



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 19, 2016 – 09:42 PM EST

PDB ID : 5KAF  
Title : RT XFEL structure of Photosystem II in the dark state at 3.0 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 : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

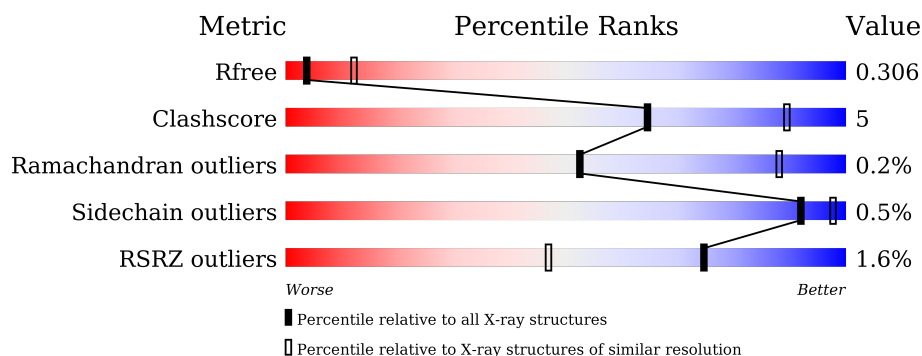
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.



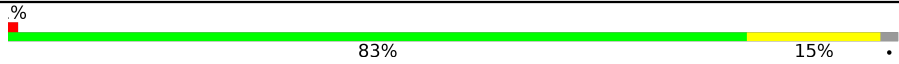
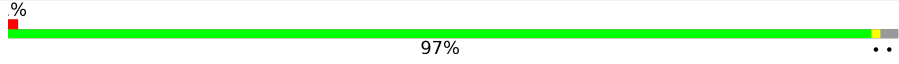
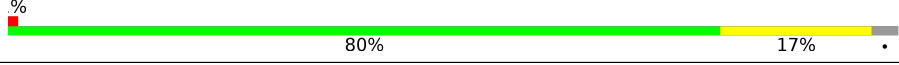
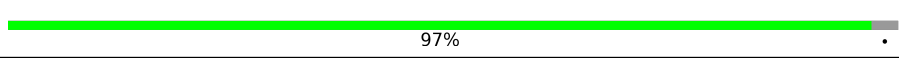
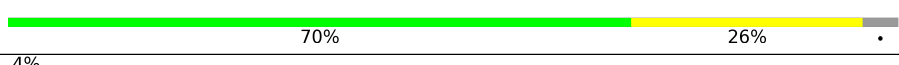
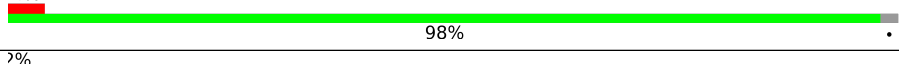
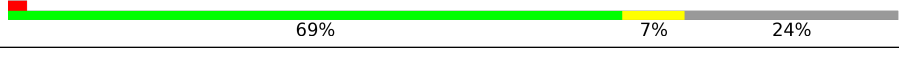

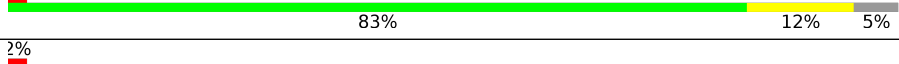
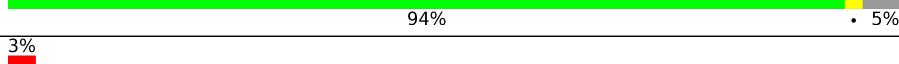

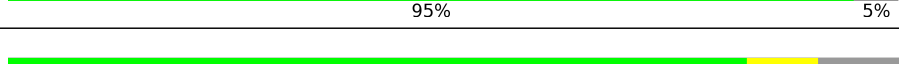
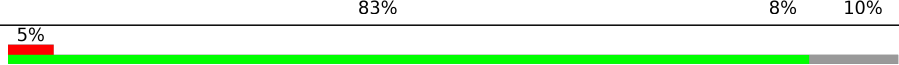
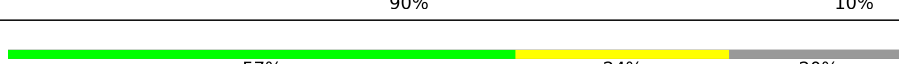

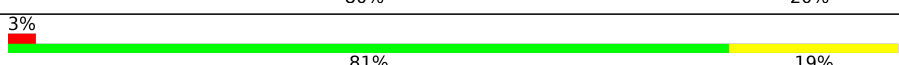
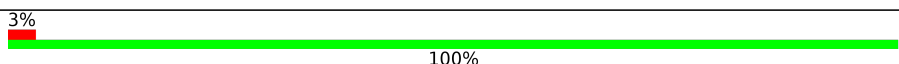
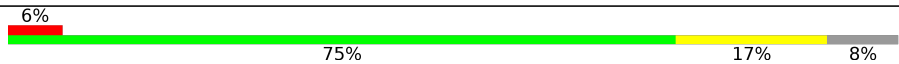
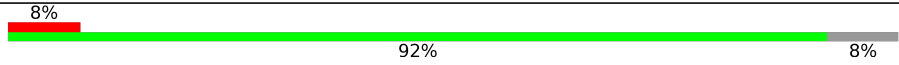

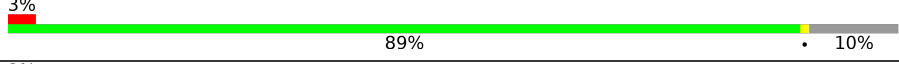
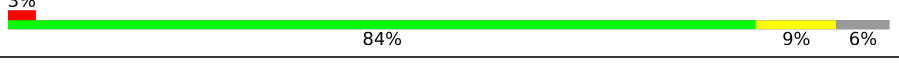
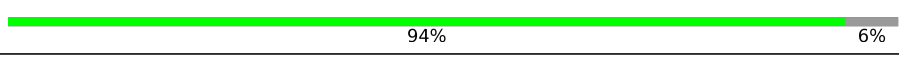


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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></div> <div>77%</div> <div>20%</div> <div>.</div> </div>
1	a	344	<div> <div></div> <div>97%</div> <div>..</div> </div>
2	B	510	<div> <div>2%</div> <div></div> <div>85%</div> <div>14%</div> <div>.</div> </div>
2	b	510	<div> <div>%</div> <div></div> <div>99%</div> <div>.</div> </div>

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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	66	
7	h	66	
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	SQD	A	619	-	-	-	X
23	SQD	I	101	-	-	-	X
23	SQD	b	601	-	-	-	X
23	SQD	c	501	-	-	-	X
25	CLA	A	606	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	609	X	-	-	-
25	CLA	A	615	X	-	-	-
25	CLA	B	601	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	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	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	D	402	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	a	606	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	609	X	-	-	-
25	CLA	a	612	X	-	-	-
25	CLA	b	604	X	-	-	X
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
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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	-	-	-
25	CLA	b	619	X	-	-	-
25	CLA	c	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	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	c	515	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	d	404	X	-	-	-
27	BCR	B	627	-	-	-	X
27	BCR	T	101	-	-	-	X
27	BCR	b	622	-	-	-	X
28	PL9	A	611	-	-	-	X
28	PL9	a	611	-	-	-	X
29	LMG	A	612	-	-	-	X
29	LMG	A	613	-	-	-	X
29	LMG	B	621	-	-	-	X
29	LMG	B	625	-	-	-	X
29	LMG	C	520	-	-	-	X
29	LMG	D	405	-	-	-	X
29	LMG	b	623	-	-	-	X
29	LMG	b	624	-	-	-	X
29	LMG	c	502	-	-	-	X
29	LMG	c	521	-	-	-	X
29	LMG	c	522	-	-	-	X
29	LMG	d	409	-	-	-	X
30	UNL	C	521	-	-	-	X
30	UNL	b	602	-	-	-	X
30	UNL	b	603	-	-	-	X
30	UNL	d	402	-	-	-	X
30	UNL	t	101	-	-	-	X
31	LHG	A	617	-	-	-	X
31	LHG	A	618	-	-	-	X
31	LHG	a	615	-	-	-	X
33	DGD	c	520	-	-	-	X
33	DGD	h	102	-	-	-	X

## 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50162 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
			2618	1715	431	457	15			
1	a	334	Total	C	N	O	S	0	0	0
			2613	1713	428	457	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
			3953	2596	658	686	13			
2	b	504	Total	C	N	O	S	3	1	0
			3960	2600	658	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
			2709	1798	441	458	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	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
			274	187	45	41	1			
6	f	34	Total	C	N	O	S	0	0	0
			274	187	45	41	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	0	0	0
			301	200	48	53			
11	l	37	Total	C	N	O	0	0	0
			301	200	48	53			

- 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
			256	171	37	47	1			
12	m	33	Total	C	N	O	S	0	0	0
			256	171	37	47	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
			1845	1154	309	378	4			
13	o	244	Total	C	N	O	S	0	0	0
			1853	1160	312	377	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	30	Total	C	N	O	S	0	0	0
			224	147	38	36	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
			279	187	45	47				
18	x	38	Total	C	N	O		0	0	0
			281	188	45	48				

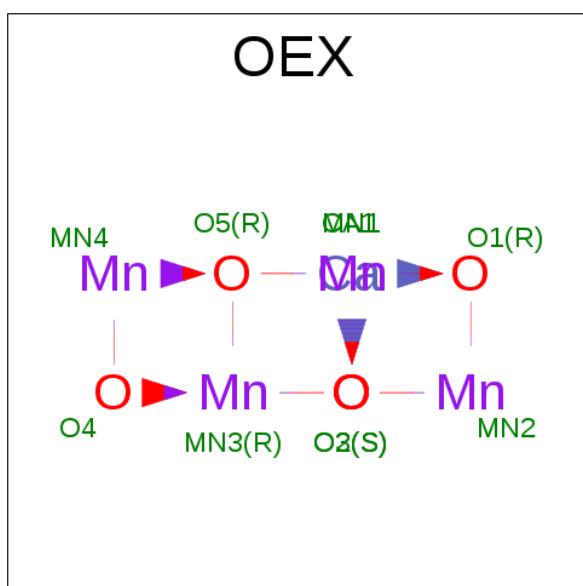
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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
			479	328	72	77	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
			273	186	47	40				

- Molecule 21 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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).

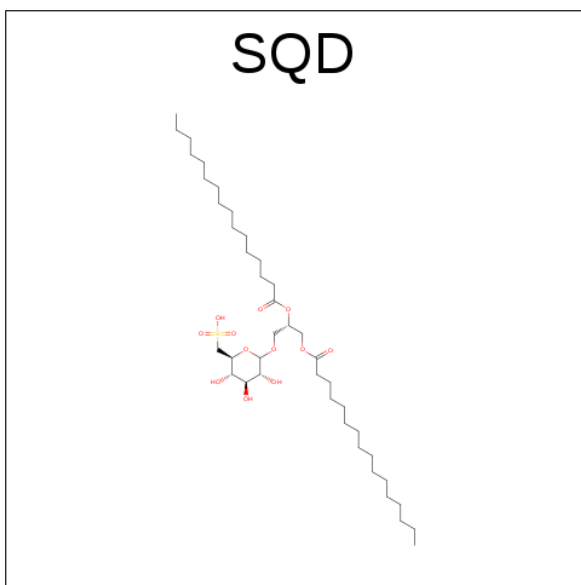
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	1	Total	Fe	0	0
			1	1		

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

- Molecule 23 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).

