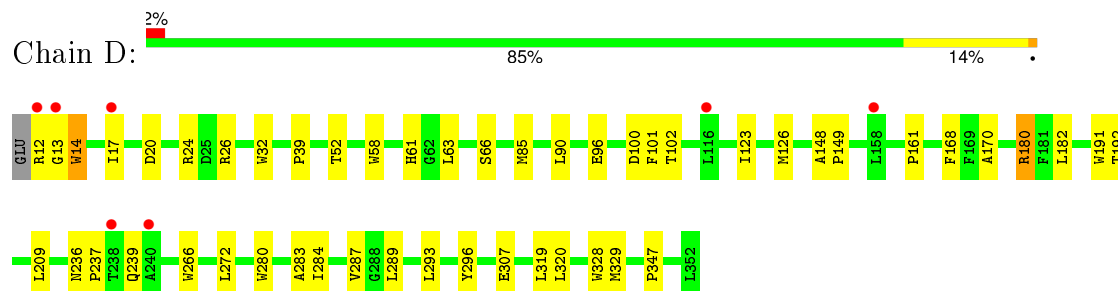
- Molecule 3: Photosystem II 44 kDa reaction center protein



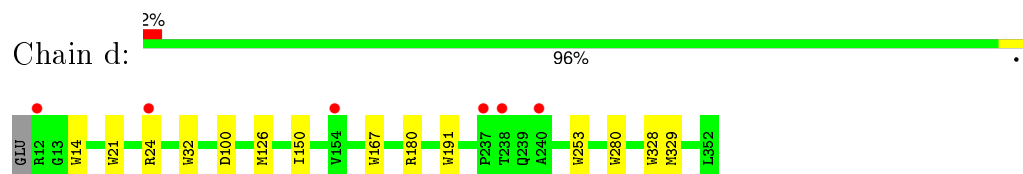
- Molecule 3: Photosystem II 44 kDa reaction center protein



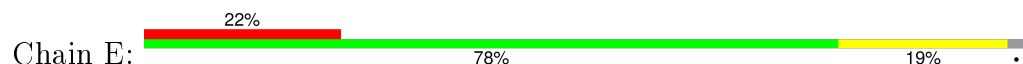
- Molecule 4: Photosystem II D2 protein



- Molecule 4: Photosystem II D2 protein

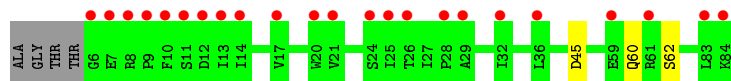
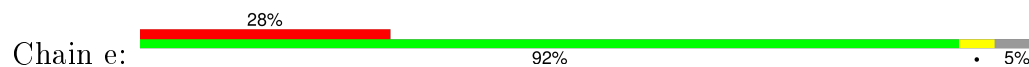


- Molecule 5: Cytochrome b559 subunit alpha





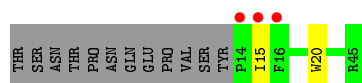
- Molecule 5: Cytochrome b559 subunit alpha



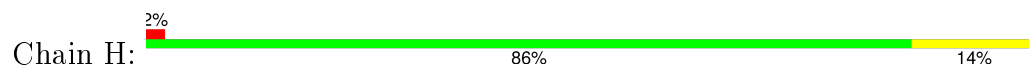
- Molecule 6: Cytochrome b559 subunit beta



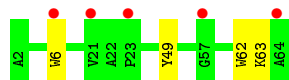
- Molecule 6: Cytochrome b559 subunit beta



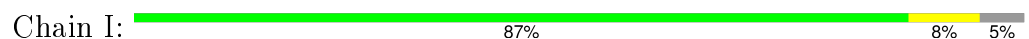
- Molecule 7: Photosystem II reaction center protein H



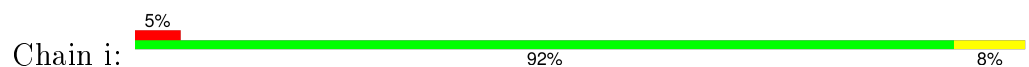
- Molecule 7: Photosystem II reaction center protein H

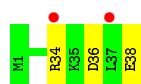


- Molecule 8: Photosystem II reaction center protein I

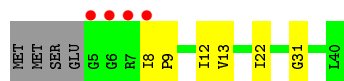
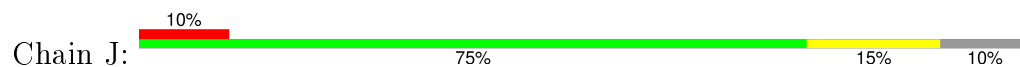


- Molecule 8: Photosystem II reaction center protein I

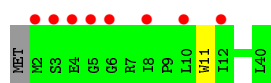
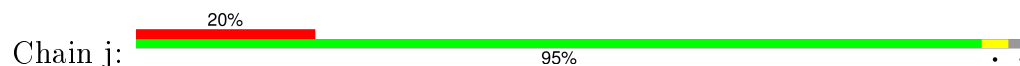




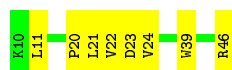
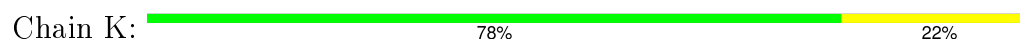
- Molecule 9: Photosystem II reaction center protein J



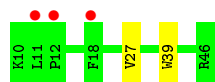
- Molecule 9: Photosystem II reaction center protein J



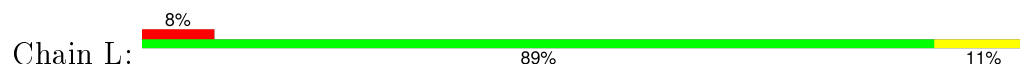
- Molecule 10: Photosystem II reaction center protein K



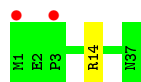
- Molecule 10: Photosystem II reaction center protein K



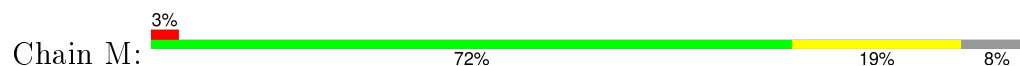
- Molecule 11: Photosystem II reaction center protein L

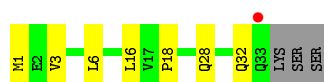


- Molecule 11: Photosystem II reaction center protein L

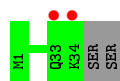


- Molecule 12: Photosystem II reaction center protein M

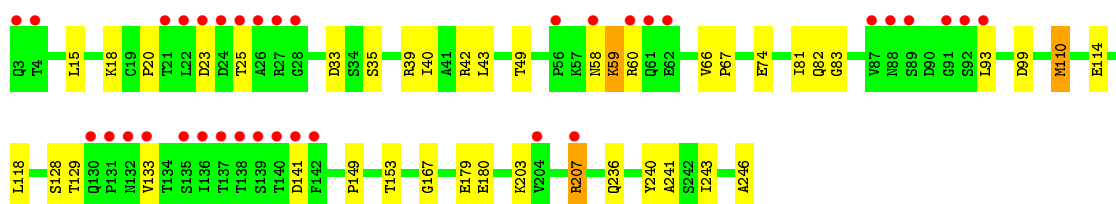
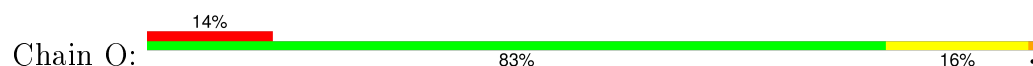




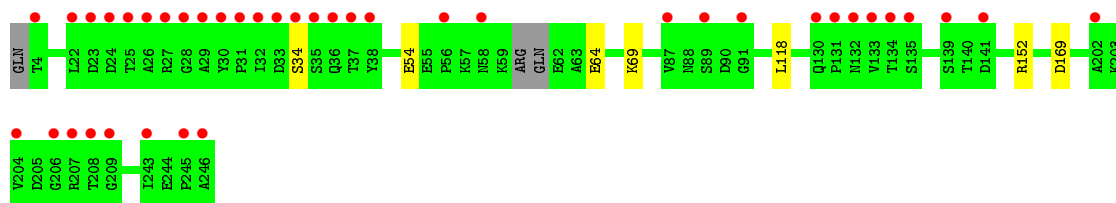
- Molecule 12: Photosystem II reaction center protein M



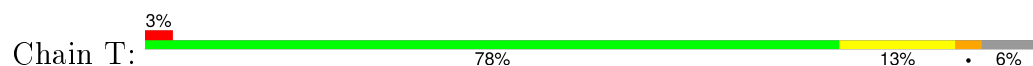
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



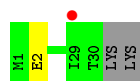
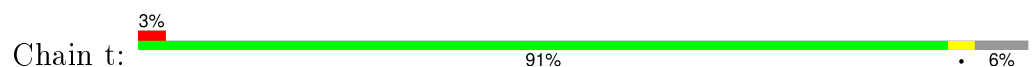
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



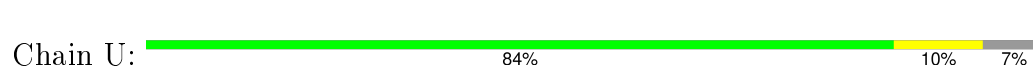
- Molecule 14: Photosystem II reaction center protein T



- Molecule 14: Photosystem II reaction center protein T



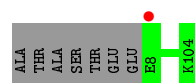
- Molecule 15: Photosystem II 12 kDa extrinsic protein



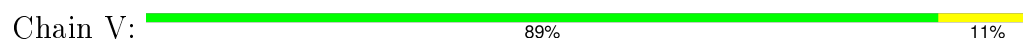




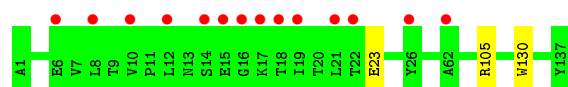
- Molecule 15: Photosystem II 12 kDa extrinsic protein



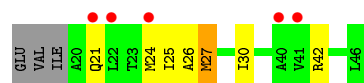
- Molecule 16: Cytochrome c-550



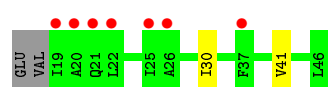
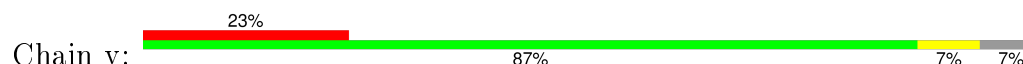
- Molecule 16: Cytochrome c-550



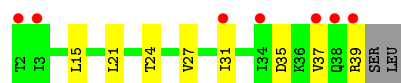
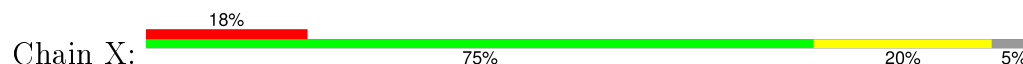
- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 17: Photosystem II reaction center protein Ycf12

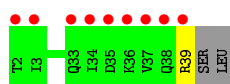


- Molecule 18: Photosystem II reaction center protein X

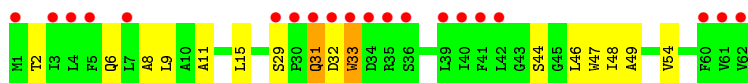
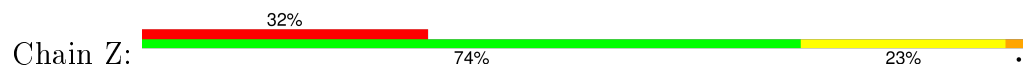


- Molecule 18: Photosystem II reaction center protein X

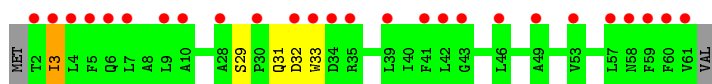
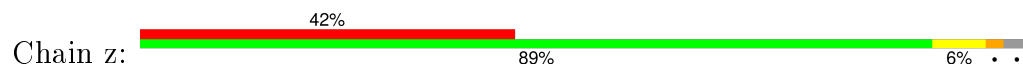




- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.19Å 228.51Å 286.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 49.02 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-1.90) 99.8 (49.02-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.86 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.156 , 0.194 0.156 , 0.193	Depositor DCC
$R_{free}$ test set	31204 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.0	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 67.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 623234 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	54036	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PL9, BCT, BCR, DGD, HSK, FE2, RRX, LHG, GOL, CL, CA, CLA, SO4, HEM, FME, UNL, HTG, MG, OEX, PHO, LMT, SQD, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.08	4/2730 (0.1%)	0.90	1/3723 (0.0%)
1	a	1.06	9/2721 (0.3%)	0.86	4/3711 (0.1%)
2	B	1.03	9/4179 (0.2%)	0.89	5/5693 (0.1%)
2	b	1.01	7/4134 (0.2%)	0.85	2/5633 (0.0%)
3	C	1.00	7/3624 (0.2%)	0.84	9/4933 (0.2%)
3	c	0.96	8/3662 (0.2%)	0.81	0/4986
4	D	1.13	5/2804 (0.2%)	0.93	3/3820 (0.1%)
4	d	1.05	8/2825 (0.3%)	0.87	2/3847 (0.1%)
5	E	0.81	0/676	0.82	0/924
5	e	0.81	0/658	0.78	1/899 (0.1%)
6	F	0.90	1/283 (0.4%)	0.71	0/386
6	f	0.92	1/265 (0.4%)	0.69	0/360
7	H	0.98	1/511 (0.2%)	0.79	0/697
7	h	0.94	2/511 (0.4%)	0.81	0/697
8	I	0.77	0/291	0.78	0/394
8	i	0.75	0/308	0.77	0/415
9	J	0.94	0/257	0.68	0/349
9	j	0.81	1/277 (0.4%)	0.69	0/376
10	K	0.76	1/303 (0.3%)	0.75	0/418
10	k	0.79	1/296 (0.3%)	0.77	0/408
11	L	1.05	0/312	0.88	0/425
11	l	1.00	0/313	0.84	1/428 (0.2%)
12	M	0.85	0/257	0.91	0/352
12	m	0.86	0/270	0.80	0/370
13	O	0.84	0/1924	0.89	0/2610
13	o	0.79	0/1900	0.86	3/2577 (0.1%)
14	T	0.93	0/255	0.86	0/346
14	t	0.99	0/255	0.92	0/346
15	U	0.93	0/781	0.90	1/1059 (0.1%)
15	u	0.95	0/786	0.91	0/1067
16	V	0.97	0/1093	0.89	1/1485 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.88	1/1084 (0.1%)	0.85	1/1475 (0.1%)
17	Y	0.55	0/197	0.66	0/263
17	y	0.50	0/197	0.75	0/264
18	X	0.72	0/286	0.75	0/387
18	x	0.67	0/286	0.75	0/387
19	Z	0.76	2/470 (0.4%)	0.74	0/645
19	z	0.68	1/442 (0.2%)	0.71	0/608
All	All	0.97	69/42423 (0.2%)	0.85	34/57763 (0.1%)

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	78	TRP	CD2-CE2	7.33	1.50	1.41
7	H	62	TRP	CD2-CE2	6.81	1.49	1.41
3	c	443	TRP	CD2-CE2	6.79	1.49	1.41
1	A	284	TRP	CD2-CE2	6.79	1.49	1.41
3	C	359	TRP	CD2-CE2	6.46	1.49	1.41

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	272	ARG	NE-CZ-NH1	-7.88	116.36	120.30
13	o	152	ARG	NE-CZ-NH1	-7.53	116.54	120.30
2	B	357	ARG	NE-CZ-NH2	-7.36	116.62	120.30
3	C	153	ASP	CB-CG-OD1	7.03	124.63	118.30
4	D	100	ASP	CB-CG-OD2	7.02	124.62	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2633	0	2544	37	0
1	a	2625	0	2538	0	0
2	B	4009	0	3879	59	0

*Continued on next page...*

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	3964	0	3817	0	0
3	C	3502	0	3431	43	0
3	c	3536	0	3460	0	0
4	D	2726	0	2629	45	0
4	d	2741	0	2654	0	0
5	E	657	0	637	22	0
5	e	639	0	617	0	0
6	F	274	0	279	7	0
6	f	257	0	269	0	0
7	H	498	0	518	7	0
7	h	498	0	518	0	0
8	I	294	0	304	6	0
8	i	311	0	326	0	0
9	J	251	0	257	5	0
9	j	271	0	270	0	0
10	K	290	0	294	7	0
10	k	286	0	285	0	0
11	L	302	0	316	7	0
11	l	300	0	314	0	0
12	M	261	0	280	21	0
12	m	271	0	293	0	0
13	O	1878	0	1853	34	0
13	o	1855	0	1823	0	0
14	T	256	0	256	4	0
14	t	256	0	256	0	0
15	U	770	0	769	6	0
15	u	772	0	766	0	0
16	V	1066	0	1075	12	0
16	v	1060	0	1053	0	0
17	Y	196	0	219	8	0
17	y	196	0	208	0	0
18	X	280	0	312	9	0
18	x	280	0	312	0	0
19	Z	459	0	484	7	0
19	z	431	0	438	0	0
20	A	10	0	0	0	0
20	a	10	0	0	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	260	0	288	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	B	1040	0	1152	61	0
23	C	845	0	936	36	0
23	D	130	0	144	7	0
23	a	260	0	288	0	0
23	b	1040	0	1152	0	0
23	c	845	0	936	0	0
23	d	130	0	144	0	0
24	A	128	0	148	5	0
24	a	128	0	148	0	0
25	A	40	0	56	2	0
25	B	120	0	168	5	0
25	C	80	0	112	5	0
25	D	40	0	56	5	0
25	K	80	0	112	9	0
25	T	40	0	56	9	0
25	a	40	0	56	0	0
25	b	120	0	168	0	0
25	c	80	0	112	0	0
25	d	40	0	56	0	0
25	k	80	0	112	0	0
25	t	40	0	56	0	0
26	A	108	0	155	5	0
26	B	54	0	78	5	0
26	D	45	0	57	3	0
26	L	54	0	78	5	0
26	a	108	0	156	0	0
26	f	33	0	39	0	0
27	A	51	0	72	3	0
27	B	51	0	72	4	0
27	C	51	0	72	2	0
27	D	51	0	72	2	0
27	Z	51	0	72	0	0
27	a	51	0	72	0	0
27	b	51	0	72	0	0
27	c	102	0	144	0	0
27	d	51	0	72	0	0
28	A	55	0	80	10	0
28	D	55	0	80	0	0
28	a	55	0	80	0	0
28	d	55	0	80	0	0
29	A	69	0	0	0	0
29	B	56	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	C	34	0	0	0	0
29	D	56	0	0	2	0
29	E	27	0	0	0	0
29	H	10	0	0	0	0
29	I	24	0	0	0	0
29	J	26	0	0	0	0
29	L	14	0	0	1	0
29	M	16	0	0	1	0
29	T	13	0	0	0	0
29	X	16	0	0	1	0
29	Z	16	0	0	0	0
29	a	56	0	0	0	0
29	b	84	0	0	0	0
29	c	40	0	0	0	0
29	d	16	0	0	0	0
29	e	11	0	0	0	0
29	i	55	0	0	0	0
29	j	28	0	0	0	0
29	t	16	0	0	0	0
29	x	16	0	0	0	0
29	z	16	0	0	0	0
30	A	35	0	46	0	0
30	B	35	0	46	4	0
30	C	35	0	46	4	0
30	F	35	0	46	0	0
30	J	24	0	35	1	0
30	M	70	0	92	3	0
30	Z	35	0	46	3	0
30	a	35	0	46	0	0
30	b	49	0	70	0	0
30	c	35	0	46	0	0
30	m	70	0	92	0	0
30	t	24	0	35	0	0
30	z	32	0	36	0	0
31	A	18	0	22	4	0
31	B	36	0	48	3	0
31	C	18	0	24	4	0
31	D	6	0	8	3	0
31	L	6	0	8	1	0
31	O	6	0	8	0	0
31	V	18	0	24	0	0
31	a	18	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	b	30	0	40	0	0
31	c	24	0	32	0	0
31	f	6	0	6	0	0
31	h	6	0	8	0	0
31	l	6	0	8	0	0
31	v	18	0	24	0	0
32	B	1	0	0	0	0
32	F	1	0	0	0	0
32	O	1	0	0	0	0
32	b	1	0	0	0	0
32	c	1	0	0	0	0
32	f	1	0	0	0	0
32	o	1	0	0	0	0
33	B	95	0	130	3	0
33	C	38	0	52	1	0
33	D	19	0	26	2	0
33	O	19	0	26	0	0
33	U	9	0	15	1	0
33	V	13	0	11	0	0
33	b	76	0	104	0	0
33	c	38	0	52	0	0
33	d	19	0	26	0	0
33	u	14	0	19	0	0
34	C	186	0	246	2	0
34	D	53	0	71	9	0
34	H	62	0	82	1	0
34	c	186	0	246	0	0
34	d	50	0	69	0	0
34	h	62	0	82	0	0
35	D	4	0	0	0	0
35	a	4	0	0	0	0
36	D	144	0	213	24	0
36	E	49	0	74	3	0
36	L	49	0	74	2	0
36	a	40	0	53	0	0
36	d	147	0	222	0	0
36	l	49	0	74	0	0
37	F	43	0	30	4	0
37	V	43	0	30	1	0
37	f	43	0	30	0	0
37	v	43	0	30	0	0
38	H	41	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	h	41	0	56	0	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	O	5	0	0	0	0
41	A	170	0	0	1	0
41	B	319	0	0	4	0
41	C	263	0	0	4	0
41	D	161	0	0	2	0
41	E	35	0	0	4	0
41	F	12	0	0	0	0
41	H	52	0	0	0	0
41	I	8	0	0	0	0
41	J	9	0	0	0	0
41	K	8	0	0	1	0
41	L	24	0	0	0	0
41	M	16	0	0	1	0
41	O	202	0	0	5	0
41	T	10	0	0	0	0
41	U	100	0	0	2	0
41	V	144	0	0	3	0
41	X	14	0	0	0	0
41	Y	6	0	0	0	0
41	Z	1	0	0	0	0
41	a	155	0	0	0	0
41	b	306	0	0	0	0
41	c	245	0	0	0	0
41	d	160	0	0	0	0
41	e	22	0	0	0	0
41	f	14	0	0	0	0
41	h	53	0	0	0	0
41	i	14	0	0	0	0
41	j	9	0	0	0	0
41	k	5	0	0	0	0
41	l	18	0	0	0	0
41	m	16	0	0	0	0
41	o	175	0	0	0	0
41	t	12	0	0	0	0
41	u	106	0	0	0	0
41	v	104	0	0	0	0
41	x	6	0	0	0	0
41	y	7	0	0	0	0
41	z	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	54036	0	51777	461	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 6.

