



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2018 – 09:34 PM EST

PDB ID : 5MX2
Title : Photosystem II depleted of the Mn₄CaO₅ cluster at 2.55 Å resolution
Authors : Zhang, M.; Bommer, M.; Chatterjee, R.; Hussain, R.; Kern, J.; Yano, J.; Dau, H.; Dobbek, H.; Zouni, A.
Deposited on : 2017-01-20
Resolution : 2.20 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

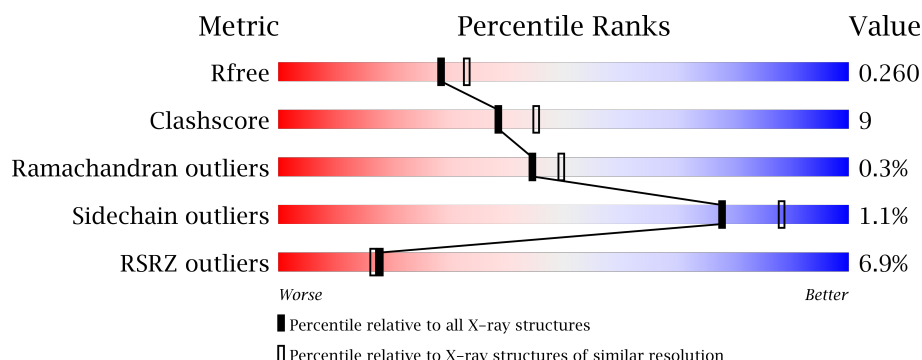
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>25%</div> <div>..</div> </div> </div>
1	a	344	<div> <div>2%</div> <div> <div></div> <div>96%</div> <div></div> <div>..</div> </div> </div>
2	B	510	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>26%</div> <div>.</div> </div> </div>
2	b	510	<div> <div>7%</div> <div> <div></div> <div>98%</div> <div></div> <div>..</div> </div> </div>
3	C	461	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
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	
15	u	134	

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Mol	Chain	Length	Quality of chain
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
22	CLA	A	403	X	-	-	-
22	CLA	A	404	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	A	412	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	C	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	C	514	X	-	-	-
22	CLA	D	402	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	H	101	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	407	X	-	-	-
22	CLA	b	603	X	-	-	X
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	b	618	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	X
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	c	514	X	-	-	-
22	CLA	d	401	X	-	-	-
22	CLA	d	402	X	-	-	-
22	CLA	d	403	X	-	-	-
25	PL9	A	408	-	-	-	X
25	PL9	a	409	-	-	-	X
26	SQD	A	411	-	-	-	X
27	LFA	A	413	-	-	-	X
27	LFA	B	623	-	-	-	X
27	LFA	B	626	-	-	-	X
27	LFA	B	627	-	-	-	X
27	LFA	D	410	-	-	-	X
27	LFA	D	413	-	-	-	X
27	LFA	b	623	-	-	-	X
27	LFA	b	626	-	-	-	X
27	LFA	d	408	-	-	-	X
27	LFA	j	101	-	-	-	X
30	LMG	B	621	-	-	-	X
30	LMG	C	501	-	-	-	X
30	LMG	C	522	-	-	-	X
30	LMG	b	624	-	-	-	X
30	LMG	c	522	-	-	-	X
32	LHG	e	101	-	-	-	X

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 50407 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	333	Total	C	N	O	S	0	0	0
			2617	1714	430	458	15			
1	a	333	Total	C	N	O	S	0	0	0
			2617	1714	430	458	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	0	0
			3980	2611	665	691	13			
2	b	503	Total	C	N	O	S	0	0	0
			3958	2599	657	689	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3455	2264	576	602	13			
3	c	448	Total	C	N	O	S	0	0	0
			3466	2270	580	603	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			
4	d	340	Total	C	N	O	S	0	0	0
			2706	1794	440	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
			656	428	106	122			
5	e	79	Total	C	N	O	0	0	0
			645	422	104	119			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	62	Total	C	N	O	S	0	0	0
			493	330	79	82	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	33	Total	C	N	O	S	0	0	0
			266	183	39	43	1			
8	i	33	Total	C	N	O	S	0	0	0
			266	183	39	43	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	33	Total	C	N	O	S	0	0	0
			238	164	34	39	1			
9	j	33	Total	C	N	O	S	0	0	0
			238	164	34	39	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	35	Total	C	N	O	0	0	0
			272	192	37	43			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	36	Total	C	N	O	0	0	0
			284	198	41	45			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	0	0
			296	197	47	52			
11	l	36	Total	C	N	O	0	0	0
			296	197	47	52			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	32	Total	C	N	O	S	0	0	0
			249	167	36	45	1			
12	m	32	Total	C	N	O	S	0	0	0
			249	167	36	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	242	Total	C	N	O	S	0	0	0
			1859	1162	314	379	4			
13	o	241	Total	C	N	O	S	0	0	0
			1852	1158	313	377	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	28	Total	C	N	O	S	0	0	0
			241	170	34	35	2			
14	t	29	Total	C	N	O	S	0	0	0
			249	176	35	36	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	0	0
			765	486	128	151			
15	u	96	Total	C	N	O	0	0	0
			765	486	128	151			

- 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	21	Total	C	N	O	S	0	0	0
			155	102	28	23	2			
17	y	23	Total	C	N	O	S	0	0	0
			171	113	30	25	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	37	Total	C	N	O	S	0	0	0
			270	182	41	47				
18	x	38	Total	C	N	O	S	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	61	Total	C	N	O	S	0	0	0
			471	323	71	75	2			
19	z	61	Total	C	N	O	S	0	0	0
			471	323	71	75	2			

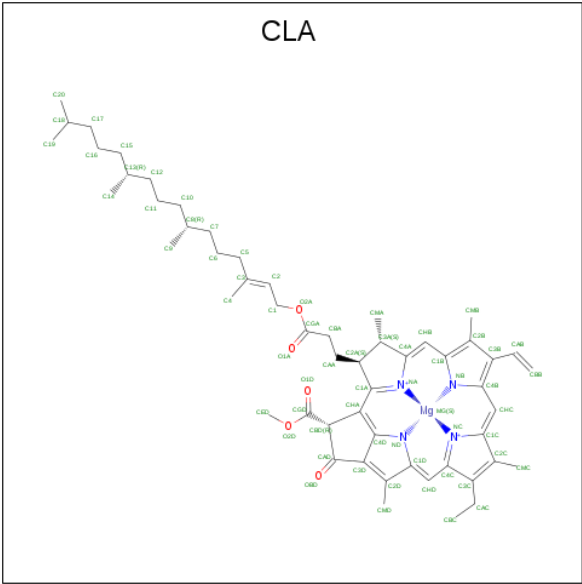
- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	35	Total	C	N	O	S	0	0	0
			282	191	49	42				
20	r	32	Total	C	N	O	S	0	0	0
			257	176	45	36				

- Molecule 21 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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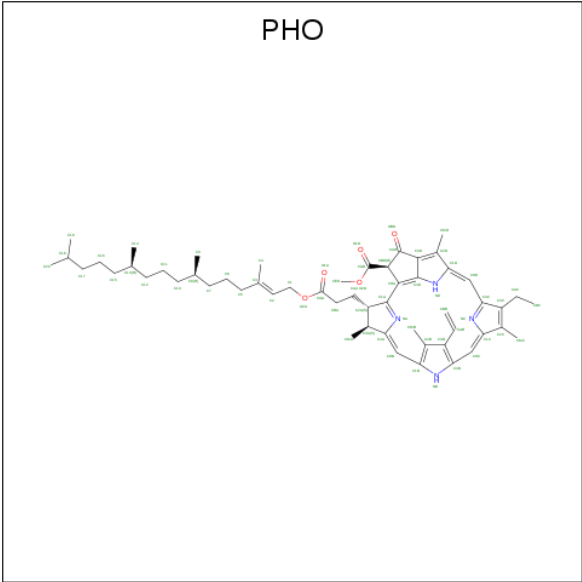
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N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

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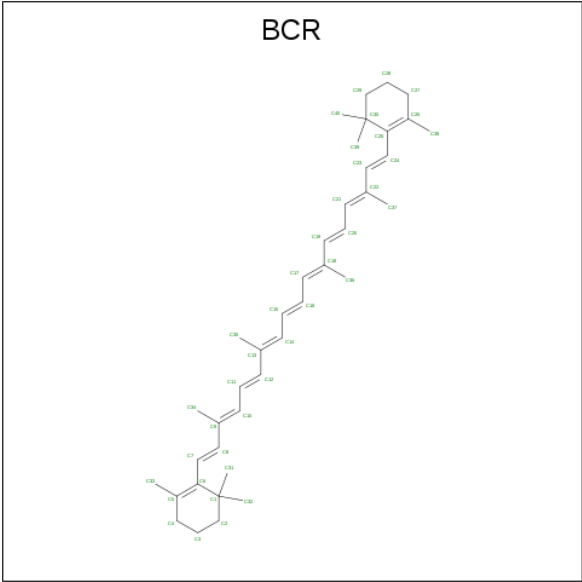
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



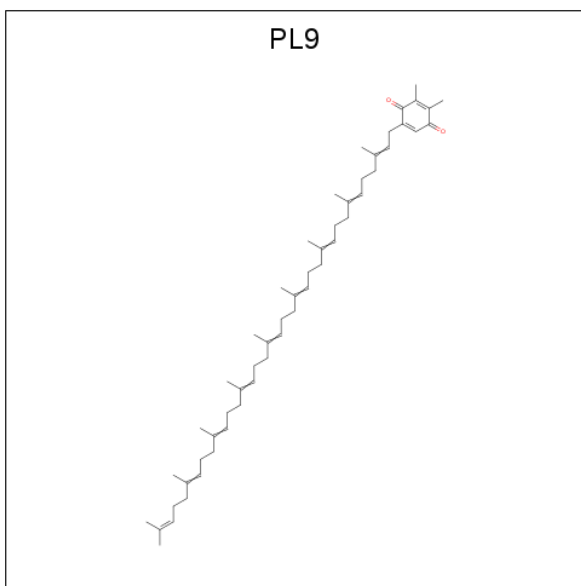
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	D	1	Total	C	N	O	0	0
			64	55	4	5		
23	a	1	Total	C	N	O	0	0
			64	55	4	5		
23	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



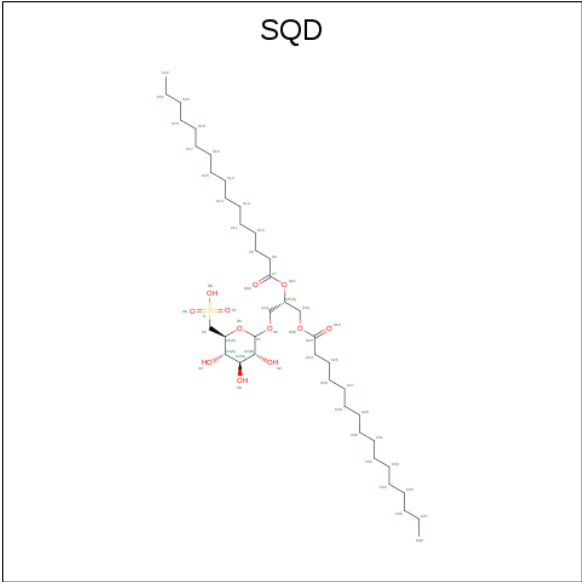
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	T	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	d	1	Total C 40 40	0	0
24	h	1	Total C 40 40	0	0
24	k	1	Total C 40 40	0	0
24	t	1	Total C 40 40	0	0

- Molecule 25 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: $C_{53}H_{80}O_2$).