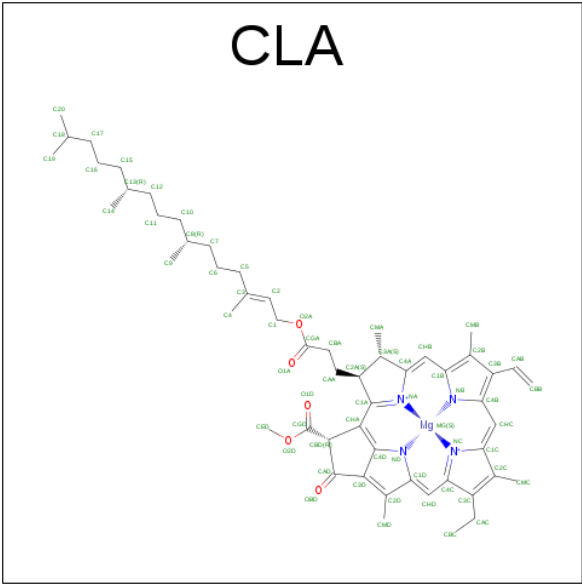


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	O	S	0	0
			52	39	12	1		
23	A	1	Total	C	O		0	0
			40	35	5			
23	B	1	Total	C	O	S	0	0
			54	41	12	1		
23	D	1	Total	C	O	S	0	0
			47	34	12	1		
23	D	1	Total	C	O	S	0	0
			43	30	12	1		
23	I	1	Total	C	O		0	0
			40	35	5			
23	b	1	Total	C	O	S	0	0
			54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

- 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: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C Mg N O 65 55 1 4 5	0	0
25	A	1	Total C Mg N O 57 47 1 4 5	0	0
25	A	1	Total C Mg N O 65 55 1 4 5	0	0
25	A	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 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	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	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	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 59	C 49	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
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

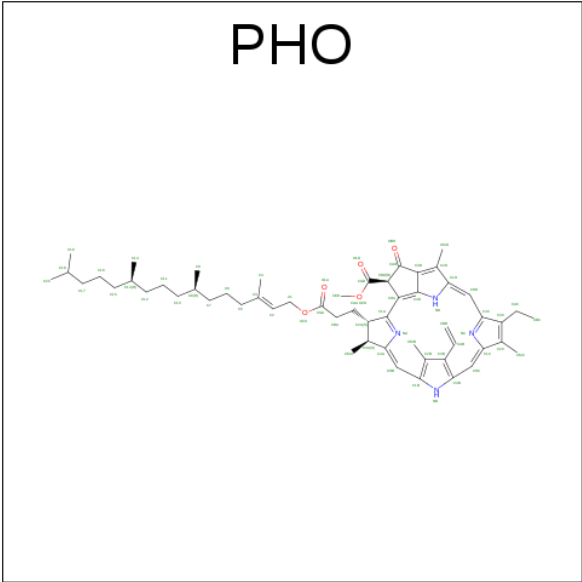
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65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

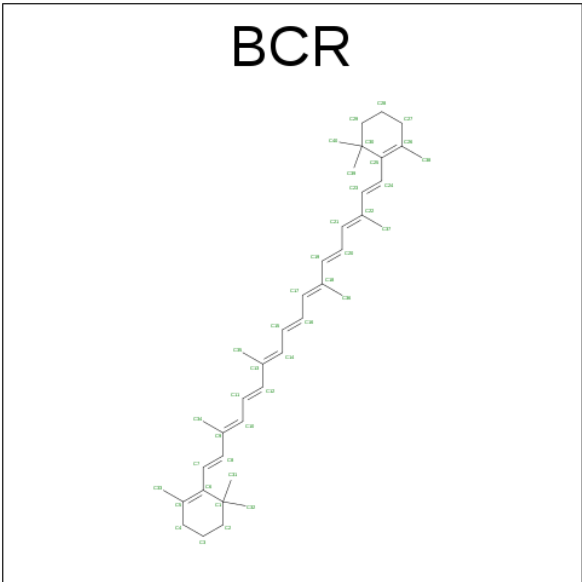
- Molecule 26 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).





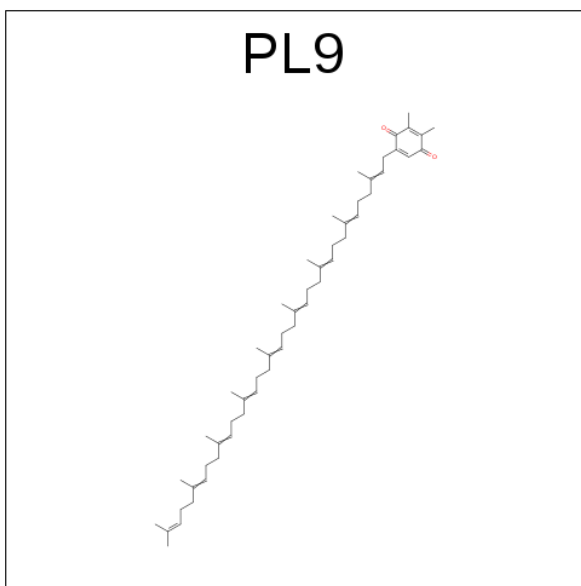
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	N	O	0	0
			64	55	4	5		
26	D	1	Total	C	N	O	0	0
			64	55	4	5		
26	a	1	Total	C	N	O	0	0
			64	55	4	5		
26	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



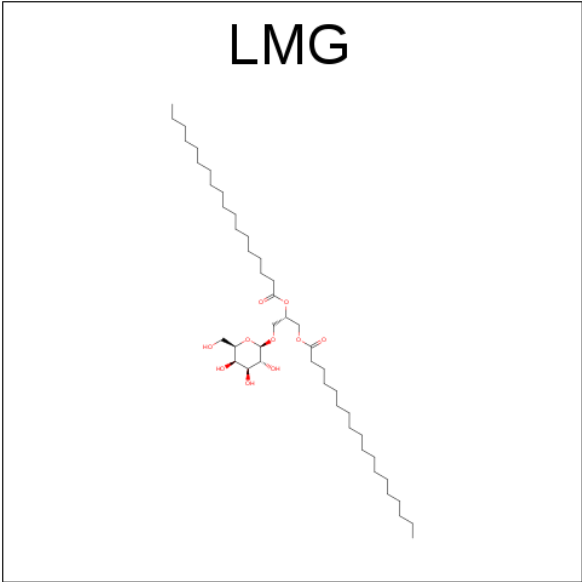
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			51	41	10		
29	A	1	Total	C	O	0	0
			51	41	10		
29	B	1	Total	C	O	0	0
			51	41	10		
29	B	1	Total	C	O	0	0
			51	41	10		
29	B	1	Total	C	O	0	0
			51	41	10		
29	C	1	Total	C	O	0	0
			51	41	10		
29	C	1	Total	C	O	0	0
			51	41	10		
29	D	1	Total	C	O	0	0
			51	41	10		
29	b	1	Total	C	O	0	0
			51	41	10		
29	b	1	Total	C	O	0	0
			51	41	10		
29	b	1	Total	C		0	0
			9	9			
29	c	1	Total	C	O	0	0
			51	41	10		
29	c	1	Total	C	O	0	0
			51	41	10		
29	c	1	Total	C	O	0	0
			51	41	10		

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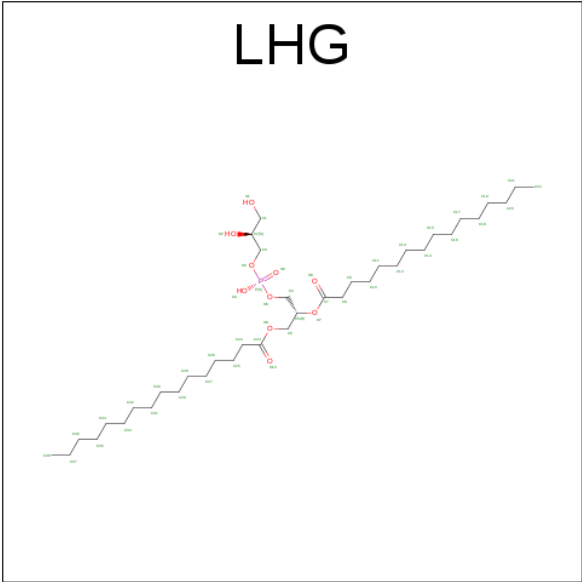
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	d	1	Total	C	O	0	0
			42	32	10		
29	d	1	Total	C	O	0	0
			40	35	5		

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

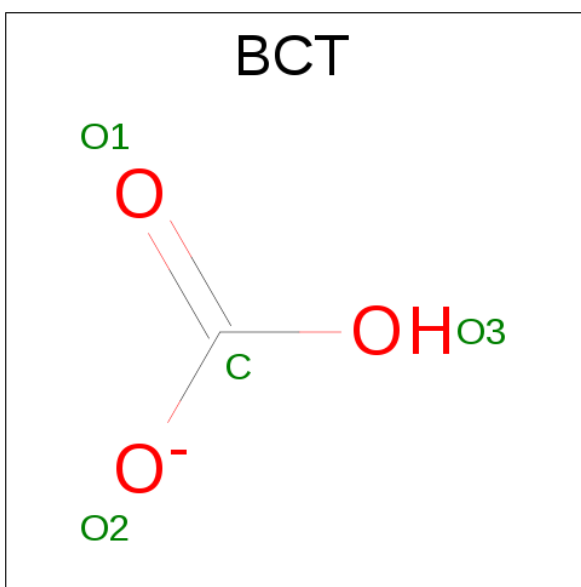
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	j	1	Total	C		0	0
			9	9			
30	d	1	Total	C		0	0
			22	22			
30	H	1	Total	C		0	0
			8	8			
30	B	3	Total	C		0	0
			28	28			
30	i	1	Total	C		0	0
			12	12			
30	C	1	Total	C		0	0
			9	9			
30	z	1	Total	C		0	0
			11	11			
30	A	1	Total	C		0	0
			7	7			
30	t	1	Total	C		0	0
			10	10			
30	m	2	Total	C		0	0
			21	21			
30	b	2	Total	C		0	0
			26	26			
30	M	2	Total	C		0	0
			23	23			

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



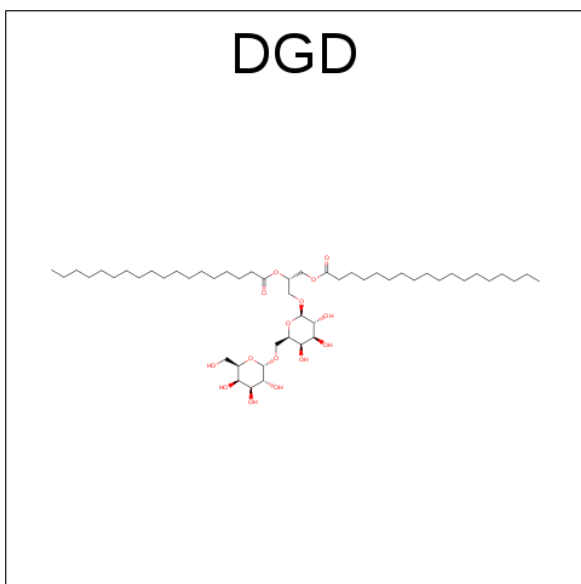
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	L	1	Total	C	O	P	0	0
			49	38	10	1		
31	a	1	Total	C	O	P	0	0
			49	38	10	1		
31	a	1	Total	C	O	P	0	0
			35	24	10	1		
31	a	1	Total	C	O	P	0	0
			42	31	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	l	1	Total	C	O	P	0	0
			49	38	10	1		

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



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

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



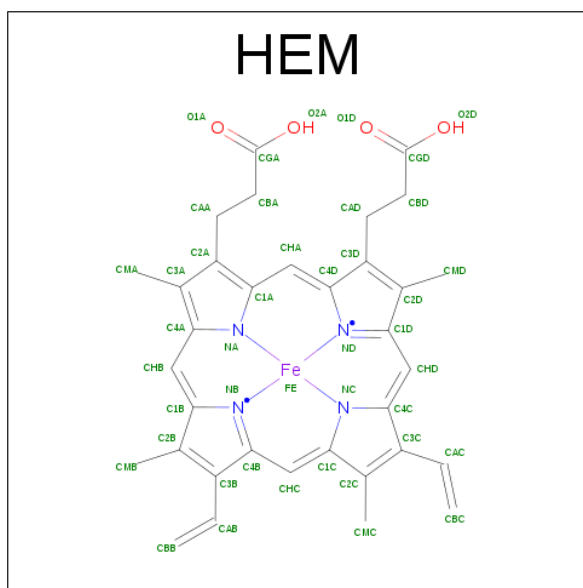
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			62	47	15		