The worst 5 of 461 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[A]:LEU:CD2	12:M:16[A]:LEU:HD23	0.97	1.49
12:M:16[A]:LEU:CD2	12:M:16[A]:LEU:CD2	0.00	1.21
36:D:409:LHG:H112	36:D:409:LHG:C38	13.80	1.17
26:L:103:SQD:H1	26:L:103:SQD:H462	1.28	1.12
36:D:409:LHG:H372	36:D:409:LHG:H131	13.21	1.10

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	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	46	35
1	a	336/344 (98%)	329 (98%)	7 (2%)	0	100	100
2	B	512/504 (102%)	503 (98%)	9 (2%)	0	100	100
2	b	508/504 (101%)	497 (98%)	11 (2%)	0	100	100
3	C	452/455 (99%)	442 (98%)	9 (2%)	1 (0%)	52	42
3	c	457/455 (100%)	442 (97%)	13 (3%)	2 (0%)	39	27
4	D	339/342 (99%)	332 (98%)	7 (2%)	0	100	100
4	d	341/342 (100%)	334 (98%)	7 (2%)	0	100	100
5	E	79/83 (95%)	78 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	e	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
7	h	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	12	3
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	32 (89%)	2 (6%)	2 (6%)	2	0
9	J	34/40 (85%)	34 (100%)	0	0	100	100
9	j	37/40 (92%)	35 (95%)	2 (5%)	0	100	100
10	K	36/37 (97%)	36 (100%)	0	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	37/37 (100%)	37 (100%)	0	0	100	100
12	M	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	247/244 (101%)	238 (96%)	8 (3%)	1 (0%)	39	27
13	o	242/244 (99%)	232 (96%)	9 (4%)	1 (0%)	39	27
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
16	V	137/137 (100%)	132 (96%)	5 (4%)	0	100	100
16	v	136/137 (99%)	129 (95%)	7 (5%)	0	100	100
17	Y	25/30 (83%)	25 (100%)	0	0	100	100
17	y	26/30 (87%)	25 (96%)	1 (4%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	55 (92%)	2 (3%)	3 (5%)	3	0
19	z	58/62 (94%)	50 (86%)	5 (9%)	3 (5%)	2	0
All	All	5224/5344 (98%)	5075 (97%)	134 (3%)	15 (0%)	46	35

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	59	LYS
19	Z	31	GLN
19	Z	32	ASP
8	i	36	ASP
19	z	31	GLN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/279 (98%)	267 (98%)	5 (2%)	66	61
1	a	271/279 (97%)	269 (99%)	2 (1%)	88	88
2	B	407/402 (101%)	404 (99%)	3 (1%)	88	88
2	b	399/402 (99%)	393 (98%)	6 (2%)	72	69
3	C	355/356 (100%)	347 (98%)	8 (2%)	58	51
3	c	358/356 (101%)	349 (98%)	9 (2%)	55	47
4	D	275/276 (100%)	273 (99%)	2 (1%)	88	88
4	d	278/276 (101%)	274 (99%)	4 (1%)	74	71
5	E	71/72 (99%)	70 (99%)	1 (1%)	74	71
5	e	68/72 (94%)	66 (97%)	2 (3%)	50	40
6	F	27/38 (71%)	26 (96%)	1 (4%)	41	29
6	f	26/38 (68%)	25 (96%)	1 (4%)	40	28
7	H	53/53 (100%)	52 (98%)	1 (2%)	65	59
7	h	53/53 (100%)	52 (98%)	1 (2%)	65	59
8	I	31/34 (91%)	31 (100%)	0	100	100
8	i	33/34 (97%)	32 (97%)	1 (3%)	48	38
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	25/28 (89%)	25 (100%)	0	100	100
10	K	29/30 (97%)	29 (100%)	0	100	100
10	k	28/30 (93%)	27 (96%)	1 (4%)	42	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	29/32 (91%)	29 (100%)	0	100	100
12	m	30/32 (94%)	30 (100%)	0	100	100
13	O	207/207 (100%)	203 (98%)	4 (2%)	65	59
13	o	206/207 (100%)	203 (98%)	3 (2%)	72	69
14	T	25/28 (89%)	24 (96%)	1 (4%)	38	26
14	t	25/28 (89%)	24 (96%)	1 (4%)	38	26
15	U	83/89 (93%)	81 (98%)	2 (2%)	57	49
15	u	83/89 (93%)	83 (100%)	0	100	100
16	V	116/117 (99%)	116 (100%)	0	100	100
16	v	115/117 (98%)	114 (99%)	1 (1%)	84	83
17	Y	19/23 (83%)	18 (95%)	1 (5%)	28	16
17	y	18/23 (78%)	16 (89%)	2 (11%)	8	2
18	X	30/33 (91%)	30 (100%)	0	100	100
18	x	30/33 (91%)	29 (97%)	1 (3%)	45	34
19	Z	47/52 (90%)	46 (98%)	1 (2%)	61	55
19	z	40/52 (77%)	38 (95%)	2 (5%)	30	18
All	All	4253/4368 (97%)	4186 (98%)	67 (2%)	72	66

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	244	GLU
2	b	479	PHE
16	v	23	GLU
1	a	261	GLN
2	b	373	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
16	V	34	GLN
2	b	53	ASN
4	d	332	GLN

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Mol	Chain	Res	Type
13	O	104	GLN
13	o	36	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 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
4	HSK	D	336[A]	-	5,10,12	0.49	0	3,12,16	2.04	2 (66%)
4	HSK	D	336[B]	-	6,11,12	0.74	0	5,14,16	2.89	3 (60%)
8	FME	I	1	8	8,9,10	0.62	0	6,9,11	1.35	0
12	FME	M	1	12	8,9,10	0.77	0	6,9,11	1.81	2 (33%)
14	FME	T	1	14	8,9,10	0.47	0	6,9,11	1.50	2 (33%)
4	HSK	d	336[A]	-	5,10,12	0.51	0	3,12,16	1.83	1 (33%)
4	HSK	d	336[B]	-	6,11,12	0.70	0	5,14,16	3.01	4 (80%)
8	FME	i	1	8	8,9,10	0.41	0	6,9,11	1.56	3 (50%)
12	FME	m	1	12	8,9,10	0.77	0	6,9,11	2.09	3 (50%)
14	FME	t	1	14	8,9,10	0.77	0	6,9,11	1.97	2 (33%)

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
4	HSK	D	336[A]	-	-	0/4/6/8	0/1/1/1
4	HSK	D	336[B]	-	-	0/4/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	0/6/9/11	0/0/0/0
12	FME	M	1	12	-	0/6/9/11	0/0/0/0
14	FME	T	1	14	-	0/6/9/11	0/0/0/0
4	HSK	d	336[A]	-	-	0/4/6/8	0/1/1/1
4	HSK	d	336[B]	-	-	0/4/6/8	0/1/1/1
8	FME	i	1	8	-	0/6/9/11	0/0/0/0
12	FME	m	1	12	-	0/6/9/11	0/0/0/0
14	FME	t	1	14	-	0/6/9/11	0/0/0/0

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	O1-CN-N	-3.70	119.43	124.76
12	m	1	FME	O1-CN-N	-2.44	121.24	124.76
8	i	1	FME	O-C-CA	-2.42	119.04	125.44
4	d	336[B]	HSK	CD2-CG-ND1	-2.33	104.96	108.24
14	t	1	FME	O-C-CA	-2.31	119.35	125.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	1	FME	7	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 276 ligands modelled in this entry, 43 are unknown and 15 are monoatomic - leaving 218 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length



