



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 19, 2016 – 10:34 PM EST

PDB ID : 5KAI
Title : NH3-bound RT XFEL structure of Photosystem II 500 ms after the 2nd illumination (2F) at 2.8 Å resolution
Authors : Young, I.D.; Ibrahim, M.; Chatterjee, R.; Gul, S.; Koroidov, S.; Brewster, A.S.; Tran, R.; Alonso-Mori, R.; Fuller, F.; Kroll, T.; Michels-Clark, T.; Laksmono, H.; Sierra, R.G.; Stan, C.A.; Saracini, C.; Bean, M.A.; Seuffert, I.; Sokaras, D.; Weng, T.-C.; Hunter, M.S.; Aquila, A.; Koglin, J.E.; Robinson, J.; Liang, M.; Boutet, S.; Lyubimov, A.Y.; Uervirojnangkoorn, M.; Moriarty, N.W.; Liebschner, D.; Afonine, P.V.; Waterman, D.G.; Evans, G.; Dobbek, H.; Weis, W.I.; Brunger, A.T.; Zwart, P.H.; Adams, P.D.; Zouni, A.; Messinger, J.; Bergmann, U.; Sauter, N.K.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2016-06-01
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

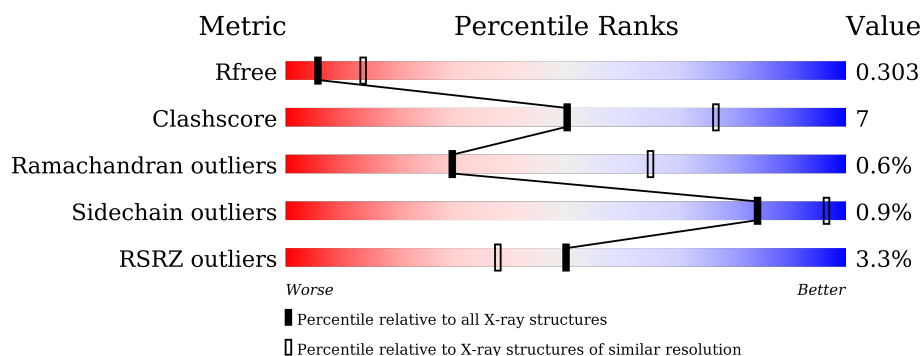
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	344	 % 75% 21% . .
1	a	344	 % 97% .
2	B	510	 2% 79% 20% .
2	b	510	 5% 98% .

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : rb-20028442

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Mol	Chain	Length	Quality of chain
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	63	
7	h	63	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	

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Mol	Chain	Length	Quality of chain
15	u	134	
16	V	163	
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	LMG	A	603	-	-	-	X
23	LMG	B	621	-	-	-	X
23	LMG	C	501	-	-	-	X
23	LMG	C	521	-	-	-	X
23	LMG	D	409	-	-	-	X
23	LMG	b	626	-	-	-	X
23	LMG	b	627	-	-	-	X
23	LMG	c	519	-	-	-	X
23	LMG	c	520	-	-	-	X
25	CLA	A	606	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	609	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	B	617	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	C	514	X	-	-	-
25	CLA	D	402	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	D	404	X	-	-	-
25	CLA	a	707	X	-	-	-
25	CLA	a	708	X	-	-	-
25	CLA	a	711	X	-	-	-
25	CLA	a	719	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	b	617	X	-	-	-
25	CLA	b	618	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	b	619	X	-	-	-
25	CLA	b	620	X	-	-	-
25	CLA	b	621	X	-	-	-
25	CLA	b	622	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	X
25	CLA	c	513	X	-	-	-
25	CLA	d	402	X	-	-	-
25	CLA	d	403	X	-	-	-
27	BCR	D	405	-	-	-	X
27	BCR	t	103	-	-	-	X
28	PL9	A	611	-	-	-	X
28	PL9	a	713	-	-	-	X
29	SQD	B	623	-	-	-	X
29	SQD	B	626	-	-	-	X
29	SQD	I	102	-	-	-	X
29	SQD	b	601	-	-	-	X
30	UNL	b	604	-	-	-	X
30	UNL	b	605	-	-	-	X
30	UNL	b	606	-	-	-	X
30	UNL	t	101	-	-	-	X
30	UNL	t	102	-	-	-	X
30	UNL	z	101	-	-	-	X
32	LHG	D	407	-	-	-	X
32	LHG	E	101	-	-	-	X
32	LHG	e	101	-	-	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50284 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2622	1717	431	459	15			
1	a	334	Total	C	N	O	S	0	0	0
			2622	1717	431	459	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	0	0
			3969	2605	661	690	13			
2	b	504	Total	C	N	O	S	0	1	0
			3968	2605	661	689	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	13			
3	c	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	13			

- 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	0	0
			2716	1800	444	460	12			
4	d	341	Total	C	N	O	S	0	0	0
			2716	1800	444	460	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
			661	432	107	122			
5	e	82	Total	C	N	O	0	0	0
			665	434	108	123			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	34	Total	C	N	O	S	0	0	0
			275	187	45	42	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
			296	200	46	49	1			
8	i	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	expression tag	UNP Q8DJZ6
i	1	FME	-	expression tag	UNP Q8DJZ6

- 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
			257	174	40	42	1			
9	j	36	Total	C	N	O	S	0	0	0
			257	174	40	42	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	l	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	0	0
			260	173	38	48	1			
12	m	33	Total	C	N	O	S	0	0	0
			260	173	38	48	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	FME	-	expression tag	UNP Q8DHA7
m	1	FME	-	expression tag	UNP Q8DHA7

- 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	0	0
			1874	1170	317	383	4			
13	o	244	Total	C	N	O	S	0	0	0
			1874	1170	317	383	4			

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	expression tag	UNP Q8DIQ0
t	1	FME	-	expression tag	UNP Q8DIQ0

- 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
			774	491	129	154				
15	u	97	Total	C	N	O		0	0	0
			774	491	129	154				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	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
			200	131	35	31	3			
17	y	30	Total	C	N	O	S	0	0	0
			224	147	38	36	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O		0	0	0
			281	188	45	48				
18	x	38	Total	C	N	O		0	0	0
			279	187	45	47				

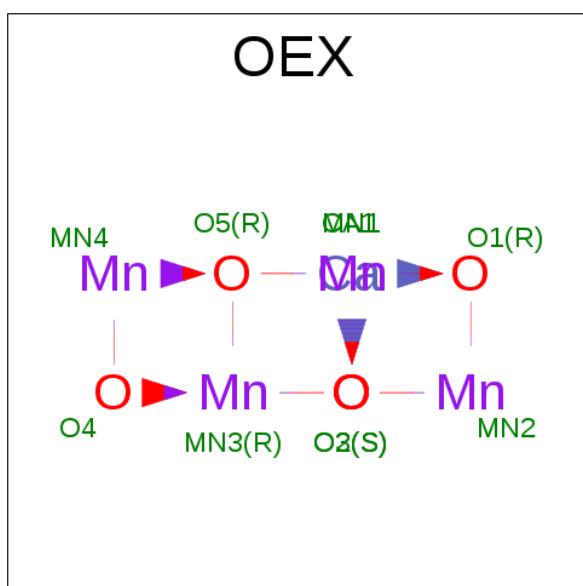
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			478	328	72	76	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O		0	0	0
			273	186	47	40				
20	r	34	Total	C	N	O		0	0	0
			270	183	47	40				

- Molecule 21 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

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

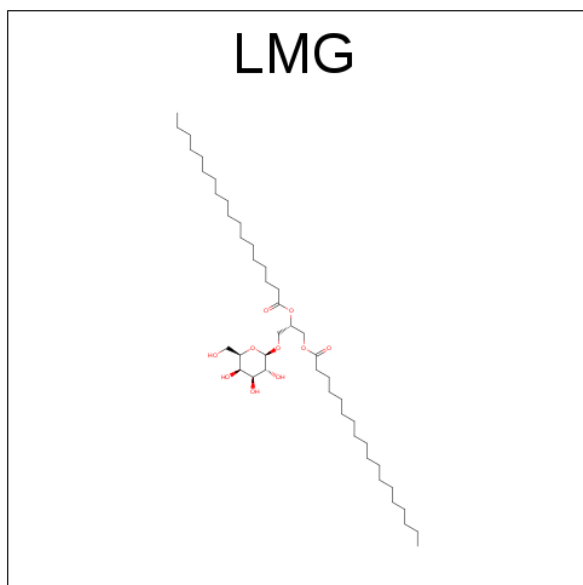
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	1	Total	Fe	0	0
			1	1		

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

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			51	41	10		
23	B	1	Total	C	O	0	0
			51	41	10		
23	C	1	Total	C	O	0	0
			51	41	10		
23	C	1	Total	C	O	0	0
			51	41	10		
23	C	1	Total	C	O	0	0
			51	41	10		
23	D	1	Total	C	O	0	0
			51	41	10		
23	M	1	Total	C	O	0	0
			51	41	10		
23	a	1	Total	C	O	0	0
			51	41	10		
23	a	1	Total	C	O	0	0
			51	41	10		
23	b	1	Total	C	O	0	0
			51	41	10		

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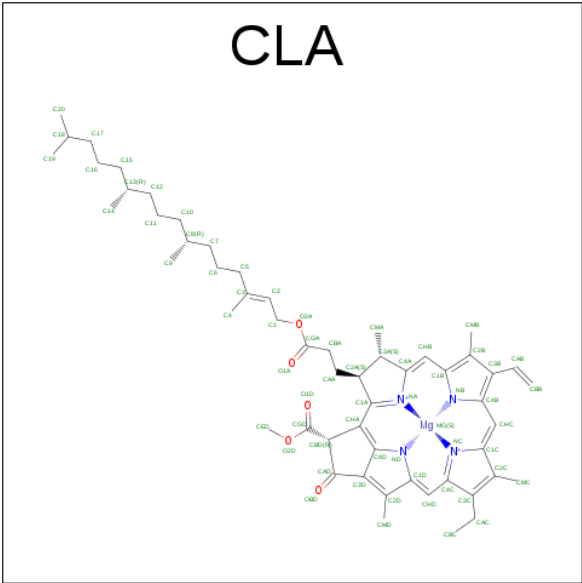
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	b	1	Total C O 51 41 10	0	0
23	b	1	Total C 9 9	0	0
23	c	1	Total C O 51 41 10	0	0
23	c	1	Total C O 51 41 10	0	0
23	d	1	Total C O 40 35 5	0	0
23	f	1	Total C O 51 41 10	0	0

- Molecule 24 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	A	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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

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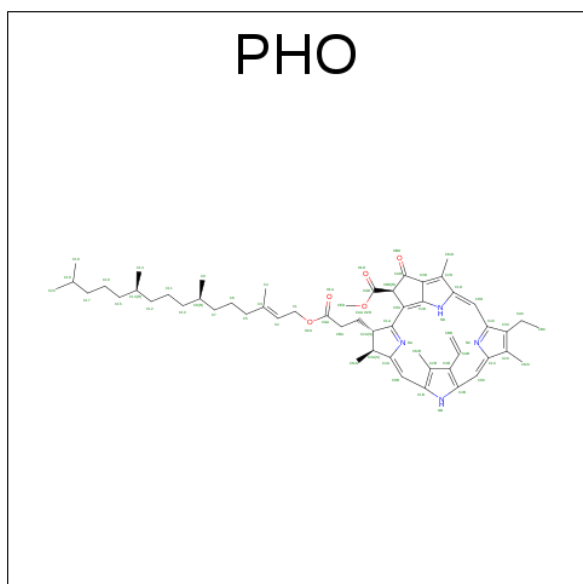
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 58	C 48	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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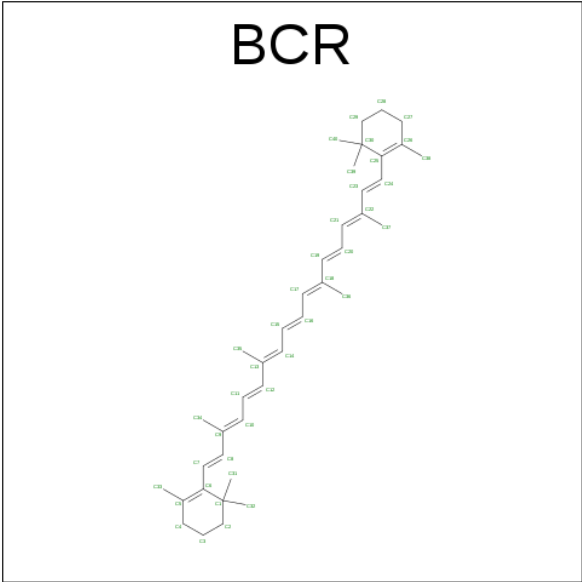
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 26 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



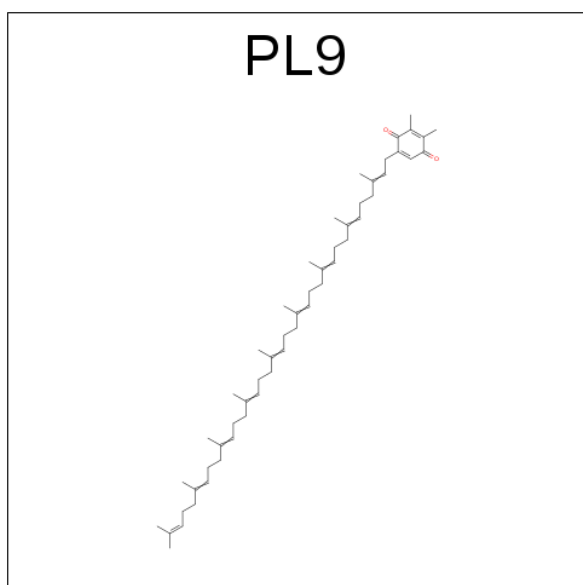
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	Y	1	Total C 40 40	0	0
27	a	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	d	1	Total C 40 40	0	0
27	h	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0
27	t	1	Total C 40 40	0	0

- 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: $C_{53}H_{80}O_2$).