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



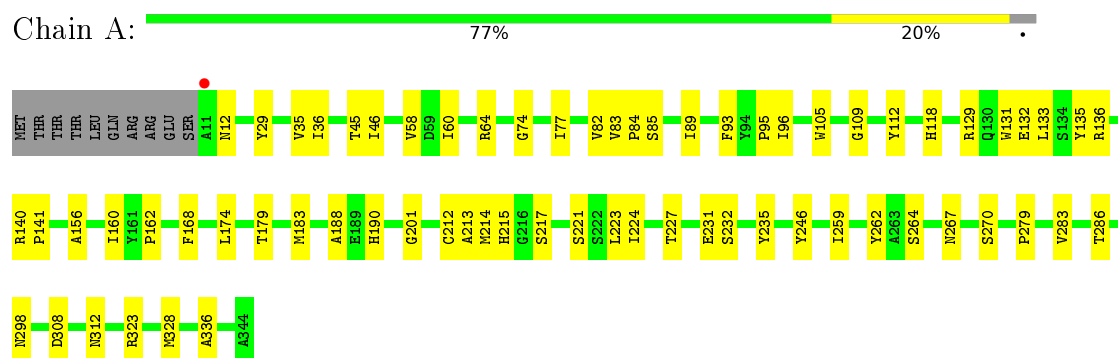
- Molecule 35 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	A	10	Total O 10 10	0	0
35	B	17	Total O 17 17	0	0
35	C	11	Total O 11 11	0	0
35	D	9	Total O 9 9	0	0
35	E	3	Total O 3 3	0	0
35	L	2	Total O 2 2	0	0
35	M	2	Total O 2 2	0	0
35	O	5	Total O 5 5	0	0
35	T	1	Total O 1 1	0	0
35	V	2	Total O 2 2	0	0
35	X	1	Total O 1 1	0	0
35	Z	1	Total O 1 1	0	0
35	a	11	Total O 11 11	0	0
35	b	12	Total O 12 12	0	0
35	c	11	Total O 11 11	0	0
35	d	9	Total O 9 9	0	0
35	i	1	Total O 1 1	0	0
35	l	2	Total O 2 2	0	0
35	o	9	Total O 9 9	0	0
35	u	2	Total O 2 2	0	0
35	v	3	Total O 3 3	0	0

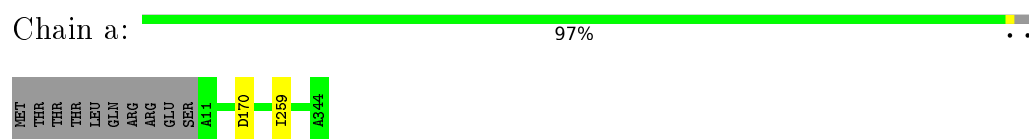
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

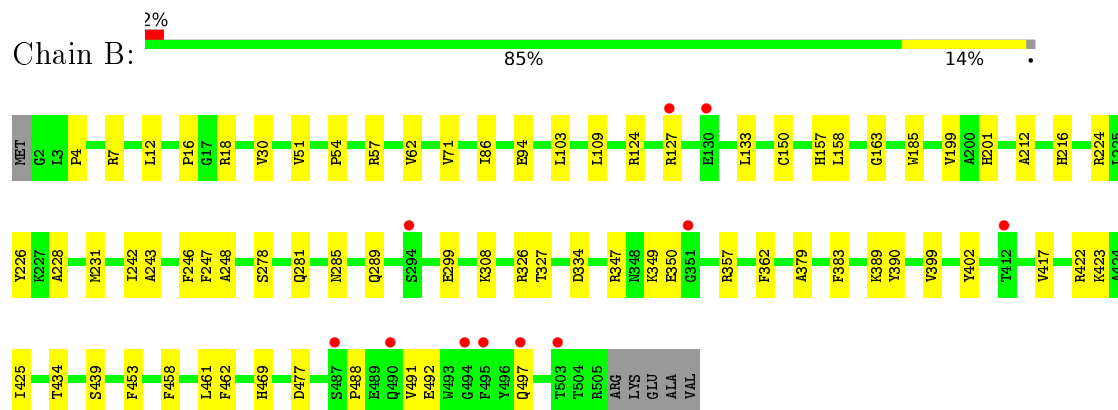
- Molecule 1: Photosystem II protein D1 1



- Molecule 1: Photosystem II protein D1 1

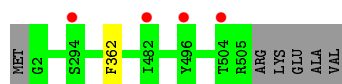


- Molecule 2: Photosystem II CP47 reaction center protein

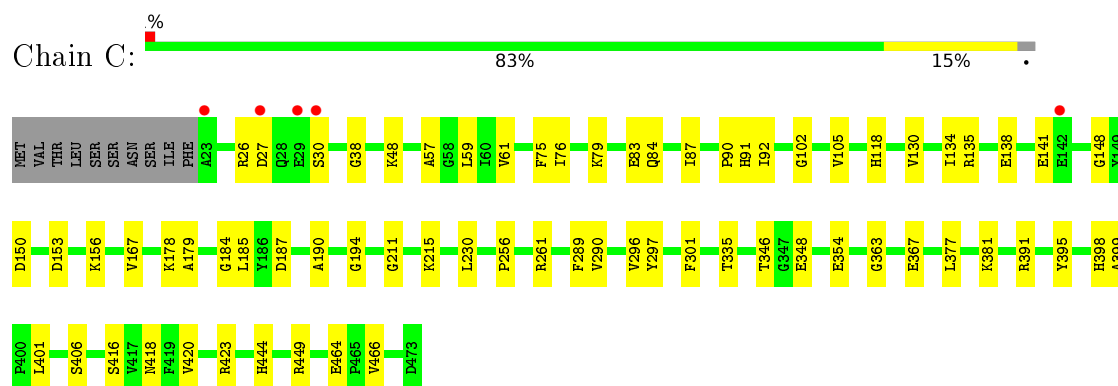


- Molecule 2: Photosystem II CP47 reaction center protein

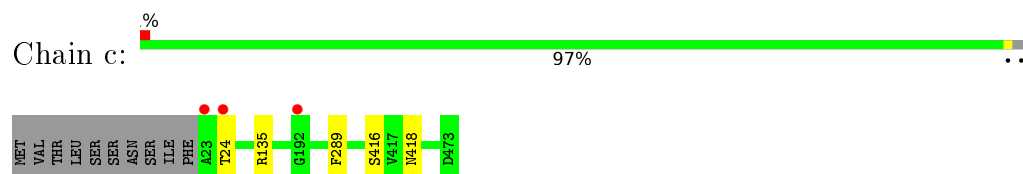




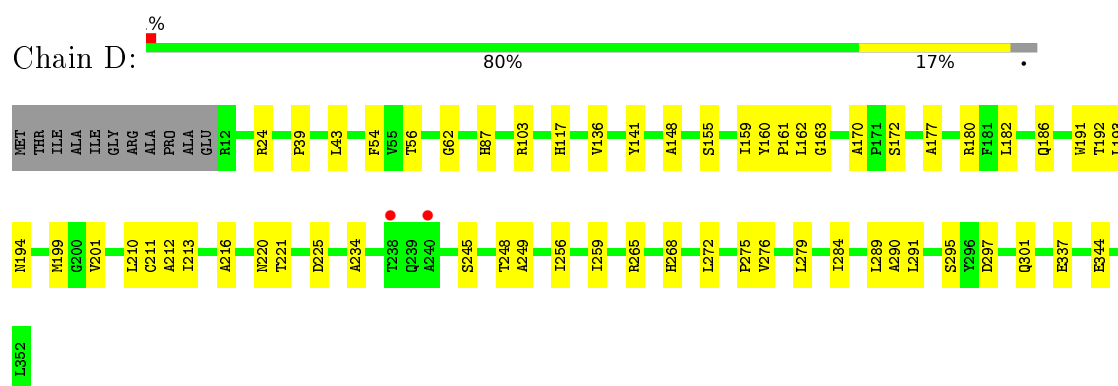
- Molecule 3: Photosystem II CP43 reaction center protein



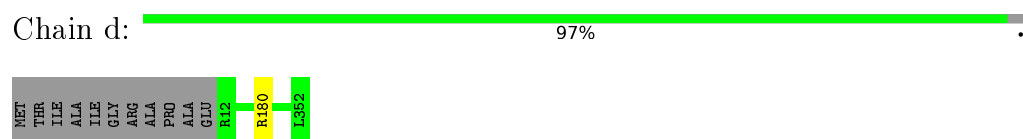
- Molecule 3: Photosystem II CP43 reaction center protein



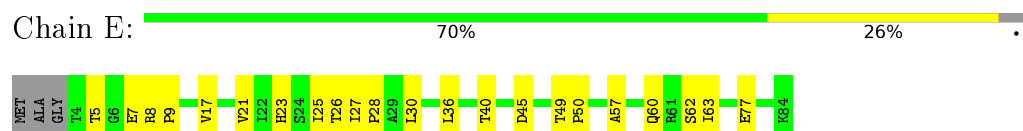
- Molecule 4: Photosystem II D2 protein



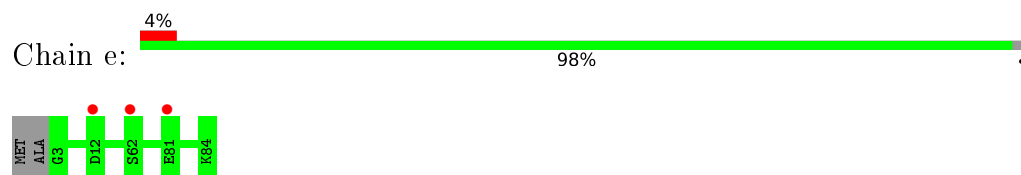
- Molecule 4: Photosystem II D2 protein



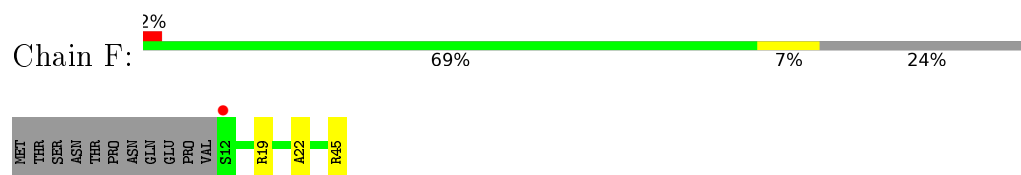
- Molecule 5: Cytochrome b559 subunit alpha



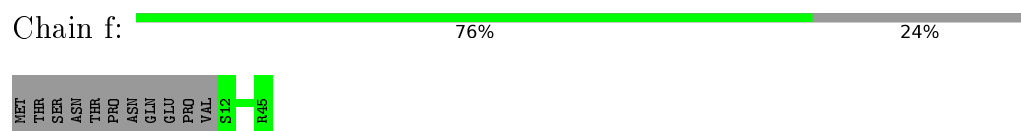
- Molecule 5: Cytochrome b559 subunit alpha



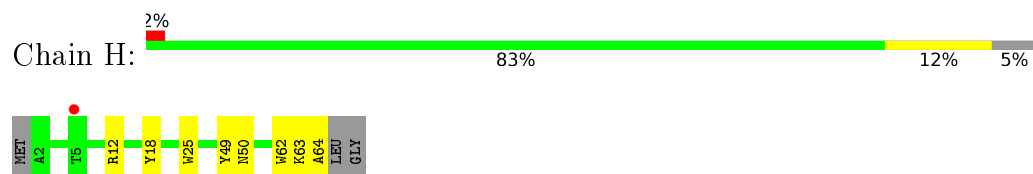
- Molecule 6: Cytochrome b559 subunit beta



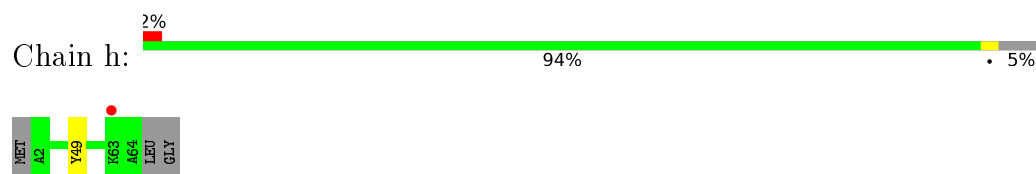
- Molecule 6: Cytochrome b559 subunit beta



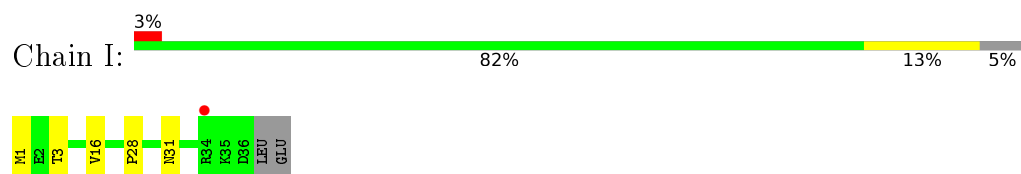
- Molecule 7: Photosystem II reaction center protein H



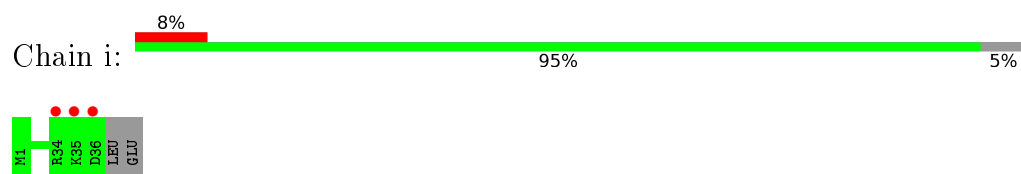
- Molecule 7: Photosystem II reaction center protein H




- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I

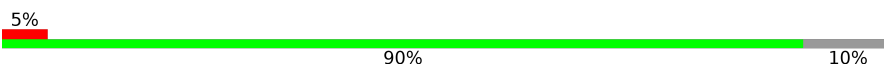


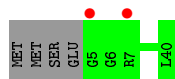
- Molecule 9: Photosystem II reaction center protein J

Chain J:  83% 8% 10%



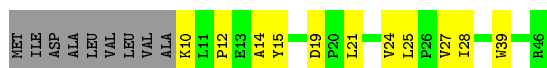
- Molecule 9: Photosystem II reaction center protein J

Chain j:  5% 90% 10%




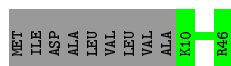
- Molecule 10: Photosystem II reaction center protein K

Chain K:  57% 24% 20%




- Molecule 10: Photosystem II reaction center protein K

Chain k:  80% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  3% 81% 19%




- Molecule 11: Photosystem II reaction center protein L

Chain l:  3% 100%



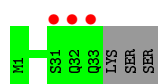
- Molecule 12: Photosystem II reaction center protein M

Chain M:  6% 75% 17% 8%

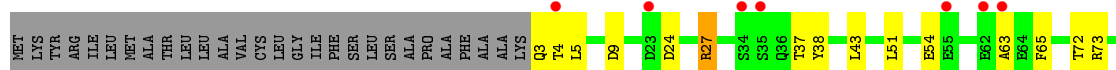
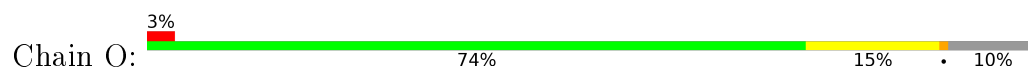


- Molecule 12: Photosystem II reaction center protein M

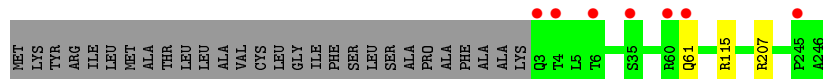
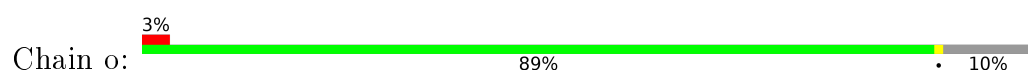
Chain m:  8% 92% 8%



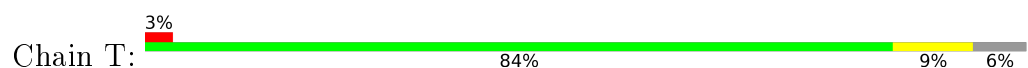
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



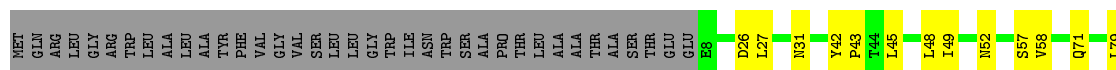
- Molecule 14: Photosystem II reaction center protein T



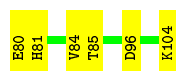
- Molecule 14: Photosystem II reaction center protein T

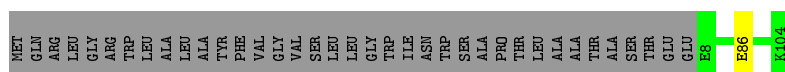


- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein

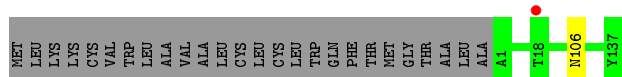
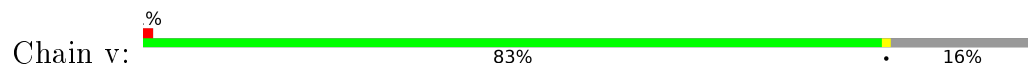




• Molecule 16: Cytochrome c-550



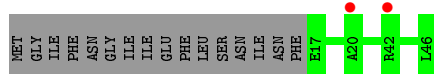
• Molecule 16: Cytochrome c-550



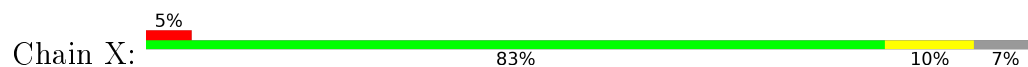
• Molecule 17: Photosystem II reaction center protein Ycf12



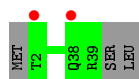
• Molecule 17: Photosystem II reaction center protein Ycf12



• Molecule 18: Photosystem II reaction center X protein

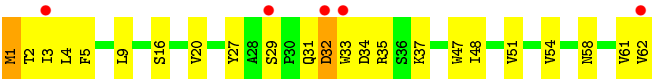


• Molecule 18: Photosystem II reaction center X protein



• Molecule 19: Photosystem II reaction center protein Z





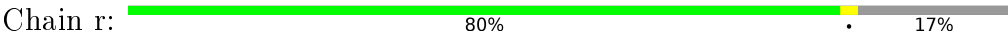
• Molecule 19: Photosystem II reaction center protein Z



• 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, $\alpha$ , $\beta$ , $\gamma$	117.73Å 223.81Å 330.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.12 – 3.00 43.12 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (43.12-3.00) 86.3 (43.12-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_2411)	Depositor
R, $R_{free}$	0.264 , 0.303 0.267 , 0.306	Depositor DCC
$R_{free}$ test set	1446 reflections (0.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.2	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 56.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	50162	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.24	0/2703	0.39	0/3687
1	a	0.24	0/2698	0.39	0/3681
2	B	0.25	0/4093	0.39	0/5580
2	b	0.25	0/4103	0.39	0/5593
3	C	0.24	0/3599	0.39	0/4900
3	c	0.24	0/3599	0.38	0/4900
4	D	0.25	0/2811	0.39	0/3830
4	d	0.25	0/2804	0.39	0/3821
5	E	0.30	0/676	0.39	0/924
5	e	0.23	0/684	0.39	0/933
6	F	0.24	0/283	0.37	0/386
6	f	0.24	0/283	0.37	0/386
7	H	0.24	0/511	0.41	0/697
7	h	0.24	0/511	0.40	0/697
8	I	0.24	0/293	0.37	0/396
8	i	0.25	0/293	0.38	0/396
9	J	0.24	0/263	0.37	0/356
9	j	0.24	0/263	0.38	0/356
10	K	0.25	0/303	0.40	0/416
10	k	0.25	0/303	0.37	0/416
11	L	0.24	0/308	0.37	0/419
11	l	0.23	0/308	0.36	0/419
12	M	0.24	0/249	0.35	0/341
12	m	0.24	0/249	0.35	0/341
13	O	0.24	0/1876	0.45	0/2549
13	o	0.24	0/1884	0.45	0/2557
14	T	0.26	0/257	0.35	0/349
14	t	0.26	0/257	0.36	0/349
15	U	0.23	0/785	0.40	0/1064
15	u	0.24	0/785	0.41	0/1064
16	V	0.23	0/1085	0.40	0/1473
16	v	0.22	0/1085	0.41	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	Y	0.27	0/225	0.54	0/301
17	y	0.24	0/225	0.37	0/301
18	X	0.23	0/282	0.35	0/381
18	x	0.24	0/284	0.37	0/384
19	Z	0.23	0/490	0.34	0/669
19	z	0.24	0/490	0.36	0/669
20	R	0.21	0/279	0.36	0/383
20	r	0.22	0/279	0.39	0/383
All	All	0.24	0/42758	0.39	0/58220

There are no bond length outliers.

There are no bond angle outliers.

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	2618	0	2515	55	0
1	a	2613	0	2506	0	0
2	B	3953	0	3802	69	0
2	b	3960	0	3811	0	0
3	C	3486	0	3407	49	0
3	c	3486	0	3407	0	0
4	D	2716	0	2621	50	0
4	d	2709	0	2612	0	0
5	E	657	0	637	21	0
5	e	665	0	651	0	0
6	F	274	0	279	4	0
6	f	274	0	279	0	0
7	H	498	0	518	5	0
7	h	498	0	518	0	0
8	I	296	0	311	3	0
8	i	296	0	311	0	0
9	J	257	0	268	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	257	0	268	0	0
10	K	293	0	305	10	0
10	k	293	0	305	0	0
11	L	301	0	309	8	0
11	l	301	0	309	0	0
12	M	256	0	269	5	0
12	m	256	0	269	0	0
13	O	1845	0	1793	25	0
13	o	1853	0	1817	0	0
14	T	258	0	261	5	0
14	t	258	0	261	0	0
15	U	774	0	773	10	0
15	u	774	0	773	0	0
16	V	1064	0	1073	11	0
16	v	1064	0	1073	0	0
17	Y	224	0	252	8	0
17	y	224	0	252	0	0
18	X	279	0	307	3	0
18	x	281	0	312	0	0
19	Z	479	0	516	15	0
19	z	479	0	516	0	0
20	R	273	0	305	10	0
20	r	273	0	305	0	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	92	0	138	3	0
23	B	54	0	78	7	0
23	D	90	0	111	1	0
23	I	40	0	67	0	0
23	b	54	0	77	0	0
23	c	54	0	78	0	0
23	f	43	0	53	0	0
24	A	2	0	0	0	0
24	a	2	0	0	0	0
25	A	252	0	269	17	0
25	B	1040	0	1152	63	0
25	C	845	0	936	50	0
25	D	130	0	144	11	0
25	a	254	0	274	0	0
25	b	1040	0	1152	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	7	0
26	a	64	0	74	0	0
26	d	64	0	74	0	0
27	A	40	0	56	5	0
27	B	160	0	224	11	0
27	C	80	0	112	4	0
27	D	40	0	56	3	0
27	H	40	0	56	4	0
27	K	40	0	56	3	0
27	T	40	0	56	6	0
27	Y	40	0	56	4	0
27	a	40	0	56	0	0
27	b	120	0	168	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	40	0	56	0	0
27	y	40	0	56	0	0
28	A	55	0	80	7	0
28	D	55	0	80	2	0
28	a	55	0	80	0	0
28	d	55	0	80	0	0
29	A	102	0	144	2	0
29	B	153	0	216	4	0
29	C	102	0	144	3	0
29	D	51	0	72	2	0
29	b	111	0	158	0	0
29	c	153	0	216	0	0
29	d	82	0	115	0	0
30	A	7	0	0	0	0
30	B	28	0	0	0	0
30	C	9	0	0	0	0
30	H	8	0	0	0	0
30	M	23	0	0	0	0
30	b	26	0	0	0	0
30	d	22	0	0	0	0
30	i	12	0	0	0	0
30	j	9	0	0	0	0
30	m	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	t	10	0	0	0	0
30	z	11	0	0	0	0
31	A	147	0	222	12	0
31	D	49	0	74	1	0
31	L	49	0	74	7	0
31	a	126	0	171	0	0
31	d	49	0	74	0	0
31	l	49	0	74	0	0
32	A	4	0	1	1	0
32	a	4	0	1	0	0
33	C	186	0	246	5	0
33	H	62	0	82	2	0
33	c	186	0	246	0	0
33	h	62	0	82	0	0
34	E	43	0	30	4	0
34	V	43	0	30	2	0
34	e	43	0	30	0	0
34	v	43	0	30	0	0
35	A	10	0	0	0	0
35	B	17	0	0	0	0
35	C	11	0	0	0	0
35	D	9	0	0	0	0
35	E	3	0	0	0	0
35	L	2	0	0	0	0
35	M	2	0	0	0	0
35	O	5	0	0	0	0
35	T	1	0	0	0	0
35	V	2	0	0	0	0
35	X	1	0	0	0	0
35	Z	1	0	0	0	0
35	a	11	0	0	0	0
35	b	12	0	0	0	0
35	c	11	0	0	0	0
35	d	9	0	0	0	0
35	i	1	0	0	0	0
35	l	2	0	0	0	0
35	o	9	0	0	0	0
35	u	2	0	0	0	0
35	v	3	0	0	0	0
All	All	50162	0	51048	448	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 5.