(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
20	OEX	A	401	1,3,41	0,15,15	0.00	-	0,32,32	0.00	-
23	CLA	A	405	-	55,73,73	1.67	11 (20%)	61,113,113	1.96	18 (29%)
23	CLA	A	406	41	55,73,73	1.68	12 (21%)	61,113,113	2.57	24 (39%)
23	CLA	A	407	41	55,73,73	1.49	9 (16%)	61,113,113	2.21	17 (27%)
24	PHO	A	408	-	67,69,69	1.69	11 (16%)	84,99,99	2.16	23 (27%)
24	PHO	A	409	-	67,69,69	1.86	13 (19%)	84,99,99	2.16	26 (30%)
23	CLA	A	410	-	55,73,73	1.69	11 (20%)	61,113,113	2.17	17 (27%)
25	BCR	A	411	-	41,41,41	1.01	0	56,56,56	1.49	11 (19%)
26	SQD	A	412	-	53,54,54	1.35	3 (5%)	61,65,65	2.50	16 (26%)
27	LMG	A	413	-	51,51,55	0.96	2 (3%)	59,59,63	1.32	4 (6%)
28	PL9	A	414	-	55,55,55	1.00	3 (5%)	68,69,69	1.58	13 (19%)
26	SQD	A	418	-	53,54,54	1.35	3 (5%)	61,65,65	1.88	12 (19%)
30	LMT	A	419	-	36,36,36	0.81	1 (2%)	47,47,47	1.39	5 (10%)
31	GOL	A	421	-	5,5,5	0.84	0	5,5,5	0.51	0
31	GOL	A	422	-	5,5,5	0.39	0	5,5,5	0.53	0
31	GOL	A	423	32	5,5,5	0.34	0	5,5,5	0.72	0
23	CLA	B	602	41	55,73,73	1.88	13 (23%)	61,113,113	2.19	15 (24%)
23	CLA	B	603	-	55,73,73	1.86	11 (20%)	61,113,113	1.78	14 (22%)
23	CLA	B	604	-	55,73,73	1.70	11 (20%)	61,113,113	2.54	19 (31%)
23	CLA	B	605	-	55,73,73	1.46	10 (18%)	61,113,113	2.27	18 (29%)
23	CLA	B	606	-	55,73,73	1.64	9 (16%)	61,113,113	2.00	16 (26%)
23	CLA	B	607	-	55,73,73	1.80	11 (20%)	61,113,113	2.17	14 (22%)
23	CLA	B	608	41	55,73,73	1.69	12 (21%)	61,113,113	1.93	17 (27%)
23	CLA	B	609	-	55,73,73	1.52	9 (16%)	61,113,113	2.44	17 (27%)
23	CLA	B	610	-	55,73,73	1.57	10 (18%)	61,113,113	2.09	15 (24%)
23	CLA	B	611	41	55,73,73	1.73	12 (21%)	61,113,113	2.12	17 (27%)
23	CLA	B	612	-	55,73,73	1.39	10 (18%)	61,113,113	2.38	18 (29%)
23	CLA	B	613	-	55,73,73	1.59	11 (20%)	61,113,113	1.95	16 (26%)
23	CLA	B	614	-	55,73,73	1.57	12 (21%)	61,113,113	1.72	15 (24%)
23	CLA	B	615	-	55,73,73	1.63	8 (14%)	61,113,113	2.01	14 (22%)
23	CLA	B	616	-	55,73,73	1.77	12 (21%)	61,113,113	2.00	16 (26%)
23	CLA	B	617	-	55,73,73	1.70	12 (21%)	61,113,113	2.03	13 (21%)
25	BCR	B	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.58	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	B	619	-	41,41,41	1.16	3 (7%)	56,56,56	1.21	7 (12%)
25	BCR	B	620	-	41,41,41	0.99	1 (2%)	56,56,56	1.68	9 (16%)
26	SQD	B	621	-	53,54,54	1.30	4 (7%)	61,65,65	2.19	11 (18%)
27	LMG	B	622	-	51,51,55	0.91	2 (3%)	59,59,63	1.61	10 (16%)
30	LMT	B	623	-	36,36,36	0.97	2 (5%)	47,47,47	1.43	8 (17%)
33	HTG	B	624	-	19,19,19	1.07	1 (5%)	22,24,24	1.52	5 (22%)
33	HTG	B	625	-	19,19,19	0.91	1 (5%)	22,24,24	1.66	4 (18%)
33	HTG	B	626	-	19,19,19	0.87	1 (5%)	22,24,24	2.25	2 (9%)
33	HTG	B	630	-	19,19,19	1.00	2 (10%)	22,24,24	1.80	2 (9%)
33	HTG	B	631	-	19,19,19	0.78	1 (5%)	22,24,24	2.38	3 (13%)
31	GOL	B	633	-	5,5,5	0.34	0	5,5,5	1.34	1 (20%)
31	GOL	B	634	-	5,5,5	0.80	0	5,5,5	0.65	0
31	GOL	B	635	-	5,5,5	0.52	0	5,5,5	1.02	0
31	GOL	B	636	-	5,5,5	0.42	0	5,5,5	0.67	0
31	GOL	B	637	-	5,5,5	0.47	0	5,5,5	1.04	0
31	GOL	B	638	-	5,5,5	0.46	0	5,5,5	0.82	0
23	CLA	C	501	-	55,73,73	1.68	12 (21%)	61,113,113	2.69	14 (22%)
23	CLA	C	502	-	55,73,73	1.70	11 (20%)	61,113,113	2.10	16 (26%)
23	CLA	C	503	-	55,73,73	1.79	11 (20%)	61,113,113	1.93	13 (21%)
23	CLA	C	504	41	55,73,73	1.70	11 (20%)	61,113,113	2.14	16 (26%)
23	CLA	C	505	-	55,73,73	1.73	12 (21%)	61,113,113	2.04	15 (24%)
23	CLA	C	506	-	55,73,73	1.79	11 (20%)	61,113,113	2.27	18 (29%)
23	CLA	C	507	41	55,73,73	1.93	13 (23%)	61,113,113	1.90	14 (22%)
23	CLA	C	508	-	55,73,73	2.02	14 (25%)	61,113,113	1.85	15 (24%)
23	CLA	C	509	-	55,73,73	1.72	12 (21%)	61,113,113	2.05	17 (27%)
23	CLA	C	510	-	55,73,73	1.75	12 (21%)	61,113,113	1.95	17 (27%)
23	CLA	C	511	3	55,73,73	1.83	14 (25%)	61,113,113	1.98	15 (24%)
23	CLA	C	512	-	55,73,73	1.82	12 (21%)	61,113,113	1.95	18 (29%)
23	CLA	C	513	-	55,73,73	1.90	11 (20%)	61,113,113	1.85	15 (24%)
25	BCR	C	514	-	41,41,41	0.87	0	56,56,56	1.30	8 (14%)
25	BCR	C	515	-	41,41,41	0.91	1 (2%)	56,56,56	1.46	4 (7%)
34	DGD	C	516	-	63,63,67	0.89	3 (4%)	77,77,81	1.39	13 (16%)
34	DGD	C	517	-	63,63,67	0.87	2 (3%)	77,77,81	1.05	4 (5%)
34	DGD	C	518	-	63,63,67	0.77	2 (3%)	77,77,81	1.31	9 (11%)
27	LMG	C	519	-	51,51,55	0.99	3 (5%)	59,59,63	1.49	9 (15%)
30	LMT	C	520	-	36,36,36	0.60	1 (2%)	47,47,47	1.53	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	HTG	C	521	-	19,19,19	0.84	1 (5%)	22,24,24	1.73	1 (4%)
33	HTG	C	522	-	19,19,19	0.93	1 (5%)	22,24,24	2.58	3 (13%)
31	GOL	C	524	-	5,5,5	0.33	0	5,5,5	1.55	1 (20%)
31	GOL	C	525	-	5,5,5	0.77	0	5,5,5	0.84	0
31	GOL	C	526	-	5,5,5	0.63	0	5,5,5	0.48	0
35	BCT	D	401	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	D	402	-	55,73,73	1.73	11 (20%)	61,113,113	2.31	24 (39%)
23	CLA	D	403	-	55,73,73	1.78	13 (23%)	61,113,113	1.86	17 (27%)
25	BCR	D	404	-	41,41,41	1.15	3 (7%)	56,56,56	2.07	20 (35%)
28	PL9	D	405	-	55,55,55	1.38	10 (18%)	68,69,69	1.71	15 (22%)
34	DGD	D	406	-	53,53,67	1.15	3 (5%)	60,61,81	1.40	8 (13%)
26	SQD	D	407	-	44,45,54	1.36	4 (9%)	52,56,65	2.45	15 (28%)
36	LHG	D	408	-	48,48,48	0.78	1 (2%)	49,54,54	1.50	6 (12%)
36	LHG	D	409	-	48,48,48	0.81	2 (4%)	49,54,54	1.13	5 (10%)
36	LHG	D	410	-	45,45,48	0.99	3 (6%)	46,51,54	1.02	3 (6%)
27	LMG	D	411	39	51,51,55	0.84	2 (3%)	59,59,63	1.05	2 (3%)
33	HTG	D	414	-	19,19,19	1.01	1 (5%)	22,24,24	1.39	1 (4%)
31	GOL	D	415	-	5,5,5	0.69	0	5,5,5	1.19	0
36	LHG	E	101	-	48,48,48	0.98	2 (4%)	49,54,54	0.96	3 (6%)
37	HEM	F	101	5,6	30,50,50	2.12	6 (20%)	24,82,82	2.88	9 (37%)
30	LMT	F	102	-	36,36,36	0.73	0	47,47,47	1.18	3 (6%)
38	RRX	H	101	-	42,42,42	1.08	3 (7%)	58,58,58	1.57	11 (18%)
34	DGD	H	102	-	63,63,67	1.09	3 (4%)	77,77,81	1.37	12 (15%)
30	LMT	J	102	-	24,24,36	0.81	1 (4%)	29,29,47	1.18	3 (10%)
25	BCR	K	101	-	41,41,41	0.87	0	56,56,56	1.69	13 (23%)
25	BCR	K	102	-	41,41,41	0.93	1 (2%)	56,56,56	1.69	11 (19%)
36	LHG	L	101	-	48,48,48	0.80	2 (4%)	49,54,54	1.52	7 (14%)
26	SQD	L	103	-	53,54,54	1.25	3 (5%)	61,65,65	2.10	11 (18%)
31	GOL	L	104	-	5,5,5	0.48	0	5,5,5	0.59	0
30	LMT	M	101	-	36,36,36	0.84	1 (2%)	47,47,47	1.30	6 (12%)
30	LMT	M	102	-	36,36,36	0.62	0	47,47,47	1.36	7 (14%)
40	SO4	O	302	-	4,4,4	0.67	0	6,6,6	0.35	0
33	HTG	O	303	-	19,19,19	1.10	2 (10%)	22,24,24	1.52	1 (4%)
31	GOL	O	304	-	5,5,5	0.50	0	5,5,5	0.58	0
25	BCR	T	101	-	41,41,41	0.87	0	56,56,56	1.62	13 (23%)
33	HTG	U	201	-	8,8,19	0.27	0	7,7,24	1.26	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	HEM	V	201	16	30,50,50	2.47	10 (33%)	24,82,82	2.76	10 (41%)
33	HTG	V	202	-	13,13,19	0.69	0	16,18,24	2.89	6 (37%)
31	GOL	V	203	-	5,5,5	0.97	0	5,5,5	0.81	0
31	GOL	V	204	-	5,5,5	0.29	0	5,5,5	0.37	0
31	GOL	V	205	-	5,5,5	0.61	0	5,5,5	0.32	0
27	LMG	Z	101	-	51,51,55	1.06	3 (5%)	59,59,63	1.37	7 (11%)
30	LMT	Z	102	-	36,36,36	0.65	1 (2%)	47,47,47	0.91	1 (2%)
26	SQD	a	401	-	53,54,54	1.45	3 (5%)	61,65,65	1.76	9 (14%)
30	LMT	a	402	-	36,36,36	0.74	1 (2%)	47,47,47	1.65	10 (21%)
20	OEX	a	404	1,3,41	0,15,15	0.00	-	0,32,32	0.00	-
35	BCT	a	408	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	a	409	-	55,73,73	1.65	9 (16%)	61,113,113	1.97	16 (26%)
23	CLA	a	410	41	55,73,73	1.61	11 (20%)	61,113,113	2.01	14 (22%)
23	CLA	a	411	41	55,73,73	1.58	12 (21%)	61,113,113	2.35	23 (37%)
24	PHO	a	412	-	67,69,69	1.83	14 (20%)	84,99,99	1.97	21 (25%)
24	PHO	a	413	-	67,69,69	1.93	16 (23%)	84,99,99	2.11	22 (26%)
23	CLA	a	414	-	55,73,73	1.68	8 (14%)	61,113,113	2.49	20 (32%)
25	BCR	a	415	-	41,41,41	1.20	3 (7%)	56,56,56	1.46	7 (12%)
26	SQD	a	416	-	53,54,54	1.32	3 (5%)	61,65,65	2.62	14 (22%)
36	LHG	a	417	-	39,39,48	1.13	2 (5%)	40,45,54	1.03	3 (7%)
27	LMG	a	418	-	51,51,55	0.90	2 (3%)	59,59,63	1.35	4 (6%)
28	PL9	a	419	-	55,55,55	0.92	3 (5%)	68,69,69	1.83	20 (29%)
31	GOL	a	422	-	5,5,5	0.64	0	5,5,5	0.74	0
31	GOL	a	423	-	5,5,5	0.58	0	5,5,5	0.52	0
31	GOL	a	424	-	5,5,5	0.61	0	5,5,5	0.76	0
33	HTG	b	601	-	19,19,19	0.93	2 (10%)	22,24,24	1.33	1 (4%)
33	HTG	b	602	-	19,19,19	0.72	0	22,24,24	1.33	2 (9%)
23	CLA	b	604	41	55,73,73	1.96	12 (21%)	61,113,113	2.10	15 (24%)
23	CLA	b	605	-	55,73,73	1.85	10 (18%)	61,113,113	2.08	16 (26%)
23	CLA	b	606	-	55,73,73	1.67	9 (16%)	61,113,113	2.40	18 (29%)
23	CLA	b	607	-	55,73,73	1.59	11 (20%)	61,113,113	2.25	19 (31%)
23	CLA	b	608	-	55,73,73	1.60	8 (14%)	61,113,113	2.38	19 (31%)
23	CLA	b	609	-	55,73,73	1.79	13 (23%)	61,113,113	1.88	15 (24%)
23	CLA	b	610	41	55,73,73	1.68	10 (18%)	61,113,113	1.84	16 (26%)
23	CLA	b	611	-	55,73,73	1.70	11 (20%)	61,113,113	2.00	13 (21%)
23	CLA	b	612	-	55,73,73	1.89	11 (20%)	61,113,113	2.00	16 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	b	613	41	55,73,73	1.81	11 (20%)	61,113,113	1.86	13 (21%)
23	CLA	b	614	-	55,73,73	1.62	8 (14%)	61,113,113	2.01	19 (31%)
23	CLA	b	615	-	55,73,73	1.56	9 (16%)	61,113,113	2.27	18 (29%)
23	CLA	b	616	-	55,73,73	1.71	9 (16%)	61,113,113	2.03	18 (29%)
23	CLA	b	617	-	55,73,73	1.61	10 (18%)	61,113,113	2.30	21 (34%)
23	CLA	b	618	-	55,73,73	1.77	11 (20%)	61,113,113	2.32	20 (32%)
23	CLA	b	619	-	55,73,73	1.85	13 (23%)	61,113,113	2.27	19 (31%)
25	BCR	b	620	-	41,41,41	1.04	2 (4%)	56,56,56	1.76	14 (25%)
25	BCR	b	621	-	41,41,41	1.14	3 (7%)	56,56,56	1.29	8 (14%)
25	BCR	b	622	-	41,41,41	0.96	1 (2%)	56,56,56	1.25	5 (8%)
27	LMG	b	623	-	51,51,55	0.83	2 (3%)	59,59,63	1.46	9 (15%)
30	LMT	b	624	-	25,25,36	0.72	1 (4%)	30,30,47	1.39	5 (16%)
30	LMT	b	625	-	24,24,36	0.53	0	29,29,47	1.26	4 (13%)
33	HTG	b	626	-	19,19,19	0.96	1 (5%)	22,24,24	1.38	4 (18%)
33	HTG	b	627	-	19,19,19	1.06	2 (10%)	22,24,24	1.99	1 (4%)
31	GOL	b	632	-	5,5,5	0.52	0	5,5,5	1.29	0
31	GOL	b	633	-	5,5,5	0.36	0	5,5,5	0.89	0
31	GOL	b	634	-	5,5,5	0.45	0	5,5,5	0.20	0
31	GOL	b	635	-	5,5,5	0.76	0	5,5,5	0.87	0
31	GOL	b	636	-	5,5,5	0.52	0	5,5,5	0.93	0
23	CLA	c	902	-	55,73,73	1.83	12 (21%)	61,113,113	2.06	15 (24%)
23	CLA	c	903	-	55,73,73	1.82	13 (23%)	61,113,113	2.04	19 (31%)
23	CLA	c	904	-	55,73,73	1.82	12 (21%)	61,113,113	1.85	18 (29%)
23	CLA	c	905	41	55,73,73	1.82	11 (20%)	61,113,113	1.93	18 (29%)
23	CLA	c	906	-	55,73,73	1.67	11 (20%)	61,113,113	2.06	19 (31%)
23	CLA	c	907	-	55,73,73	1.77	12 (21%)	61,113,113	1.91	16 (26%)
23	CLA	c	908	41	55,73,73	1.78	14 (25%)	61,113,113	2.29	19 (31%)
23	CLA	c	909	-	55,73,73	1.90	13 (23%)	61,113,113	1.65	13 (21%)
23	CLA	c	910	-	55,73,73	1.97	12 (21%)	61,113,113	1.99	18 (29%)
23	CLA	c	911	-	55,73,73	1.81	11 (20%)	61,113,113	1.74	14 (22%)
23	CLA	c	912	3	55,73,73	1.87	10 (18%)	61,113,113	2.12	18 (29%)
23	CLA	c	913	-	55,73,73	1.96	11 (20%)	61,113,113	1.86	16 (26%)
23	CLA	c	914	-	55,73,73	2.01	12 (21%)	61,113,113	1.81	12 (19%)
25	BCR	c	915	-	41,41,41	0.85	1 (2%)	56,56,56	1.29	5 (8%)
25	BCR	c	916	-	41,41,41	0.95	1 (2%)	56,56,56	1.39	7 (12%)
34	DGD	c	917	-	63,63,67	0.88	3 (4%)	77,77,81	1.30	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DGD	c	918	-	63,63,67	0.97	4 (6%)	77,77,81	1.25	10 (12%)