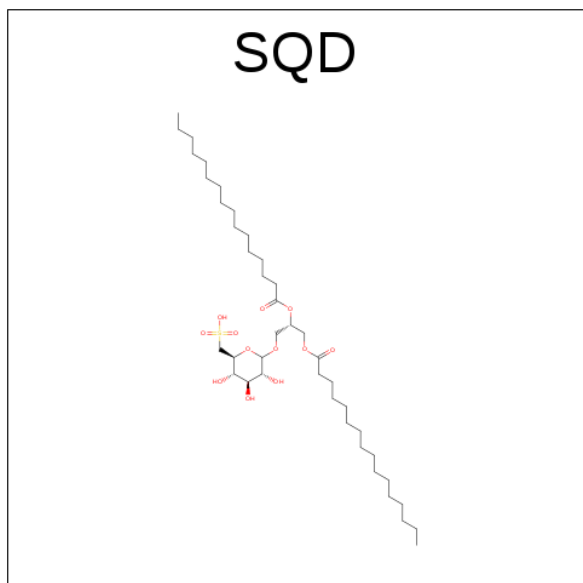
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 55 53 2	0	0
28	D	1	Total C O 55 53 2	0	0

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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		

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).

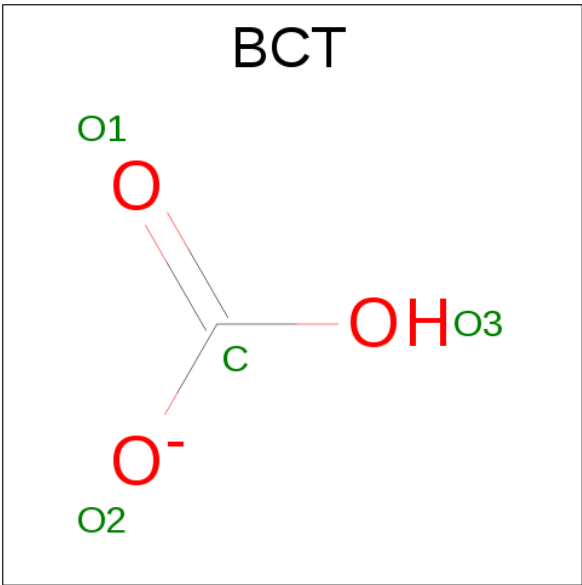


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	S	0	0
			52	39	12	1		
29	A	1	Total	C	O		0	0
			40	35	5			
29	B	1	Total	C	O	S	0	0
			47	34	12	1		
29	B	1	Total	C	O	S	0	0
			54	41	12	1		
29	D	1	Total	C	O	S	0	0
			43	30	12	1		
29	I	1	Total	C	O		0	0
			40	35	5			
29	a	1	Total	C	O	S	0	0
			54	41	12	1		
29	b	1	Total	C	O	S	0	0
			54	41	12	1		
29	f	1	Total	C	O	S	0	0
			41	28	12	1		

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

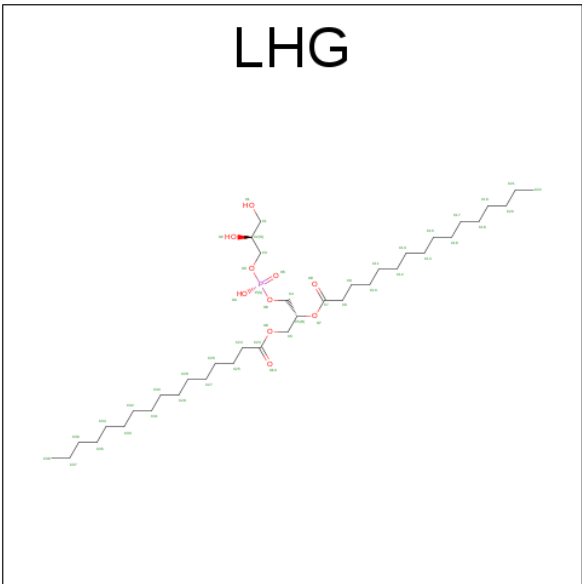
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	j	1	Total C 9 9	0	0
30	i	1	Total C 22 22	0	0
30	d	1	Total C 22 22	0	0
30	H	1	Total C 8 8	0	0
30	B	3	Total C 29 29	0	0
30	I	1	Total C 9 9	0	0
30	a	3	Total C 24 24	0	0
30	z	1	Total C 11 11	0	0
30	A	1	Total C 7 7	0	0
30	t	2	Total C 15 15	0	0
30	m	2	Total C 17 17	0	0
30	b	4	Total C 48 48	0	0
30	M	2	Total C 22 22	0	0

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



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

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



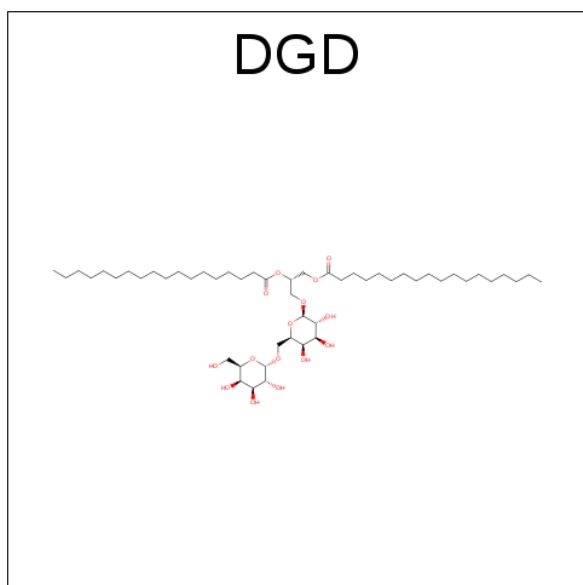
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	O	P	0	0
			49	38	10	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	E	1	Total	C	O	P	0	0
			49	38	10	1		
32	L	1	Total	C	O	P	0	0
			49	38	10	1		
32	a	1	Total	C	O	P	0	0
			39	28	10	1		
32	b	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	e	1	Total	C	O	P	0	0
			42	31	10	1		

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



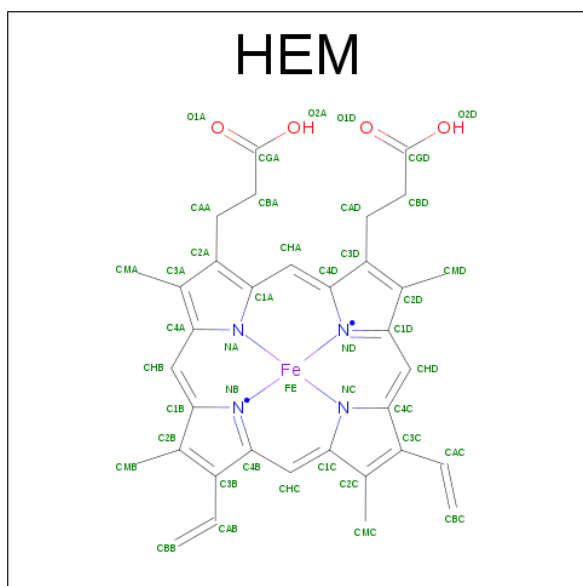
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			62	47	15		
33	C	1	Total	C	O	0	0
			62	47	15		

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

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



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

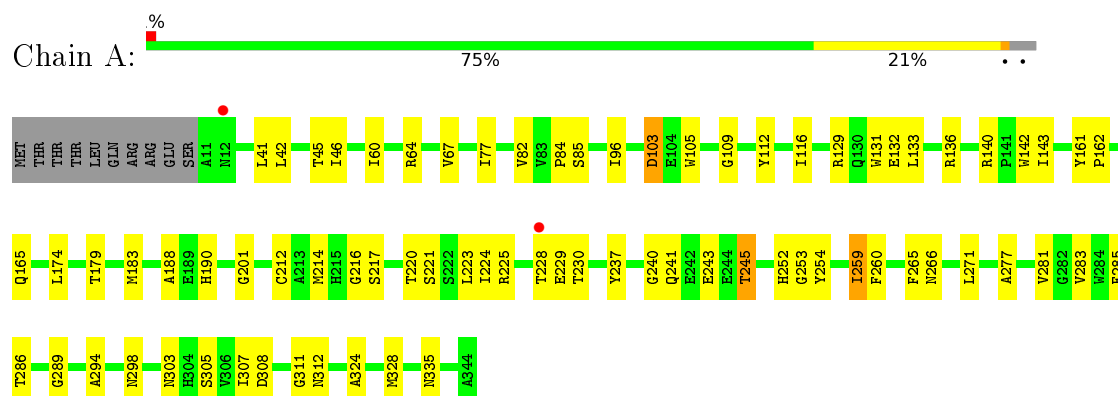
- Molecule 35 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	A	14	Total O 14 14	0	0
35	B	5	Total O 5 5	0	0
35	C	2	Total O 2 2	0	0
35	D	5	Total O 5 5	0	0
35	H	1	Total O 1 1	0	0
35	K	1	Total O 1 1	0	0
35	L	1	Total O 1 1	0	0
35	M	1	Total O 1 1	0	0
35	O	9	Total O 9 9	0	0
35	U	1	Total O 1 1	0	0
35	V	6	Total O 6 6	0	0
35	a	13	Total O 13 13	0	0
35	b	12	Total O 12 12	0	0
35	c	8	Total O 8 8	0	0
35	d	11	Total O 11 11	0	0
35	e	1	Total O 1 1	0	0
35	h	1	Total O 1 1	0	0
35	l	1	Total O 1 1	0	0
35	o	5	Total O 5 5	0	0
35	u	5	Total O 5 5	0	0
35	v	3	Total O 3 3	0	0
35	z	1	Total O 1 1	0	0

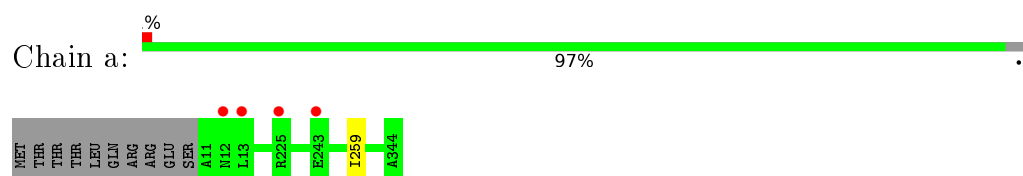
3 Residue-property plots [i](#)

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

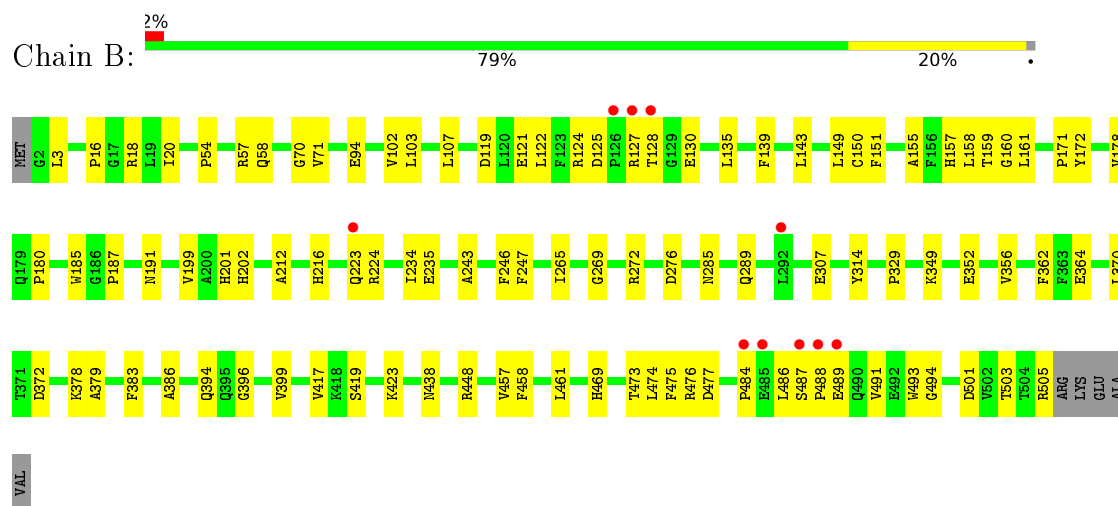
• Molecule 1: Photosystem II protein D1 1