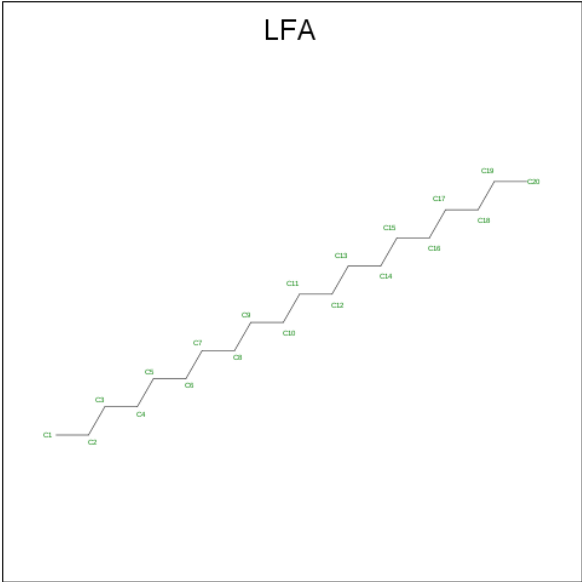
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	O	0	0
			55	53	2		
25	D	1	Total	C	O	0	0
			55	53	2		
25	a	1	Total	C	O	0	0
			55	53	2		
25	d	1	Total	C	O	0	0
			55	53	2		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	D	1	Total	C	O	S	0	0
			43	30	12	1		
26	L	1	Total	C	O	S	0	0
			48	35	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O		0	0
			50	41	9			
26	b	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 27 is EICOSANE (three-letter code: LFA) (formula: C₂₀H₄₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	1	Total	C	0	0
			14	14		
27	A	1	Total	C	0	0
			11	11		
27	B	1	Total	C	0	0
			10	10		
27	B	1	Total	C	0	0
			16	16		
27	B	1	Total	C	0	0
			13	13		
27	B	1	Total	C	0	0
			15	15		
27	B	1	Total	C	0	0
			9	9		
27	B	1	Total	C	0	0
			10	10		
27	B	1	Total	C	0	0
			14	14		
27	B	1	Total	C	0	0
			12	12		
27	C	1	Total	C	0	0
			15	15		
27	D	1	Total	C	0	0
			15	15		
27	D	1	Total	C	0	0
			8	8		
27	D	1	Total	C	0	0
			10	10		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	I	1	Total C 14 14	0	0
27	J	1	Total C 11 11	0	0
27	M	1	Total C 10 10	0	0
27	M	1	Total C 16 16	0	0
27	T	1	Total C 12 12	0	0
27	a	1	Total C 7 7	0	0
27	b	1	Total C 15 15	0	0
27	b	1	Total C 10 10	0	0
27	b	1	Total C 12 12	0	0
27	b	1	Total C 16 16	0	0
27	b	1	Total C 12 12	0	0
27	b	1	Total C 11 11	0	0
27	b	1	Total C 9 9	0	0
27	b	1	Total C 15 15	0	0
27	c	1	Total C 9 9	0	0
27	c	1	Total C 15 15	0	0
27	d	1	Total C 15 15	0	0
27	d	1	Total C 9 9	0	0
27	d	1	Total C 16 16	0	0
27	i	1	Total C 16 16	0	0
27	i	1	Total C 7 7	0	0

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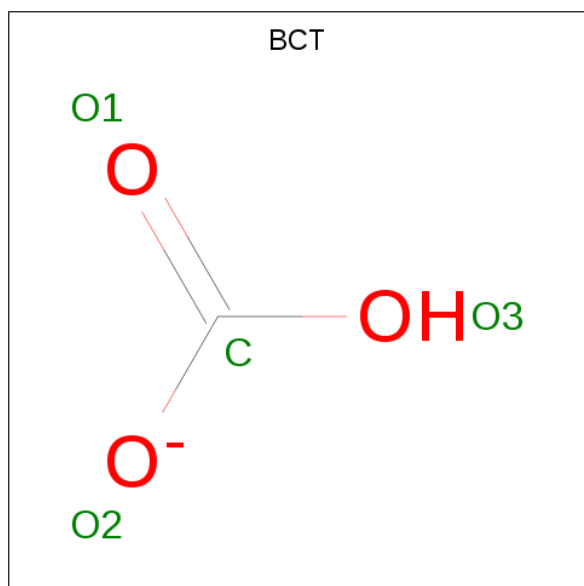
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	j	1	Total C 15 15	0	0
27	m	1	Total C 10 10	0	0
27	m	1	Total C 15 15	0	0
27	t	1	Total C 15 15	0	0

- Molecule 28 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

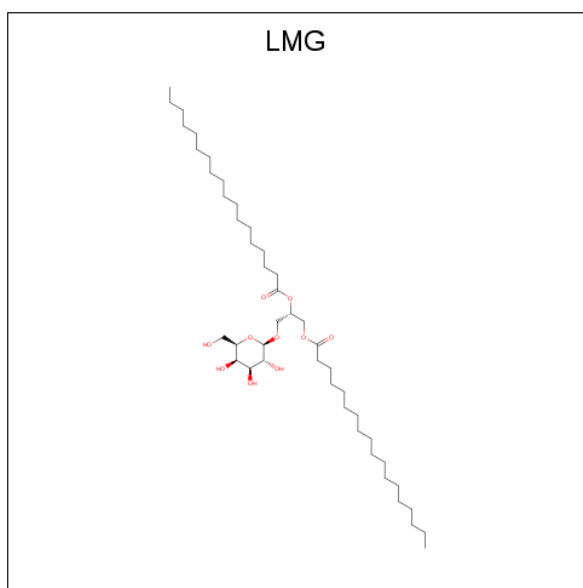
- Molecule 29 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter

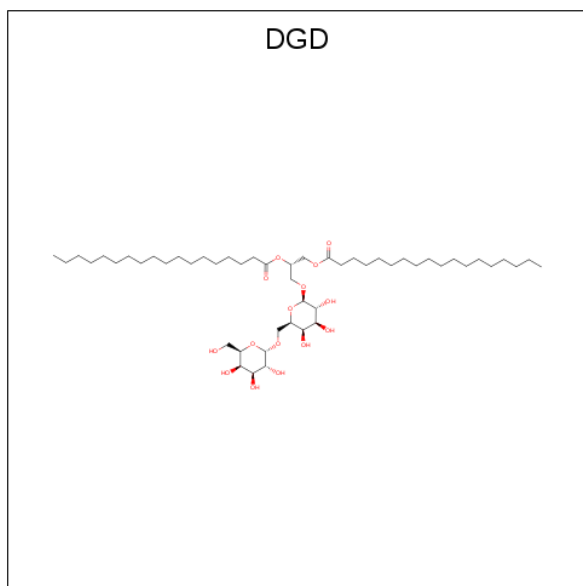
code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	B	1	Total	C	O	0	0
			51	41	10		
30	B	1	Total	C	O	0	0
			36	26	10		
30	C	1	Total	C	O	0	0
			51	41	10		
30	C	1	Total	C	O	0	0
			48	38	10		
30	C	1	Total	C	O	0	0
			44	34	10		
30	D	1	Total	C	O	0	0
			51	41	10		
30	b	1	Total	C	O	0	0
			39	29	10		
30	c	1	Total	C	O	0	0
			51	41	10		
30	c	1	Total	C	O	0	0
			51	41	10		
30	c	1	Total	C	O	0	0
			41	31	10		
30	f	1	Total	C	O	0	0
			51	41	10		
30	m	1	Total	C	O	0	0
			51	41	10		

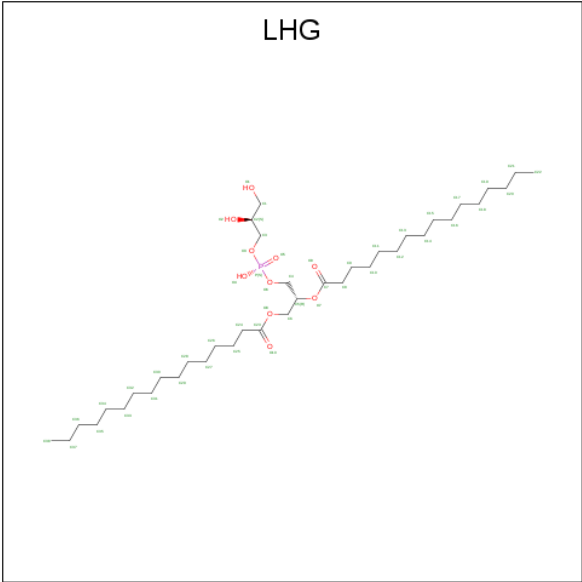
- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD)

(formula: C₅₁H₉₆O₁₅).



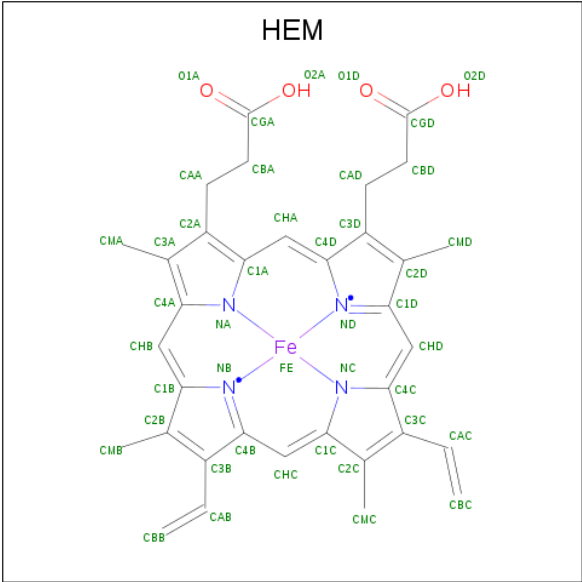
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	C	1	Total	C	O	0	0
			62	47	15		
31	C	1	Total	C	O	0	0
			56	41	15		
31	C	1	Total	C	O	0	0
			62	47	15		
31	H	1	Total	C	O	0	0
			60	45	15		
31	c	1	Total	C	O	0	0
			62	47	15		
31	c	1	Total	C	O	0	0
			55	40	15		
31	c	1	Total	C	O	0	0
			62	47	15		
31	h	1	Total	C	O	0	0
			62	47	15		

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



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	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		
32	L	1	Total	C	O	P	0	0
			49	38	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		
32	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	A	70	Total	O	0	0
			70	70		
34	B	84	Total	O	0	0
			84	84		
34	C	62	Total	O	0	0
			62	62		
34	D	72	Total	O	0	0
			72	72		
34	E	5	Total	O	0	0
			5	5		
34	F	1	Total	O	0	0
			1	1		
34	H	17	Total	O	0	0
			17	17		
34	J	1	Total	O	0	0
			1	1		

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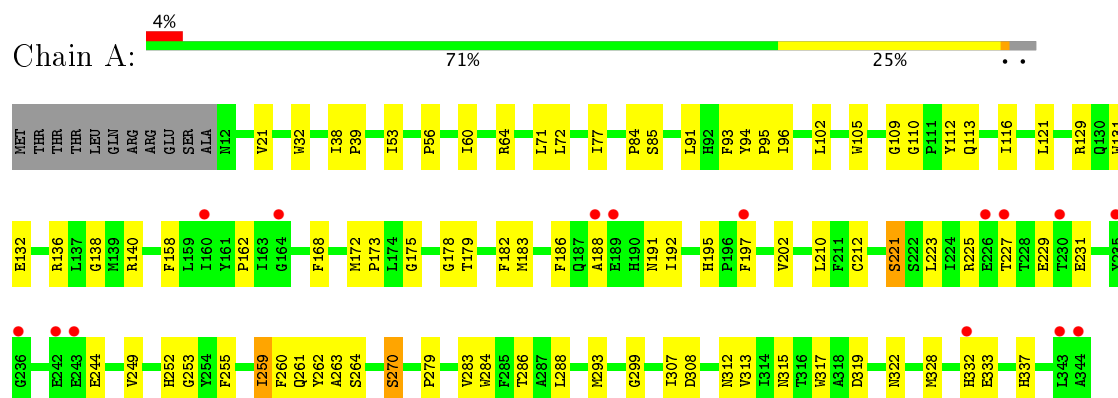
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	K	1	Total 1	O 1	0	0
34	L	5	Total 5	O 5	0	0
34	M	3	Total 3	O 3	0	0
34	O	30	Total 30	O 30	0	0
34	T	2	Total 2	O 2	0	0
34	U	2	Total 2	O 2	0	0
34	V	12	Total 12	O 12	0	0
34	X	3	Total 3	O 3	0	0
34	a	77	Total 77	O 77	0	0
34	b	72	Total 72	O 72	0	0
34	c	65	Total 65	O 65	0	0
34	d	51	Total 51	O 51	0	0
34	e	5	Total 5	O 5	0	0
34	f	2	Total 2	O 2	0	0
34	h	3	Total 3	O 3	0	0
34	l	5	Total 5	O 5	0	0
34	m	2	Total 2	O 2	0	0
34	o	25	Total 25	O 25	0	0
34	t	3	Total 3	O 3	0	0
34	u	12	Total 12	O 12	0	0
34	v	11	Total 11	O 11	0	0