34	DGD	c	919	-	63,63,67	1.03	6 (9%)	77,77,81	1.39	11 (14%)
27	LMG	c	920	-	51,51,55	1.08	4 (7%)	59,59,63	1.29	8 (13%)
27	LMG	c	921	-	51,51,55	1.06	3 (5%)	59,59,63	1.27	6 (10%)
30	LMT	c	922	-	36,36,36	0.73	1 (2%)	47,47,47	1.04	4 (8%)
33	HTG	c	923	-	19,19,19	0.94	2 (10%)	22,24,24	1.97	1 (4%)
33	HTG	c	924	-	19,19,19	0.94	1 (5%)	22,24,24	2.60	5 (22%)
31	GOL	c	927	-	5,5,5	0.59	0	5,5,5	0.43	0
31	GOL	c	928	-	5,5,5	0.27	0	5,5,5	0.77	0
31	GOL	c	929	-	5,5,5	0.48	0	5,5,5	0.79	0
31	GOL	c	930	-	5,5,5	0.41	0	5,5,5	0.68	0
33	HTG	d	401	-	19,19,19	1.01	2 (10%)	22,24,24	1.73	2 (9%)
23	CLA	d	402	-	55,73,73	1.62	7 (12%)	61,113,113	2.33	17 (27%)
23	CLA	d	403	-	55,73,73	1.82	13 (23%)	61,113,113	2.16	16 (26%)
25	BCR	d	404	-	41,41,41	0.99	3 (7%)	56,56,56	1.82	15 (26%)
28	PL9	d	405	-	55,55,55	1.37	9 (16%)	68,69,69	1.70	14 (20%)
34	DGD	d	406	-	50,50,67	1.16	3 (6%)	58,58,81	1.37	11 (18%)
36	LHG	d	407	-	48,48,48	0.78	2 (4%)	49,54,54	1.44	6 (12%)
36	LHG	d	408	-	48,48,48	0.77	2 (4%)	49,54,54	1.32	8 (16%)
36	LHG	d	409	-	48,48,48	0.90	3 (6%)	49,54,54	1.07	4 (8%)
27	LMG	d	410	39	51,51,55	0.98	3 (5%)	59,59,63	1.15	8 (13%)
37	HEM	f	101	5,6	30,50,50	2.00	7 (23%)	24,82,82	3.07	12 (50%)
26	SQD	f	102	-	30,32,54	1.51	3 (10%)	33,36,65	1.95	7 (21%)
31	GOL	f	104	32	5,5,5	0.49	0	5,5,5	0.42	0
38	RRX	h	101	-	42,42,42	0.94	0	58,58,58	1.30	8 (13%)
34	DGD	h	102	-	63,63,67	0.96	3 (4%)	77,77,81	1.29	9 (11%)
31	GOL	h	103	-	5,5,5	0.32	0	5,5,5	0.27	0
25	BCR	k	101	-	41,41,41	0.84	1 (2%)	56,56,56	1.48	10 (17%)
25	BCR	k	102	-	41,41,41	0.97	2 (4%)	56,56,56	1.31	4 (7%)
36	LHG	l	101	-	48,48,48	0.82	2 (4%)	49,54,54	1.10	5 (10%)
31	GOL	l	102	-	5,5,5	0.45	0	5,5,5	1.01	0
30	LMT	m	101	-	36,36,36	0.73	0	47,47,47	1.43	9 (19%)
30	LMT	m	102	-	36,36,36	0.71	1 (2%)	47,47,47	1.17	3 (6%)
25	BCR	t	101	-	41,41,41	0.99	2 (4%)	56,56,56	1.85	13 (23%)
30	LMT	t	102	-	24,24,36	0.66	0	29,29,47	1.43	4 (13%)
33	HTG	u	201	-	10,13,19	0.75	1 (10%)	8,14,24	3.03	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	HEM	v	201	16	30,50,50	2.54	11 (36%)	24,82,82	2.58	10 (41%)
31	GOL	v	202	-	5,5,5	0.56	0	5,5,5	0.47	0
31	GOL	v	203	-	5,5,5	0.71	0	5,5,5	0.45	0
31	GOL	v	204	-	5,5,5	0.32	0	5,5,5	0.60	0
30	LMT	z	101	-	32,32,36	0.69	1 (3%)	42,42,47	1.01	3 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	OEX	A	401	1,3,41	-	0/0/68/68	0/0/6/6
23	CLA	A	405	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	A	406	41	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	A	407	41	2/2/20/25	0/37/135/135	0/0/9/9
24	PHO	A	408	-	-	0/53/103/103	0/1/6/6
24	PHO	A	409	-	-	0/53/103/103	0/1/6/6
23	CLA	A	410	-	1/1/20/25	0/37/135/135	0/0/9/9
25	BCR	A	411	-	-	0/29/63/63	0/2/2/2
26	SQD	A	412	-	-	0/49/69/69	0/1/1/1
27	LMG	A	413	-	-	0/46/66/70	0/1/1/1
28	PL9	A	414	-	-	0/53/73/73	0/1/1/1
26	SQD	A	418	-	-	0/49/69/69	0/1/1/1
30	LMT	A	419	-	-	0/21/61/61	0/2/2/2
31	GOL	A	421	-	-	0/4/4/4	0/0/0/0
31	GOL	A	422	-	-	0/4/4/4	0/0/0/0
31	GOL	A	423	32	-	0/4/4/4	0/0/0/0
23	CLA	B	602	41	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	B	603	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	607	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	608	41	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	609	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	B	610	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	B	611	41	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	612	-	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	617	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
26	SQD	B	621	-	-	0/49/69/69	0/1/1/1
27	LMG	B	622	-	-	0/46/66/70	0/1/1/1
30	LMT	B	623	-	-	0/21/61/61	0/2/2/2
33	HTG	B	624	-	-	0/10/30/30	0/1/1/1
33	HTG	B	625	-	-	0/10/30/30	0/1/1/1
33	HTG	B	626	-	-	0/10/30/30	0/1/1/1
33	HTG	B	630	-	-	0/10/30/30	0/1/1/1
33	HTG	B	631	-	-	0/10/30/30	0/1/1/1
31	GOL	B	633	-	-	0/4/4/4	0/0/0/0
31	GOL	B	634	-	-	0/4/4/4	0/0/0/0
31	GOL	B	635	-	-	0/4/4/4	0/0/0/0
31	GOL	B	636	-	-	0/4/4/4	0/0/0/0
31	GOL	B	637	-	-	0/4/4/4	0/0/0/0
31	GOL	B	638	-	-	0/4/4/4	0/0/0/0
23	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	502	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	504	41	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	505	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	C	506	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	C	507	41	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	508	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	511	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	512	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	513	-	1/1/20/25	0/37/135/135	0/0/9/9
25	BCR	C	514	-	-	0/29/63/63	0/2/2/2
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
34	DGD	C	516	-	-	0/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	DGD	C	517	-	-	0/51/91/95	0/2/2/2
34	DGD	C	518	-	-	0/51/91/95	0/2/2/2
27	LMG	C	519	-	-	0/46/66/70	0/1/1/1
30	LMT	C	520	-	-	0/21/61/61	0/2/2/2
33	HTG	C	521	-	-	0/10/30/30	0/1/1/1
33	HTG	C	522	-	-	0/10/30/30	0/1/1/1
31	GOL	C	524	-	-	0/4/4/4	0/0/0/0
31	GOL	C	525	-	-	0/4/4/4	0/0/0/0
31	GOL	C	526	-	-	0/4/4/4	0/0/0/0
35	BCT	D	401	21	-	0/0/0/0	0/0/0/0
23	CLA	D	402	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	D	403	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	D	404	-	-	0/29/63/63	0/2/2/2
28	PL9	D	405	-	-	0/53/73/73	0/1/1/1
34	DGD	D	406	-	-	0/47/68/95	0/1/1/2
26	SQD	D	407	-	-	0/40/60/69	0/1/1/1
36	LHG	D	408	-	-	0/53/53/53	0/0/0/0
36	LHG	D	409	-	-	0/53/53/53	0/0/0/0
36	LHG	D	410	-	-	0/50/50/53	0/0/0/0
27	LMG	D	411	39	-	0/46/66/70	0/1/1/1
33	HTG	D	414	-	-	0/10/30/30	0/1/1/1
31	GOL	D	415	-	-	0/4/4/4	0/0/0/0
36	LHG	E	101	-	-	0/53/53/53	0/0/0/0
37	HEM	F	101	5,6	-	0/10/54/54	0/0/8/8
30	LMT	F	102	-	-	0/21/61/61	0/2/2/2
38	RRX	H	101	-	-	0/29/65/65	0/2/2/2
34	DGD	H	102	-	-	0/51/91/95	0/2/2/2
30	LMT	J	102	-	-	0/15/35/61	0/1/1/2
25	BCR	K	101	-	-	0/29/63/63	0/2/2/2
25	BCR	K	102	-	-	0/29/63/63	0/2/2/2
36	LHG	L	101	-	-	0/53/53/53	0/0/0/0
26	SQD	L	103	-	-	0/49/69/69	0/1/1/1
31	GOL	L	104	-	-	0/4/4/4	0/0/0/0
30	LMT	M	101	-	-	0/21/61/61	0/2/2/2
30	LMT	M	102	-	-	0/21/61/61	0/2/2/2
40	SO4	O	302	-	-	0/0/0/0	0/0/0/0
33	HTG	O	303	-	-	0/10/30/30	0/1/1/1
31	GOL	O	304	-	-	0/4/4/4	0/0/0/0
25	BCR	T	101	-	-	0/29/63/63	0/2/2/2
33	HTG	U	201	-	-	0/6/6/30	0/0/0/1
37	HEM	V	201	16	-	0/10/54/54	0/0/8/8
33	HTG	V	202	-	-	0/3/24/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GOL	V	203	-	-	0/4/4/4	0/0/0/0
31	GOL	V	204	-	-	0/4/4/4	0/0/0/0
31	GOL	V	205	-	-	0/4/4/4	0/0/0/0
27	LMG	Z	101	-	-	0/46/66/70	0/1/1/1
30	LMT	Z	102	-	-	0/21/61/61	0/2/2/2
26	SQD	a	401	-	-	0/49/69/69	0/1/1/1
30	LMT	a	402	-	-	0/21/61/61	0/2/2/2
20	OEX	a	404	1,3,41	-	0/0/68/68	0/0/6/6
35	BCT	a	408	21	-	0/0/0/0	0/0/0/0
23	CLA	a	409	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	a	410	41	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	a	411	41	2/2/20/25	0/37/135/135	0/0/9/9
24	PHO	a	412	-	-	0/53/103/103	0/1/6/6
24	PHO	a	413	-	-	0/53/103/103	0/1/6/6
23	CLA	a	414	-	1/1/20/25	0/37/135/135	0/0/9/9
25	BCR	a	415	-	-	0/29/63/63	0/2/2/2
26	SQD	a	416	-	-	0/49/69/69	0/1/1/1
36	LHG	a	417	-	-	0/44/44/53	0/0/0/0
27	LMG	a	418	-	-	0/46/66/70	0/1/1/1
28	PL9	a	419	-	-	0/53/73/73	0/1/1/1
31	GOL	a	422	-	-	0/4/4/4	0/0/0/0
31	GOL	a	423	-	-	0/4/4/4	0/0/0/0
31	GOL	a	424	-	-	0/4/4/4	0/0/0/0
33	HTG	b	601	-	-	0/10/30/30	0/1/1/1
33	HTG	b	602	-	-	0/10/30/30	0/1/1/1
23	CLA	b	604	41	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	609	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	610	41	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	611	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	b	612	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	b	613	41	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	614	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	618	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	619	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	b	620	-	-	0/29/63/63	0/2/2/2
25	BCR	b	621	-	-	0/29/63/63	0/2/2/2
25	BCR	b	622	-	-	0/29/63/63	0/2/2/2
27	LMG	b	623	-	-	0/46/66/70	0/1/1/1
30	LMT	b	624	-	-	0/17/37/61	0/1/1/2
30	LMT	b	625	-	-	0/15/35/61	0/1/1/2
33	HTG	b	626	-	-	0/10/30/30	0/1/1/1
33	HTG	b	627	-	-	0/10/30/30	0/1/1/1
31	GOL	b	632	-	-	0/4/4/4	0/0/0/0
31	GOL	b	633	-	-	0/4/4/4	0/0/0/0
31	GOL	b	634	-	-	0/4/4/4	0/0/0/0
31	GOL	b	635	-	-	0/4/4/4	0/0/0/0
31	GOL	b	636	-	-	0/4/4/4	0/0/0/0
23	CLA	c	902	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	903	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	904	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	c	905	41	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	906	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	c	907	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	c	908	41	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	909	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	c	910	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	911	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	912	3	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	c	913	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	914	-	2/2/20/25	0/37/135/135	0/0/9/9
25	BCR	c	915	-	-	0/29/63/63	0/2/2/2
25	BCR	c	916	-	-	0/29/63/63	0/2/2/2
34	DGD	c	917	-	-	0/51/91/95	0/2/2/2
34	DGD	c	918	-	-	0/51/91/95	0/2/2/2
34	DGD	c	919	-	-	0/51/91/95	0/2/2/2
27	LMG	c	920	-	-	0/46/66/70	0/1/1/1
27	LMG	c	921	-	-	0/46/66/70	0/1/1/1
30	LMT	c	922	-	-	0/21/61/61	0/2/2/2
33	HTG	c	923	-	-	0/10/30/30	0/1/1/1
33	HTG	c	924	-	-	0/10/30/30	0/1/1/1
31	GOL	c	927	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GOL	c	928	-	-	0/4/4/4	0/0/0/0
31	GOL	c	929	-	-	0/4/4/4	0/0/0/0
31	GOL	c	930	-	-	0/4/4/4	0/0/0/0
33	HTG	d	401	-	-	0/10/30/30	0/1/1/1
23	CLA	d	402	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	d	403	-	1/1/20/25	0/37/135/135	0/0/9/9
25	BCR	d	404	-	-	0/29/63/63	0/2/2/2
28	PL9	d	405	-	-	0/53/73/73	0/1/1/1
34	DGD	d	406	-	-	0/44/64/95	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	LMG	d	410	39	-	0/46/66/70	0/1/1/1
37	HEM	f	101	5,6	-	0/10/54/54	0/0/8/8
26	SQD	f	102	-	-	2/33/33/69	0/0/0/1
31	GOL	f	104	32	-	0/4/4/4	0/0/0/0
38	RRX	h	101	-	-	0/29/65/65	0/2/2/2
34	DGD	h	102	-	-	0/51/91/95	0/2/2/2
31	GOL	h	103	-	-	0/4/4/4	0/0/0/0
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
25	BCR	k	102	-	-	0/29/63/63	0/2/2/2
36	LHG	l	101	-	-	0/53/53/53	0/0/0/0
31	GOL	l	102	-	-	0/4/4/4	0/0/0/0
30	LMT	m	101	-	-	0/21/61/61	0/2/2/2
30	LMT	m	102	-	-	0/21/61/61	0/2/2/2
25	BCR	t	101	-	-	0/29/63/63	0/2/2/2
30	LMT	t	102	-	-	0/15/35/61	0/1/1/2
33	HTG	u	201	-	-	0/12/14/30	0/0/0/1
37	HEM	v	201	16	-	0/10/54/54	0/0/8/8
31	GOL	v	202	-	-	0/4/4/4	0/0/0/0
31	GOL	v	203	-	-	0/4/4/4	0/0/0/0
31	GOL	v	204	-	-	0/4/4/4	0/0/0/0
30	LMT	z	101	-	-	0/15/55/61	0/2/2/2