The worst 5 of 448 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:HIS:HE1	25:B:606:CLA:NA	1.76	0.83
31:A:618:LHG:HC31	5:E:9:PRO:HB3	1.61	0.81
31:A:616:LHG:O4	4:D:141:TYR:OH	1.98	0.80
25:A:607:CLA:HAB	25:D:403:CLA:H72	28.85	0.74
29:C:519:LMG:H191	10:K:27:VAL:HG11	1.70	0.74

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	332/344 (96%)	320 (96%)	11 (3%)	1 (0%)	46	84
1	a	332/344 (96%)	320 (96%)	11 (3%)	1 (0%)	46	84
2	B	502/510 (98%)	483 (96%)	19 (4%)	0	100	100
2	b	503/510 (99%)	486 (97%)	17 (3%)	0	100	100
3	C	449/461 (97%)	436 (97%)	12 (3%)	1 (0%)	52	88
3	c	449/461 (97%)	430 (96%)	17 (4%)	2 (0%)	39	80
4	D	339/352 (96%)	328 (97%)	11 (3%)	0	100	100
4	d	339/352 (96%)	324 (96%)	15 (4%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	78 (98%)	2 (2%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	61/66 (92%)	57 (93%)	3 (5%)	1 (2%)	12	48
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	I	34/38 (90%)	32 (94%)	2 (6%)	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%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	M	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
12	m	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
13	O	242/272 (89%)	228 (94%)	14 (6%)	0	100	100
13	o	242/272 (89%)	232 (96%)	9 (4%)	1 (0%)	39	80
14	T	28/32 (88%)	27 (96%)	1 (4%)	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%)	90 (95%)	5 (5%)	0	100	100
16	V	135/163 (83%)	128 (95%)	7 (5%)	0	100	100
16	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
17	Y	28/46 (61%)	25 (89%)	2 (7%)	1 (4%)	4	24
17	y	28/46 (61%)	28 (100%)	0	0	100	100
18	X	36/41 (88%)	36 (100%)	0	0	100	100
18	x	36/41 (88%)	32 (89%)	4 (11%)	0	100	100
19	Z	60/62 (97%)	55 (92%)	3 (5%)	2 (3%)	5	26
19	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
20	R	32/41 (78%)	32 (100%)	0	0	100	100
20	r	32/41 (78%)	32 (100%)	0	0	100	100
All	All	5240/5700 (92%)	5040 (96%)	190 (4%)	10 (0%)	52	88

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	Y	18	VAL
19	Z	32	ASP

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Mol	Chain	Res	Type
13	o	61	GLN
3	C	416	SER
7	H	63	LYS

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/280 (96%)	269 (100%)	0	100	100
1	a	268/280 (96%)	267 (100%)	1 (0%)	93	98
2	B	398/407 (98%)	397 (100%)	1 (0%)	94	98
2	b	400/407 (98%)	399 (100%)	1 (0%)	94	98
3	C	352/362 (97%)	350 (99%)	2 (1%)	90	97
3	c	352/362 (97%)	349 (99%)	3 (1%)	84	95
4	D	276/283 (98%)	275 (100%)	1 (0%)	93	98
4	d	274/283 (97%)	273 (100%)	1 (0%)	93	98
5	E	71/73 (97%)	71 (100%)	0	100	100
5	e	72/73 (99%)	72 (100%)	0	100	100
6	F	27/39 (69%)	27 (100%)	0	100	100
6	f	27/39 (69%)	27 (100%)	0	100	100
7	H	53/55 (96%)	52 (98%)	1 (2%)	65	90
7	h	53/55 (96%)	52 (98%)	1 (2%)	65	90
8	I	32/34 (94%)	32 (100%)	0	100	100
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
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	34/35 (97%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	28/32 (88%)	28 (100%)	0	100	100
12	m	28/32 (88%)	28 (100%)	0	100	100
13	O	200/228 (88%)	198 (99%)	2 (1%)	82	95
13	o	202/228 (89%)	200 (99%)	2 (1%)	82	95
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	94
16	V	117/138 (85%)	117 (100%)	0	100	100
16	v	117/138 (85%)	116 (99%)	1 (1%)	84	95
17	Y	23/37 (62%)	23 (100%)	0	100	100
17	y	23/37 (62%)	23 (100%)	0	100	100
18	X	30/34 (88%)	30 (100%)	0	100	100
18	x	31/34 (91%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	65	90
19	z	52/52 (100%)	51 (98%)	1 (2%)	65	90
20	R	29/33 (88%)	29 (100%)	0	100	100
20	r	29/33 (88%)	28 (97%)	1 (3%)	44	81
All	All	4313/4654 (93%)	4292 (100%)	21 (0%)	92	98

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	362	PHE
3	c	289	PHE
15	u	86	GLU
1	a	170	ASP
16	v	106	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
19	Z	31	GLN

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Mol	Chain	Res	Type
2	b	216	HIS
12	m	5	GLN
13	O	196	GLN
4	d	332	GLN