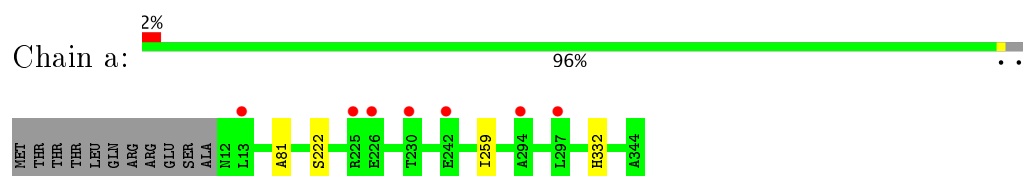
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

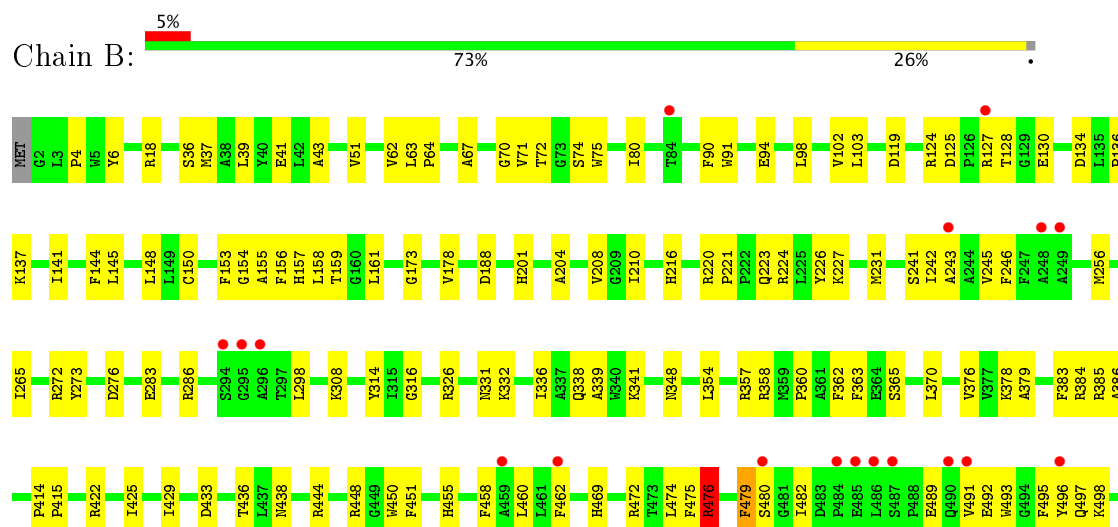
• Molecule 1: Photosystem II protein D1 1



• Molecule 1: Photosystem II protein D1 1



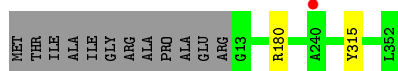
• Molecule 2: Photosystem II CP47 reaction center protein





- Molecule 4: Photosystem II D2 protein

Chain d: 96%



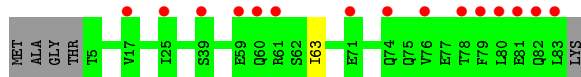
- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 7% 62% 35%



- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 18% 93% 6%



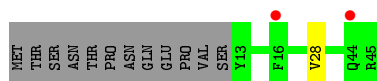
- Molecule 6: Cytochrome b559 subunit beta

Chain F: 2% 44% 29% 27%



- Molecule 6: Cytochrome b559 subunit beta

Chain f: 4% 71% 27%



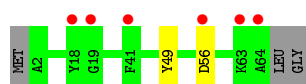
- Molecule 7: Photosystem II reaction center protein H

Chain H: 73% 21% 6%



- Molecule 7: Photosystem II reaction center protein H

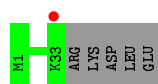
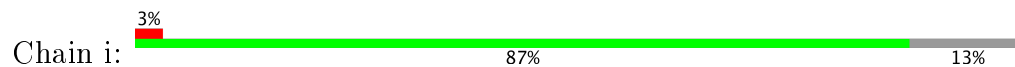
Chain h: 9% 92% 5%



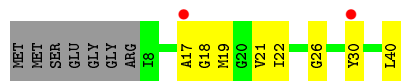
- Molecule 8: Photosystem II reaction center protein I



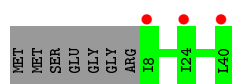
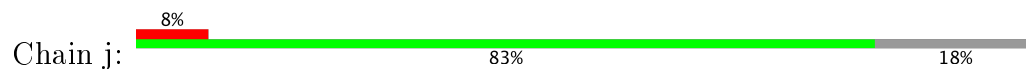
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



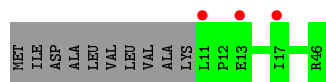
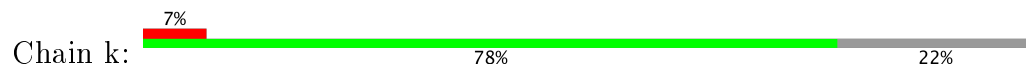
- Molecule 9: Photosystem II reaction center protein J



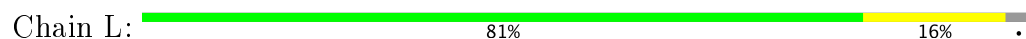
- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K

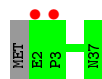


- Molecule 11: Photosystem II reaction center protein L





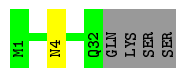
- Molecule 11: Photosystem II reaction center protein L



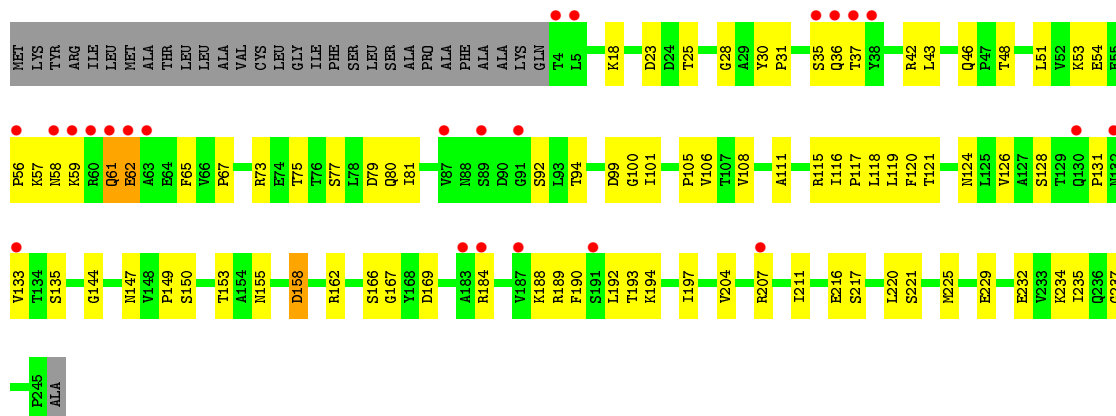
- Molecule 12: Photosystem II reaction center protein M



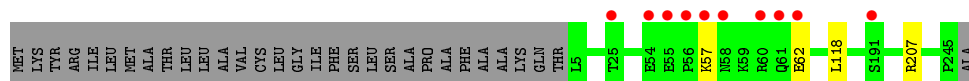
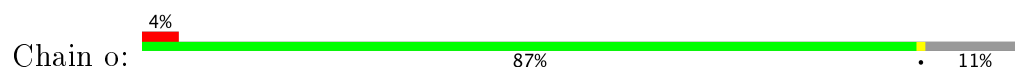
- Molecule 12: Photosystem II reaction center protein M



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



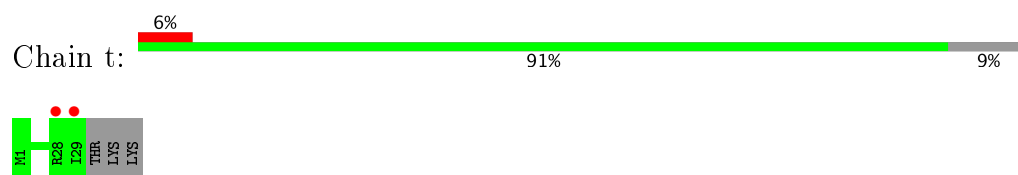
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



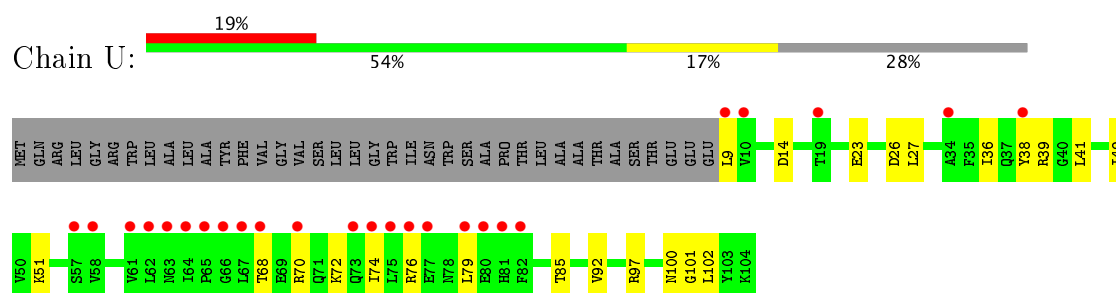
- Molecule 14: Photosystem II reaction center protein T



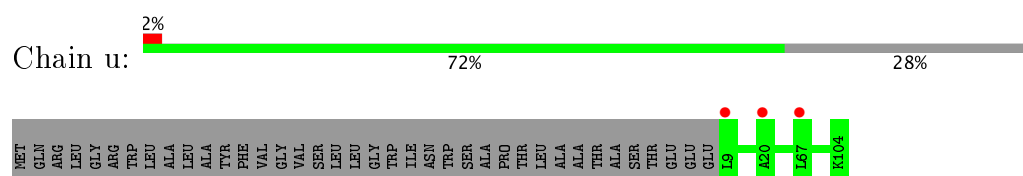
- Molecule 14: Photosystem II reaction center protein T



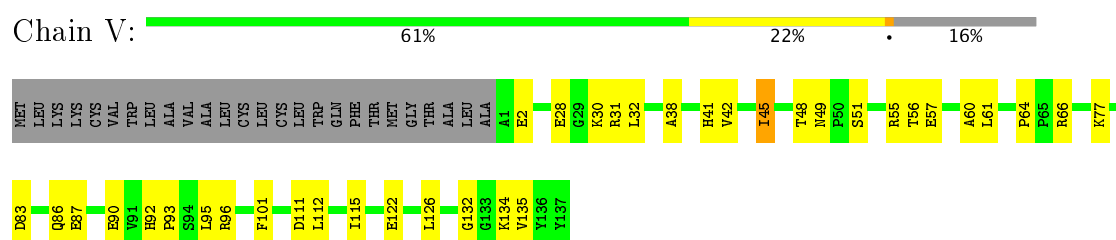
- Molecule 15: Photosystem II 12 kDa extrinsic protein



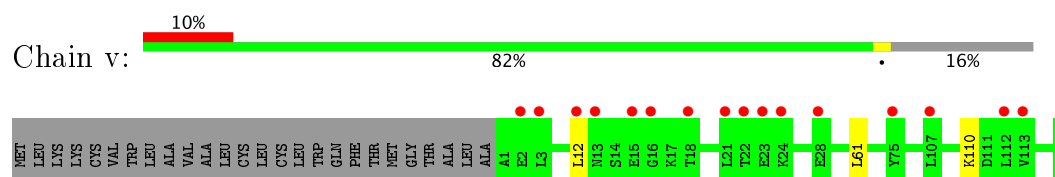
- Molecule 15: Photosystem II 12 kDa extrinsic protein