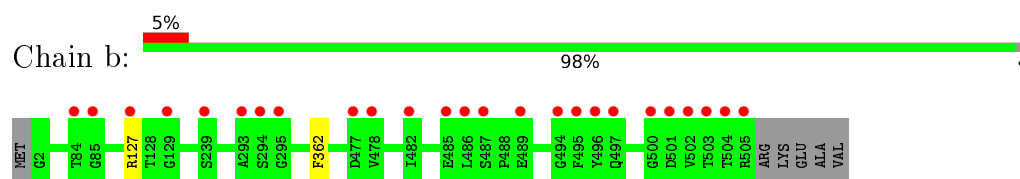
• Molecule 1: Photosystem II protein D1 1



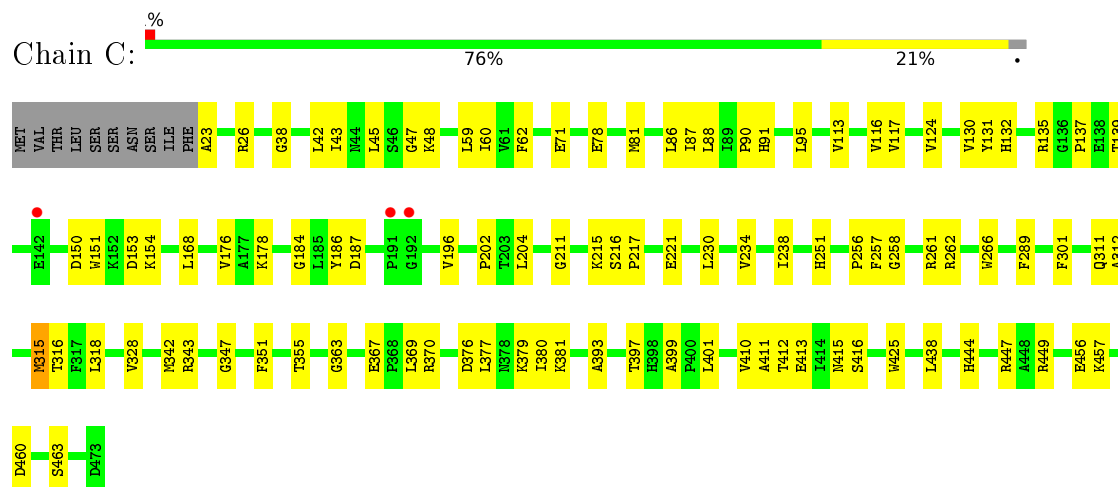
• Molecule 2: Photosystem II CP47 reaction center protein



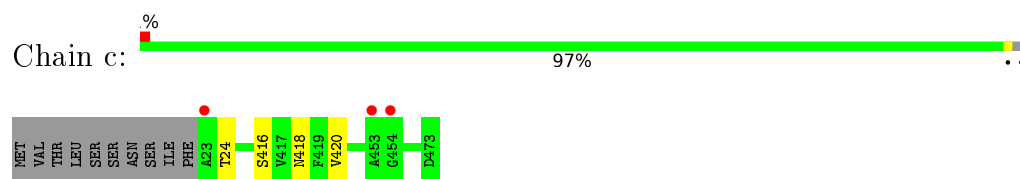
• Molecule 2: Photosystem II CP47 reaction center protein



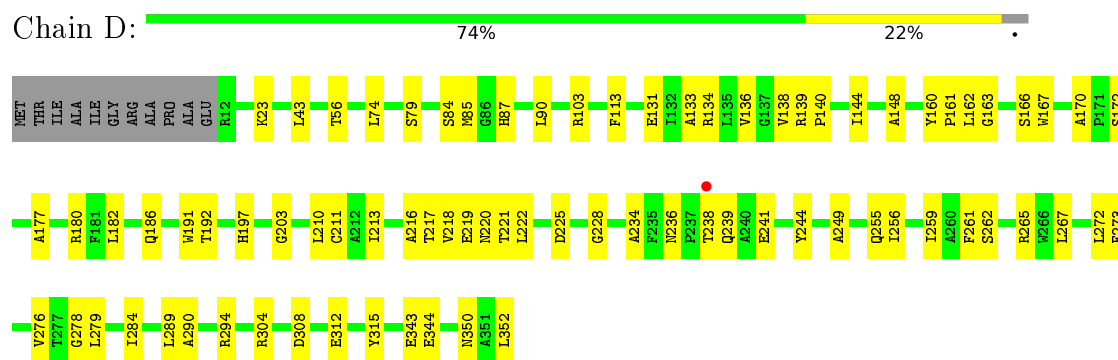
- Molecule 3: Photosystem II CP43 reaction center protein



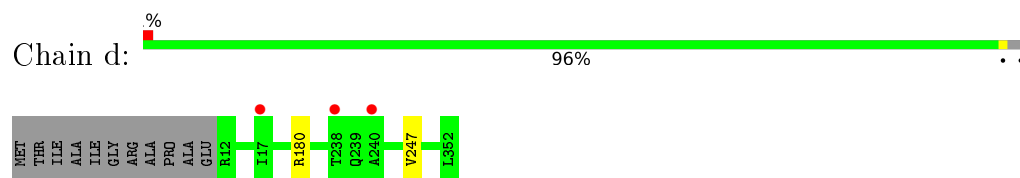
- Molecule 3: Photosystem II CP43 reaction center protein



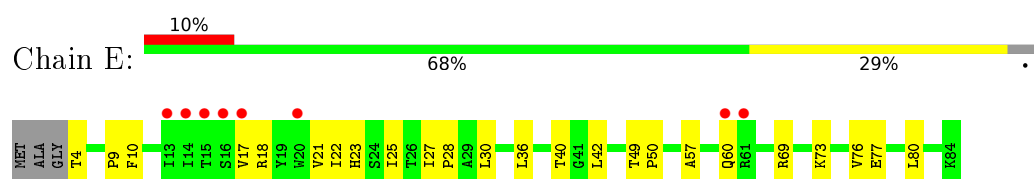
- Molecule 4: Photosystem II D2 protein



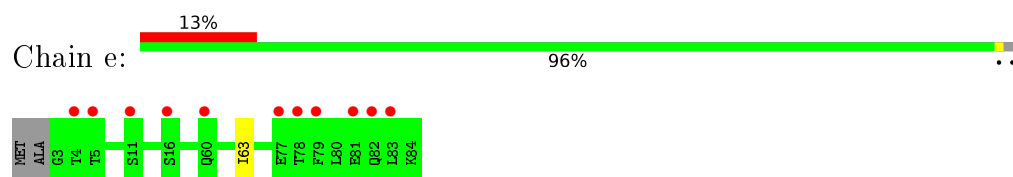
- Molecule 4: Photosystem II D2 protein



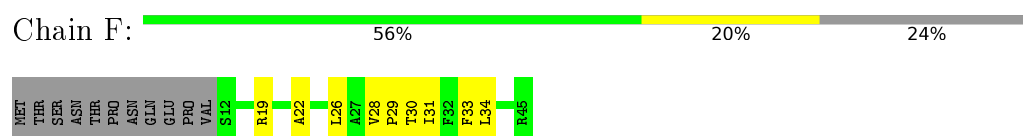
- Molecule 5: Cytochrome b559 subunit alpha



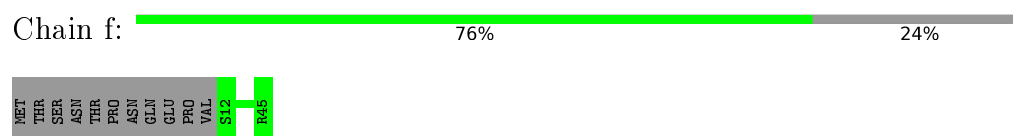
- Molecule 5: Cytochrome b559 subunit alpha



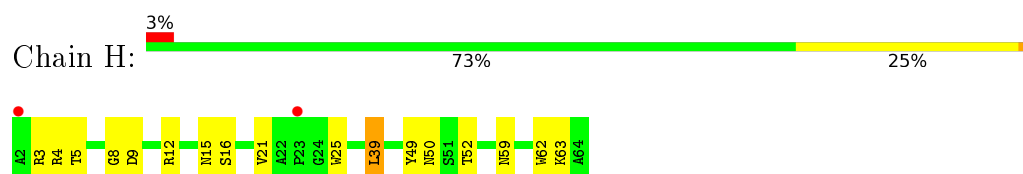
- Molecule 6: Cytochrome b559 subunit beta



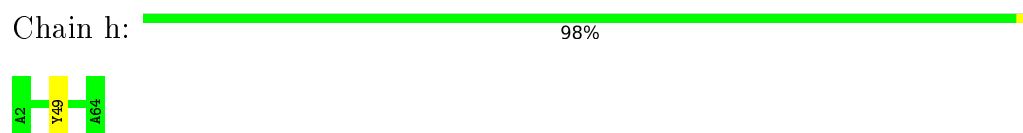
- Molecule 6: Cytochrome b559 subunit beta



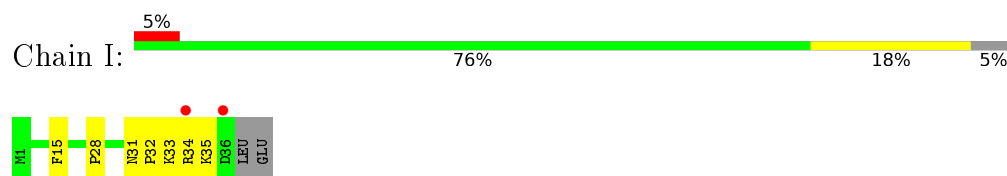
- Molecule 7: Photosystem II reaction center protein H



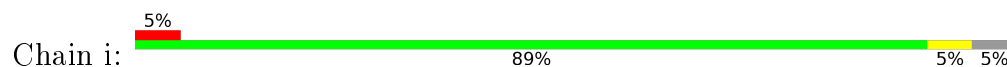
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I

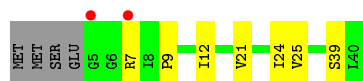


- Molecule 8: Photosystem II reaction center protein I

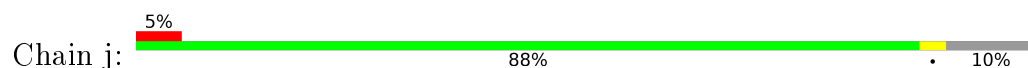




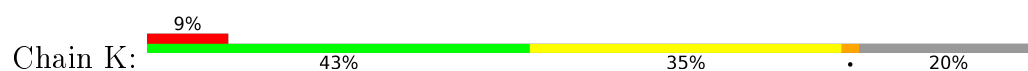
- Molecule 9: Photosystem II reaction center protein J



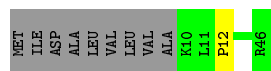
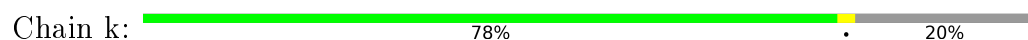
- Molecule 9: Photosystem II reaction center protein J



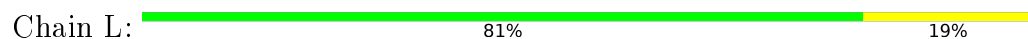
- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L

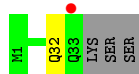
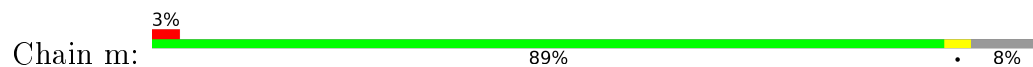


- Molecule 12: Photosystem II reaction center protein M

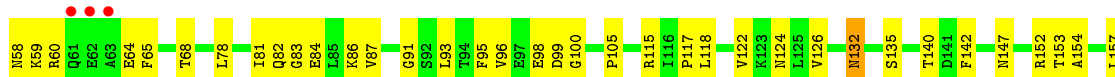
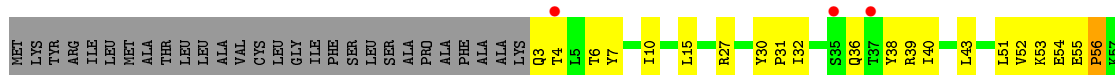




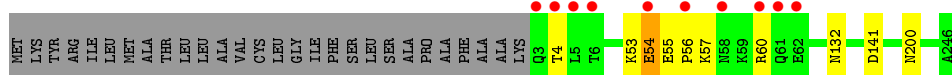
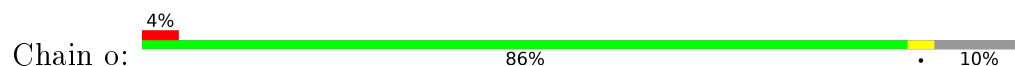
- Molecule 12: Photosystem II reaction center protein M



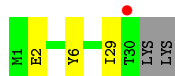
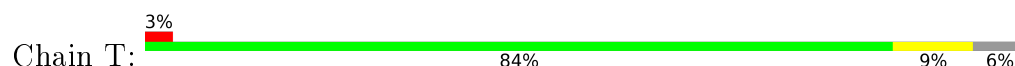
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