### 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	0.79	0	5,9,11	0.88	0
12	FME	M	1	12	8,9,10	0.87	0	5,9,11	0.82	0
14	FME	T	1	14	8,9,10	0.86	0	5,9,11	0.92	0
8	FME	i	1	8	8,9,10	0.86	0	5,9,11	0.88	0
12	FME	m	1	12	8,9,10	0.86	0	5,9,11	0.92	0
14	FME	t	1	14	8,9,10	0.87	0	5,9,11	0.91	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	1	FME	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 174 ligands modelled in this entry, 17 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	SQD	A	603	-	51,52,54	0.96	4 (7%)	60,63,65	1.93	11 (18%)
25	CLA	A	606	-	57,73,73	1.13	5 (8%)	61,113,113	1.17	5 (8%)
25	CLA	A	607	35	49,65,73	1.23	5 (10%)	51,103,113	1.18	5 (9%)
26	PHO	A	608	-	67,69,69	1.24	9 (13%)	86,99,99	1.06	7 (8%)
25	CLA	A	609	-	57,73,73	1.13	5 (8%)	61,113,113	1.12	6 (9%)
27	BCR	A	610	-	41,41,41	1.12	2 (4%)	56,56,56	1.20	5 (8%)
28	PL9	A	611	-	54,55,55	0.86	2 (3%)	68,69,69	1.45	14 (20%)
29	LMG	A	612	-	51,51,55	0.71	0	59,59,63	1.31	6 (10%)
29	LMG	A	613	-	51,51,55	0.70	0	59,59,63	1.51	8 (13%)
25	CLA	A	615	35	57,73,73	1.14	4 (7%)	61,113,113	1.10	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LHG	A	616	-	48,48,48	0.61	0	49,54,54	1.28	6 (12%)
31	LHG	A	617	-	48,48,48	0.60	0	49,54,54	1.25	6 (12%)
31	LHG	A	618	-	48,48,48	0.65	1 (2%)	49,54,54	1.25	7 (14%)
23	SQD	A	619	-	39,39,54	0.86	2 (5%)	41,41,65	1.17	2 (4%)
32	BCT	A	620	22	0,3,3	0.00	-	0,3,3	0.00	-
25	CLA	B	601	35	57,73,73	1.14	4 (7%)	61,113,113	1.11	6 (9%)
25	CLA	B	602	-	57,73,73	1.14	5 (8%)	61,113,113	1.08	5 (8%)
25	CLA	B	603	-	57,73,73	1.14	5 (8%)	61,113,113	1.10	6 (9%)
25	CLA	B	604	-	57,73,73	1.14	4 (7%)	61,113,113	1.17	7 (11%)
25	CLA	B	605	-	57,73,73	1.15	5 (8%)	61,113,113	1.09	5 (8%)
25	CLA	B	606	-	57,73,73	1.14	4 (7%)	61,113,113	1.14	7 (11%)
25	CLA	B	607	35	57,73,73	1.13	5 (8%)	61,113,113	1.09	5 (8%)
25	CLA	B	608	-	57,73,73	1.13	4 (7%)	61,113,113	1.11	6 (9%)
25	CLA	B	609	-	57,73,73	1.14	4 (7%)	61,113,113	1.10	7 (11%)
25	CLA	B	610	35	57,73,73	1.14	4 (7%)	61,113,113	1.08	5 (8%)
25	CLA	B	611	-	57,73,73	1.14	4 (7%)	61,113,113	1.13	7 (11%)
25	CLA	B	612	-	57,73,73	1.13	4 (7%)	61,113,113	1.15	6 (9%)
25	CLA	B	613	-	57,73,73	1.13	4 (7%)	61,113,113	1.16	6 (9%)
25	CLA	B	614	-	57,73,73	1.13	4 (7%)	61,113,113	1.09	6 (9%)
25	CLA	B	615	-	57,73,73	1.15	4 (7%)	61,113,113	1.13	6 (9%)
25	CLA	B	616	-	57,73,73	1.13	6 (10%)	61,113,113	1.16	6 (9%)
27	BCR	B	617	-	41,41,41	1.16	2 (4%)	56,56,56	1.28	7 (12%)
27	BCR	B	618	-	41,41,41	1.12	2 (4%)	56,56,56	1.24	6 (10%)
27	BCR	B	619	-	41,41,41	1.12	2 (4%)	56,56,56	1.27	8 (14%)
29	LMG	B	620	-	51,51,55	0.72	0	59,59,63	1.34	7 (11%)
29	LMG	B	621	-	51,51,55	0.72	1 (1%)	59,59,63	1.39	8 (13%)
29	LMG	B	625	-	51,51,55	0.82	2 (3%)	59,59,63	1.42	8 (13%)
23	SQD	B	626	-	53,54,54	0.94	4 (7%)	62,65,65	1.93	12 (19%)
27	BCR	B	627	-	41,41,41	1.13	2 (4%)	56,56,56	1.29	8 (14%)
25	CLA	C	501	-	57,73,73	1.13	4 (7%)	61,113,113	1.12	6 (9%)
25	CLA	C	502	-	57,73,73	1.14	5 (8%)	61,113,113	1.11	5 (8%)
25	CLA	C	503	-	57,73,73	1.14	4 (7%)	61,113,113	1.11	6 (9%)
25	CLA	C	504	35	57,73,73	1.13	5 (8%)	61,113,113	1.11	6 (9%)
25	CLA	C	505	-	57,73,73	1.14	4 (7%)	61,113,113	1.12	7 (11%)
25	CLA	C	506	-	57,73,73	1.14	4 (7%)	61,113,113	1.10	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	C	507	35	57,73,73	1.13	4 (7%)	61,113,113	1.14	7 (11%)
25	CLA	C	508	-	57,73,73	1.14	5 (8%)	61,113,113	1.12	6 (9%)
25	CLA	C	509	-	57,73,73	1.13	4 (7%)	61,113,113	1.14	6 (9%)
25	CLA	C	510	-	57,73,73	1.14	4 (7%)	61,113,113	1.11	5 (8%)
25	CLA	C	511	3	57,73,73	1.14	4 (7%)	61,113,113	1.13	6 (9%)
25	CLA	C	512	-	57,73,73	1.13	4 (7%)	61,113,113	1.16	7 (11%)
25	CLA	C	513	-	57,73,73	1.14	4 (7%)	61,113,113	1.10	6 (9%)
27	BCR	C	514	-	41,41,41	1.14	2 (4%)	56,56,56	1.26	7 (12%)
27	BCR	C	515	-	41,41,41	1.14	2 (4%)	56,56,56	1.24	7 (12%)
33	DGD	C	516	-	63,63,67	0.84	1 (1%)	77,77,81	1.43	7 (9%)
33	DGD	C	517	-	63,63,67	0.89	1 (1%)	77,77,81	1.37	8 (10%)
33	DGD	C	518	-	63,63,67	0.85	1 (1%)	77,77,81	1.41	9 (11%)
29	LMG	C	519	-	51,51,55	0.71	0	59,59,63	1.33	6 (10%)
29	LMG	C	520	-	51,51,55	0.77	1 (1%)	59,59,63	1.35	6 (10%)
26	PHO	D	401	-	67,69,69	1.24	7 (10%)	86,99,99	1.07	7 (8%)
25	CLA	D	402	-	57,73,73	1.14	4 (7%)	61,113,113	1.08	6 (9%)
25	CLA	D	403	-	57,73,73	1.14	4 (7%)	61,113,113	1.11	6 (9%)
27	BCR	D	404	-	41,41,41	1.13	2 (4%)	56,56,56	1.24	7 (12%)
29	LMG	D	405	-	51,51,55	0.72	0	59,59,63	1.32	7 (11%)
31	LHG	D	406	-	48,48,48	0.61	0	49,54,54	1.25	6 (12%)
28	PL9	D	407	-	54,55,55	0.85	3 (5%)	68,69,69	1.45	16 (23%)
23	SQD	D	408	-	46,47,54	1.00	4 (8%)	55,58,65	2.02	12 (21%)
23	SQD	D	409	-	42,43,54	1.06	5 (11%)	51,54,65	2.00	10 (19%)
34	HEM	E	101	5,6	24,50,50	1.94	5 (20%)	16,82,82	1.39	3 (18%)
27	BCR	H	102	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	7 (12%)
33	DGD	H	103	-	63,63,67	0.86	1 (1%)	77,77,81	1.36	9 (11%)
23	SQD	I	101	-	39,39,54	0.84	2 (5%)	41,41,65	1.20	2 (4%)
27	BCR	K	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.27	8 (14%)
31	LHG	L	101	-	48,48,48	0.62	0	49,54,54	1.25	6 (12%)
27	BCR	T	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.28	7 (12%)
34	HEM	V	201	16	24,50,50	2.02	5 (20%)	16,82,82	1.35	3 (18%)
27	BCR	Y	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.17	3 (5%)
21	OEX	a	601	1,3,35	0,15,15	0.00	-	0,32,32	0.00	-
32	BCT	a	605	22	0,3,3	0.00	-	0,3,3	0.00	-
25	CLA	a	606	-	57,73,73	1.13	5 (8%)	61,113,113	1.14	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	a	607	35	51,67,73	1.21	5 (9%)	53,105,113	1.16	4 (7%)
26	PHO	a	608	-	67,69,69	1.23	7 (10%)	86,99,99	1.05	8 (9%)
25	CLA	a	609	-	57,73,73	1.13	4 (7%)	61,113,113	1.10	5 (8%)
27	BCR	a	610	-	41,41,41	1.11	2 (4%)	56,56,56	1.20	5 (8%)
28	PL9	a	611	-	54,55,55	0.81	2 (3%)	68,69,69	1.42	13 (19%)
25	CLA	a	612	35	57,73,73	1.14	4 (7%)	61,113,113	1.10	6 (9%)
31	LHG	a	613	-	48,48,48	0.61	0	49,54,54	1.29	6 (12%)
31	LHG	a	614	-	34,34,48	0.72	0	35,40,54	1.20	3 (8%)
31	LHG	a	615	-	41,41,48	0.67	0	42,47,54	1.31	6 (14%)
23	SQD	b	601	-	53,54,54	0.95	5 (9%)	62,65,65	1.76	9 (14%)
25	CLA	b	604	35	57,73,73	1.14	5 (8%)	61,113,113	1.12	6 (9%)
25	CLA	b	605	-	57,73,73	1.14	4 (7%)	61,113,113	1.09	5 (8%)
25	CLA	b	606	-	57,73,73	1.13	5 (8%)	61,113,113	1.11	5 (8%)
25	CLA	b	607	-	57,73,73	1.13	4 (7%)	61,113,113	1.19	7 (11%)
25	CLA	b	608	-	57,73,73	1.15	4 (7%)	61,113,113	1.10	5 (8%)
25	CLA	b	609	-	57,73,73	1.13	5 (8%)	61,113,113	1.14	6 (9%)
25	CLA	b	610	35	57,73,73	1.13	4 (7%)	61,113,113	1.09	5 (8%)
25	CLA	b	611	-	57,73,73	1.13	5 (8%)	61,113,113	1.12	6 (9%)
25	CLA	b	612	-	57,73,73	1.14	4 (7%)	61,113,113	1.11	7 (11%)
25	CLA	b	613	35	57,73,73	1.14	4 (7%)	61,113,113	1.08	5 (8%)
25	CLA	b	614	-	57,73,73	1.14	4 (7%)	61,113,113	1.14	7 (11%)
25	CLA	b	615	-	57,73,73	1.14	5 (8%)	61,113,113	1.14	6 (9%)
25	CLA	b	616	-	57,73,73	1.13	4 (7%)	61,113,113	1.13	6 (9%)
25	CLA	b	617	-	57,73,73	1.14	4 (7%)	61,113,113	1.11	7 (11%)
25	CLA	b	618	-	57,73,73	1.14	4 (7%)	61,113,113	1.15	7 (11%)
25	CLA	b	619	-	57,73,73	1.13	5 (8%)	61,113,113	1.16	5 (8%)
27	BCR	b	620	-	41,41,41	1.15	2 (4%)	56,56,56	1.24	5 (8%)
27	BCR	b	621	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	3 (5%)
27	BCR	b	622	-	41,41,41	1.11	2 (4%)	56,56,56	1.25	5 (8%)
29	LMG	b	623	-	51,51,55	0.71	0	59,59,63	1.36	7 (11%)
29	LMG	b	624	-	51,51,55	0.74	0	59,59,63	1.31	7 (11%)
29	LMG	b	625	-	8,8,55	0.15	0	7,7,63	0.91	0
23	SQD	c	501	-	53,54,54	0.95	5 (9%)	62,65,65	1.83	9 (14%)
29	LMG	c	502	-	51,51,55	0.75	0	59,59,63	1.33	6 (10%)
25	CLA	c	503	-	57,73,73	1.13	4 (7%)	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	c	504	-	57,73,73	1.15	5 (8%)	61,113,113	1.10	6 (9%)
25	CLA	c	505	-	57,73,73	1.14	4 (7%)	61,113,113	1.12	6 (9%)
25	CLA	c	506	35	57,73,73	1.13	4 (7%)	61,113,113	1.12	6 (9%)
25	CLA	c	507	-	57,73,73	1.14	4 (7%)	61,113,113	1.12	7 (11%)
25	CLA	c	508	-	57,73,73	1.14	4 (7%)	61,113,113	1.12	6 (9%)
25	CLA	c	509	35	57,73,73	1.13	4 (7%)	61,113,113	1.15	7 (11%)
25	CLA	c	510	-	50,66,73	1.21	4 (8%)	52,104,113	1.20	7 (13%)
25	CLA	c	511	-	57,73,73	1.14	5 (8%)	61,113,113	1.13	7 (11%)
25	CLA	c	512	-	57,73,73	1.13	4 (7%)	61,113,113	1.14	6 (9%)
25	CLA	c	513	3	57,73,73	1.13	4 (7%)	61,113,113	1.15	6 (9%)
25	CLA	c	514	-	57,73,73	1.12	4 (7%)	61,113,113	1.20	6 (9%)
25	CLA	c	515	-	57,73,73	1.13	4 (7%)	61,113,113	1.11	7 (11%)
27	BCR	c	516	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	6 (10%)
27	BCR	c	517	-	41,41,41	1.13	2 (4%)	56,56,56	1.21	6 (10%)
33	DGD	c	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.43	10 (12%)
33	DGD	c	519	-	63,63,67	0.88	2 (3%)	77,77,81	1.39	10 (12%)
33	DGD	c	520	-	63,63,67	0.86	1 (1%)	77,77,81	1.41	11 (14%)
29	LMG	c	521	-	51,51,55	0.70	0	59,59,63	1.33	6 (10%)
29	LMG	c	522	-	51,51,55	0.78	1 (1%)	59,59,63	1.36	7 (11%)
26	PHO	d	401	-	67,69,69	1.24	8 (11%)	86,99,99	1.08	8 (9%)
25	CLA	d	403	-	57,73,73	1.14	4 (7%)	61,113,113	1.09	7 (11%)
25	CLA	d	404	-	57,73,73	1.12	4 (7%)	61,113,113	1.15	6 (9%)
27	BCR	d	405	-	41,41,41	1.10	2 (4%)	56,56,56	1.23	4 (7%)
29	LMG	d	406	-	42,42,55	0.78	0	50,50,63	1.32	8 (16%)
31	LHG	d	407	-	48,48,48	0.61	0	49,54,54	1.26	6 (12%)
28	PL9	d	408	-	54,55,55	0.86	3 (5%)	68,69,69	1.43	13 (19%)
29	LMG	d	409	-	39,39,55	0.56	0	41,41,63	1.27	3 (7%)
34	HEM	e	101	5,6	24,50,50	1.93	4 (16%)	16,82,82	1.35	1 (6%)
23	SQD	f	101	-	42,43,54	1.06	4 (9%)	51,54,65	2.01	11 (21%)
27	BCR	h	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.30	7 (12%)
33	DGD	h	102	-	63,63,67	0.85	0	77,77,81	1.33	8 (10%)
27	BCR	k	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	4 (7%)
31	LHG	l	101	-	48,48,48	0.61	1 (2%)	49,54,54	1.24	6 (12%)
34	HEM	v	201	16	24,50,50	2.03	5 (20%)	16,82,82	1.36	1 (6%)
27	BCR	y	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.18	4 (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
21	OEX	A	601	1,3,35	-	0/0/68/68	0/0/6/6
23	SQD	A	603	-	-	0/47/67/69	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	3/3/18/25	0/28/126/135	0/0/9/9
26	PHO	A	608	-	-	0/53/103/103	0/1/6/6
25	CLA	A	609	-	3/3/20/25	0/37/135/135	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	LMG	A	612	-	-	0/46/66/70	0/1/1/1
29	LMG	A	613	-	-	0/46/66/70	0/1/1/1
25	CLA	A	615	35	3/3/20/25	0/37/135/135	0/0/9/9
31	LHG	A	616	-	-	0/53/53/53	0/0/0/0
31	LHG	A	617	-	-	0/53/53/53	0/0/0/0
31	LHG	A	618	-	-	0/53/53/53	0/0/0/0
23	SQD	A	619	-	-	0/41/41/69	0/0/0/1
32	BCT	A	620	22	-	0/0/0/0	0/0/0/0
25	CLA	B	601	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	602	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	603	-	3/3/20/25	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	-	2/2/20/25	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	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	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	B	610	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	611	-	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
27	BCR	B	617	-	-	0/29/63/63	0/2/2/2
27	BCR	B	618	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	B	619	-	-	0/29/63/63	0/2/2/2
29	LMG	B	620	-	-	0/46/66/70	0/1/1/1
29	LMG	B	621	-	-	0/46/66/70	0/1/1/1
29	LMG	B	625	-	-	0/46/66/70	0/1/1/1
23	SQD	B	626	-	-	2/49/69/69	0/1/1/1
27	BCR	B	627	-	-	0/29/63/63	0/2/2/2
25	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	502	-	2/2/20/25	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	3/3/20/25	0/37/135/135	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
25	CLA	C	508	-	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	2/2/20/25	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
29	LMG	C	519	-	-	0/46/66/70	0/1/1/1
29	LMG	C	520	-	-	0/46/66/70	0/1/1/1
26	PHO	D	401	-	-	0/53/103/103	0/1/6/6
25	CLA	D	402	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	D	403	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	D	404	-	-	0/29/63/63	0/2/2/2
29	LMG	D	405	-	-	0/46/66/70	0/1/1/1
31	LHG	D	406	-	-	0/53/53/53	0/0/0/0
28	PL9	D	407	-	-	0/53/73/73	0/1/1/1
23	SQD	D	408	-	-	0/42/62/69	0/1/1/1
23	SQD	D	409	-	-	0/38/58/69	0/1/1/1
34	HEM	E	101	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	SQD	I	101	-	-	0/41/41/69	0/0/0/1
27	BCR	K	101	-	-	0/29/63/63	0/2/2/2
31	LHG	L	101	-	-	0/53/53/53	0/0/0/0
27	BCR	T	101	-	-	0/29/63/63	0/2/2/2
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
21	OEX	a	601	1,3,35	-	0/0/68/68	0/0/6/6
32	BCT	a	605	22	-	0/0/0/0	0/0/0/0
25	CLA	a	606	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	a	607	35	3/3/18/25	0/30/128/135	0/0/9/9
26	PHO	a	608	-	-	0/53/103/103	0/1/6/6
25	CLA	a	609	-	3/3/20/25	0/37/135/135	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
25	CLA	a	612	35	3/3/20/25	0/37/135/135	0/0/9/9
31	LHG	a	613	-	-	0/53/53/53	0/0/0/0
31	LHG	a	614	-	-	0/39/39/53	0/0/0/0
31	LHG	a	615	-	-	0/46/46/53	0/0/0/0
23	SQD	b	601	-	-	0/49/69/69	0/1/1/1
25	CLA	b	604	35	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	-	2/2/20/25	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	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	612	-	2/2/20/25	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	-	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
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
27	BCR	b	620	-	-	0/29/63/63	0/2/2/2
27	BCR	b	621	-	-	0/29/63/63	0/2/2/2
27	BCR	b	622	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	b	623	-	-	0/46/66/70	0/1/1/1
29	LMG	b	624	-	-	0/46/66/70	0/1/1/1
29	LMG	b	625	-	-	0/6/6/70	0/0/0/1
23	SQD	c	501	-	-	0/49/69/69	0/1/1/1
29	LMG	c	502	-	-	0/46/66/70	0/1/1/1
25	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	504	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	c	505	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	506	35	3/3/20/25	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	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	509	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	510	-	3/3/18/25	0/29/127/135	0/0/9/9
25	CLA	c	511	-	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	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	514	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	515	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	c	516	-	-	0/29/63/63	0/2/2/2
27	BCR	c	517	-	-	0/29/63/63	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
33	DGD	c	520	-	-	0/51/91/95	0/2/2/2
29	LMG	c	521	-	-	0/46/66/70	0/1/1/1
29	LMG	c	522	-	-	0/46/66/70	0/1/1/1
26	PHO	d	401	-	-	0/53/103/103	0/1/6/6
25	CLA	d	403	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	d	404	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	d	405	-	-	0/29/63/63	0/2/2/2
29	LMG	d	406	-	-	0/37/57/70	0/1/1/1
31	LHG	d	407	-	-	0/53/53/53	0/0/0/0
28	PL9	d	408	-	-	0/53/73/73	0/1/1/1
29	LMG	d	409	-	-	1/41/41/70	0/0/0/1
34	HEM	e	101	5,6	-	0/6/54/54	0/0/8/8
23	SQD	f	101	-	-	0/38/58/69	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
31	LHG	l	101	-	-	0/53/53/53	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