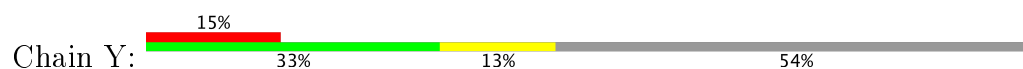
- Molecule 16: Cytochrome c-550

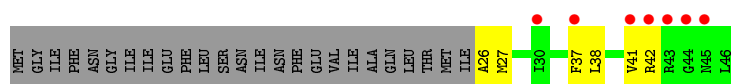


- Molecule 16: Cytochrome c-550

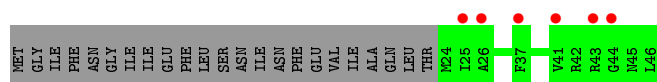


- Molecule 17: Photosystem II reaction center protein Ycf12

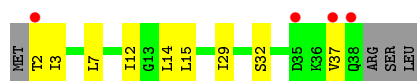




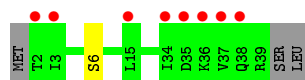
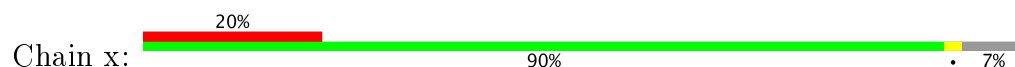
- Molecule 17: Photosystem II reaction center protein Ycf12



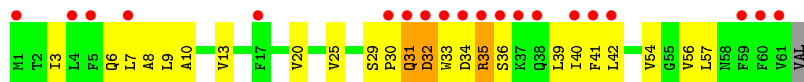
- Molecule 18: Photosystem II reaction center X protein



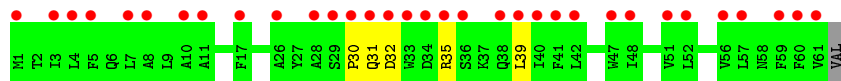
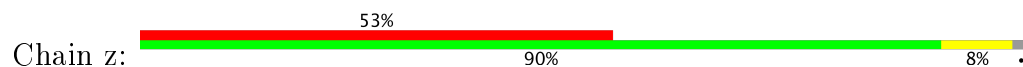
- Molecule 18: Photosystem II reaction center X protein



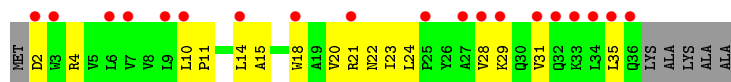
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z

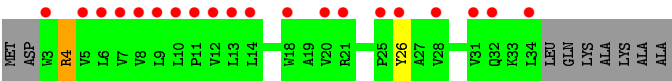


- Molecule 20: Photosystem II protein Y



- 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, α , β , γ	116.33Å 219.62Å 304.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.65 – 2.20 49.65 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.6 (49.65-2.20) 92.6 (49.65-2.20)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.211 , 0.260 0.209 , 0.260	Depositor DCC
R_{free} test set	18223 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.673	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	50407	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, LFA, DGD, CL, CLA, PL9, FE, HEM, BCT, PHO, SQD, 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	0.54	0/2702	0.52	0/3685
1	a	0.53	0/2702	0.51	0/3685
2	B	0.54	0/4120	0.54	1/5614 (0.0%)
2	b	0.51	1/4098 (0.0%)	0.53	2/5586 (0.0%)
3	C	0.48	0/3568	0.51	0/4858
3	c	0.50	2/3579 (0.1%)	0.54	1/4872 (0.0%)
4	D	0.57	0/2801	0.54	1/3818 (0.0%)
4	d	0.52	0/2801	0.53	0/3818
5	E	0.41	0/675	0.48	0/922
5	e	0.58	1/664 (0.2%)	0.52	0/907
6	F	0.41	0/278	0.44	0/379
6	f	0.40	0/278	0.44	0/379
7	H	0.50	0/506	0.51	0/690
7	h	0.43	0/511	0.50	0/697
8	I	0.48	0/273	0.49	0/370
8	i	0.47	0/273	0.48	0/370
9	J	0.51	0/244	0.46	0/332
9	j	0.38	0/244	0.47	0/332
10	K	0.38	0/282	0.46	0/391
10	k	0.42	0/294	0.48	0/405
11	L	0.55	0/303	0.55	0/412
11	l	0.56	0/303	0.50	0/412
12	M	0.52	0/252	0.50	0/344
12	m	0.45	0/252	0.47	0/344
13	O	0.45	0/1890	0.56	1/2564 (0.0%)
13	o	0.46	0/1883	0.54	0/2554
14	T	0.60	0/250	0.41	0/338
14	t	0.51	0/258	0.45	0/349
15	U	0.33	0/776	0.49	0/1052
15	u	0.45	0/776	0.52	0/1052
16	V	0.43	0/1085	0.50	0/1473
16	v	0.40	0/1085	0.49	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.28	0/156	0.43	0/207
17	y	0.31	0/172	0.47	0/228
18	X	0.38	0/273	0.45	0/370
18	x	0.31	0/284	0.43	0/384
19	Z	0.31	0/482	0.49	0/659
19	z	0.36	0/482	0.66	1/659 (0.2%)
20	R	0.31	0/288	0.44	0/395
20	r	0.37	0/263	0.69	1/361 (0.3%)
All	All	0.49	4/42406 (0.0%)	0.52	8/57740 (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
1	a	0	1
19	z	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	63	ILE	C-N	-10.84	1.13	1.34
3	c	399	ALA	C-N	-7.65	1.19	1.34
2	b	2	GLY	C-N	-5.82	1.20	1.34
3	c	78	GLU	C-N	-5.37	1.21	1.34

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	135	ARG	NE-CZ-NH1	9.25	124.93	120.30
19	z	39	LEU	CA-CB-CG	9.14	136.31	115.30
2	B	476	ARG	NE-CZ-NH2	6.77	123.69	120.30
4	D	233	ARG	NE-CZ-NH1	6.47	123.54	120.30
20	r	4	ARG	NE-CZ-NH2	6.45	123.53	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	81	ALA	Peptide
19	z	35	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2617	0	2514	83	0
1	a	2617	0	2514	0	0
2	B	3980	0	3841	125	0
2	b	3958	0	3815	0	0
3	C	3455	0	3376	100	0
3	c	3466	0	3389	0	0
4	D	2706	0	2608	92	0
4	d	2706	0	2608	0	0
5	E	656	0	638	34	0
5	e	645	0	628	0	0
6	F	269	0	277	13	0
6	f	269	0	277	0	0
7	H	493	0	513	12	0
7	h	498	0	518	0	0
8	I	266	0	282	4	0
8	i	266	0	282	0	0
9	J	238	0	249	5	0
9	j	238	0	249	0	0
10	K	272	0	279	10	0
10	k	284	0	292	0	0
11	L	296	0	304	8	0
11	l	296	0	304	0	0
12	M	249	0	268	6	0
12	m	249	0	268	0	0
13	O	1859	0	1833	66	0
13	o	1852	0	1826	0	0
14	T	241	0	244	9	0
14	t	249	0	255	0	0
15	U	765	0	767	16	0
15	u	765	0	767	0	0
16	V	1064	0	1073	27	0
16	v	1064	0	1073	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Y	155	0	175	4	0
17	y	171	0	195	0	0
18	X	270	0	299	7	0
18	x	281	0	312	0	0
19	Z	471	0	507	21	0
19	z	471	0	507	0	0
20	R	282	0	313	15	0
20	r	257	0	290	0	0
21	A	2	0	0	1	0
21	a	2	0	0	0	0
22	A	260	0	288	17	0
22	B	975	0	1080	67	0
22	C	845	0	936	84	0
22	D	130	0	144	10	0
22	H	65	0	72	1	0
22	a	195	0	216	0	0
22	b	1040	0	1152	0	0
22	c	845	0	936	0	0
22	d	195	0	216	0	0
23	A	64	0	74	2	0
23	D	64	0	74	2	0
23	a	128	0	148	0	0
24	A	40	0	56	1	0
24	B	120	0	168	8	0
24	C	80	0	112	9	0
24	D	40	0	56	4	0
24	H	40	0	56	4	0
24	K	80	0	112	11	0
24	T	40	0	56	1	0
24	a	40	0	56	0	0
24	b	120	0	168	0	0
24	c	120	0	168	0	0
24	d	40	0	56	0	0
24	h	40	0	56	0	0
24	k	40	0	56	0	0
24	t	40	0	56	0	0
25	A	55	0	80	6	0
25	D	55	0	80	8	0
25	a	55	0	80	0	0
25	d	55	0	80	0	0
26	A	108	0	156	4	0
26	D	43	0	53	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	L	48	0	63	4	0
26	a	104	0	153	0	0
26	b	54	0	78	0	0
26	f	43	0	53	0	0
27	A	25	0	42	1	0
27	B	99	0	187	13	0
27	C	15	0	29	3	0
27	D	33	0	57	4	0
27	I	14	0	24	0	0
27	J	11	0	18	3	0
27	M	26	0	47	3	0
27	T	12	0	23	0	0
27	a	7	0	10	0	0
27	b	100	0	183	0	0
27	c	24	0	43	0	0
27	d	40	0	77	0	0
27	i	23	0	41	0	0
27	j	15	0	29	0	0
27	m	25	0	45	0	0
27	t	15	0	29	0	0
28	A	1	0	0	0	0
28	a	1	0	0	0	0
29	A	4	0	0	0	0
29	a	4	0	0	0	0
30	B	87	0	114	1	0
30	C	143	0	196	15	0
30	D	51	0	72	1	0
30	b	39	0	48	0	0
30	c	143	0	196	0	0
30	f	51	0	72	0	0
30	m	51	0	72	0	0
31	C	180	0	234	16	0
31	H	60	0	78	3	0
31	c	179	0	232	0	0
31	h	62	0	82	0	0
32	D	147	0	222	37	0
32	E	42	0	57	6	0
32	L	49	0	74	6	0
32	b	49	0	74	0	0
32	d	98	0	148	0	0
32	e	42	0	57	0	0
32	l	49	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	E	43	0	30	11	0
33	V	43	0	30	1	0
33	e	43	0	30	0	0
33	v	43	0	30	0	0
34	A	70	0	0	8	0
34	B	84	0	0	3	0
34	C	62	0	0	7	0
34	D	72	0	0	4	0
34	E	5	0	0	1	0
34	F	1	0	0	0	0
34	H	17	0	0	1	0
34	J	1	0	0	0	0
34	K	1	0	0	0	0
34	L	5	0	0	1	0
34	M	3	0	0	0	0
34	O	30	0	0	6	0
34	T	2	0	0	0	0
34	U	2	0	0	0	0
34	V	12	0	0	3	0
34	X	3	0	0	0	0
34	a	77	0	0	0	0
34	b	72	0	0	0	0
34	c	65	0	0	0	0
34	d	51	0	0	0	0
34	e	5	0	0	0	0
34	f	2	0	0	0	0
34	h	3	0	0	0	0
34	l	5	0	0	0	0
34	m	2	0	0	0	0
34	o	25	0	0	0	0
34	t	3	0	0	0	0
34	u	12	0	0	0	0
34	v	11	0	0	0	0
All	All	50407	0	51279	757	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 9.