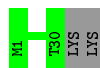
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 14: Photosystem II reaction center protein T

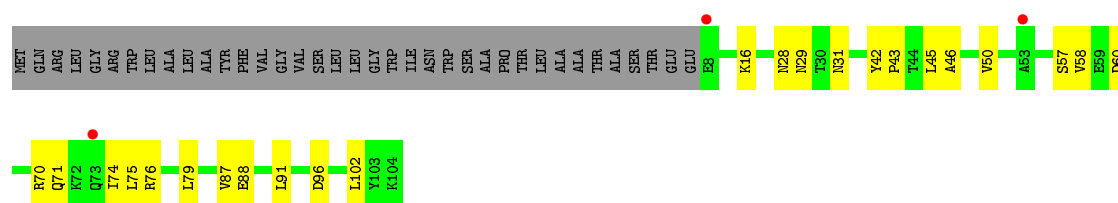


- Molecule 14: Photosystem II reaction center protein T



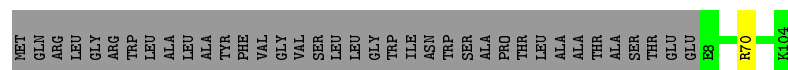
- Molecule 15: Photosystem II 12 kDa extrinsic protein





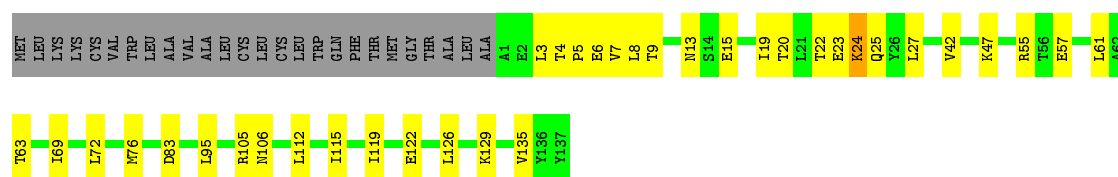
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 72% 28%



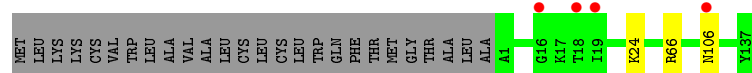
- Molecule 16: Cytochrome c-550

Chain V: 62% 21% 16%



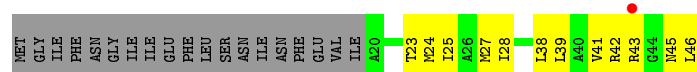
- Molecule 16: Cytochrome c-550

Chain v: 2% 82% 16%



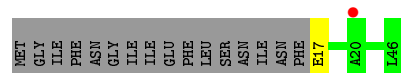
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 2% 33% 26% 41%



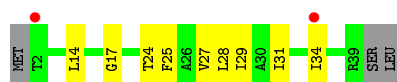
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 2% 63% 35%

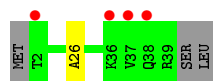
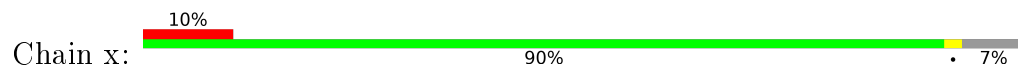


- Molecule 18: Photosystem II reaction center X protein

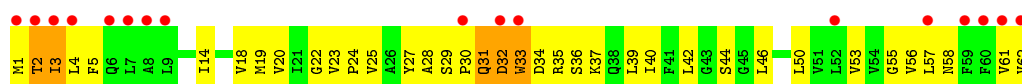
Chain X: 5% 71% 22% 7%



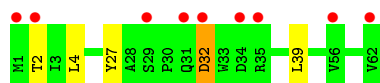
- Molecule 18: Photosystem II reaction center X protein



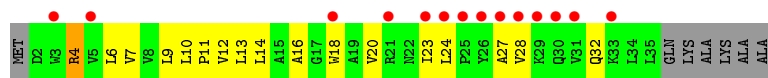
- Molecule 19: Photosystem II reaction center protein Z



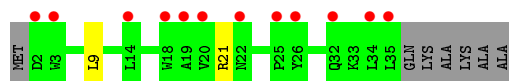
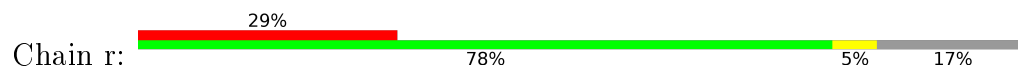
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.91Å 224.27Å 331.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.57 – 2.80 43.57 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (43.57-2.80) 87.7 (43.57-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_2411)	Depositor
R, R_{free}	0.250 , 0.300 0.253 , 0.303	Depositor DCC
R_{free} test set	1792 reflections (0.96%)	DCC
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	50284	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/2707	0.42	0/3692
1	a	0.25	0/2707	0.40	0/3692
2	B	0.26	0/4109	0.41	0/5600
2	b	0.25	0/4111	0.41	0/5603
3	C	0.25	0/3599	0.40	0/4900
3	c	0.26	0/3599	0.43	0/4900
4	D	0.25	0/2811	0.40	0/3830
4	d	0.25	0/2811	0.40	0/3830
5	E	0.26	0/680	0.42	0/928
5	e	0.32	1/684 (0.1%)	0.40	0/933
6	F	0.25	0/284	0.40	0/387
6	f	0.24	0/284	0.36	0/387
7	H	0.27	0/511	0.44	0/697
7	h	0.24	0/511	0.41	0/697
8	I	0.26	0/293	0.40	0/396
8	i	0.56	1/293 (0.3%)	0.54	0/396
9	J	0.24	0/263	0.38	0/356
9	j	0.24	0/263	0.38	0/356
10	K	0.30	0/303	0.50	0/416
10	k	0.43	0/303	0.45	0/416
11	L	0.27	0/311	0.43	0/422
11	l	0.24	0/311	0.38	0/422
12	M	0.24	0/253	0.35	0/346
12	m	0.24	0/253	0.33	0/346
13	O	0.26	0/1905	0.46	0/2583
13	o	0.27	0/1905	0.52	1/2583 (0.0%)
14	T	0.27	0/257	0.36	0/349
14	t	0.26	0/257	0.36	0/349
15	U	0.24	0/785	0.43	0/1064
15	u	0.26	0/785	0.48	0/1064
16	V	0.23	0/1085	0.43	0/1473
16	v	0.23	0/1085	0.44	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.23	0/201	0.41	0/268
17	y	0.35	0/225	0.45	0/301
18	X	0.25	0/284	0.42	0/384
18	x	0.24	0/282	0.39	0/381
19	Z	0.30	0/490	0.51	0/669
19	z	0.35	0/489	0.52	0/669
20	R	0.27	0/279	0.52	0/383
20	r	0.25	0/276	0.51	0/379
All	All	0.26	2/42844 (0.0%)	0.42	1/58320 (0.0%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	33	LYS	CB-CG	-6.06	1.36	1.52
5	e	63	ILE	C-N	5.53	1.44	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	54	GLU	C-N-CA	5.75	136.08	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	o	4	THR	Peptide

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2622	0	2519	70	0
1	a	2622	0	2519	0	0
2	B	3969	0	3828	92	0
2	b	3968	0	3829	0	0
3	C	3486	0	3407	82	0
3	c	3486	0	3407	0	0
4	D	2716	0	2621	68	0
4	d	2716	0	2621	0	0
5	E	661	0	648	27	0
5	e	665	0	651	0	0
6	F	275	0	282	9	0
6	f	275	0	282	0	0
7	H	498	0	518	18	0
7	h	498	0	518	0	0
8	I	296	0	311	7	0
8	i	296	0	311	0	0
9	J	257	0	268	4	0
9	j	257	0	268	0	0
10	K	293	0	305	12	0
10	k	293	0	305	0	0
11	L	304	0	316	7	0
11	l	304	0	316	0	0
12	M	260	0	275	6	0
12	m	260	0	275	0	0
13	O	1874	0	1846	63	0
13	o	1874	0	1846	0	0
14	T	258	0	261	3	0
14	t	258	0	261	0	0
15	U	774	0	773	18	0
15	u	774	0	773	0	0
16	V	1064	0	1073	32	0
16	v	1064	0	1073	0	0
17	Y	200	0	226	8	0
17	y	224	0	252	0	0
18	X	281	0	312	10	0
18	x	279	0	307	0	0
19	Z	479	0	516	38	0
19	z	478	0	516	0	0
20	R	273	0	305	24	0
20	r	270	0	296	0	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	51	0	72	2	0
23	B	51	0	72	1	0
23	C	153	0	216	1	0
23	D	51	0	72	3	0
23	M	51	0	72	3	0
23	a	102	0	144	0	0
23	b	111	0	158	0	0
23	c	102	0	144	0	0
23	d	40	0	61	0	0
23	f	51	0	72	0	0
24	A	2	0	0	0	0
24	a	2	0	0	0	0
25	A	184	0	192	4	0
25	B	1040	0	1152	59	0
25	C	845	0	936	48	0
25	D	195	0	216	12	0
25	a	260	0	288	0	0
25	b	1022	0	1115	0	0
25	c	838	0	919	0	0
25	d	130	0	144	0	0
26	A	64	0	74	2	0
26	D	64	0	74	3	0
26	a	128	0	148	0	0
27	A	40	0	56	4	0
27	B	120	0	168	4	0
27	C	80	0	112	5	0
27	D	40	0	56	4	0
27	H	40	0	56	3	0
27	K	40	0	56	3	0
27	Y	40	0	56	0	0
27	a	40	0	56	0	0
27	b	160	0	224	0	0
27	c	80	0	112	0	0
27	d	40	0	56	0	0
27	h	40	0	56	0	0
27	k	80	0	112	0	0
27	t	40	0	56	0	0
28	A	55	0	80	5	0
28	D	55	0	80	2	0
28	a	55	0	80	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	d	55	0	80	0	0
29	A	92	0	138	3	0
29	B	101	0	135	6	0
29	D	43	0	53	4	0
29	I	40	0	67	3	0
29	a	54	0	78	0	0
29	b	54	0	77	0	0
29	f	41	0	49	0	0
30	A	7	0	0	0	0
30	B	29	0	0	0	0
30	H	8	0	0	0	0
30	I	9	0	0	0	0
30	M	22	0	0	0	0
30	a	24	0	0	0	0
30	b	48	0	0	0	0
30	d	22	0	0	0	0
30	i	22	0	0	0	0
30	j	9	0	0	0	0
30	m	17	0	0	0	0
30	t	15	0	0	0	0
30	z	11	0	0	0	0
31	A	4	0	1	0	0
31	a	4	0	1	0	0
32	B	49	0	74	2	0
32	D	98	0	148	10	0
32	E	49	0	74	4	0
32	L	49	0	74	4	0
32	a	39	0	51	0	0
32	b	49	0	74	0	0
32	d	98	0	148	0	0
32	e	42	0	57	0	0
33	C	186	0	246	7	0
33	H	62	0	82	0	0
33	c	186	0	246	0	0
33	h	62	0	82	0	0
34	E	43	0	30	5	0
34	V	43	0	30	3	0
34	e	43	0	30	0	0
34	v	43	0	30	0	0
35	A	14	0	0	0	0
35	B	5	0	0	0	0
35	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	D	5	0	0	1	0
35	H	1	0	0	0	0
35	K	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	O	9	0	0	2	0
35	U	1	0	0	0	0
35	V	6	0	0	1	0
35	a	13	0	0	0	0
35	b	12	0	0	0	0
35	c	8	0	0	0	0
35	d	11	0	0	0	0
35	e	1	0	0	0	0
35	h	1	0	0	0	0
35	l	1	0	0	0	0
35	o	5	0	0	0	0
35	u	5	0	0	0	0
35	v	3	0	0	0	0
35	z	1	0	0	0	0
All	All	50284	0	51204	625	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 625 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)
7:H:4:ARG:NH2	7:H:9:ASP:OD2	1.66	1.23
13:O:54:GLU:HA	13:O:55:GLU:HB2	4.70	1.02
1:A:225:ARG:HD3	2:B:484:PRO:HD3	1.58	0.83
13:O:55:GLU:OE1	13:O:56:PRO:HD3	7.09	0.81
2:B:269:GLY:O	2:B:448:ARG:NH2	2.13	0.80