The worst 5 of 1061 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	v	201	HEM	C3B-C4B	-8.05	1.44	1.51
26	A	412	SQD	C6-S	-7.78	1.66	1.77
37	F	101	HEM	C3B-C4B	-7.41	1.45	1.51
26	a	416	SQD	C6-S	-7.37	1.67	1.77
37	V	201	HEM	C3B-C4B	-7.27	1.45	1.51

The worst 5 of 2018 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	501	CLA	O2D-CGD-O1D	-9.91	103.33	123.79
23	c	907	CLA	CHD-C4C-C3C	-6.86	114.33	124.94
26	A	412	SQD	O7-S-C6	-6.60	101.37	106.94
23	b	619	CLA	CHD-C4C-C3C	-6.57	114.78	124.94
23	C	502	CLA	CHD-C4C-C3C	-6.54	114.83	124.94

5 of 168 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	c	914	CLA	NC
23	c	914	CLA	NA
23	A	406	CLA	NA
23	d	402	CLA	ND
23	d	402	CLA	NA

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	f	102	SQD	C7-O47-C45-C44
26	f	102	SQD	C45-O47-C7-O49

There are no ring outliers.

83 monomers are involved in 254 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	405	CLA	4	0
23	A	406	CLA	4	0
23	A	407	CLA	1	0
24	A	408	PHO	2	0
24	A	409	PHO	3	0
23	A	410	CLA	3	0
25	A	411	BCR	2	0
26	A	412	SQD	4	0
27	A	413	LMG	3	0
28	A	414	PL9	10	0
26	A	418	SQD	1	0
31	A	422	GOL	1	0
31	A	423	GOL	3	0
23	B	602	CLA	1	0
23	B	604	CLA	3	0
23	B	605	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	606	CLA	7	0
23	B	607	CLA	5	0
23	B	608	CLA	3	0
23	B	609	CLA	4	0
23	B	610	CLA	1	0
23	B	611	CLA	4	0
23	B	612	CLA	5	0
23	B	613	CLA	6	0
23	B	614	CLA	4	0
23	B	615	CLA	7	0
23	B	616	CLA	4	0
23	B	617	CLA	11	0
25	B	619	BCR	3	0
25	B	620	BCR	2	0
26	B	621	SQD	5	0
27	B	622	LMG	4	0
30	B	623	LMT	4	0
33	B	626	HTG	2	0
33	B	631	HTG	1	0
31	B	633	GOL	2	0
31	B	635	GOL	1	0
23	C	501	CLA	4	0
23	C	502	CLA	2	0
23	C	503	CLA	3	0
23	C	504	CLA	4	0
23	C	505	CLA	1	0
23	C	506	CLA	5	0
23	C	507	CLA	2	0
23	C	508	CLA	2	0
23	C	509	CLA	4	0
23	C	510	CLA	4	0
23	C	511	CLA	5	0
23	C	512	CLA	3	0
23	C	513	CLA	3	0
25	C	514	BCR	1	0
25	C	515	BCR	4	0
34	C	517	DGD	2	0
27	C	519	LMG	2	0
30	C	520	LMT	4	0
33	C	521	HTG	1	0
31	C	524	GOL	4	0
23	D	402	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	D	403	CLA	6	0
25	D	404	BCR	5	0
34	D	406	DGD	9	0
26	D	407	SQD	3	0
36	D	408	LHG	2	0
36	D	409	LHG	9	0
36	D	410	LHG	13	0
27	D	411	LMG	2	0
33	D	414	HTG	2	0
31	D	415	GOL	3	0
36	E	101	LHG	3	0
37	F	101	HEM	4	0
38	H	101	RRX	4	0
34	H	102	DGD	1	0
30	J	102	LMT	1	0
25	K	101	BCR	5	0
25	K	102	BCR	4	0
36	L	101	LHG	2	0
26	L	103	SQD	5	0
31	L	104	GOL	1	0
30	M	101	LMT	3	0
25	T	101	BCR	9	0
33	U	201	HTG	1	0
37	V	201	HEM	1	0
30	Z	102	LMT	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	334/344 (97%)	-0.14	5 (1%) 76 79	16, 23, 46, 69	0
1	a	334/344 (97%)	0.03	14 (4%) 40 44	19, 24, 50, 76	0
2	B	504/504 (100%)	0.11	39 (7%) 16 18	18, 27, 54, 88	0
2	b	501/504 (99%)	0.14	47 (9%) 11 12	20, 29, 58, 119	0
3	C	451/455 (99%)	-0.07	14 (3%) 52 56	21, 31, 46, 81	0
3	c	455/455 (100%)	0.18	26 (5%) 27 30	23, 34, 48, 79	0
4	D	340/342 (99%)	-0.20	7 (2%) 67 70	17, 24, 40, 70	0
4	d	340/342 (99%)	-0.16	6 (1%) 71 74	19, 26, 45, 80	0
5	E	81/83 (97%)	0.97	18 (22%) 1 1	27, 40, 62, 82	0
5	e	79/83 (95%)	1.24	23 (29%) 1 0	32, 44, 72, 82	0
6	F	34/44 (77%)	0.23	5 (14%) 3 3	26, 34, 63, 74	0
6	f	32/44 (72%)	0.38	3 (9%) 11 12	29, 37, 76, 86	0
7	H	63/63 (100%)	-0.05	1 (1%) 74 78	24, 33, 43, 70	0
7	h	63/63 (100%)	0.41	5 (7%) 15 17	27, 37, 51, 81	0
8	I	35/38 (92%)	-0.08	0 100 100	27, 34, 64, 86	0
8	i	37/38 (97%)	0.24	2 (5%) 29 33	26, 34, 71, 83	0
9	J	36/40 (90%)	0.18	4 (11%) 7 8	26, 38, 65, 79	0
9	j	39/40 (97%)	0.64	8 (20%) 1 1	30, 42, 68, 84	0
10	K	37/37 (100%)	-0.14	0 100 100	32, 38, 47, 63	0
10	k	37/37 (100%)	0.34	3 (8%) 15 16	36, 42, 55, 69	0
11	L	37/37 (100%)	-0.10	3 (8%) 15 16	17, 22, 65, 75	0
11	l	37/37 (100%)	0.16	2 (5%) 29 33	19, 23, 64, 95	0
12	M	32/36 (88%)	-0.14	1 (3%) 52 56	21, 24, 40, 56	0
12	m	33/36 (91%)	0.03	2 (6%) 25 27	20, 25, 48, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	244/244 (100%)	0.34	35 (14%) 4 4	18, 33, 66, 120	0
13	o	241/244 (98%)	0.42	40 (16%) 2 2	20, 35, 71, 87	0
14	T	29/32 (90%)	0.03	1 (3%) 49 52	19, 23, 49, 85	0
14	t	29/32 (90%)	0.03	1 (3%) 49 52	20, 23, 47, 72	0
15	U	97/104 (93%)	-0.10	0 100 100	23, 30, 52, 58	0
15	u	97/104 (93%)	-0.33	1 (1%) 84 86	24, 30, 40, 66	0
16	V	137/137 (100%)	-0.35	0 100 100	22, 28, 43, 51	0
16	v	137/137 (100%)	0.48	14 (10%) 9 10	26, 37, 52, 72	0
17	Y	27/30 (90%)	1.10	5 (18%) 2 2	37, 47, 70, 77	0
17	y	28/30 (93%)	1.21	7 (25%) 1 1	45, 55, 73, 77	0
18	X	38/40 (95%)	0.74	7 (18%) 2 2	32, 39, 65, 69	0
18	x	38/40 (95%)	0.97	9 (23%) 1 1	34, 42, 83, 94	0
19	Z	62/62 (100%)	1.51	20 (32%) 1 0	37, 46, 75, 92	0
19	z	60/62 (96%)	2.02	26 (43%) 0 0	47, 57, 88, 95	0
All	All	5235/5344 (97%)	0.15	404 (7%) 16 18	16, 30, 59, 120	0

The worst 5 of 404 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	494	GLY	8.4
2	b	496	TYR	8.2
18	x	37	VAL	8.0
13	o	246	ALA	7.5
13	O	60	ARG	7.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	HSK	D	336[B]	11/12	0.98	0.09	-	23,26,27,29	8
14	FME	T	1	10/11	0.97	0.08	-	24,27,43,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
12	FME	M	1	10/11	0.96	0.11	-	27,34,51,59	0
14	FME	t	1	10/11	0.95	0.09	-	20,23,41,50	0
8	FME	I	1	10/11	0.97	0.12	-	27,34,38,39	0
4	HSK	D	336[A]	10/12	0.98	0.09	-	26,28,31,34	7
12	FME	m	1	10/11	0.92	0.12	-	31,38,54,60	0
8	FME	i	1	10/11	0.98	0.11	-	30,32,37,39	0
4	HSK	d	336[A]	10/12	0.96	0.10	-	30,33,40,44	7
4	HSK	d	336[B]	11/12	0.96	0.10	-	30,31,37,38	8