The worst 5 of 757 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)
3:C:189:TRP:HE1	3:C:295:THR:HG22	4.55	0.89
2:B:357:ARG:NH2	4:D:337:GLU:O	2.84	0.88
32:D:408:LHG:H151	32:D:408:LHG:H352	1.53	0.88
11:L:7:ARG:NH2	26:L:101:SQD:O8	2.09	0.85
2:B:128:THR:HG22	2:B:130:GLU:H	5.68	0.85

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	331/344 (96%)	321 (97%)	9 (3%)	1 (0%)	44	49
1	a	331/344 (96%)	319 (96%)	11 (3%)	1 (0%)	44	49
2	B	503/510 (99%)	478 (95%)	25 (5%)	0	100	100
2	b	501/510 (98%)	479 (96%)	22 (4%)	0	100	100
3	C	445/461 (96%)	433 (97%)	11 (2%)	1 (0%)	51	58
3	c	446/461 (97%)	430 (96%)	15 (3%)	1 (0%)	51	58
4	D	338/352 (96%)	327 (97%)	11 (3%)	0	100	100
4	d	338/352 (96%)	321 (95%)	17 (5%)	0	100	100
5	E	79/84 (94%)	76 (96%)	3 (4%)	0	100	100
5	e	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
6	F	31/45 (69%)	31 (100%)	0	0	100	100
6	f	31/45 (69%)	30 (97%)	1 (3%)	0	100	100
7	H	60/66 (91%)	56 (93%)	4 (7%)	0	100	100
7	h	61/66 (92%)	55 (90%)	6 (10%)	0	100	100
8	I	31/38 (82%)	30 (97%)	1 (3%)	0	100	100
8	i	31/38 (82%)	31 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	31/40 (78%)	30 (97%)	1 (3%)	0	100	100
9	j	31/40 (78%)	30 (97%)	1 (3%)	0	100	100
10	K	33/46 (72%)	32 (97%)	1 (3%)	0	100	100
10	k	34/46 (74%)	33 (97%)	1 (3%)	0	100	100
11	L	34/37 (92%)	34 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	30/36 (83%)	30 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	240/272 (88%)	222 (92%)	15 (6%)	3 (1%)	14	11
13	o	239/272 (88%)	223 (93%)	14 (6%)	2 (1%)	22	21
14	T	26/32 (81%)	26 (100%)	0	0	100	100
14	t	27/32 (84%)	25 (93%)	2 (7%)	0	100	100
15	U	94/134 (70%)	90 (96%)	4 (4%)	0	100	100
15	u	94/134 (70%)	89 (95%)	5 (5%)	0	100	100
16	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	25	24
16	v	135/163 (83%)	127 (94%)	8 (6%)	0	100	100
17	Y	19/46 (41%)	18 (95%)	1 (5%)	0	100	100
17	y	21/46 (46%)	21 (100%)	0	0	100	100
18	X	35/41 (85%)	34 (97%)	1 (3%)	0	100	100
18	x	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
19	Z	59/62 (95%)	54 (92%)	2 (3%)	3 (5%)	2	1
19	z	59/62 (95%)	53 (90%)	3 (5%)	3 (5%)	2	1
20	R	33/41 (80%)	32 (97%)	0	1 (3%)	5	2
20	r	30/41 (73%)	30 (100%)	0	0	100	100
All	All	5173/5700 (91%)	4951 (96%)	205 (4%)	17 (0%)	44	49

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	57	LYS
19	Z	32	ASP
19	Z	35	ARG
3	c	416	SER
19	z	30	PRO

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%)	87	93
1	a	270/280 (96%)	268 (99%)	2 (1%)	87	93
2	B	403/407 (99%)	400 (99%)	3 (1%)	87	93
2	b	401/407 (98%)	399 (100%)	2 (0%)	91	96
3	C	349/362 (96%)	346 (99%)	3 (1%)	82	91
3	c	350/362 (97%)	345 (99%)	5 (1%)	71	84
4	D	275/283 (97%)	273 (99%)	2 (1%)	87	93
4	d	275/283 (97%)	273 (99%)	2 (1%)	87	93
5	E	71/73 (97%)	71 (100%)	0	100	100
5	e	70/73 (96%)	70 (100%)	0	100	100
6	F	27/39 (69%)	27 (100%)	0	100	100
6	f	27/39 (69%)	26 (96%)	1 (4%)	39	49
7	H	53/55 (96%)	51 (96%)	2 (4%)	38	47
7	h	53/55 (96%)	51 (96%)	2 (4%)	38	47
8	I	30/35 (86%)	29 (97%)	1 (3%)	43	54
8	i	30/35 (86%)	30 (100%)	0	100	100
9	J	23/28 (82%)	22 (96%)	1 (4%)	33	41
9	j	23/28 (82%)	23 (100%)	0	100	100
10	K	28/37 (76%)	27 (96%)	1 (4%)	40	50
10	k	29/37 (78%)	29 (100%)	0	100	100
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	29/33 (88%)	29 (100%)	0	100	100
12	m	29/33 (88%)	28 (97%)	1 (3%)	42	53
13	O	206/228 (90%)	202 (98%)	4 (2%)	62	76
13	o	205/228 (90%)	203 (99%)	2 (1%)	80	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	25/29 (86%)	25 (100%)	0	100	100
14	t	26/29 (90%)	26 (100%)	0	100	100
15	U	83/112 (74%)	82 (99%)	1 (1%)	75	86
15	u	83/112 (74%)	83 (100%)	0	100	100
16	V	117/138 (85%)	117 (100%)	0	100	100
16	v	117/138 (85%)	114 (97%)	3 (3%)	51	64
17	Y	15/37 (40%)	15 (100%)	0	100	100
17	y	17/37 (46%)	17 (100%)	0	100	100
18	X	30/34 (88%)	29 (97%)	1 (3%)	43	54
18	x	31/34 (91%)	30 (97%)	1 (3%)	44	56
19	Z	51/52 (98%)	50 (98%)	1 (2%)	60	74
19	z	51/52 (98%)	51 (100%)	0	100	100
20	R	30/33 (91%)	29 (97%)	1 (3%)	43	54
20	r	27/33 (82%)	25 (93%)	2 (7%)	16	17
All	All	4297/4660 (92%)	4251 (99%)	46 (1%)	78	88