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	332/344 (96%)	324 (98%)	7 (2%)	1 (0%)	46	79
1	a	332/344 (96%)	325 (98%)	6 (2%)	1 (0%)	46	79
2	B	502/510 (98%)	482 (96%)	19 (4%)	1 (0%)	52	84
2	b	503/510 (99%)	484 (96%)	19 (4%)	0	100	100
3	C	449/461 (97%)	431 (96%)	17 (4%)	1 (0%)	52	84
3	c	449/461 (97%)	430 (96%)	17 (4%)	2 (0%)	39	74
4	D	339/352 (96%)	325 (96%)	14 (4%)	0	100	100
4	d	339/352 (96%)	323 (95%)	16 (5%)	0	100	100
5	E	79/84 (94%)	76 (96%)	3 (4%)	0	100	100
5	e	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
6	F	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	61/63 (97%)	54 (88%)	7 (12%)	0	100	100
7	h	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
8	I	34/38 (90%)	29 (85%)	5 (15%)	0	100	100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	32 (94%)	1 (3%)	1 (3%)	6	19
10	K	35/46 (76%)	33 (94%)	1 (3%)	1 (3%)	6	19
10	k	35/46 (76%)	32 (91%)	2 (6%)	1 (3%)	6	19
11	L	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	l	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	M	31/36 (86%)	29 (94%)	1 (3%)	1 (3%)	5	17
12	m	31/36 (86%)	29 (94%)	1 (3%)	1 (3%)	5	17
13	O	242/272 (89%)	230 (95%)	10 (4%)	2 (1%)	24	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	223 (92%)	15 (6%)	4 (2%)	11	36
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
15	u	95/134 (71%)	88 (93%)	7 (7%)	0	100	100
16	V	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
16	v	135/163 (83%)	125 (93%)	10 (7%)	0	100	100
17	Y	25/46 (54%)	23 (92%)	2 (8%)	0	100	100
17	y	28/46 (61%)	28 (100%)	0	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	36/41 (88%)	32 (89%)	3 (8%)	1 (3%)	6	21
19	Z	60/62 (97%)	51 (85%)	1 (2%)	8 (13%)	0	1
19	z	60/62 (97%)	53 (88%)	4 (7%)	3 (5%)	3	8
20	R	32/41 (78%)	29 (91%)	3 (9%)	0	100	100
20	r	32/41 (78%)	30 (94%)	1 (3%)	1 (3%)	5	17
All	All	5237/5694 (92%)	4987 (95%)	220 (4%)	30 (1%)	30	65

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	Z	30	PRO
19	Z	31	GLN
19	Z	33	TRP
19	Z	61	VAL
3	c	24	THR

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	270/280 (96%)	268 (99%)	2 (1%)	88	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	270/280 (96%)	270 (100%)	0	100	100
2	B	402/407 (99%)	397 (99%)	5 (1%)	78	95
2	b	402/407 (99%)	400 (100%)	2 (0%)	92	98
3	C	352/362 (97%)	350 (99%)	2 (1%)	90	98
3	c	352/362 (97%)	350 (99%)	2 (1%)	90	98
4	D	276/283 (98%)	274 (99%)	2 (1%)	88	97
4	d	276/283 (98%)	274 (99%)	2 (1%)	88	97
5	E	72/73 (99%)	72 (100%)	0	100	100
5	e	72/73 (99%)	72 (100%)	0	100	100
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	53/53 (100%)	51 (96%)	2 (4%)	40	74
7	h	53/53 (100%)	52 (98%)	1 (2%)	65	91
8	I	32/34 (94%)	32 (100%)	0	100	100
8	i	32/34 (94%)	31 (97%)	1 (3%)	47	81
9	J	24/28 (86%)	23 (96%)	1 (4%)	36	71
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	29/32 (91%)	29 (100%)	0	100	100
12	m	29/32 (91%)	29 (100%)	0	100	100
13	O	207/228 (91%)	206 (100%)	1 (0%)	92	98
13	o	207/228 (91%)	202 (98%)	5 (2%)	57	87
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	84/112 (75%)	84 (100%)	0	100	100
15	u	84/112 (75%)	83 (99%)	1 (1%)	78	95
16	V	117/138 (85%)	116 (99%)	1 (1%)	84	96
16	v	117/138 (85%)	114 (97%)	3 (3%)	54	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Y	20/37 (54%)	19 (95%)	1 (5%)	30	64
17	y	23/37 (62%)	22 (96%)	1 (4%)	35	70
18	X	31/34 (91%)	31 (100%)	0	100	100
18	x	30/34 (88%)	30 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	65	91
19	z	52/52 (100%)	49 (94%)	3 (6%)	25	57
20	R	29/33 (88%)	28 (97%)	1 (3%)	44	78
20	r	28/33 (85%)	27 (96%)	1 (4%)	42	76
All	All	4339/4650 (93%)	4298 (99%)	41 (1%)	84	96