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
29	UNL	T	102	13/-	0.78	0.54	33.26	66,70,83,87	0
29	UNL	A	420	4/-	0.93	0.53	32.42	64,66,66,66	0
29	UNL	t	103	16/-	0.71	0.46	19.49	63,74,94,95	0
29	UNL	a	403	6/-	0.92	0.42	16.55	57,62,66,66	0
31	GOL	b	633	6/6	0.93	0.24	11.67	41,46,49,52	0
40	SO4	O	302	5/5	0.82	0.29	11.42	78,87,95,105	0
31	GOL	D	415	6/6	0.96	0.19	9.24	35,36,42,46	0
30	LMT	b	625	24/35	0.78	0.25	9.04	35,61,99,100	0
29	UNL	d	411	16/-	0.86	0.32	8.70	39,49,63,66	0
29	UNL	b	628	36/-	0.82	0.26	8.33	44,65,101,106	0
33	HTG	b	602	19/19	0.67	0.27	7.84	50,93,111,117	0
31	GOL	L	104	6/6	0.91	0.26	7.25	44,52,54,55	0
34	DGD	D	406	53/66	0.54	0.29	6.99	53,77,92,103	0
31	GOL	l	102	6/6	0.89	0.38	6.94	37,55,57,57	0
29	UNL	D	413	16/-	0.89	0.26	6.87	39,47,65,65	0
33	HTG	d	401	19/19	0.56	0.30	6.49	55,101,111,114	0
31	GOL	a	422	6/6	0.94	0.10	6.47	30,38,44,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
29	UNL	C	523	34/-	0.69	0.28	6.33	52,77,88,93	0
29	UNL	b	631	16/-	0.72	0.23	5.73	59,66,77,79	0
30	LMT	J	102	24/35	0.74	0.19	5.52	45,55,79,83	0
29	UNL	i	103	13/-	0.65	0.29	5.49	58,65,76,78	0
31	GOL	C	526	6/6	0.89	0.14	5.46	38,43,51,57	0
29	UNL	b	630	16/-	0.75	0.39	5.16	51,62,73,74	0
34	DGD	d	406	50/66	0.62	0.26	5.05	56,75,94,97	0
30	LMT	F	102	35/35	0.71	0.36	5.00	53,84,91,96	0
30	LMT	t	102	24/35	0.78	0.26	5.00	33,55,94,95	0
31	GOL	V	204	6/6	0.95	0.26	4.95	39,52,59,59	0
29	UNL	E	103	12/-	0.60	0.29	4.84	65,73,83,88	0
31	GOL	c	928	6/6	0.94	0.22	4.74	42,51,54,54	0
29	UNL	B	629	14/-	0.66	0.27	4.65	61,70,89,90	0
31	GOL	a	423	6/6	0.96	0.14	4.44	33,34,35,45	0
33	HTG	V	202	13/19	0.92	0.26	4.26	43,48,76,84	0
29	UNL	E	102	15/-	0.62	0.23	4.24	57,64,83,83	0
28	PL9	A	414	55/55	0.76	0.26	4.13	47,66,93,96	0
33	HTG	C	522	19/19	0.75	0.34	4.13	50,79,92,94	0
26	SQD	B	621	54/54	0.63	0.27	3.80	48,65,108,109	0
29	UNL	B	632	16/-	0.78	0.32	3.77	50,59,73,73	0
30	LMT	M	101	35/35	0.68	0.24	3.69	43,61,77,90	0
31	GOL	f	104	6/6	0.91	0.33	3.65	46,51,51,54	0
27	LMG	A	413	51/55	0.79	0.24	3.64	42,57,76,78	0
36	LHG	d	407	49/49	0.94	0.23	3.56	27,36,46,49	0
29	UNL	j	102	16/-	0.80	0.17	3.56	52,61,69,69	0
29	UNL	D	412	40/-	0.79	0.20	3.53	39,60,96,99	0
26	SQD	L	103	54/54	0.71	0.24	3.49	43,64,89,96	0
23	CLA	B	602	65/65	0.92	0.18	3.47	29,41,78,95	0
26	SQD	a	401	54/54	0.76	0.18	3.43	45,59,85,90	0
31	GOL	V	205	6/6	0.97	0.23	3.39	33,36,37,41	0
31	GOL	A	421	6/6	0.96	0.13	3.33	30,37,38,41	0
31	GOL	a	424	6/6	0.85	0.19	3.31	42,56,59,74	0
26	SQD	A	418	54/54	0.81	0.19	3.21	42,59,81,86	0
31	GOL	A	423	6/6	0.98	0.25	3.17	39,43,45,53	0
33	HTG	u	201	14/19	0.83	0.25	3.12	46,64,90,96	0
31	GOL	B	633	6/6	0.95	0.13	3.01	34,39,47,52	0
33	HTG	b	626	19/19	0.96	0.17	2.98	29,40,73,75	0
27	LMG	c	921	51/55	0.74	0.27	2.96	38,80,95,111	0
33	HTG	D	414	19/19	0.70	0.31	2.92	66,93,106,107	0
39	MG	j	101	1/1	0.99	0.16	2.88	35,35,35,35	0
34	DGD	C	518	62/66	0.96	0.15	2.86	20,30,68,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
25	BCR	T	101	40/40	0.96	0.16	2.77	24,32,47,53	0
31	GOL	b	632	6/6	0.95	0.11	2.74	35,42,46,47	0
29	UNL	x	101	16/-	0.91	0.16	2.72	36,45,70,73	0
29	UNL	z	102	16/-	0.76	0.22	2.71	51,70,89,92	0
23	CLA	b	604	65/65	0.93	0.17	2.66	34,47,73,81	0
30	LMT	A	419	35/35	0.87	0.15	2.63	37,56,73,94	0
28	PL9	a	419	55/55	0.75	0.23	2.58	52,74,98,109	0
27	LMG	D	411	51/55	0.93	0.17	2.55	23,35,91,99	0
25	BCR	B	619	40/40	0.95	0.19	2.43	19,26,42,45	0
30	LMT	C	520	35/35	0.83	0.30	2.43	52,71,83,89	0
29	UNL	A	417	13/-	0.81	0.35	2.38	56,59,66,66	0
29	UNL	X	101	16/-	0.91	0.12	2.37	34,39,58,60	0
36	LHG	D	410	46/49	0.97	0.14	2.33	24,32,82,87	0
31	GOL	A	422	6/6	0.89	0.13	2.33	42,55,58,67	0
31	GOL	C	524	6/6	0.91	0.17	2.29	36,45,47,53	0
33	HTG	U	201	9/19	0.79	0.23	2.25	54,59,82,98	0
25	BCR	D	404	40/40	0.96	0.16	2.21	24,29,55,57	0
30	LMT	m	102	35/35	0.76	0.19	2.21	41,54,72,84	0
30	LMT	c	922	35/35	0.78	0.32	2.13	61,73,85,90	0
27	LMG	d	410	51/55	0.91	0.12	2.13	29,36,80,91	0
31	GOL	c	930	6/6	0.95	0.21	2.11	49,54,57,59	0
25	BCR	B	618	40/40	0.96	0.15	2.08	20,26,29,30	0
36	LHG	D	408	49/49	0.93	0.16	2.05	26,35,45,45	0
27	LMG	Z	101	51/55	0.73	0.27	1.99	41,76,102,113	0
30	LMT	Z	102	35/35	0.78	0.28	1.97	41,87,102,107	0
26	SQD	D	407	45/54	0.82	0.28	1.96	50,78,94,101	0
34	DGD	C	516	62/66	0.94	0.20	1.96	22,32,85,87	0
30	LMT	a	402	35/35	0.84	0.17	1.93	37,54,69,80	0
29	UNL	J	104	12/-	0.85	0.17	1.87	53,65,72,74	0
33	HTG	c	924	19/19	0.78	0.41	1.86	53,85,97,100	0
23	CLA	C	505	65/65	0.96	0.14	1.86	26,31,47,51	0
27	LMG	a	418	51/55	0.75	0.22	1.84	43,60,68,73	0
29	UNL	a	421	10/-	0.89	0.29	1.80	53,57,61,64	0
25	BCR	C	515	40/40	0.96	0.14	1.80	28,34,41,44	0
28	PL9	d	405	55/55	0.95	0.16	1.78	19,25,30,34	0
33	HTG	b	601	19/19	0.87	0.14	1.78	43,51,62,68	0
31	GOL	B	638	6/6	0.93	0.10	1.78	35,47,49,53	0
30	LMT	M	102	35/35	0.64	0.24	1.71	35,52,60,63	0
30	LMT	b	624	25/35	0.71	0.21	1.70	51,71,94,98	0
36	LHG	d	409	49/49	0.96	0.16	1.69	27,32,85,91	0
27	LMG	B	622	51/55	0.87	0.18	1.67	28,37,53,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	A	407	65/65	0.97	0.16	1.66	18,21,80,92	0
25	BCR	A	411	40/40	0.97	0.12	1.64	21,26,33,36	0
36	LHG	a	417	40/49	0.69	0.25	1.64	60,109,148,151	0
29	UNL	a	420	40/-	0.57	0.33	1.64	53,72,88,94	0
34	DGD	c	919	62/66	0.91	0.14	1.64	25,35,60,71	0
25	BCR	b	621	40/40	0.96	0.20	1.63	21,28,43,46	0
33	HTG	B	630	19/19	0.84	0.15	1.60	39,52,66,79	0
31	GOL	b	636	6/6	0.87	0.12	1.55	45,56,58,60	0
23	CLA	C	509	65/65	0.96	0.13	1.54	27,31,47,51	0
23	CLA	B	611	65/65	0.96	0.14	1.52	19,25,34,39	0
26	SQD	a	416	54/54	0.91	0.17	1.50	37,55,88,90	0
36	LHG	L	101	49/49	0.94	0.14	1.49	22,31,44,49	0
29	UNL	j	103	12/-	0.71	0.25	1.47	55,65,70,71	0
25	BCR	b	620	40/40	0.97	0.16	1.47	23,27,33,33	0
24	PHO	a	413	64/64	0.97	0.13	1.46	19,25,30,35	0
31	GOL	c	927	6/6	0.86	0.13	1.46	43,53,60,68	0
36	LHG	d	408	49/49	0.95	0.14	1.45	22,27,42,47	0
34	DGD	H	102	62/66	0.91	0.20	1.43	24,31,40,45	0
23	CLA	C	508	65/65	0.96	0.13	1.43	24,29,73,81	0
31	GOL	B	636	6/6	0.95	0.14	1.42	33,43,47,56	0
23	CLA	b	611	65/65	0.98	0.18	1.42	22,27,39,43	0
27	LMG	b	623	51/55	0.88	0.19	1.41	30,39,52,63	0
31	GOL	b	635	6/6	0.81	0.14	1.40	40,43,46,48	0
25	BCR	d	404	40/40	0.94	0.10	1.36	25,33,56,58	0
36	LHG	l	101	49/49	0.92	0.17	1.36	22,31,47,57	0
29	UNL	A	415	36/-	0.60	0.25	1.36	58,67,75,79	0
23	CLA	c	914	65/65	0.90	0.15	1.35	38,53,90,98	0
36	LHG	D	409	49/49	0.96	0.12	1.29	22,28,40,44	0
23	CLA	A	410	65/65	0.96	0.11	1.26	20,24,99,105	0
31	GOL	C	525	6/6	0.98	0.15	1.26	26,26,27,29	0
34	DGD	C	517	62/66	0.94	0.14	1.23	22,31,78,92	0
23	CLA	b	614	65/65	0.97	0.17	1.23	20,24,36,45	0
30	LMT	z	101	32/35	0.80	0.24	1.20	46,85,90,100	0
34	DGD	h	102	62/66	0.88	0.18	1.18	27,35,45,52	0
23	CLA	c	909	65/65	0.97	0.18	1.17	25,30,82,98	0
33	HTG	B	625	19/19	0.94	0.15	1.14	31,38,71,75	0
23	CLA	B	608	65/65	0.97	0.14	1.10	17,20,34,37	0
36	LHG	E	101	49/49	0.82	0.21	1.08	50,80,94,97	0
23	CLA	C	503	65/65	0.96	0.12	1.07	26,31,38,39	0