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	X	14	LEU
2	b	495	PHE
18	x	6	SER
19	Z	31	GLN
1	a	332	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	312	ASN
3	c	332	GLN
13	o	200	ASN
2	b	282	GLN
3	c	418	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 189 ligands modelled in this entry, 6 are monoatomic - leaving 183 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$
22	CLA	A	403	-	56,73,73	1.32	3 (5%)	65,113,113	1.26	5 (7%)
22	CLA	A	404	34	56,73,73	1.17	3 (5%)	65,113,113	1.21	7 (10%)
23	PHO	A	405	-	67,69,69	0.78	3 (4%)	87,99,99	1.02	5 (5%)
22	CLA	A	406	-	56,73,73	1.42	6 (10%)	65,113,113	1.38	5 (7%)
24	BCR	A	407	-	41,41,41	0.81	0	56,56,56	1.56	12 (21%)
25	PL9	A	408	-	55,55,55	0.61	2 (3%)	69,69,69	1.92	20 (28%)
26	SQD	A	409	-	53,54,54	1.12	4 (7%)	63,65,65	1.80	12 (19%)
27	LFA	A	410	-	13,13,19	0.10	0	12,12,18	0.33	0
26	SQD	A	411	-	53,54,54	1.14	4 (7%)	63,65,65	1.51	9 (14%)
22	CLA	A	412	34	56,73,73	1.18	4 (7%)	65,113,113	1.33	4 (6%)
27	LFA	A	413	-	10,10,19	0.08	0	9,9,18	0.42	0
29	BCT	A	415	28	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	B	601	-	56,73,73	1.13	3 (5%)	65,113,113	1.25	6 (9%)
22	CLA	B	602	-	56,73,73	1.13	4 (7%)	65,113,113	1.37	7 (10%)
22	CLA	B	603	-	56,73,73	1.27	2 (3%)	65,113,113	1.36	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	604	-	56,73,73	1.16	2 (3%)	65,113,113	1.14	5 (7%)
22	CLA	B	605	-	56,73,73	1.22	4 (7%)	65,113,113	1.33	5 (7%)
22	CLA	B	606	34	56,73,73	1.37	5 (8%)	65,113,113	1.32	9 (13%)
22	CLA	B	607	-	56,73,73	1.49	4 (7%)	65,113,113	1.15	4 (6%)
22	CLA	B	608	-	56,73,73	1.14	4 (7%)	65,113,113	1.47	5 (7%)
22	CLA	B	609	34	56,73,73	1.44	5 (8%)	65,113,113	1.28	7 (10%)
22	CLA	B	610	-	56,73,73	1.22	4 (7%)	65,113,113	1.41	7 (10%)
22	CLA	B	611	-	56,73,73	1.19	3 (5%)	65,113,113	1.26	5 (7%)
22	CLA	B	612	-	56,73,73	1.20	4 (7%)	65,113,113	1.37	7 (10%)
22	CLA	B	613	-	56,73,73	1.32	5 (8%)	65,113,113	1.14	6 (9%)
22	CLA	B	614	-	56,73,73	1.30	4 (7%)	65,113,113	1.32	8 (12%)
22	CLA	B	615	-	56,73,73	1.24	4 (7%)	65,113,113	1.25	7 (10%)
24	BCR	B	616	-	41,41,41	0.84	1 (2%)	56,56,56	1.70	12 (21%)
24	BCR	B	617	-	41,41,41	0.84	2 (4%)	56,56,56	1.61	12 (21%)
24	BCR	B	618	-	41,41,41	0.90	1 (2%)	56,56,56	1.97	14 (25%)
30	LMG	B	619	-	51,51,55	0.91	2 (3%)	59,59,63	1.07	2 (3%)
27	LFA	B	620	-	9,9,19	0.14	0	8,8,18	0.43	0
30	LMG	B	621	-	36,36,55	1.03	2 (5%)	44,44,63	1.27	5 (11%)
27	LFA	B	622	-	15,15,19	0.10	0	14,14,18	0.32	0
27	LFA	B	623	-	12,12,19	0.09	0	11,11,18	0.23	0
27	LFA	B	624	-	14,14,19	0.08	0	13,13,18	0.31	0
27	LFA	B	625	-	8,8,19	0.10	0	7,7,18	0.31	0
27	LFA	B	626	-	9,9,19	0.11	0	8,8,18	0.45	0
27	LFA	B	627	-	13,13,19	0.10	0	12,12,18	0.51	0
27	LFA	B	628	-	11,11,19	0.09	0	10,10,18	0.37	0
30	LMG	C	501	-	51,51,55	0.87	2 (3%)	59,59,63	1.12	3 (5%)
22	CLA	C	502	-	56,73,73	1.25	5 (8%)	65,113,113	1.35	6 (9%)
22	CLA	C	503	-	56,73,73	1.16	3 (5%)	65,113,113	1.23	7 (10%)
22	CLA	C	504	-	56,73,73	1.18	3 (5%)	65,113,113	1.27	6 (9%)
22	CLA	C	505	34	56,73,73	1.16	4 (7%)	65,113,113	1.33	8 (12%)
22	CLA	C	506	-	56,73,73	1.27	4 (7%)	65,113,113	1.18	5 (7%)
22	CLA	C	507	-	56,73,73	1.31	5 (8%)	65,113,113	1.39	7 (10%)
22	CLA	C	508	34	56,73,73	1.15	4 (7%)	65,113,113	1.23	7 (10%)
22	CLA	C	509	-	56,73,73	1.11	4 (7%)	65,113,113	1.30	7 (10%)
22	CLA	C	510	-	56,73,73	1.09	4 (7%)	65,113,113	1.42	6 (9%)
22	CLA	C	511	-	56,73,73	1.16	3 (5%)	65,113,113	1.31	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	C	512	3	56,73,73	1.02	3 (5%)	65,113,113	1.37	6 (9%)
22	CLA	C	513	-	56,73,73	1.14	4 (7%)	65,113,113	1.33	6 (9%)
22	CLA	C	514	-	56,73,73	1.10	4 (7%)	65,113,113	1.35	7 (10%)
24	BCR	C	515	-	41,41,41	0.81	1 (2%)	56,56,56	1.79	17 (30%)
24	BCR	C	516	-	41,41,41	0.97	3 (7%)	56,56,56	1.73	10 (17%)
31	DGD	C	517	-	63,63,67	0.82	2 (3%)	77,77,81	1.25	7 (9%)
31	DGD	C	518	-	57,57,67	0.84	2 (3%)	71,71,81	1.31	10 (14%)
31	DGD	C	519	-	63,63,67	0.81	3 (4%)	77,77,81	1.12	7 (9%)
30	LMG	C	520	-	48,48,55	0.92	2 (4%)	56,56,63	1.18	5 (8%)
27	LFA	C	521	-	14,14,19	0.08	0	13,13,18	0.33	0
30	LMG	C	522	-	44,44,55	1.04	3 (6%)	52,52,63	1.62	9 (17%)
23	PHO	D	401	-	67,69,69	0.78	2 (2%)	87,99,99	0.99	5 (5%)
22	CLA	D	402	-	56,73,73	1.14	3 (5%)	65,113,113	1.18	7 (10%)
22	CLA	D	403	-	56,73,73	1.25	5 (8%)	65,113,113	1.31	7 (10%)
24	BCR	D	404	-	41,41,41	0.88	2 (4%)	56,56,56	1.89	13 (23%)
25	PL9	D	405	-	55,55,55	0.68	3 (5%)	69,69,69	1.59	14 (20%)
32	LHG	D	406	-	48,48,48	0.87	3 (6%)	49,54,54	1.23	4 (8%)
32	LHG	D	407	-	48,48,48	0.85	3 (6%)	49,54,54	1.21	4 (8%)
32	LHG	D	408	-	48,48,48	0.85	3 (6%)	49,54,54	1.05	2 (4%)
30	LMG	D	409	-	51,51,55	0.94	2 (3%)	59,59,63	0.97	2 (3%)
27	LFA	D	410	-	14,14,19	0.09	0	13,13,18	0.25	0
26	SQD	D	411	-	42,43,54	1.26	4 (9%)	52,54,65	2.02	12 (23%)
27	LFA	D	412	-	7,7,19	0.12	0	6,6,18	0.33	0
27	LFA	D	413	-	9,9,19	0.16	0	8,8,18	0.51	0
32	LHG	E	101	-	41,41,48	0.99	2 (4%)	42,47,54	1.13	3 (7%)
33	HEM	E	102	5,6	28,50,50	1.58	2 (7%)	17,82,82	1.99	5 (29%)
22	CLA	H	101	34	56,73,73	1.24	4 (7%)	65,113,113	1.25	4 (6%)
24	BCR	H	102	-	41,41,41	0.74	0	56,56,56	1.86	13 (23%)
31	DGD	H	103	-	61,61,67	0.83	2 (3%)	75,75,81	1.23	5 (6%)
27	LFA	I	101	-	13,13,19	0.09	0	12,12,18	0.36	0
27	LFA	J	101	-	10,10,19	0.11	0	9,9,18	0.36	0
24	BCR	K	101	-	41,41,41	0.78	2 (4%)	56,56,56	1.64	11 (19%)
24	BCR	K	102	-	41,41,41	0.84	1 (2%)	56,56,56	1.90	13 (23%)
26	SQD	L	101	-	47,48,54	1.22	4 (8%)	57,59,65	4.73	11 (19%)
32	LHG	L	102	-	48,48,48	0.93	2 (4%)	49,54,54	1.15	3 (6%)
27	LFA	M	101	-	9,9,19	0.15	0	8,8,18	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LFA	M	102	-	15,15,19	0.16	0	14,14,18	0.64	0
24	BCR	T	101	-	41,41,41	0.89	1 (2%)	56,56,56	2.03	16 (28%)
27	LFA	T	102	-	11,11,19	0.11	0	10,10,18	0.41	0
33	HEM	V	201	16	28,50,50	1.59	2 (7%)	17,82,82	1.99	5 (29%)
22	CLA	a	404	-	56,73,73	1.15	4 (7%)	65,113,113	1.25	7 (10%)
22	CLA	a	405	34	56,73,73	1.22	4 (7%)	65,113,113	1.15	6 (9%)
23	PHO	a	406	-	67,69,69	0.74	2 (2%)	87,99,99	1.03	6 (6%)
22	CLA	a	407	-	56,73,73	1.12	4 (7%)	65,113,113	1.35	7 (10%)
24	BCR	a	408	-	41,41,41	0.86	1 (2%)	56,56,56	1.44	12 (21%)
25	PL9	a	409	-	55,55,55	0.58	1 (1%)	69,69,69	1.73	16 (23%)
26	SQD	a	410	-	53,54,54	1.12	4 (7%)	63,65,65	1.57	12 (19%)
27	LFA	a	411	-	6,6,19	0.11	0	5,5,18	0.21	0
26	SQD	a	412	-	50,50,54	0.88	2 (4%)	58,58,65	1.20	6 (10%)
29	BCT	a	413	28	0,3,3	0.00	-	0,3,3	0.00	-
23	PHO	a	414	-	67,69,69	0.76	2 (2%)	87,99,99	0.96	4 (4%)
26	SQD	b	601	-	53,54,54	1.13	4 (7%)	63,65,65	1.68	14 (22%)
27	LFA	b	602	-	14,14,19	0.10	0	13,13,18	0.43	0
22	CLA	b	603	34	56,73,73	1.22	3 (5%)	65,113,113	1.29	6 (9%)
22	CLA	b	604	-	56,73,73	1.11	5 (8%)	65,113,113	1.37	7 (10%)
22	CLA	b	605	-	56,73,73	1.15	5 (8%)	65,113,113	1.26	6 (9%)
22	CLA	b	606	-	56,73,73	1.23	4 (7%)	65,113,113	1.34	8 (12%)
22	CLA	b	607	-	56,73,73	1.34	5 (8%)	65,113,113	1.20	7 (10%)
22	CLA	b	608	-	56,73,73	1.30	5 (8%)	65,113,113	1.30	7 (10%)
22	CLA	b	609	34	56,73,73	1.16	6 (10%)	65,113,113	1.29	10 (15%)
22	CLA	b	610	-	56,73,73	1.28	5 (8%)	65,113,113	1.27	7 (10%)
22	CLA	b	611	-	56,73,73	1.22	5 (8%)	65,113,113	1.29	7 (10%)
22	CLA	b	612	34	56,73,73	1.38	5 (8%)	65,113,113	1.31	8 (12%)
22	CLA	b	613	-	56,73,73	1.28	2 (3%)	65,113,113	1.36	4 (6%)
22	CLA	b	614	-	56,73,73	1.22	5 (8%)	65,113,113	1.43	6 (9%)
22	CLA	b	615	-	56,73,73	1.25	6 (10%)	65,113,113	1.30	7 (10%)
22	CLA	b	616	-	56,73,73	1.30	4 (7%)	65,113,113	1.20	5 (7%)
22	CLA	b	617	-	56,73,73	1.15	3 (5%)	65,113,113	1.26	7 (10%)
22	CLA	b	618	-	56,73,73	1.27	5 (8%)	65,113,113	1.28	8 (12%)
24	BCR	b	619	-	41,41,41	0.83	1 (2%)	56,56,56	1.79	12 (21%)
24	BCR	b	620	-	41,41,41	0.77	0	56,56,56	1.51	10 (17%)
24	BCR	b	621	-	41,41,41	0.82	1 (2%)	56,56,56	1.86	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LFA	b	622	-	9,9,19	0.11	0	8,8,18	0.32	0
27	LFA	b	623	-	11,11,19	0.10	0	10,10,18	0.38	0
30	LMG	b	624	-	39,39,55	1.10	3 (7%)	47,47,63	1.18	6 (12%)
27	LFA	b	625	-	15,15,19	0.09	0	14,14,18	0.39	0
27	LFA	b	626	-	11,11,19	0.11	0	10,10,18	0.29	0
27	LFA	b	627	-	10,10,19	0.10	0	9,9,18	0.35	0
32	LHG	b	628	-	48,48,48	0.88	3 (6%)	49,54,54	1.15	5 (10%)
27	LFA	b	629	-	8,8,19	0.11	0	7,7,18	0.32	0
27	LFA	b	630	-	14,14,19	0.08	0	13,13,18	0.37	0
30	LMG	c	501	-	51,51,55	0.85	2 (3%)	59,59,63	1.27	4 (6%)
22	CLA	c	502	-	56,73,73	1.08	4 (7%)	65,113,113	1.28	7 (10%)
22	CLA	c	503	-	56,73,73	1.15	4 (7%)	65,113,113	1.31	7 (10%)
22	CLA	c	504	-	56,73,73	1.16	3 (5%)	65,113,113	1.32	7 (10%)
22	CLA	c	505	34	56,73,73	1.09	3 (5%)	65,113,113	1.23	6 (9%)
22	CLA	c	506	-	56,73,73	1.28	3 (5%)	65,113,113	1.26	4 (6%)
22	CLA	c	507	-	56,73,73	1.14	4 (7%)	65,113,113	1.36	6 (9%)
22	CLA	c	508	34	56,73,73	1.15	5 (8%)	65,113,113	1.27	8 (12%)
22	CLA	c	509	-	56,73,73	1.18	5 (8%)	65,113,113	1.25	6 (9%)
22	CLA	c	510	-	56,73,73	1.18	4 (7%)	65,113,113	1.37	5 (7%)
22	CLA	c	511	-	56,73,73	1.23	4 (7%)	65,113,113	1.26	5 (7%)
22	CLA	c	512	3	56,73,73	1.23	4 (7%)	65,113,113	1.35	8 (12%)
22	CLA	c	513	-	56,73,73	1.20	4 (7%)	65,113,113	1.27	6 (9%)
22	CLA	c	514	-	56,73,73	1.08	5 (8%)	65,113,113	1.35	7 (10%)
24	BCR	c	515	-	41,41,41	0.84	2 (4%)	56,56,56	1.38	6 (10%)
31	DGD	c	516	-	63,63,67	0.82	3 (4%)	77,77,81	1.16	7 (9%)
31	DGD	c	517	-	56,56,67	0.87	2 (3%)	70,70,81	1.13	5 (7%)
31	DGD	c	518	-	63,63,67	0.83	3 (4%)	77,77,81	1.07	2 (2%)
30	LMG	c	519	-	51,51,55	0.89	2 (3%)	59,59,63	1.19	6 (10%)
27	LFA	c	520	-	8,8,19	0.11	0	7,7,18	0.36	0
27	LFA	c	521	-	14,14,19	0.08	0	13,13,18	0.34	0
30	LMG	c	522	-	41,41,55	1.02	2 (4%)	49,49,63	1.64	11 (22%)
24	BCR	c	523	-	41,41,41	0.82	1 (2%)	56,56,56	1.84	13 (23%)
24	BCR	c	524	-	41,41,41	0.77	0	56,56,56	1.73	12 (21%)
22	CLA	d	401	34	56,73,73	1.16	4 (7%)	65,113,113	1.39	6 (9%)
22	CLA	d	402	-	56,73,73	1.22	3 (5%)	65,113,113	1.18	3 (4%)
22	CLA	d	403	-	56,73,73	1.22	4 (7%)	65,113,113	1.47	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	d	404	-	41,41,41	0.89	1 (2%)	56,56,56	2.21	18 (32%)
25	PL9	d	405	-	55,55,55	0.62	2 (3%)	69,69,69	1.69	15 (21%)
32	LHG	d	406	-	48,48,48	0.91	3 (6%)	49,54,54	1.22	4 (8%)
32	LHG	d	407	-	48,48,48	0.89	2 (4%)	49,54,54	1.14	3 (6%)
27	LFA	d	408	-	14,14,19	0.10	0	13,13,18	0.42	0
27	LFA	d	409	-	8,8,19	0.12	0	7,7,18	0.26	0
27	LFA	d	410	-	15,15,19	0.08	0	14,14,18	0.36	0
32	LHG	e	101	-	41,41,48	0.96	2 (4%)	42,47,54	1.09	3 (7%)
33	HEM	e	102	5,6	28,50,50	1.51	2 (7%)	17,82,82	1.44	3 (17%)
30	LMG	f	101	-	51,51,55	0.88	2 (3%)	59,59,63	1.11	5 (8%)
26	SQD	f	102	-	42,43,54	1.26	4 (9%)	52,54,65	1.92	12 (23%)
24	BCR	h	101	-	41,41,41	0.76	0	56,56,56	1.82	12 (21%)
31	DGD	h	102	-	63,63,67	0.80	2 (3%)	77,77,81	1.04	5 (6%)
27	LFA	i	101	-	15,15,19	0.10	0	14,14,18	0.38	0
27	LFA	i	102	-	6,6,19	0.12	0	5,5,18	0.16	0
27	LFA	j	101	-	14,14,19	0.09	0	13,13,18	0.43	0
24	BCR	k	101	-	41,41,41	0.84	1 (2%)	56,56,56	1.83	13 (23%)
32	LHG	l	101	-	48,48,48	0.85	3 (6%)	49,54,54	1.26	5 (10%)
27	LFA	m	101	-	9,9,19	0.12	0	8,8,18	0.43	0
27	LFA	m	102	-	14,14,19	0.11	0	13,13,18	0.40	0
30	LMG	m	103	-	51,51,55	0.82	2 (3%)	59,59,63	1.39	8 (13%)
27	LFA	t	101	-	14,14,19	0.11	0	13,13,18	0.52	0
24	BCR	t	102	-	41,41,41	0.84	1 (2%)	56,56,56	1.93	14 (25%)
33	HEM	v	201	16	28,50,50	1.60	2 (7%)	17,82,82	2.16	4 (23%)