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	R	4	ARG
3	c	420	VAL
19	z	27	TYR
2	b	127	ARG
2	b	362	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
15	U	29	ASN
1	a	261	GLN
13	o	147	ASN
16	V	106	ASN
1	a	335	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.88	0	5,9,11	1.21	0
12	FME	M	1	12	8,9,10	0.83	0	5,9,11	0.89	0
14	FME	T	1	14	8,9,10	0.88	0	5,9,11	0.97	0
8	FME	i	1	8	8,9,10	0.87	0	5,9,11	0.93	0
12	FME	m	1	12	8,9,10	0.87	0	5,9,11	0.92	0
14	FME	t	1	14	8,9,10	0.87	0	5,9,11	0.89	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	0/6/9/11	0/0/0/0
12	FME	M	1	12	-	0/6/9/11	0/0/0/0
14	FME	T	1	14	-	0/6/9/11	0/0/0/0
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.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 180 ligands modelled in this entry, 23 are unknown and 6 are monoatomic - leaving 151 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	OEX	A	601	1,3,35	0,15,15	0.00	-	0,32,32	0.00	-
23	LMG	A	603	-	51,51,55	0.93	2 (3%)	59,59,63	1.40	8 (13%)
25	CLA	A	606	-	57,73,73	1.14	5 (8%)	61,113,113	1.12	5 (8%)
25	CLA	A	607	35	57,73,73	1.15	5 (8%)	61,113,113	1.09	5 (8%)
26	PHO	A	608	-	67,69,69	1.23	7 (10%)	86,99,99	1.08	8 (9%)
25	CLA	A	609	-	46,62,73	1.26	4 (8%)	47,99,113	1.20	5 (10%)
27	BCR	A	610	-	41,41,41	1.10	2 (4%)	56,56,56	1.20	5 (8%)
28	PL9	A	611	-	54,55,55	0.85	2 (3%)	68,69,69	1.44	14 (20%)
29	SQD	A	612	-	51,52,54	0.96	5 (9%)	60,63,65	2.04	10 (16%)
29	SQD	A	614	-	39,39,54	0.87	2 (5%)	41,41,65	1.20	3 (7%)
31	BCT	A	615	22	0,3,3	0.00	-	0,3,3	0.00	-
25	CLA	B	602	35	57,73,73	1.14	4 (7%)	61,113,113	1.14	5 (8%)
25	CLA	B	603	-	57,73,73	1.14	5 (8%)	61,113,113	1.11	5 (8%)
25	CLA	B	604	-	57,73,73	1.13	4 (7%)	61,113,113	1.13	6 (9%)
25	CLA	B	605	-	57,73,73	1.14	4 (7%)	61,113,113	1.22	7 (11%)
25	CLA	B	606	-	57,73,73	1.14	4 (7%)	61,113,113	1.07	6 (9%)
25	CLA	B	607	-	57,73,73	1.14	4 (7%)	61,113,113	1.14	6 (9%)
25	CLA	B	608	35	57,73,73	1.13	4 (7%)	61,113,113	1.09	6 (9%)
25	CLA	B	609	-	57,73,73	1.13	5 (8%)	61,113,113	1.12	5 (8%)
25	CLA	B	610	-	57,73,73	1.15	4 (7%)	61,113,113	1.13	7 (11%)
25	CLA	B	611	35	57,73,73	1.14	4 (7%)	61,113,113	1.12	6 (9%)
25	CLA	B	612	-	57,73,73	1.13	4 (7%)	61,113,113	1.18	7 (11%)
25	CLA	B	613	-	57,73,73	1.13	5 (8%)	61,113,113	1.18	6 (9%)
25	CLA	B	614	-	57,73,73	1.14	4 (7%)	61,113,113	1.16	7 (11%)
25	CLA	B	615	-	57,73,73	1.14	5 (8%)	61,113,113	1.12	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	616	-	57,73,73	1.14	4 (7%)	61,113,113	1.15	6 (9%)
25	CLA	B	617	-	57,73,73	1.12	5 (8%)	61,113,113	1.20	7 (11%)
27	BCR	B	618	-	41,41,41	1.12	2 (4%)	56,56,56	1.28	8 (14%)
27	BCR	B	619	-	41,41,41	1.11	2 (4%)	56,56,56	1.20	5 (8%)
27	BCR	B	620	-	41,41,41	1.13	2 (4%)	56,56,56	1.23	5 (8%)
23	LMG	B	621	-	51,51,55	0.73	1 (1%)	59,59,63	1.37	9 (15%)
29	SQD	B	623	-	46,47,54	1.01	3 (6%)	55,58,65	2.07	13 (23%)
32	LHG	B	625	-	48,48,48	0.62	0	49,54,54	1.28	6 (12%)
29	SQD	B	626	-	53,54,54	0.94	5 (9%)	62,65,65	2.16	9 (14%)
23	LMG	C	501	-	51,51,55	0.72	0	59,59,63	1.31	6 (10%)
25	CLA	C	502	-	57,73,73	1.14	4 (7%)	61,113,113	1.11	6 (9%)
25	CLA	C	503	-	57,73,73	1.14	5 (8%)	61,113,113	1.13	7 (11%)
25	CLA	C	504	-	57,73,73	1.13	5 (8%)	61,113,113	1.15	7 (11%)
25	CLA	C	505	35	57,73,73	1.13	5 (8%)	61,113,113	1.11	5 (8%)
25	CLA	C	506	-	57,73,73	1.13	4 (7%)	61,113,113	1.13	7 (11%)
25	CLA	C	507	-	57,73,73	1.14	4 (7%)	61,113,113	1.08	7 (11%)
25	CLA	C	508	35	57,73,73	1.13	4 (7%)	61,113,113	1.15	6 (9%)
25	CLA	C	509	-	57,73,73	1.12	4 (7%)	61,113,113	1.16	7 (11%)
25	CLA	C	510	-	57,73,73	1.14	4 (7%)	61,113,113	1.12	6 (9%)
25	CLA	C	511	-	57,73,73	1.13	5 (8%)	61,113,113	1.16	7 (11%)
25	CLA	C	512	3	57,73,73	1.12	4 (7%)	61,113,113	1.18	7 (11%)
25	CLA	C	513	-	57,73,73	1.12	4 (7%)	61,113,113	1.20	6 (9%)
25	CLA	C	514	-	57,73,73	1.12	5 (8%)	61,113,113	1.19	7 (11%)
27	BCR	C	515	-	41,41,41	1.11	2 (4%)	56,56,56	1.25	8 (14%)
27	BCR	C	516	-	41,41,41	1.13	2 (4%)	56,56,56	1.23	5 (8%)
33	DGD	C	517	-	63,63,67	0.83	1 (1%)	77,77,81	1.42	9 (11%)
33	DGD	C	518	-	63,63,67	0.90	4 (6%)	77,77,81	1.45	11 (14%)
33	DGD	C	519	-	63,63,67	0.86	1 (1%)	77,77,81	1.42	10 (12%)
23	LMG	C	520	-	51,51,55	0.73	0	59,59,63	1.31	6 (10%)
23	LMG	C	521	-	51,51,55	0.78	1 (1%)	59,59,63	1.36	5 (8%)
26	PHO	D	401	-	67,69,69	1.23	8 (11%)	86,99,99	1.07	7 (8%)
25	CLA	D	402	35	57,73,73	1.13	5 (8%)	61,113,113	1.13	4 (6%)
25	CLA	D	403	-	57,73,73	1.15	5 (8%)	61,113,113	1.07	5 (8%)
25	CLA	D	404	-	57,73,73	1.15	4 (7%)	61,113,113	1.13	7 (11%)
27	BCR	D	405	-	41,41,41	1.19	2 (4%)	56,56,56	1.26	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	PL9	D	406	-	54,55,55	0.85	2 (3%)	68,69,69	1.46	15 (22%)
32	LHG	D	407	-	48,48,48	0.60	1 (2%)	49,54,54	1.26	6 (12%)
32	LHG	D	408	-	48,48,48	0.60	0	49,54,54	1.25	6 (12%)
23	LMG	D	409	-	51,51,55	0.72	0	59,59,63	1.30	7 (11%)
29	SQD	D	410	-	42,43,54	1.06	5 (11%)	51,54,65	2.04	9 (17%)
32	LHG	E	101	-	48,48,48	0.67	1 (2%)	49,54,54	1.22	6 (12%)
34	HEM	E	102	5,6	24,50,50	2.03	5 (20%)	16,82,82	1.38	2 (12%)
27	BCR	H	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.33	7 (12%)
33	DGD	H	103	-	63,63,67	0.85	1 (1%)	77,77,81	1.35	7 (9%)
29	SQD	I	102	-	39,39,54	0.84	2 (5%)	41,41,65	1.23	2 (4%)
27	BCR	K	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	5 (8%)
32	LHG	L	101	-	48,48,48	0.61	1 (2%)	49,54,54	1.26	6 (12%)
23	LMG	M	101	-	51,51,55	0.73	0	59,59,63	1.32	6 (10%)
34	HEM	V	201	16	24,50,50	2.05	5 (20%)	16,82,82	1.33	2 (12%)
27	BCR	Y	101	-	41,41,41	1.13	3 (7%)	56,56,56	1.18	4 (7%)
23	LMG	a	701	-	51,51,55	0.79	0	59,59,63	1.32	7 (11%)
21	OEX	a	702	1,3,35	0,15,15	0.00	-	0,32,32	0.00	-
31	BCT	a	706	22	0,3,3	0.00	-	0,3,3	0.00	-
25	CLA	a	707	-	57,73,73	1.14	4 (7%)	61,113,113	1.13	4 (6%)
25	CLA	a	708	35	57,73,73	1.14	5 (8%)	61,113,113	1.11	5 (8%)
26	PHO	a	709	-	67,69,69	1.24	7 (10%)	86,99,99	1.06	8 (9%)
26	PHO	a	710	-	67,69,69	1.23	7 (10%)	86,99,99	1.08	7 (8%)
25	CLA	a	711	-	57,73,73	1.14	4 (7%)	61,113,113	1.10	6 (9%)
27	BCR	a	712	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	5 (8%)
28	PL9	a	713	-	54,55,55	0.83	2 (3%)	68,69,69	1.42	12 (17%)
29	SQD	a	714	-	53,54,54	0.94	4 (7%)	62,65,65	1.95	11 (17%)
23	LMG	a	715	-	51,51,55	0.74	0	59,59,63	1.32	6 (10%)
25	CLA	a	719	35	57,73,73	1.14	4 (7%)	61,113,113	1.09	4 (6%)
32	LHG	a	720	-	38,38,48	0.67	0	39,44,54	1.18	3 (7%)
29	SQD	b	601	-	53,54,54	0.94	3 (5%)	62,65,65	2.17	10 (16%)
27	BCR	b	602	-	41,41,41	1.12	2 (4%)	56,56,56	1.24	7 (12%)
25	CLA	b	607	35	57,73,73	1.13	4 (7%)	61,113,113	1.16	6 (9%)
25	CLA	b	608	-	57,73,73	1.13	4 (7%)	61,113,113	1.08	6 (9%)
25	CLA	b	609	-	57,73,73	1.13	4 (7%)	61,113,113	1.12	6 (9%)
25	CLA	b	610	-	57,73,73	1.13	4 (7%)	61,113,113	1.23	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	611	-	57,73,73	1.14	5 (8%)	61,113,113	1.08	5 (8%)
25	CLA	b	612	-	57,73,73	1.13	5 (8%)	61,113,113	1.15	5 (8%)
25	CLA	b	613	35	57,73,73	1.13	5 (8%)	61,113,113	1.11	5 (8%)
25	CLA	b	614	-	57,73,73	1.13	5 (8%)	61,113,113	1.12	5 (8%)
25	CLA	b	615	-	57,73,73	1.14	4 (7%)	61,113,113	1.11	6 (9%)
25	CLA	b	616	35	57,73,73	1.14	4 (7%)	61,113,113	1.09	6 (9%)
25	CLA	b	617	-	57,73,73	1.12	5 (8%)	61,113,113	1.19	7 (11%)
25	CLA	b	618	-	57,73,73	1.15	4 (7%)	61,113,113	1.14	6 (9%)
25	CLA	b	619	-	57,73,73	1.12	4 (7%)	61,113,113	1.19	7 (11%)
25	CLA	b	620	-	57,73,73	1.14	5 (8%)	61,113,113	1.10	4 (6%)
25	CLA	b	621	-	57,73,73	1.13	5 (8%)	61,113,113	1.17	6 (9%)
25	CLA	b	622	-	39,55,73	1.34	4 (10%)	42,91,113	1.37	6 (14%)
27	BCR	b	623	-	41,41,41	1.16	3 (7%)	56,56,56	1.27	8 (14%)
27	BCR	b	624	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	6 (10%)
27	BCR	b	625	-	41,41,41	1.13	2 (4%)	56,56,56	1.25	7 (12%)
23	LMG	b	626	-	51,51,55	0.80	3 (5%)	59,59,63	1.53	9 (15%)
23	LMG	b	627	-	51,51,55	0.77	0	59,59,63	1.27	4 (6%)
23	LMG	b	628	-	8,8,55	0.16	0	7,7,63	0.91	0
32	LHG	b	629	-	48,48,48	0.61	1 (2%)	49,54,54	1.24	6 (12%)
25	CLA	c	501	-	57,73,73	1.14	5 (8%)	61,113,113	1.11	6 (9%)
25	CLA	c	502	-	57,73,73	1.14	5 (8%)	61,113,113	1.12	7 (11%)
25	CLA	c	503	-	57,73,73	1.14	4 (7%)	61,113,113	1.14	5 (8%)
25	CLA	c	504	35	50,66,73	1.21	4 (8%)	52,104,113	1.21	6 (11%)
25	CLA	c	505	-	57,73,73	1.14	4 (7%)	61,113,113	1.09	7 (11%)
25	CLA	c	506	-	57,73,73	1.13	5 (8%)	61,113,113	1.11	6 (9%)
25	CLA	c	507	35	57,73,73	1.13	4 (7%)	61,113,113	1.15	7 (11%)
25	CLA	c	508	-	57,73,73	1.13	4 (7%)	61,113,113	1.12	7 (11%)
25	CLA	c	509	-	57,73,73	1.13	5 (8%)	61,113,113	1.16	6 (9%)
25	CLA	c	510	-	57,73,73	1.13	4 (7%)	61,113,113	1.15	5 (8%)
25	CLA	c	511	3	57,73,73	1.13	5 (8%)	61,113,113	1.16	6 (9%)
25	CLA	c	512	-	57,73,73	1.11	4 (7%)	61,113,113	1.21	6 (9%)
25	CLA	c	513	-	57,73,73	1.12	4 (7%)	61,113,113	1.16	6 (9%)
27	BCR	c	514	-	41,41,41	1.15	2 (4%)	56,56,56	1.26	7 (12%)
27	BCR	c	515	-	41,41,41	1.13	2 (4%)	56,56,56	1.23	5 (8%)
33	DGD	c	516	-	63,63,67	0.85	1 (1%)	77,77,81	1.41	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	DGD	c	517	-	63,63,67	0.93	2 (3%)	77,77,81	1.42	10 (12%)
33	DGD	c	518	-	63,63,67	0.85	1 (1%)	77,77,81	1.42	10 (12%)
23	LMG	c	519	-	51,51,55	0.71	0	59,59,63	1.32	5 (8%)
23	LMG	c	520	-	51,51,55	0.81	1 (1%)	59,59,63	1.36	6 (10%)
25	CLA	d	402	-	57,73,73	1.15	4 (7%)	61,113,113	1.09	5 (8%)
25	CLA	d	403	-	57,73,73	1.12	4 (7%)	61,113,113	1.17	6 (9%)
27	BCR	d	404	-	41,41,41	1.15	3 (7%)	56,56,56	1.24	7 (12%)
28	PL9	d	405	-	54,55,55	0.82	2 (3%)	68,69,69	1.43	14 (20%)
32	LHG	d	406	-	48,48,48	0.61	0	49,54,54	1.28	7 (14%)
32	LHG	d	407	-	48,48,48	0.61	0	49,54,54	1.25	6 (12%)
23	LMG	d	408	-	39,39,55	0.53	0	41,41,63	1.27	3 (7%)
32	LHG	e	101	-	41,41,48	0.67	1 (2%)	42,47,54	1.33	7 (16%)
34	HEM	e	102	5,6	24,50,50	2.12	5 (20%)	16,82,82	1.44	2 (12%)
23	LMG	f	101	-	51,51,55	0.70	0	59,59,63	1.36	7 (11%)
29	SQD	f	102	-	40,41,54	1.08	5 (12%)	49,52,65	1.99	9 (18%)
27	BCR	h	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	7 (12%)
33	DGD	h	102	-	63,63,67	0.87	0	77,77,81	1.30	7 (9%)
27	BCR	k	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.15	2 (3%)
27	BCR	k	102	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	6 (10%)
27	BCR	t	103	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	7 (12%)
34	HEM	v	201	16	24,50,50	2.04	5 (20%)	16,82,82	1.32	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	OEX	A	601	1,3,35	-	0/0/68/68	0/0/6/6
23	LMG	A	603	-	-	0/46/66/70	0/1/1/1
25	CLA	A	606	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	A	607	35	3/3/20/25	0/37/135/135	0/0/9/9
26	PHO	A	608	-	-	0/53/103/103	0/1/6/6
25	CLA	A	609	-	3/3/17/25	0/24/122/135	0/0/9/9
27	BCR	A	610	-	-	0/29/63/63	0/2/2/2
28	PL9	A	611	-	-	0/53/73/73	0/1/1/1
29	SQD	A	612	-	-	0/47/67/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	A	614	-	-	0/41/41/69	0/0/0/1
31	BCT	A	615	22	-	0/0/0/0	0/0/0/0
25	CLA	B	602	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	603	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	607	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	608	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	609	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	610	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	B	611	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	617	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	B	618	-	-	0/29/63/63	0/2/2/2
27	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	BCR	B	620	-	-	0/29/63/63	0/2/2/2
23	LMG	B	621	-	-	0/46/66/70	0/1/1/1
29	SQD	B	623	-	-	0/42/62/69	0/1/1/1
32	LHG	B	625	-	-	0/53/53/53	0/0/0/0
29	SQD	B	626	-	-	1/49/69/69	0/1/1/1
23	LMG	C	501	-	-	0/46/66/70	0/1/1/1
25	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	505	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	506	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	C	507	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	C	508	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	511	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	512	3	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	513	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	514	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	C	515	-	-	0/29/63/63	0/2/2/2
27	BCR	C	516	-	-	0/29/63/63	0/2/2/2
33	DGD	C	517	-	-	0/51/91/95	0/2/2/2
33	DGD	C	518	-	-	0/51/91/95	0/2/2/2
33	DGD	C	519	-	-	0/51/91/95	0/2/2/2
23	LMG	C	520	-	-	0/46/66/70	0/1/1/1
23	LMG	C	521	-	-	0/46/66/70	0/1/1/1
26	PHO	D	401	-	-	0/53/103/103	0/1/6/6
25	CLA	D	402	35	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	D	403	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	D	404	-	2/2/20/25	0/37/135/135	0/0/9/9
27	BCR	D	405	-	-	0/29/63/63	0/2/2/2
28	PL9	D	406	-	-	0/53/73/73	0/1/1/1
32	LHG	D	407	-	-	0/53/53/53	0/0/0/0
32	LHG	D	408	-	-	0/53/53/53	0/0/0/0
23	LMG	D	409	-	-	0/46/66/70	0/1/1/1
29	SQD	D	410	-	-	0/38/58/69	0/1/1/1
32	LHG	E	101	-	-	0/53/53/53	0/0/0/0
34	HEM	E	102	5,6	-	0/6/54/54	0/0/8/8
27	BCR	H	102	-	-	0/29/63/63	0/2/2/2
33	DGD	H	103	-	-	0/51/91/95	0/2/2/2
29	SQD	I	102	-	-	0/41/41/69	0/0/0/1
27	BCR	K	101	-	-	0/29/63/63	0/2/2/2
32	LHG	L	101	-	-	0/53/53/53	0/0/0/0
23	LMG	M	101	-	-	0/46/66/70	0/1/1/1
34	HEM	V	201	16	-	0/6/54/54	0/0/8/8
27	BCR	Y	101	-	-	0/29/63/63	0/2/2/2
23	LMG	a	701	-	-	0/46/66/70	0/1/1/1
21	OEX	a	702	1,3,35	-	0/0/68/68	0/0/6/6
31	BCT	a	706	22	-	0/0/0/0	0/0/0/0
25	CLA	a	707	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	a	708	35	3/3/20/25	0/37/135/135	0/0/9/9
26	PHO	a	709	-	-	0/53/103/103	0/1/6/6
26	PHO	a	710	-	-	0/53/103/103	0/1/6/6
25	CLA	a	711	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	a	712	-	-	0/29/63/63	0/2/2/2
28	PL9	a	713	-	-	0/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	a	714	-	-	0/49/69/69	0/1/1/1
23	LMG	a	715	-	-	0/46/66/70	0/1/1/1
25	CLA	a	719	35	3/3/20/25	0/37/135/135	0/0/9/9
32	LHG	a	720	-	-	0/43/43/53	0/0/0/0
29	SQD	b	601	-	-	0/49/69/69	0/1/1/1
27	BCR	b	602	-	-	0/29/63/63	0/2/2/2
25	CLA	b	607	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	609	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	610	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	611	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	b	612	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	613	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	615	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	b	616	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	618	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	619	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	620	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	621	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	622	-	3/3/16/25	0/16/114/135	0/0/9/9
27	BCR	b	623	-	-	0/29/63/63	0/2/2/2
27	BCR	b	624	-	-	0/29/63/63	0/2/2/2
27	BCR	b	625	-	-	0/29/63/63	0/2/2/2
23	LMG	b	626	-	-	0/46/66/70	0/1/1/1
23	LMG	b	627	-	-	0/46/66/70	0/1/1/1
23	LMG	b	628	-	-	0/6/6/70	0/0/0/1
32	LHG	b	629	-	-	0/53/53/53	0/0/0/0
25	CLA	c	501	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	502	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	504	35	3/3/18/25	0/29/127/135	0/0/9/9
25	CLA	c	505	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	c	506	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	c	507	35	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	508	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	510	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	511	3	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	512	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	513	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	c	514	-	-	0/29/63/63	0/2/2/2
27	BCR	c	515	-	-	0/29/63/63	0/2/2/2
33	DGD	c	516	-	-	0/51/91/95	0/2/2/2
33	DGD	c	517	-	-	0/51/91/95	0/2/2/2
33	DGD	c	518	-	-	0/51/91/95	0/2/2/2
23	LMG	c	519	-	-	0/46/66/70	0/1/1/1
23	LMG	c	520	-	-	0/46/66/70	0/1/1/1
25	CLA	d	402	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	d	403	-	2/2/20/25	0/37/135/135	0/0/9/9
27	BCR	d	404	-	-	0/29/63/63	0/2/2/2
28	PL9	d	405	-	-	0/53/73/73	0/1/1/1
32	LHG	d	406	-	-	0/53/53/53	0/0/0/0
32	LHG	d	407	-	-	0/53/53/53	0/0/0/0
23	LMG	d	408	-	-	0/41/41/70	0/0/0/1
32	LHG	e	101	-	-	0/46/46/53	0/0/0/0
34	HEM	e	102	5,6	-	0/6/54/54	0/0/8/8
23	LMG	f	101	-	-	0/46/66/70	0/1/1/1
29	SQD	f	102	-	-	0/36/56/69	0/1/1/1
27	BCR	h	101	-	-	0/29/63/63	0/2/2/2
33	DGD	h	102	-	-	0/51/91/95	0/2/2/2
27	BCR	k	101	-	-	0/29/63/63	0/2/2/2
27	BCR	k	102	-	-	0/29/63/63	0/2/2/2
27	BCR	t	103	-	-	0/29/63/63	0/2/2/2
34	HEM	v	201	16	-	0/6/54/54	0/0/8/8