27	LMG	c	920	51/55	0.82	0.23	1.07	30,65,100,104	0
33	HTG	b	627	19/19	0.74	0.34	1.06	53,94,104,105	0
31	GOL	v	204	6/6	0.95	0.25	1.06	46,50,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
23	CLA	a	411	65/65	0.98	0.14	1.05	18,23,106,117	0
31	GOL	V	203	6/6	0.95	0.15	1.03	26,32,36,38	0
26	SQD	A	412	54/54	0.94	0.14	1.03	35,54,71,74	0
23	CLA	c	911	65/65	0.97	0.22	1.02	24,30,41,45	0
23	CLA	a	410	65/65	0.98	0.13	1.01	17,20,28,34	0
24	PHO	A	409	64/64	0.97	0.14	1.01	19,22,29,37	0
23	CLA	c	910	65/65	0.97	0.18	1.00	25,31,49,52	0
23	CLA	b	610	65/65	0.97	0.15	0.99	18,23,32,35	0
23	CLA	B	616	65/65	0.97	0.10	0.98	23,28,48,50	0
27	LMG	C	519	51/55	0.86	0.19	0.98	29,59,97,105	0
23	CLA	C	510	65/65	0.96	0.15	0.96	22,28,38,41	0
25	BCR	t	101	40/40	0.95	0.14	0.95	23,30,42,44	0
23	CLA	b	617	65/65	0.96	0.14	0.93	20,25,71,83	0
23	CLA	B	610	65/65	0.88	0.13	0.93	23,28,33,35	0
23	CLA	B	606	65/65	0.97	0.15	0.90	17,23,35,40	0
23	CLA	C	504	65/65	0.96	0.15	0.90	23,28,62,68	0
23	CLA	B	612	65/65	0.96	0.13	0.87	18,21,34,37	0
23	CLA	B	613	65/65	0.97	0.14	0.86	19,24,31,34	0
23	CLA	b	612	65/65	0.89	0.13	0.85	26,30,36,38	0
23	CLA	B	609	65/65	0.97	0.16	0.84	18,24,31,34	0
23	CLA	B	605	65/65	0.97	0.18	0.81	19,22,53,55	0
30	LMT	m	101	35/35	0.74	0.22	0.80	32,51,61,62	0
23	CLA	C	501	65/65	0.96	0.14	0.79	25,32,46,53	0
23	CLA	b	616	65/65	0.98	0.20	0.78	20,24,46,50	0
23	CLA	B	614	65/65	0.97	0.17	0.78	18,23,48,54	0
30	LMT	B	623	35/35	0.75	0.24	0.77	43,79,117,129	0
31	GOL	B	635	6/6	0.94	0.12	0.75	38,47,49,50	0
31	GOL	B	637	6/6	0.93	0.13	0.74	36,38,45,54	0
23	CLA	b	613	65/65	0.96	0.13	0.74	24,28,35,40	0
28	PL9	D	405	55/55	0.97	0.10	0.72	18,23,31,38	0
25	BCR	b	622	40/40	0.95	0.10	0.70	25,33,43,45	0
23	CLA	d	402	65/65	0.98	0.12	0.70	18,21,39,44	0
25	BCR	K	101	40/40	0.95	0.10	0.68	30,35,40,43	0
34	DGD	c	917	62/66	0.94	0.16	0.68	24,33,77,80	0
23	CLA	c	905	65/65	0.94	0.18	0.68	24,31,64,66	0
31	GOL	b	634	6/6	0.96	0.12	0.68	32,39,44,46	0
23	CLA	b	607	65/65	0.96	0.16	0.66	20,25,54,59	0
23	CLA	c	903	65/65	0.95	0.19	0.63	22,29,42,55	0
23	CLA	a	409	65/65	0.98	0.12	0.60	18,21,31,43	0
23	CLA	b	608	65/65	0.98	0.11	0.55	20,24,33,34	0
23	CLA	B	604	65/65	0.97	0.14	0.52	17,22,34,41	0
23	CLA	c	904	65/65	0.94	0.15	0.51	24,37,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	SQD	f	102	33/54	0.81	0.21	0.51	63,73,113,114	0
31	GOL	v	203	6/6	0.95	0.15	0.51	31,35,41,43	0
31	GOL	c	929	6/6	0.99	0.14	0.47	25,27,30,30	0
25	BCR	k	102	40/40	0.88	0.13	0.47	29,41,48,50	0
24	PHO	A	408	64/64	0.97	0.11	0.46	16,21,25,27	0
23	CLA	a	414	65/65	0.97	0.09	0.44	19,25,99,104	0
23	CLA	C	502	65/65	0.97	0.14	0.44	21,26,39,48	0
23	CLA	b	606	65/65	0.96	0.12	0.43	20,26,37,42	0
34	DGD	c	918	62/66	0.92	0.15	0.42	27,35,79,91	0
23	CLA	c	902	65/65	0.94	0.13	0.38	27,34,46,50	0
23	CLA	A	406	65/65	0.97	0.09	0.38	13,18,29,39	0
23	CLA	b	615	65/65	0.96	0.14	0.37	19,27,33,38	0
23	CLA	B	603	65/65	0.92	0.14	0.35	23,26,34,37	0
23	CLA	c	913	65/65	0.93	0.12	0.35	33,45,67,72	0
24	PHO	a	412	64/64	0.98	0.12	0.32	17,22,26,27	0
23	CLA	C	506	65/65	0.90	0.13	0.32	25,38,94,97	0
38	RRX	H	101	41/41	0.88	0.14	0.31	25,30,44,47	0
23	CLA	c	908	65/65	0.94	0.12	0.28	26,32,52,55	0
23	CLA	b	609	65/65	0.92	0.11	0.27	23,31,57,63	0
33	HTG	O	303	19/19	0.97	0.09	0.27	27,32,50,52	0
23	CLA	C	513	65/65	0.93	0.13	0.27	35,46,78,83	0
25	BCR	K	102	40/40	0.96	0.08	0.26	28,31,39,42	0
29	UNL	J	103	14/-	0.77	0.16	0.26	61,66,73,76	0
23	CLA	C	512	65/65	0.94	0.10	0.26	34,41,69,74	0
23	CLA	A	405	65/65	0.97	0.10	0.25	14,19,25,42	0
35	BCT	a	408	4/4	0.96	0.09	0.25	30,32,37,46	0
23	CLA	B	617	65/65	0.96	0.10	0.24	20,28,79,83	0
37	HEM	f	101	43/43	0.98	0.19	0.23	39,47,61,77	0
23	CLA	D	402	65/65	0.96	0.11	0.20	13,18,36,39	0
39	MG	J	101	1/1	0.99	0.09	0.19	28,28,28,28	0
33	HTG	B	624	19/19	0.96	0.09	0.13	27,33,41,51	0
23	CLA	D	403	65/65	0.96	0.11	0.13	22,28,73,79	0
23	CLA	B	615	65/65	0.96	0.11	0.11	19,24,67,74	0
25	BCR	B	620	40/40	0.95	0.09	0.09	22,31,41,44	0
25	BCR	c	916	40/40	0.94	0.10	0.06	28,36,45,47	0
23	CLA	b	605	65/65	0.93	0.12	0.06	24,29,36,39	0
23	CLA	B	607	65/65	0.94	0.10	0.00	21,27,55,61	0
38	RRX	h	101	41/41	0.88	0.12	-0.04	27,35,49,54	0
22	CL	a	407	1/1	0.99	0.12	-0.09	27,27,27,27	0
35	BCT	D	401	4/4	0.98	0.08	-0.09	32,35,41,51	0
23	CLA	c	906	65/65	0.96	0.10	-0.12	26,31,46,50	0
23	CLA	b	619	65/65	0.96	0.12	-0.19	25,32,89,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
25	BCR	k	101	40/40	0.93	0.09	-0.22	33,39,47,49	0
23	CLA	C	507	65/65	0.95	0.10	-0.27	26,33,56,61	0
37	HEM	V	201	43/43	0.99	0.07	-0.29	22,24,28,33	0
23	CLA	d	403	65/65	0.97	0.08	-0.33	25,32,83,90	0
25	BCR	a	415	40/40	0.96	0.07	-0.34	21,25,30,31	0
25	BCR	c	915	40/40	0.92	0.10	-0.36	44,51,59,60	0
37	HEM	F	101	43/43	0.97	0.12	-0.42	36,42,49,52	0
23	CLA	c	912	65/65	0.95	0.09	-0.48	29,37,45,50	0
23	CLA	C	511	65/65	0.95	0.09	-0.48	27,34,40,42	0
23	CLA	b	618	65/65	0.95	0.08	-0.52	24,30,49,53	0
23	CLA	c	907	65/65	0.94	0.09	-0.56	28,36,76,80	0
21	FE2	a	405	1/1	0.99	0.06	-0.60	27,27,27,27	0
37	HEM	v	201	43/43	0.98	0.08	-0.66	25,31,35,38	0
25	BCR	C	514	40/40	0.95	0.07	-0.70	33,42,46,46	0
22	CL	A	404	1/1	0.99	0.13	-0.76	22,22,22,22	0
21	FE2	A	402	1/1	1.00	0.06	-0.86	26,26,26,26	0
31	GOL	B	634	6/6	0.96	0.10	-0.89	29,29,34,37	0
31	GOL	v	202	6/6	0.96	0.10	-0.94	35,36,40,41	0
20	OEX	a	404	10/10	1.00	0.07	-1.51	22,26,28,29	0
20	OEX	A	401	10/10	1.00	0.07	-1.52	21,23,27,28	0
22	CL	A	403	1/1	0.99	0.06	-1.71	25,25,25,25	0
32	CA	O	301	1/1	0.95	0.14	-1.92	49,49,49,49	0
32	CA	o	301	1/1	0.95	0.11	-2.03	51,51,51,51	0
32	CA	c	901	1/1	0.96	0.07	-4.10	46,46,46,46	0
22	CL	a	406	1/1	0.99	0.04	-4.85	29,29,29,29	0
29	UNL	b	629	16/-	0.89	0.11	-	43,48,56,60	0
29	UNL	e	800	11/-	0.76	0.29	-	53,60,68,68	0
33	HTG	C	521	19/19	0.92	0.18	-	56,63,76,80	0
29	UNL	c	926	10/-	0.75	0.17	-	65,67,71,72	0
29	UNL	A	416	16/-	0.90	0.14	-	41,46,73,73	0
31	GOL	h	103	6/6	0.56	0.28	-	78,83,83,84	0
29	UNL	i	104	10/-	0.74	0.28	-	67,72,77,78	0
29	UNL	I	102	11/-	0.83	0.22	-	62,65,66,68	0
29	UNL	H	103	10/-	0.75	0.23	-	60,69,74,76	0
32	CA	F	103	1/1	0.96	0.15	-	55,55,55,55	0
32	CA	b	603	1/1	0.90	0.09	-	82,82,82,82	0
32	CA	B	601	1/1	0.82	0.09	-	81,81,81,81	0
29	UNL	B	627	16/-	0.83	0.14	-	43,47,69,69	0
29	UNL	i	102	16/-	0.79	0.23	-	54,65,83,84	0
29	UNL	L	102	14/-	0.89	0.22	-	52,58,66,69	0
33	HTG	B	626	19/19	0.74	0.41	-	48,87,92,93	0
32	CA	f	103	1/1	0.97	0.19	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	HTG	c	923	19/19	0.85	0.24	-	64,75,82,83	0
33	HTG	B	631	19/19	0.69	0.26	-	49,111,120,125	0
31	GOL	O	304	6/6	0.79	0.17	-	52,60,61,63	0
29	UNL	c	925	30/-	0.74	0.18	-	59,72,89,95	0
29	UNL	I	101	13/-	0.78	0.22	-	44,53,61,63	0
29	UNL	B	628	10/-	0.86	0.27	-	52,56,70,74	0
29	UNL	Z	103	16/-	0.74	0.21	-	48,63,81,81	0
29	UNL	M	103	16/-	0.85	0.23	-	49,58,77,79	0
29	UNL	i	101	16/-	0.92	0.13	-	40,46,56,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.