The worst 5 of 457 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	v	201	HEM	C3C-C2C	-4.96	1.34	1.40
34	V	201	HEM	C3C-C2C	-4.91	1.34	1.40
34	E	101	HEM	C3B-C2B	-4.11	1.35	1.40
34	v	201	HEM	C3B-C2B	-4.04	1.35	1.40
34	E	101	HEM	C3C-C2C	-4.03	1.35	1.40

The worst 5 of 950 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	603	SQD	O9-S-O7	-4.66	100.79	113.96
29	A	613	LMG	O1-C1-C2	-4.65	102.28	108.00
33	c	518	DGD	O3G-C3G-C2G	-4.56	100.14	110.99
23	D	408	SQD	O9-S-O7	-4.56	101.08	113.96
23	B	626	SQD	O9-S-O7	-4.55	101.11	113.96

5 of 198 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	c	515	CLA	NC
25	c	515	CLA	ND
25	c	515	CLA	NA
25	b	614	CLA	NC
25	b	614	CLA	ND

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	d	409	LMG	C8-O7-C10-C11
23	B	626	SQD	C45-O47-C7-O49
23	B	626	SQD	C45-O47-C7-C8

There are no ring outliers.

74 monomers are involved in 226 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	603	SQD	1	0
25	A	606	CLA	3	0
25	A	607	CLA	3	0
26	A	608	PHO	2	0
25	A	609	CLA	10	0
27	A	610	BCR	5	0
28	A	611	PL9	7	0
29	A	613	LMG	2	0
25	A	615	CLA	1	0
31	A	616	LHG	2	0
31	A	617	LHG	7	0
31	A	618	LHG	3	0
23	A	619	SQD	2	0
32	A	620	BCT	1	0
25	B	601	CLA	3	0
25	B	602	CLA	4	0
25	B	603	CLA	2	0
25	B	604	CLA	2	0
25	B	605	CLA	4	0
25	B	606	CLA	6	0
25	B	607	CLA	4	0
25	B	608	CLA	6	0
25	B	609	CLA	6	0
25	B	610	CLA	4	0
25	B	611	CLA	3	0
25	B	612	CLA	7	0
25	B	613	CLA	4	0
25	B	614	CLA	6	0
25	B	615	CLA	7	0
25	B	616	CLA	3	0
27	B	617	BCR	2	0
27	B	618	BCR	2	0
27	B	619	BCR	2	0
29	B	620	LMG	1	0
29	B	621	LMG	1	0
29	B	625	LMG	2	0
23	B	626	SQD	7	0
27	B	627	BCR	5	0
25	C	501	CLA	6	0
25	C	502	CLA	1	0
25	C	503	CLA	11	0
25	C	504	CLA	3	0
25	C	505	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	506	CLA	2	0
25	C	507	CLA	5	0
25	C	508	CLA	6	0
25	C	509	CLA	6	0
25	C	510	CLA	4	0
25	C	511	CLA	3	0
25	C	512	CLA	4	0
25	C	513	CLA	3	0
27	C	514	BCR	1	0
27	C	515	BCR	3	0
33	C	516	DGD	1	0
33	C	517	DGD	2	0
33	C	518	DGD	2	0
29	C	519	LMG	1	0
29	C	520	LMG	2	0
26	D	401	PHO	7	0
25	D	402	CLA	3	0
25	D	403	CLA	8	0
27	D	404	BCR	3	0
29	D	405	LMG	2	0
31	D	406	LHG	1	0
28	D	407	PL9	2	0
23	D	408	SQD	1	0
34	E	101	HEM	4	0
27	H	102	BCR	4	0
33	H	103	DGD	2	0
27	K	101	BCR	3	0
31	L	101	LHG	7	0
27	T	101	BCR	6	0
34	V	201	HEM	2	0
27	Y	101	BCR	4	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%)	-0.35	1 (0%) 94 84	28, 38, 60, 76	0
1	a	334/344 (97%)	-0.43	0 100 100	28, 38, 60, 76	0
2	B	504/510 (98%)	-0.17	11 (2%) 65 35	27, 41, 66, 86	0
2	b	504/510 (98%)	-0.22	4 (0%) 87 67	29, 42, 67, 85	0
3	C	451/461 (97%)	-0.26	5 (1%) 82 58	30, 45, 61, 75	0
3	c	451/461 (97%)	-0.23	3 (0%) 89 70	31, 46, 63, 93	0
4	D	341/352 (96%)	-0.39	2 (0%) 90 73	28, 39, 56, 67	0
4	d	341/352 (96%)	-0.37	0 100 100	29, 40, 55, 78	0
5	E	81/84 (96%)	-0.05	0 100 100	39, 54, 72, 89	0
5	e	82/84 (97%)	0.24	3 (3%) 45 19	43, 61, 75, 80	0
6	F	34/45 (75%)	-0.35	1 (2%) 55 26	40, 50, 63, 77	0
6	f	34/45 (75%)	-0.42	0 100 100	39, 51, 69, 72	0
7	H	63/66 (95%)	0.03	1 (1%) 74 47	39, 47, 57, 63	0
7	h	63/66 (95%)	-0.10	1 (1%) 74 47	35, 47, 58, 68	0
8	I	35/38 (92%)	0.09	1 (2%) 55 26	29, 44, 71, 73	0
8	i	35/38 (92%)	0.05	3 (8%) 13 4	33, 43, 74, 94	0
9	J	36/40 (90%)	-0.25	0 100 100	44, 58, 68, 75	0
9	j	36/40 (90%)	0.00	2 (5%) 28 11	49, 57, 72, 79	0
10	K	37/46 (80%)	-0.00	0 100 100	45, 59, 75, 89	0
10	k	37/46 (80%)	-0.07	0 100 100	47, 56, 72, 79	0
11	L	37/37 (100%)	-0.34	1 (2%) 58 28	32, 38, 62, 84	0
11	l	37/37 (100%)	-0.35	1 (2%) 58 28	29, 38, 69, 81	0
12	M	32/36 (88%)	-0.14	2 (6%) 23 9	33, 38, 56, 74	0
12	m	32/36 (88%)	0.03	3 (9%) 11 4	31, 41, 59, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	244/272 (89%)	-0.06	8 (3%) 50 22	30, 47, 81, 111	0
13	o	244/272 (89%)	-0.06	7 (2%) 55 26	31, 46, 80, 127	0
14	T	29/32 (90%)	-0.38	1 (3%) 49 21	30, 39, 60, 74	0
14	t	29/32 (90%)	-0.47	0 100 100	31, 36, 63, 66	0
15	U	97/134 (72%)	-0.03	0 100 100	36, 49, 69, 75	0
15	u	97/134 (72%)	-0.27	0 100 100	32, 44, 58, 76	0
16	V	137/163 (84%)	-0.18	0 100 100	34, 47, 59, 74	0
16	v	137/163 (84%)	-0.03	1 (0%) 89 70	34, 54, 67, 81	0
17	Y	30/46 (65%)	0.52	3 (10%) 9 4	60, 73, 84, 87	0
17	y	30/46 (65%)	0.15	2 (6%) 21 7	49, 65, 78, 83	0
18	X	38/41 (92%)	0.14	2 (5%) 30 12	41, 50, 65, 79	0
18	x	38/41 (92%)	0.19	2 (5%) 30 12	46, 55, 74, 76	0
19	Z	62/62 (100%)	0.48	5 (8%) 15 5	52, 69, 88, 98	0
19	z	62/62 (100%)	0.56	8 (12%) 5 2	51, 72, 97, 105	0
20	R	34/41 (82%)	0.88	2 (5%) 26 10	65, 73, 83, 86	0
20	r	34/41 (82%)	0.59	0 100 100	65, 78, 86, 90	0
All	All	5313/5700 (93%)	-0.18	86 (1%) 74 47	27, 45, 72, 127	0

The worst 5 of 86 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	O	35	SER	6.9
13	o	3	GLN	6.1
12	M	33	GLN	5.2
16	v	18	THR	4.9
12	m	31	SER	4.7