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
22	CLA	A	403	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	A	404	34	3/3/20/25	0/37/135/135	0/0/9/9
23	PHO	A	405	-	-	0/53/103/103	0/1/6/6
22	CLA	A	406	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	A	407	-	-	0/29/63/63	0/2/2/2
25	PL9	A	408	-	-	0/53/73/73	0/1/1/1
26	SQD	A	409	-	-	0/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LFA	A	410	-	-	0/11/11/17	0/0/0/0
26	SQD	A	411	-	-	0/49/69/69	0/1/1/1
22	CLA	A	412	34	3/3/20/25	0/37/135/135	0/0/9/9
27	LFA	A	413	-	-	0/8/8/17	0/0/0/0
29	BCT	A	415	28	-	0/0/0/0	0/0/0/0
22	CLA	B	601	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	602	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	606	34	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	607	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	609	34	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	610	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	B	616	-	-	0/29/63/63	0/2/2/2
24	BCR	B	617	-	-	0/29/63/63	0/2/2/2
24	BCR	B	618	-	-	0/29/63/63	0/2/2/2
30	LMG	B	619	-	-	0/46/66/70	0/1/1/1
27	LFA	B	620	-	-	0/7/7/17	0/0/0/0
30	LMG	B	621	-	-	0/31/51/70	0/1/1/1
27	LFA	B	622	-	-	0/13/13/17	0/0/0/0
27	LFA	B	623	-	-	0/10/10/17	0/0/0/0
27	LFA	B	624	-	-	0/12/12/17	0/0/0/0
27	LFA	B	625	-	-	0/6/6/17	0/0/0/0
27	LFA	B	626	-	-	0/7/7/17	0/0/0/0
27	LFA	B	627	-	-	0/11/11/17	0/0/0/0
27	LFA	B	628	-	-	0/9/9/17	0/0/0/0
30	LMG	C	501	-	-	0/46/66/70	0/1/1/1
22	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	505	34	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	508	34	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	511	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	512	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	513	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	514	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	C	515	-	-	0/29/63/63	0/2/2/2
24	BCR	C	516	-	-	0/29/63/63	0/2/2/2
31	DGD	C	517	-	-	0/51/91/95	0/2/2/2
31	DGD	C	518	-	-	0/45/85/95	0/2/2/2
31	DGD	C	519	-	-	0/51/91/95	0/2/2/2
30	LMG	C	520	-	-	0/43/63/70	0/1/1/1
27	LFA	C	521	-	-	0/12/12/17	0/0/0/0
30	LMG	C	522	-	-	1/39/59/70	0/1/1/1
23	PHO	D	401	-	-	0/53/103/103	0/1/6/6
22	CLA	D	402	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	D	403	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	D	404	-	-	0/29/63/63	0/2/2/2
25	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
32	LHG	D	408	-	-	0/53/53/53	0/0/0/0
30	LMG	D	409	-	-	0/46/66/70	0/1/1/1
27	LFA	D	410	-	-	0/12/12/17	0/0/0/0
26	SQD	D	411	-	-	0/38/58/69	0/1/1/1
27	LFA	D	412	-	-	0/5/5/17	0/0/0/0
27	LFA	D	413	-	-	0/7/7/17	0/0/0/0
32	LHG	E	101	-	-	0/46/46/53	0/0/0/0
33	HEM	E	102	5,6	-	0/6/54/54	0/0/8/8
22	CLA	H	101	34	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	H	102	-	-	0/29/63/63	0/2/2/2
31	DGD	H	103	-	-	0/49/89/95	0/2/2/2
27	LFA	I	101	-	-	0/11/11/17	0/0/0/0
27	LFA	J	101	-	-	0/8/8/17	0/0/0/0
24	BCR	K	101	-	-	0/29/63/63	0/2/2/2
24	BCR	K	102	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	L	101	-	-	0/43/63/69	0/1/1/1
32	LHG	L	102	-	-	0/53/53/53	0/0/0/0
27	LFA	M	101	-	-	0/7/7/17	0/0/0/0
27	LFA	M	102	-	-	0/13/13/17	0/0/0/0
24	BCR	T	101	-	-	0/29/63/63	0/2/2/2
27	LFA	T	102	-	-	0/9/9/17	0/0/0/0
33	HEM	V	201	16	-	0/6/54/54	0/0/8/8
22	CLA	a	404	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	a	405	34	3/3/20/25	0/37/135/135	0/0/9/9
23	PHO	a	406	-	-	0/53/103/103	0/1/6/6
22	CLA	a	407	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	a	408	-	-	0/29/63/63	0/2/2/2
25	PL9	a	409	-	-	0/53/73/73	0/1/1/1
26	SQD	a	410	-	-	0/49/69/69	0/1/1/1
27	LFA	a	411	-	-	0/4/4/17	0/0/0/0
26	SQD	a	412	-	-	0/44/64/69	0/1/1/1
29	BCT	a	413	28	-	0/0/0/0	0/0/0/0
23	PHO	a	414	-	-	0/53/103/103	0/1/6/6
26	SQD	b	601	-	-	0/49/69/69	0/1/1/1
27	LFA	b	602	-	-	0/12/12/17	0/0/0/0
22	CLA	b	603	34	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	604	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	609	34	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	610	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	612	34	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	618	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	b	619	-	-	0/29/63/63	0/2/2/2
24	BCR	b	620	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	b	621	-	-	0/29/63/63	0/2/2/2
27	LFA	b	622	-	-	0/7/7/17	0/0/0/0
27	LFA	b	623	-	-	0/9/9/17	0/0/0/0
30	LMG	b	624	-	-	0/34/54/70	0/1/1/1
27	LFA	b	625	-	-	0/13/13/17	0/0/0/0
27	LFA	b	626	-	-	0/9/9/17	0/0/0/0
27	LFA	b	627	-	-	0/8/8/17	0/0/0/0
32	LHG	b	628	-	-	0/53/53/53	0/0/0/0
27	LFA	b	629	-	-	0/6/6/17	0/0/0/0
27	LFA	b	630	-	-	0/12/12/17	0/0/0/0
30	LMG	c	501	-	-	0/46/66/70	0/1/1/1
22	CLA	c	502	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	504	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	505	34	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	506	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	507	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	508	34	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	510	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	511	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	512	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	513	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	514	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	c	515	-	-	0/29/63/63	0/2/2/2
31	DGD	c	516	-	-	0/51/91/95	0/2/2/2
31	DGD	c	517	-	-	0/44/84/95	0/2/2/2
31	DGD	c	518	-	-	0/51/91/95	0/2/2/2
30	LMG	c	519	-	-	0/46/66/70	0/1/1/1
27	LFA	c	520	-	-	0/6/6/17	0/0/0/0
27	LFA	c	521	-	-	0/12/12/17	0/0/0/0
30	LMG	c	522	-	-	0/36/56/70	0/1/1/1
24	BCR	c	523	-	-	0/29/63/63	0/2/2/2
24	BCR	c	524	-	-	0/29/63/63	0/2/2/2
22	CLA	d	401	34	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	d	402	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	d	403	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	d	404	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	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
27	LFA	d	408	-	-	0/12/12/17	0/0/0/0
27	LFA	d	409	-	-	0/6/6/17	0/0/0/0
27	LFA	d	410	-	-	0/13/13/17	0/0/0/0
32	LHG	e	101	-	-	0/46/46/53	0/0/0/0
33	HEM	e	102	5,6	-	0/6/54/54	0/0/8/8
30	LMG	f	101	-	-	0/46/66/70	0/1/1/1
26	SQD	f	102	-	-	0/38/58/69	0/1/1/1
24	BCR	h	101	-	-	0/29/63/63	0/2/2/2
31	DGD	h	102	-	-	0/51/91/95	0/2/2/2
27	LFA	i	101	-	-	0/13/13/17	0/0/0/0
27	LFA	i	102	-	-	0/4/4/17	0/0/0/0
27	LFA	j	101	-	-	0/12/12/17	0/0/0/0
24	BCR	k	101	-	-	0/29/63/63	0/2/2/2
32	LHG	l	101	-	-	0/53/53/53	0/0/0/0
27	LFA	m	101	-	-	0/7/7/17	0/0/0/0
27	LFA	m	102	-	-	0/12/12/17	0/0/0/0
30	LMG	m	103	-	-	0/46/66/70	0/1/1/1
27	LFA	t	101	-	-	0/12/12/17	0/0/0/0
24	BCR	t	102	-	-	0/29/63/63	0/2/2/2
33	HEM	v	201	16	-	0/6/54/54	0/0/8/8

The worst 5 of 432 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	606	CLA	C3B-C2B	-6.89	1.31	1.40
33	v	201	HEM	C3C-C2C	-6.52	1.31	1.40
22	A	406	CLA	C3B-C2B	-6.41	1.31	1.40
33	V	201	HEM	C3C-C2C	-6.39	1.31	1.40
22	B	607	CLA	C3B-C2B	-6.28	1.32	1.40

The worst 5 of 1060 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	101	SQD	O9-S-C6	-25.87	84.72	106.83
26	L	101	SQD	O8-S-O9	-11.66	84.64	111.37
26	L	101	SQD	O9-S-O7	-9.68	80.32	113.86
22	B	608	CLA	C1C-NC-C4C	-8.23	102.32	107.06
22	d	403	CLA	C1C-NC-C4C	-8.20	102.34	107.06

5 of 210 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	b	614	CLA	NC
22	b	614	CLA	ND
22	b	614	CLA	NA
22	b	617	CLA	NC
22	b	617	CLA	ND

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	C	522	LMG	C7-O1-C1-O6

There are no ring outliers.