The worst 5 of 469 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	e	102	HEM	C3B-C2B	-5.24	1.33	1.40
34	V	201	HEM	C3C-C2C	-5.10	1.33	1.40
34	E	102	HEM	C3C-C2C	-5.02	1.34	1.40
34	v	201	HEM	C3C-C2C	-4.96	1.34	1.40
34	e	102	HEM	C3C-C2C	-4.93	1.34	1.40

The worst 5 of 945 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	612	SQD	O9-S-O7	-4.75	100.56	113.96
29	B	626	SQD	O9-S-O7	-4.71	100.66	113.96
29	B	623	SQD	O9-S-O7	-4.64	100.84	113.96
29	f	102	SQD	O9-S-O7	-4.54	101.13	113.96
29	D	410	SQD	O9-S-O7	-4.51	101.21	113.96

5 of 196 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	C	513	CLA	NC
25	C	513	CLA	ND
25	C	513	CLA	NA
25	C	508	CLA	NC
25	C	508	CLA	NA

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	B	626	SQD	C45-O47-C7-C8

There are no ring outliers.

69 monomers are involved in 200 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	603	LMG	2	0
25	A	606	CLA	1	0
25	A	607	CLA	2	0
26	A	608	PHO	2	0
25	A	609	CLA	1	0
27	A	610	BCR	4	0
28	A	611	PL9	5	0
29	A	612	SQD	2	0
29	A	614	SQD	1	0
25	B	602	CLA	4	0
25	B	603	CLA	1	0
25	B	604	CLA	4	0
25	B	605	CLA	3	0
25	B	606	CLA	1	0
25	B	607	CLA	7	0
25	B	608	CLA	2	0
25	B	609	CLA	3	0
25	B	610	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	611	CLA	3	0
25	B	612	CLA	8	0
25	B	613	CLA	2	0
25	B	614	CLA	3	0
25	B	615	CLA	6	0
25	B	616	CLA	4	0
25	B	617	CLA	6	0
27	B	618	BCR	2	0
27	B	619	BCR	1	0
27	B	620	BCR	1	0
23	B	621	LMG	1	0
29	B	623	SQD	1	0
32	B	625	LHG	2	0
29	B	626	SQD	5	0
25	C	502	CLA	2	0
25	C	503	CLA	2	0
25	C	504	CLA	3	0
25	C	505	CLA	6	0
25	C	506	CLA	3	0
25	C	507	CLA	3	0
25	C	508	CLA	2	0
25	C	509	CLA	10	0
25	C	510	CLA	4	0
25	C	511	CLA	6	0
25	C	512	CLA	6	0
25	C	513	CLA	3	0
25	C	514	CLA	2	0
27	C	515	BCR	2	0
27	C	516	BCR	3	0
33	C	517	DGD	3	0
33	C	518	DGD	4	0
33	C	519	DGD	2	0
23	C	520	LMG	1	0
26	D	401	PHO	3	0
25	D	402	CLA	6	0
25	D	403	CLA	5	0
25	D	404	CLA	1	0
27	D	405	BCR	4	0
28	D	406	PL9	2	0
32	D	407	LHG	4	0
32	D	408	LHG	6	0
23	D	409	LMG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	D	410	SQD	4	0
32	E	101	LHG	4	0
34	E	102	HEM	5	0
27	H	102	BCR	3	0
29	I	102	SQD	3	0
27	K	101	BCR	3	0
32	L	101	LHG	4	0
23	M	101	LMG	3	0
34	V	201	HEM	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.31	2 (0%) 90 86	38, 46, 69, 82	0
1	a	334/344 (97%)	-0.21	4 (1%) 81 73	35, 48, 71, 82	0
2	B	504/510 (98%)	-0.11	10 (1%) 68 58	38, 50, 74, 98	0
2	b	504/510 (98%)	-0.11	25 (4%) 32 21	38, 50, 76, 94	0
3	C	451/461 (97%)	-0.14	3 (0%) 89 84	41, 54, 71, 90	0
3	c	451/461 (97%)	-0.10	3 (0%) 89 84	39, 55, 74, 90	0
4	D	341/352 (96%)	-0.35	1 (0%) 94 92	37, 48, 63, 82	0
4	d	341/352 (96%)	-0.20	3 (0%) 85 79	40, 50, 67, 85	0
5	E	81/84 (96%)	0.30	8 (9%) 9 4	47, 67, 79, 85	0
5	e	82/84 (97%)	0.71	11 (13%) 4 2	52, 70, 85, 87	0
6	F	34/45 (75%)	-0.16	0 100 100	54, 64, 78, 84	0
6	f	34/45 (75%)	-0.35	0 100 100	56, 63, 77, 80	0
7	H	63/63 (100%)	0.13	2 (3%) 51 39	43, 55, 68, 73	0
7	h	63/63 (100%)	0.02	0 100 100	48, 56, 64, 68	0
8	I	35/38 (92%)	0.14	2 (5%) 27 17	43, 53, 83, 94	0
8	i	35/38 (92%)	0.13	2 (5%) 27 17	44, 51, 82, 89	0
9	J	36/40 (90%)	-0.01	2 (5%) 28 18	56, 64, 86, 99	0
9	j	36/40 (90%)	0.12	2 (5%) 28 18	55, 66, 85, 89	0
10	K	37/46 (80%)	0.34	4 (10%) 8 3	62, 68, 83, 89	0
10	k	37/46 (80%)	0.19	0 100 100	60, 70, 84, 89	0
11	L	37/37 (100%)	-0.32	0 100 100	34, 45, 82, 93	0
11	l	37/37 (100%)	-0.43	1 (2%) 58 45	36, 47, 81, 90	0
12	M	32/36 (88%)	-0.40	1 (3%) 52 40	38, 47, 71, 83	0
12	m	32/36 (88%)	-0.30	1 (3%) 52 40	36, 47, 71, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.03	9 (3%) 45 33	42, 57, 87, 106	0
13	o	244/272 (89%)	-0.06	10 (4%) 41 29	43, 56, 89, 116	0
14	T	29/32 (90%)	-0.08	1 (3%) 49 36	37, 46, 69, 87	0
14	t	29/32 (90%)	-0.52	0 100 100	38, 48, 70, 79	0
15	U	97/134 (72%)	0.04	3 (3%) 52 40	45, 58, 75, 86	0
15	u	97/134 (72%)	-0.20	0 100 100	47, 55, 69, 84	0
16	V	137/163 (84%)	-0.13	0 100 100	45, 55, 67, 85	0
16	v	137/163 (84%)	0.18	4 (2%) 55 43	49, 63, 79, 100	0
17	Y	27/46 (58%)	0.35	1 (3%) 45 33	68, 75, 87, 95	0
17	y	30/46 (65%)	0.39	1 (3%) 50 38	69, 79, 89, 90	0
18	X	38/41 (92%)	0.25	2 (5%) 30 20	52, 60, 82, 93	0
18	x	38/41 (92%)	0.25	4 (10%) 8 4	54, 63, 80, 92	0
19	Z	62/62 (100%)	0.87	17 (27%) 1 0	62, 76, 100, 113	0
19	z	62/62 (100%)	0.65	9 (14%) 3 2	67, 82, 101, 112	0
20	R	34/41 (82%)	1.68	14 (41%) 0 0	70, 82, 94, 95	0
20	r	34/41 (82%)	1.58	12 (35%) 0 0	70, 84, 94, 101	0
All	All	5310/5694 (93%)	-0.06	174 (3%) 50 38	34, 53, 81, 116	0