## 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( $\text{\AA}^2$ )	Q<0.9
14	FME	T	1	10/11	0.93	0.13	-	44,47,53,54	0
12	FME	M	1	10/11	0.93	0.29	-	30,43,53,54	0
8	FME	I	1	10/11	0.91	0.29	-	43,56,63,71	0
14	FME	t	1	10/11	0.92	0.25	-	39,42,63,72	0
8	FME	i	1	10/11	0.91	0.22	-	35,50,56,61	0
12	FME	m	1	10/11	0.91	0.23	-	26,45,55,64	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
30	UNL	b	603	13/-	0.77	0.29	6.75	39,48,61,62	0
29	LMG	C	520	51/55	0.74	0.39	4.83	49,62,82,100	0
30	UNL	b	602	13/-	0.87	0.25	4.82	30,36,41,45	0
30	UNL	C	521	9/-	0.84	0.28	4.66	36,42,46,49	0
29	LMG	d	409	40/55	0.79	0.31	4.24	40,55,76,77	0
31	LHG	a	615	42/49	0.77	0.32	4.21	54,78,89,100	0
29	LMG	b	624	51/55	0.76	0.32	4.14	45,64,76,86	0
29	LMG	c	522	51/55	0.80	0.37	4.10	36,68,83,90	0
23	SQD	b	601	54/54	0.81	0.28	3.64	39,60,90,97	0
30	UNL	t	101	10/-	0.76	0.28	3.63	26,41,47,47	0
28	PL9	A	611	55/55	0.74	0.37	3.50	39,58,75,79	0
29	LMG	A	612	51/55	0.80	0.33	3.46	34,59,76,85	0
29	LMG	D	405	51/55	0.89	0.27	3.45	34,53,88,92	0
29	LMG	B	625	51/55	0.81	0.26	3.14	28,52,74,78	0
23	SQD	I	101	40/54	0.70	0.39	3.11	31,52,84,89	0
28	PL9	a	611	55/55	0.84	0.29	3.08	40,59,72,73	0
27	BCR	b	622	40/40	0.87	0.25	3.01	33,43,52,54	0
29	LMG	B	621	51/55	0.80	0.30	2.95	32,56,71,74	0
29	LMG	A	613	51/55	0.80	0.30	2.79	31,53,78,84	0
33	DGD	c	520	62/66	0.87	0.27	2.76	36,47,72,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
29	LMG	c	502	51/55	0.78	0.31	2.71	34,57,80,83	0
25	CLA	C	504	65/65	0.86	0.27	2.60	33,51,70,78	0
29	LMG	c	521	51/55	0.80	0.32	2.60	33,65,83,88	0
23	SQD	c	501	54/54	0.84	0.32	2.60	38,58,76,77	0
23	SQD	A	619	40/54	0.79	0.28	2.49	25,48,67,69	0
29	LMG	b	623	51/55	0.82	0.30	2.49	29,48,71,74	0
31	LHG	A	617	49/49	0.87	0.33	2.47	33,55,78,82	0
27	BCR	T	101	40/40	0.87	0.28	2.43	31,43,58,62	0
33	DGD	h	102	62/66	0.82	0.29	2.42	35,47,63,73	0
25	CLA	b	604	65/65	0.84	0.28	2.40	44,59,76,88	0
30	UNL	d	402	22/-	0.82	0.31	2.33	26,43,60,78	0
27	BCR	B	627	40/40	0.86	0.26	2.33	30,41,49,53	0
25	CLA	c	505	65/65	0.87	0.27	2.31	32,51,62,68	0
31	LHG	A	618	49/49	0.74	0.29	2.25	41,72,85,94	0
27	BCR	y	101	40/40	0.83	0.29	1.97	50,63,70,74	0
25	CLA	c	504	65/65	0.89	0.26	1.88	32,46,59,65	0
27	BCR	d	405	40/40	0.88	0.23	1.84	29,43,56,62	0
24	CL	a	603	1/1	0.82	0.23	1.67	59,59,59,59	0
28	PL9	D	407	55/55	0.90	0.23	1.67	26,35,45,50	0
33	DGD	H	103	62/66	0.85	0.27	1.67	26,41,53,61	0
27	BCR	Y	101	40/40	0.84	0.26	1.65	46,60,72,76	0
33	DGD	c	519	62/66	0.87	0.26	1.59	37,57,86,95	0
27	BCR	B	618	40/40	0.88	0.25	1.59	28,40,48,52	0
33	DGD	C	518	62/66	0.88	0.25	1.58	33,48,65,74	0
25	CLA	a	609	65/65	0.90	0.25	1.55	19,34,71,81	0
28	PL9	d	408	55/55	0.92	0.21	1.54	21,33,43,45	0
23	SQD	A	603	52/54	0.86	0.29	1.51	38,60,78,82	0
25	CLA	C	512	65/65	0.83	0.30	1.51	42,58,68,79	0
25	CLA	B	601	65/65	0.85	0.29	1.51	41,59,84,96	0
27	BCR	b	620	40/40	0.89	0.23	1.42	33,45,53,54	0
30	UNL	z	101	11/-	0.82	0.28	1.39	31,53,58,60	0
27	BCR	B	619	40/40	0.88	0.21	1.39	33,44,58,60	0
31	LHG	D	406	49/49	0.92	0.24	1.38	25,40,50,59	0
25	CLA	B	608	65/65	0.89	0.28	1.36	29,37,47,52	0
27	BCR	D	404	40/40	0.88	0.25	1.33	28,46,63,67	0
25	CLA	c	511	65/65	0.89	0.24	1.33	38,46,55,57	0
27	BCR	C	514	40/40	0.85	0.29	1.31	45,56,64,66	0
25	CLA	B	606	65/65	0.86	0.28	1.30	29,44,65,84	0
25	CLA	d	404	65/65	0.87	0.24	1.29	32,46,73,91	0
27	BCR	C	515	40/40	0.88	0.23	1.21	32,42,52,53	0
25	CLA	c	510	58/65	0.88	0.24	1.18	34,46,59,67	0
25	CLA	c	514	65/65	0.85	0.27	1.10	45,59,78,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
25	CLA	A	615	65/65	0.92	0.22	1.08	22,34,43,47	0
25	CLA	c	515	65/65	0.83	0.30	1.06	45,60,78,81	0
31	LHG	d	407	49/49	0.93	0.20	1.06	20,37,47,51	0
25	CLA	C	509	65/65	0.89	0.25	1.04	33,46,59,67	0
25	CLA	b	608	65/65	0.92	0.19	1.02	30,40,46,51	0
29	LMG	d	406	42/55	0.91	0.21	1.01	38,48,63,73	0
25	CLA	D	403	65/65	0.88	0.24	1.00	21,37,63,69	0
25	CLA	b	609	65/65	0.90	0.23	0.99	21,35,59,81	0
25	CLA	B	603	65/65	0.90	0.25	0.98	28,37,45,47	0
27	BCR	c	516	40/40	0.86	0.32	0.96	33,63,70,72	0
23	SQD	B	626	54/54	0.84	0.23	0.96	33,52,85,90	0
23	SQD	D	409	43/54	0.79	0.29	0.95	37,68,89,98	0
25	CLA	A	606	65/65	0.89	0.22	0.92	26,34,45,48	0
25	CLA	C	503	65/65	0.87	0.25	0.92	37,49,58,65	0
25	CLA	A	609	65/65	0.92	0.23	0.91	17,29,79,89	0
25	CLA	C	502	65/65	0.87	0.26	0.87	35,51,62,69	0
29	LMG	C	519	51/55	0.82	0.28	0.86	42,61,73,85	0
33	DGD	C	516	62/66	0.91	0.21	0.85	21,39,63,71	0
27	BCR	K	101	40/40	0.88	0.24	0.83	45,53,60,66	0
27	BCR	B	617	40/40	0.92	0.20	0.81	32,41,49,50	0
26	PHO	d	401	64/64	0.92	0.21	0.81	24,39,45,49	0
25	CLA	D	402	65/65	0.90	0.22	0.80	24,36,48,59	0
30	UNL	m	102	16/-	0.83	0.27	0.80	37,45,51,54	0
27	BCR	k	101	40/40	0.84	0.26	0.80	37,53,59,61	0
31	LHG	L	101	49/49	0.90	0.23	0.79	29,41,51,57	0
23	SQD	D	408	47/54	0.80	0.27	0.76	17,53,103,121	0
29	LMG	B	620	51/55	0.86	0.24	0.76	27,46,67,75	0
25	CLA	c	506	65/65	0.89	0.23	0.75	36,49,70,74	0
27	BCR	H	102	40/40	0.80	0.32	0.75	34,51,59,65	0
25	CLA	C	511	65/65	0.85	0.26	0.69	45,57,66,70	0
25	CLA	b	617	65/65	0.89	0.22	0.69	34,45,63,73	0
26	PHO	A	608	64/64	0.93	0.21	0.68	23,32,37,43	0
31	LHG	a	614	35/49	0.90	0.23	0.68	36,47,56,58	0
25	CLA	C	501	65/65	0.92	0.21	0.68	34,42,49,54	0
25	CLA	c	508	65/65	0.87	0.25	0.65	34,49,72,78	0
25	CLA	B	605	65/65	0.92	0.19	0.64	24,34,40,42	0
27	BCR	A	610	40/40	0.92	0.20	0.62	22,34,44,47	0
25	CLA	b	605	65/65	0.90	0.22	0.58	31,43,56,58	0
31	LHG	l	101	49/49	0.90	0.21	0.57	30,45,54,56	0
25	CLA	C	505	65/65	0.91	0.21	0.57	33,41,55,62	0
25	CLA	B	607	65/65	0.92	0.20	0.55	26,36,44,54	0
25	CLA	b	619	65/65	0.90	0.24	0.55	30,44,72,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
25	CLA	b	606	65/65	0.93	0.20	0.53	24,36,50,58	0
25	CLA	B	602	65/65	0.94	0.22	0.47	29,39,47,52	0
33	DGD	C	517	62/66	0.92	0.22	0.45	39,51,74,83	0
25	CLA	A	607	57/65	0.93	0.20	0.44	29,37,49,67	0
25	CLA	C	513	65/65	0.88	0.29	0.44	41,62,74,83	0
25	CLA	B	616	65/65	0.89	0.24	0.43	32,44,70,76	0
31	LHG	a	613	49/49	0.93	0.20	0.43	26,43,56,60	0
25	CLA	b	610	65/65	0.93	0.19	0.42	23,37,51,54	0
25	CLA	c	503	65/65	0.93	0.21	0.41	27,40,46,52	0
25	CLA	B	614	65/65	0.88	0.22	0.40	32,42,63,82	0
25	CLA	c	512	65/65	0.91	0.23	0.40	31,47,56,64	0
23	SQD	f	101	43/54	0.87	0.25	0.38	51,70,77,84	0
27	BCR	b	621	40/40	0.90	0.22	0.37	31,42,57,59	0
25	CLA	B	613	65/65	0.92	0.23	0.34	19,33,48,69	0
25	CLA	c	507	65/65	0.90	0.21	0.33	32,44,61,64	0
25	CLA	b	611	65/65	0.89	0.24	0.30	27,41,54,57	0
27	BCR	c	517	40/40	0.92	0.20	0.28	19,39,50,52	0
33	DGD	c	518	62/66	0.90	0.21	0.26	28,46,63,79	0
26	PHO	a	608	64/64	0.93	0.20	0.25	19,28,38,42	0
25	CLA	C	510	65/65	0.89	0.24	0.23	41,51,58,60	0
25	CLA	C	508	65/65	0.90	0.22	0.22	38,49,82,90	0
27	BCR	h	101	40/40	0.84	0.27	0.19	31,45,55,62	0
25	CLA	b	613	65/65	0.92	0.20	0.18	24,35,43,45	0
25	CLA	b	618	65/65	0.90	0.20	0.17	28,40,47,56	0
25	CLA	C	507	65/65	0.89	0.22	0.16	32,42,52,67	0
25	CLA	B	604	65/65	0.90	0.23	0.15	28,37,57,65	0
26	PHO	D	401	64/64	0.92	0.21	0.14	27,37,47,54	0
25	CLA	d	403	65/65	0.92	0.19	0.13	24,36,45,50	0
25	CLA	B	610	65/65	0.92	0.21	0.12	25,33,39,45	0
25	CLA	B	611	65/65	0.93	0.22	0.11	21,31,38,44	0
27	BCR	a	610	40/40	0.93	0.19	0.06	19,32,45,47	0
31	LHG	A	616	49/49	0.92	0.20	0.05	24,41,54,58	0
25	CLA	a	606	65/65	0.93	0.18	-0.01	23,31,38,39	0
25	CLA	b	607	65/65	0.91	0.20	-0.01	24,34,48,53	0
25	CLA	c	509	65/65	0.91	0.20	-0.02	30,39,51,55	0
25	CLA	B	612	65/65	0.93	0.20	-0.08	26,35,42,46	0
25	CLA	B	615	65/65	0.92	0.19	-0.09	27,41,51,57	0
25	CLA	b	612	65/65	0.91	0.19	-0.15	28,41,55,61	0
25	CLA	B	609	65/65	0.89	0.20	-0.18	24,44,52,58	0
25	CLA	b	616	65/65	0.92	0.20	-0.20	25,33,51,62	0
25	CLA	a	612	65/65	0.94	0.17	-0.22	17,29,37,39	0
25	CLA	c	513	65/65	0.89	0.22	-0.23	42,52,58,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
25	CLA	C	506	65/65	0.90	0.20	-0.23	32,47,64,68	0
30	UNL	M	102	17/-	0.88	0.22	-0.29	31,37,49,51	0
25	CLA	a	607	59/65	0.94	0.17	-0.34	27,37,55,72	0
34	HEM	v	201	43/43	0.94	0.17	-0.40	32,41,48,52	0
25	CLA	b	615	65/65	0.94	0.18	-0.41	22,32,41,50	0
34	HEM	E	101	43/43	0.92	0.20	-0.46	42,54,67,69	0
34	HEM	V	201	43/43	0.93	0.17	-0.49	31,44,52,56	0
25	CLA	b	614	65/65	0.93	0.18	-0.57	25,35,41,50	0
34	HEM	e	101	43/43	0.89	0.21	-0.57	50,62,69,70	0
30	UNL	B	624	11/-	0.88	0.18	-0.71	26,31,38,41	0
32	BCT	A	620	4/4	0.95	0.15	-1.37	26,36,37,44	0
24	CL	a	604	1/1	0.93	0.14	-1.70	42,42,42,42	0
32	BCT	a	605	4/4	0.96	0.10	-1.99	44,47,49,50	0
24	CL	A	604	1/1	0.93	0.10	-2.11	43,43,43,43	0
24	CL	A	605	1/1	0.96	0.13	-2.23	44,44,44,44	0
21	OEX	A	601	10/10	0.98	0.10	-2.52	33,40,45,46	0
22	FE2	a	602	1/1	0.91	0.08	-3.25	62,62,62,62	0
21	OEX	a	601	10/10	0.98	0.08	-4.14	40,44,48,51	0
22	FE2	A	602	1/1	0.96	0.05	-6.60	46,46,46,46	0
30	UNL	B	623	11/-	0.81	0.23	-	35,40,47,48	0
29	LMG	b	625	9/55	0.65	0.42	-	40,46,52,55	0
30	UNL	H	101	8/-	0.84	0.20	-	29,35,43,47	0
30	UNL	j	101	9/-	0.80	0.28	-	40,49,60,63	0
30	UNL	B	622	6/-	0.86	0.24	-	26,42,50,56	0
30	UNL	M	101	6/-	0.83	0.31	-	41,46,52,65	0
30	UNL	m	101	5/-	0.80	0.28	-	26,32,37,41	0
30	UNL	i	101	12/-	0.84	0.29	-	24,39,51,51	0
30	UNL	A	614	7/-	0.89	0.19	-	32,38,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.