The worst 5 of 174 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	56	PRO	5.5
20	R	28	VAL	5.4
16	v	18	THR	5.4
14	T	30	THR	5.3
3	C	142	GLU	5.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	FME	I	1	10/11	0.90	0.28	-	50,60,70,76	0
12	FME	M	1	10/11	0.92	0.30	-	54,63,77,87	0
12	FME	m	1	10/11	0.94	0.12	-	52,59,74,79	0
14	FME	t	1	10/11	0.94	0.12	-	42,56,71,77	0
14	FME	T	1	10/11	0.92	0.15	-	51,58,70,77	0
8	FME	i	1	10/11	0.90	0.34	-	49,61,69,69	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	UNL	b	606	13/-	0.80	0.25	7.03	45,51,57,59	0
23	LMG	c	520	51/55	0.82	0.40	6.84	61,75,95,100	0
29	SQD	I	102	40/54	0.65	0.49	6.35	44,69,94,102	0
23	LMG	c	519	51/55	0.82	0.30	4.44	42,75,90,91	0
30	UNL	b	604	11/-	0.85	0.27	4.01	38,48,57,59	0
23	LMG	b	626	51/55	0.80	0.30	3.65	38,56,72,77	0
27	BCR	D	405	40/40	0.87	0.24	3.41	48,61,77,81	0
23	LMG	C	501	51/55	0.77	0.31	3.41	46,67,81,88	0
30	UNL	z	101	11/-	0.81	0.29	3.32	48,65,72,72	0
23	LMG	C	521	51/55	0.81	0.34	3.23	49,71,81,91	0
23	LMG	b	627	51/55	0.84	0.31	3.22	51,70,80,82	0
25	CLA	c	512	65/65	0.87	0.25	3.20	60,67,89,91	0
30	UNL	b	605	13/-	0.87	0.21	3.15	42,54,62,62	0
32	LHG	E	101	49/49	0.80	0.28	3.15	48,77,92,95	0
28	PL9	A	611	55/55	0.82	0.29	3.01	46,68,78,83	0
23	LMG	B	621	51/55	0.80	0.25	2.83	52,70,78,88	0
29	SQD	B	623	47/54	0.74	0.27	2.64	44,61,109,124	0
30	UNL	t	102	5/-	0.93	0.20	2.58	32,38,43,47	0
23	LMG	A	603	51/55	0.81	0.26	2.39	40,62,77,83	0
32	LHG	D	407	49/49	0.94	0.23	2.30	34,49,59,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	LHG	e	101	42/49	0.76	0.31	2.21	57,76,98,101	0
29	SQD	b	601	54/54	0.83	0.24	2.20	45,66,94,105	0
30	UNL	t	101	10/-	0.92	0.17	2.18	26,44,49,50	0
29	SQD	B	626	54/54	0.88	0.25	2.08	46,67,90,99	0
27	BCR	t	103	40/40	0.88	0.23	2.07	36,47,60,63	0
23	LMG	D	409	51/55	0.91	0.20	2.06	39,61,82,88	0
28	PL9	a	713	55/55	0.86	0.25	2.01	57,68,77,84	0
25	CLA	b	607	65/65	0.86	0.26	1.99	48,63,81,91	0
25	CLA	c	513	65/65	0.87	0.24	1.85	57,68,82,96	0
30	UNL	d	401	22/-	0.82	0.23	1.85	39,54,63,66	0
29	SQD	A	614	40/54	0.84	0.22	1.73	47,59,68,72	0
23	LMG	C	520	51/55	0.78	0.27	1.64	43,74,86,89	0
28	PL9	D	406	55/55	0.91	0.22	1.64	31,43,52,55	0
27	BCR	B	618	40/40	0.93	0.18	1.62	37,52,60,63	0
27	BCR	d	404	40/40	0.90	0.23	1.58	45,59,70,77	0
25	CLA	D	404	65/65	0.89	0.22	1.51	34,44,80,84	0
27	BCR	b	602	40/40	0.89	0.22	1.50	45,53,70,76	0
27	BCR	k	102	40/40	0.86	0.26	1.49	53,65,81,84	0
33	DGD	c	517	62/66	0.89	0.22	1.46	54,61,81,92	0
23	LMG	d	408	40/55	0.79	0.24	1.46	47,61,84,89	0
27	BCR	B	619	40/40	0.93	0.20	1.45	35,47,51,52	0
27	BCR	k	101	40/40	0.84	0.24	1.43	53,69,78,78	0
28	PL9	d	405	55/55	0.93	0.20	1.38	32,41,53,56	0
25	CLA	C	514	65/65	0.86	0.24	1.37	44,73,81,89	0
30	UNL	a	717	7/-	0.84	0.26	1.31	48,53,61,67	0
27	BCR	b	623	40/40	0.92	0.19	1.23	42,53,60,61	0
25	CLA	A	607	65/65	0.93	0.19	1.15	31,46,91,99	0
25	CLA	C	513	65/65	0.88	0.23	1.13	52,66,80,86	0
23	LMG	a	701	51/55	0.85	0.23	1.13	42,64,87,90	0
23	LMG	a	715	51/55	0.82	0.24	1.07	47,65,85,91	0
32	LHG	D	408	49/49	0.92	0.21	1.05	42,59,72,84	0
25	CLA	C	505	65/65	0.89	0.22	1.05	48,63,71,79	0
25	CLA	b	613	65/65	0.92	0.19	1.04	37,44,55,58	0
30	UNL	B	624	11/-	0.92	0.20	1.02	34,49,52,53	0
23	LMG	f	101	51/55	0.90	0.20	1.02	48,58,84,93	0
29	SQD	f	102	41/54	0.87	0.30	0.99	54,73,85,89	0
27	BCR	c	514	40/40	0.89	0.25	0.98	61,67,74,75	0
23	LMG	M	101	51/55	0.88	0.20	0.92	34,58,74,77	0
25	CLA	c	503	65/65	0.90	0.21	0.92	48,61,68,73	0
25	CLA	B	606	65/65	0.93	0.18	0.91	37,45,52,53	0
27	BCR	b	624	40/40	0.90	0.20	0.90	38,49,58,59	0
26	PHO	a	710	64/64	0.93	0.22	0.89	38,46,55,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	CLA	B	602	65/65	0.87	0.21	0.89	44,62,75,80	0
25	CLA	C	509	65/65	0.92	0.21	0.88	46,55,91,100	0
33	DGD	c	518	62/66	0.92	0.19	0.88	44,57,76,81	0
25	CLA	B	609	65/65	0.93	0.25	0.84	32,45,51,59	0
25	CLA	c	505	65/65	0.92	0.19	0.76	41,52,60,69	0
30	UNL	m	102	12/-	0.91	0.19	0.76	41,47,50,52	0
32	LHG	d	406	49/49	0.94	0.19	0.73	32,53,61,65	0
27	BCR	Y	101	40/40	0.91	0.20	0.73	46,66,71,72	0
29	SQD	A	612	52/54	0.92	0.20	0.71	45,67,80,92	0
25	CLA	B	607	65/65	0.90	0.20	0.71	41,50,64,75	0
25	CLA	c	510	65/65	0.92	0.21	0.69	43,54,63,68	0
25	CLA	a	707	65/65	0.91	0.18	0.69	33,47,51,53	0
25	CLA	A	606	65/65	0.91	0.19	0.68	29,43,48,53	0
25	CLA	C	511	65/65	0.89	0.24	0.68	44,57,64,70	0
29	SQD	D	410	43/54	0.88	0.29	0.66	56,75,87,96	0
26	PHO	D	401	64/64	0.94	0.20	0.63	37,46,55,59	0
32	LHG	B	625	49/49	0.93	0.20	0.63	41,51,58,61	0
25	CLA	C	503	65/65	0.92	0.23	0.60	43,56,62,68	0
27	BCR	c	515	40/40	0.91	0.18	0.58	38,53,64,72	0
25	CLA	a	711	65/65	0.92	0.19	0.57	34,46,79,87	0
27	BCR	h	101	40/40	0.88	0.22	0.56	40,54,68,71	0
27	BCR	H	102	40/40	0.84	0.25	0.56	41,54,62,62	0
25	CLA	C	506	65/65	0.91	0.19	0.55	41,51,57,60	0
27	BCR	C	516	40/40	0.91	0.20	0.54	42,51,58,58	0
25	CLA	c	506	65/65	0.91	0.21	0.52	47,57,79,92	0
25	CLA	C	510	65/65	0.92	0.20	0.51	45,57,64,68	0
25	CLA	b	609	65/65	0.94	0.19	0.51	34,45,55,61	0
33	DGD	C	517	62/66	0.92	0.20	0.50	36,46,65,71	0
25	CLA	b	616	65/65	0.92	0.20	0.48	34,42,50,56	0
32	LHG	d	407	49/49	0.94	0.18	0.47	36,46,54,61	0
33	DGD	C	518	62/66	0.91	0.19	0.46	51,62,81,88	0
33	DGD	h	102	62/66	0.90	0.23	0.46	41,55,63,66	0
29	SQD	a	714	54/54	0.92	0.22	0.46	48,68,83,90	0
33	DGD	c	516	62/66	0.92	0.20	0.46	34,50,68,76	0
25	CLA	b	620	65/65	0.93	0.17	0.46	35,52,61,64	0
25	CLA	b	610	65/65	0.91	0.22	0.45	37,47,59,62	0
25	CLA	B	604	65/65	0.93	0.20	0.45	33,44,54,57	0
27	BCR	a	712	40/40	0.93	0.16	0.44	26,44,53,54	0
25	CLA	B	603	65/65	0.93	0.21	0.44	42,52,59,62	0
26	PHO	a	709	64/64	0.95	0.19	0.43	26,41,47,50	0
32	LHG	b	629	49/49	0.94	0.16	0.40	36,50,57,64	0
32	LHG	a	720	39/49	0.92	0.20	0.40	41,54,65,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	UNL	M	103	16/-	0.88	0.21	0.40	41,51,57,58	0
27	BCR	B	620	40/40	0.91	0.18	0.39	39,48,56,71	0
25	CLA	D	402	65/65	0.92	0.18	0.39	31,41,47,51	0
33	DGD	C	519	62/66	0.92	0.17	0.36	43,56,67,76	0
25	CLA	d	403	65/65	0.89	0.20	0.36	45,54,65,66	0
25	CLA	c	504	58/65	0.90	0.19	0.36	52,59,66,67	0
25	CLA	B	608	65/65	0.93	0.17	0.35	30,42,52,56	0
25	CLA	C	507	65/65	0.91	0.20	0.35	44,55,75,88	0
25	CLA	B	611	65/65	0.94	0.19	0.34	40,47,55,60	0
25	CLA	b	612	65/65	0.91	0.17	0.31	32,46,56,69	0
25	CLA	A	609	54/65	0.94	0.16	0.29	34,43,60,71	0
25	CLA	C	502	65/65	0.93	0.20	0.29	38,50,57,64	0
27	BCR	b	625	40/40	0.92	0.16	0.28	36,49,55,58	0
25	CLA	C	508	65/65	0.89	0.20	0.28	41,50,57,66	0
25	CLA	B	610	65/65	0.90	0.19	0.27	36,51,58,63	0
25	CLA	B	615	65/65	0.92	0.17	0.27	38,48,67,73	0
25	CLA	C	504	65/65	0.93	0.20	0.25	43,57,62,68	0
33	DGD	H	103	62/66	0.91	0.21	0.24	39,49,59,62	0
27	BCR	C	515	40/40	0.88	0.23	0.23	53,63,72,76	0
26	PHO	A	608	64/64	0.95	0.18	0.21	32,40,46,50	0
25	CLA	b	618	65/65	0.95	0.20	0.19	32,43,50,52	0
25	CLA	a	719	65/65	0.94	0.16	0.17	32,43,49,54	0
25	CLA	b	619	65/65	0.94	0.20	0.16	31,42,59,67	0
32	LHG	L	101	49/49	0.94	0.17	0.16	39,50,57,64	0
25	CLA	b	608	65/65	0.93	0.19	0.15	39,49,60,64	0
25	CLA	c	502	65/65	0.93	0.21	0.15	45,55,67,81	0
25	CLA	B	614	65/65	0.93	0.20	0.12	34,43,57,69	0
34	HEM	V	201	43/43	0.95	0.16	0.12	41,51,57,63	0
25	CLA	b	611	65/65	0.95	0.16	0.07	30,46,52,56	0
25	CLA	c	508	65/65	0.93	0.19	0.06	46,57,72,82	0
25	CLA	C	512	65/65	0.91	0.19	0.06	52,60,69,71	0
25	CLA	B	605	65/65	0.92	0.22	0.04	35,47,62,73	0
25	CLA	b	617	65/65	0.93	0.19	0.02	36,45,50,57	0
25	CLA	B	613	65/65	0.94	0.19	0.02	36,43,55,59	0
25	CLA	c	501	65/65	0.94	0.19	0.01	37,49,55,59	0
27	BCR	K	101	40/40	0.90	0.20	0.01	51,60,70,75	0
25	CLA	a	708	65/65	0.95	0.16	-0.02	37,47,89,101	0
25	CLA	b	615	65/65	0.92	0.17	-0.11	42,50,55,60	0
25	CLA	c	509	65/65	0.93	0.19	-0.12	49,57,70,73	0
25	CLA	D	403	65/65	0.94	0.16	-0.17	33,42,54,61	0
25	CLA	b	614	65/65	0.94	0.22	-0.17	39,48,58,60	0
25	CLA	d	402	65/65	0.93	0.16	-0.20	35,45,51,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	CLA	B	617	65/65	0.89	0.20	-0.25	39,52,80,84	0
34	HEM	E	102	43/43	0.93	0.21	-0.26	52,66,76,80	0
30	UNL	I	101	9/-	0.84	0.20	-0.26	44,52,61,61	0
25	CLA	B	612	65/65	0.93	0.19	-0.31	32,42,49,54	0
25	CLA	b	621	65/65	0.92	0.17	-0.40	38,49,55,60	0
25	CLA	c	507	65/65	0.93	0.17	-0.54	41,50,61,67	0
25	CLA	B	616	65/65	0.92	0.16	-0.56	42,51,60,64	0
27	BCR	A	610	40/40	0.94	0.15	-0.57	31,44,52,56	0
34	HEM	e	102	43/43	0.93	0.20	-0.58	60,71,81,91	0
25	CLA	b	622	47/65	0.93	0.16	-0.67	40,48,58,64	0
25	CLA	c	511	65/65	0.90	0.18	-0.74	50,62,71,74	0
34	HEM	v	201	43/43	0.95	0.15	-0.87	46,58,64,72	0
24	CL	A	605	1/1	0.94	0.14	-1.27	51,51,51,51	0
31	BCT	a	706	4/4	0.98	0.09	-1.49	50,56,56,59	0
31	BCT	A	615	4/4	0.97	0.10	-1.72	46,49,51,54	0
24	CL	a	705	1/1	0.97	0.12	-2.05	50,50,50,50	0
21	OEX	A	601	10/10	0.98	0.11	-2.11	42,54,59,60	0
21	OEX	a	702	10/10	0.97	0.11	-2.52	44,52,59,60	0
24	CL	a	704	1/1	0.93	0.12	-3.34	59,59,59,59	0
22	FE2	A	602	1/1	0.97	0.03	-3.97	60,60,60,60	0
24	CL	A	604	1/1	0.99	0.06	-5.11	39,39,39,39	0
22	FE2	a	703	1/1	0.95	0.03	-7.24	60,60,60,60	0
30	UNL	j	101	9/-	0.85	0.24	-	52,61,65,65	0
30	UNL	a	718	13/-	0.85	0.21	-	45,54,61,62	0
30	UNL	i	101	22/-	0.85	0.22	-	36,50,58,62	0
30	UNL	M	102	6/-	0.88	0.31	-	45,51,51,53	0
30	UNL	m	101	5/-	0.88	0.23	-	36,39,42,45	0
30	UNL	a	716	4/-	0.82	0.31	-	31,46,50,51	0
30	UNL	B	622	6/-	0.85	0.26	-	40,51,56,56	0
30	UNL	B	601	12/-	0.85	0.18	-	31,49,56,56	0
30	UNL	b	603	11/-	0.83	0.24	-	44,54,62,62	0
30	UNL	A	613	7/-	0.89	0.18	-	34,49,53,55	0
23	LMG	b	628	9/55	0.87	0.22	-	36,50,54,54	0
30	UNL	H	101	8/-	0.87	0.18	-	43,53,58,64	0

6.5 Other polymers ⓘ

There are no such residues in this entry.