85 monomers are involved in 321 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	403	CLA	3	0
22	A	404	CLA	7	0
23	A	405	PHO	2	0
22	A	406	CLA	4	0
24	A	407	BCR	1	0
25	A	408	PL9	6	0
26	A	409	SQD	2	0
26	A	411	SQD	2	0
22	A	412	CLA	3	0
27	A	413	LFA	1	0
22	B	601	CLA	1	0
22	B	602	CLA	4	0
22	B	603	CLA	5	0
22	B	604	CLA	13	0
22	B	605	CLA	8	0
22	B	606	CLA	6	0
22	B	607	CLA	11	0
22	B	608	CLA	9	0
22	B	609	CLA	1	0
22	B	610	CLA	2	0
22	B	611	CLA	9	0
22	B	612	CLA	3	0
22	B	613	CLA	3	0
22	B	614	CLA	5	0
22	B	615	CLA	5	0
24	B	616	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	617	BCR	4	0
24	B	618	BCR	1	0
30	B	619	LMG	1	0
27	B	622	LFA	2	0
27	B	623	LFA	5	0
27	B	624	LFA	1	0
27	B	625	LFA	1	0
27	B	626	LFA	2	0
27	B	627	LFA	1	0
27	B	628	LFA	1	0
30	C	501	LMG	9	0
22	C	502	CLA	12	0
22	C	503	CLA	6	0
22	C	504	CLA	11	0
22	C	505	CLA	10	0
22	C	506	CLA	8	0
22	C	507	CLA	5	0
22	C	508	CLA	7	0
22	C	509	CLA	10	0
22	C	510	CLA	6	0
22	C	511	CLA	11	0
22	C	512	CLA	8	0
22	C	513	CLA	2	0
22	C	514	CLA	3	0
24	C	515	BCR	6	0
24	C	516	BCR	3	0
31	C	517	DGD	9	0
31	C	518	DGD	6	0
31	C	519	DGD	1	0
30	C	520	LMG	2	0
27	C	521	LFA	3	0
30	C	522	LMG	4	0
23	D	401	PHO	2	0
22	D	402	CLA	3	0
22	D	403	CLA	7	0
24	D	404	BCR	4	0
25	D	405	PL9	8	0
32	D	406	LHG	11	0
32	D	407	LHG	16	0
32	D	408	LHG	10	0
30	D	409	LMG	1	0
27	D	410	LFA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	D	411	SQD	1	0
27	D	412	LFA	1	0
27	D	413	LFA	1	0
32	E	101	LHG	6	0
33	E	102	HEM	11	0
22	H	101	CLA	1	0
24	H	102	BCR	4	0
31	H	103	DGD	3	0
27	J	101	LFA	3	0
24	K	101	BCR	7	0
24	K	102	BCR	4	0
26	L	101	SQD	4	0
32	L	102	LHG	6	0
27	M	101	LFA	1	0
27	M	102	LFA	2	0
24	T	101	BCR	1	0
33	V	201	HEM	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	c	1
5	e	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	c	399:ALA	C	400:PRO	N	1.19
1	e	63:ILE	C	64:PRO	N	1.13

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, 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	333/344 (96%)	0.32	15 (4%) 34 32	17, 24, 47, 70	0
1	a	333/344 (96%)	0.14	7 (2%) 64 61	16, 24, 48, 66	0
2	B	505/510 (99%)	0.15	23 (4%) 33 32	16, 25, 55, 73	0
2	b	503/510 (98%)	0.20	35 (6%) 17 16	19, 30, 59, 90	0
3	C	447/461 (96%)	0.23	23 (5%) 29 27	20, 32, 50, 83	0
3	c	448/461 (97%)	0.07	12 (2%) 55 52	21, 32, 46, 67	0
4	D	340/352 (96%)	0.07	7 (2%) 64 61	16, 25, 42, 62	0
4	d	340/352 (96%)	0.06	1 (0%) 93 93	17, 28, 48, 67	0
5	E	81/84 (96%)	0.59	6 (7%) 15 14	29, 46, 59, 76	0
5	e	79/84 (94%)	0.91	15 (18%) 1 1	34, 50, 68, 87	0
6	F	33/45 (73%)	0.02	1 (3%) 51 48	32, 39, 49, 58	0
6	f	33/45 (73%)	-0.03	2 (6%) 22 21	39, 44, 61, 63	0
7	H	62/66 (93%)	-0.00	0 100 100	25, 30, 36, 45	0
7	h	63/66 (95%)	0.46	6 (9%) 9 8	34, 39, 50, 55	0
8	I	33/38 (86%)	-0.17	0 100 100	23, 28, 35, 43	0
8	i	33/38 (86%)	-0.22	1 (3%) 51 48	21, 28, 39, 45	0
9	J	33/40 (82%)	0.41	2 (6%) 22 21	33, 41, 49, 54	0
9	j	33/40 (82%)	0.34	3 (9%) 10 9	33, 41, 49, 56	0
10	K	35/46 (76%)	0.51	3 (8%) 11 10	41, 47, 69, 76	0
10	k	36/46 (78%)	0.16	3 (8%) 12 11	35, 45, 66, 77	0
11	L	36/37 (97%)	-0.30	0 100 100	18, 22, 46, 54	0
11	l	36/37 (97%)	-0.15	2 (5%) 25 24	17, 23, 43, 55	0
12	M	32/36 (88%)	-0.09	0 100 100	19, 24, 45, 51	0
12	m	32/36 (88%)	0.02	0 100 100	20, 25, 48, 52	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	242/272 (88%)	0.48	24 (9%) 8 7	24, 43, 69, 124	0
13	o	241/272 (88%)	0.11	10 (4%) 38 36	25, 39, 68, 122	0
14	T	28/32 (87%)	0.06	1 (3%) 43 41	19, 23, 42, 72	0
14	t	29/32 (90%)	0.09	2 (6%) 18 16	20, 24, 46, 57	0
15	U	96/134 (71%)	1.33	25 (26%) 1 1	45, 61, 83, 90	0
15	u	96/134 (71%)	0.31	3 (3%) 49 47	32, 40, 51, 54	0
16	V	137/163 (84%)	0.00	0 100 100	32, 40, 50, 61	0
16	v	137/163 (84%)	0.55	16 (11%) 5 4	34, 43, 59, 75	0
17	Y	21/46 (45%)	1.76	7 (33%) 0 0	54, 65, 81, 85	0
17	y	23/46 (50%)	1.19	6 (26%) 1 1	50, 58, 79, 82	0
18	X	37/41 (90%)	0.32	4 (10%) 6 6	32, 38, 53, 65	0
18	x	38/41 (92%)	0.93	8 (21%) 1 1	38, 49, 68, 84	0
19	Z	61/62 (98%)	1.78	20 (32%) 0 0	50, 64, 121, 133	0
19	z	61/62 (98%)	2.46	33 (54%) 0 0	51, 72, 114, 128	0
20	R	35/41 (85%)	2.23	19 (54%) 0 0	49, 61, 81, 84	0
20	r	32/41 (78%)	2.40	20 (62%) 0 0	56, 65, 90, 97	0
All	All	5253/5700 (92%)	0.30	365 (6%) 18 16	16, 33, 65, 133	0

The worst 5 of 365 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Z	33	TRP	12.3
19	z	31	GLN	9.6
19	Z	30	PRO	8.5
13	O	58	ASN	7.9
3	C	29	GLU	7.5

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
27	LFA	b	623	12/20	0.76	0.22	9.72	25,36,38,39	0
27	LFA	D	413	10/20	0.91	0.17	7.24	22,23,26,28	0
30	LMG	c	522	41/55	0.79	0.30	7.02	21,46,54,60	0
30	LMG	C	522	44/55	0.82	0.29	6.66	32,42,53,58	0
27	LFA	b	626	12/20	0.74	0.24	6.38	29,36,43,47	0
30	LMG	B	621	36/55	0.80	0.25	4.94	28,50,59,63	0
25	PL9	a	409	55/55	0.87	0.20	4.89	38,48,59,65	0
30	LMG	b	624	39/55	0.78	0.23	4.55	34,53,60,66	0
27	LFA	B	626	10/20	0.79	0.20	4.39	20,29,38,40	0
25	PL9	A	408	55/55	0.84	0.20	4.31	34,43,53,56	0
26	SQD	A	411	54/54	0.79	0.20	4.03	27,47,71,83	0
27	LFA	D	410	15/20	0.88	0.17	3.42	23,28,40,47	0
22	CLA	b	603	65/65	0.82	0.24	3.14	33,57,78,85	0
27	LFA	j	101	15/20	0.85	0.21	2.89	41,45,51,56	0
27	LFA	B	623	13/20	0.87	0.16	2.77	21,31,34,36	0
27	LFA	d	408	15/20	0.88	0.18	2.43	25,32,37,37	0
27	LFA	B	627	14/20	0.87	0.17	2.31	20,31,36,39	0
27	LFA	A	413	11/20	0.76	0.17	2.22	27,32,46,47	0
22	CLA	c	507	65/65	0.92	0.13	2.20	25,32,52,58	0
32	LHG	e	101	42/49	0.89	0.16	2.15	40,62,80,94	0
30	LMG	C	501	51/55	0.81	0.21	2.07	26,40,50,53	0
26	SQD	a	412	50/54	0.86	0.16	1.91	28,43,70,76	0
32	LHG	d	406	49/49	0.95	0.12	1.82	18,24,32,36	0
27	LFA	B	628	12/20	0.92	0.20	1.76	23,28,37,37	0
27	LFA	C	521	15/20	0.80	0.16	1.75	26,34,39,42	0
24	BCR	t	102	40/40	0.89	0.17	1.75	21,26,38,40	0
30	LMG	c	501	51/55	0.83	0.18	1.72	25,39,51,60	0
27	LFA	B	624	15/20	0.78	0.15	1.67	28,37,47,48	0
26	SQD	b	601	54/54	0.80	0.18	1.62	25,39,62,65	0
27	LFA	d	410	16/20	0.82	0.16	1.58	28,35,44,45	0
27	LFA	m	102	15/20	0.85	0.20	1.58	25,29,37,37	0
22	CLA	C	513	65/65	0.89	0.16	1.55	34,41,54,63	0
22	CLA	D	403	65/65	0.92	0.16	1.51	17,24,62,66	0
27	LFA	t	101	15/20	0.89	0.18	1.51	25,31,42,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	CLA	d	403	65/65	0.93	0.15	1.49	22,30,57,63	0
27	LFA	B	620	10/20	0.91	0.14	1.48	22,24,28,33	0
30	LMG	B	619	51/55	0.81	0.18	1.46	15,31,42,47	0
31	DGD	H	103	60/66	0.85	0.22	1.45	22,29,40,45	0
24	BCR	b	619	40/40	0.92	0.16	1.43	18,28,34,35	0
22	CLA	a	407	65/65	0.94	0.13	1.41	13,19,56,60	0
22	CLA	A	406	65/65	0.95	0.13	1.39	11,20,54,60	0
24	BCR	d	404	40/40	0.91	0.14	1.38	25,36,53,56	0
22	CLA	B	615	65/65	0.92	0.15	1.37	19,25,70,79	0
32	LHG	d	407	49/49	0.95	0.16	1.36	21,37,60,63	0
22	CLA	c	505	65/65	0.94	0.23	1.35	21,33,49,53	0
30	LMG	C	520	48/55	0.75	0.23	1.35	38,53,67,71	0
26	SQD	L	101	48/54	0.82	0.17	1.34	21,42,66,69	0
27	LFA	b	622	10/20	0.89	0.14	1.25	27,31,37,38	0
24	BCR	B	616	40/40	0.91	0.15	1.25	19,25,31,32	0
25	PL9	D	405	55/55	0.91	0.15	1.23	12,21,26,28	0
24	BCR	K	101	40/40	0.86	0.17	1.21	37,48,53,55	0
22	CLA	b	618	65/65	0.90	0.15	1.19	23,32,58,64	0
32	LHG	E	101	42/49	0.84	0.17	1.09	31,54,67,71	0
26	SQD	f	102	43/54	0.92	0.23	1.05	51,66,77,86	0
24	BCR	c	515	40/40	0.93	0.12	1.02	19,29,38,41	0
22	CLA	c	514	65/65	0.91	0.17	0.95	33,45,61,67	0
22	CLA	b	607	65/65	0.94	0.14	0.90	18,23,30,32	0
32	LHG	D	408	49/49	0.93	0.16	0.87	16,33,53,57	0
26	SQD	D	411	43/54	0.88	0.21	0.87	38,50,58,69	0
24	BCR	T	101	40/40	0.90	0.14	0.86	22,29,34,37	0
31	DGD	h	102	62/66	0.85	0.20	0.85	23,33,40,45	0
22	CLA	b	608	65/65	0.92	0.13	0.85	22,29,42,53	0
22	CLA	c	509	65/65	0.94	0.18	0.85	24,30,59,66	0
24	BCR	c	523	40/40	0.90	0.15	0.81	39,46,52,55	0
32	LHG	D	407	49/49	0.94	0.13	0.81	18,24,30,37	0
22	CLA	B	604	65/65	0.94	0.16	0.81	15,21,25,29	0
22	CLA	c	513	65/65	0.90	0.15	0.79	36,42,55,62	0
24	BCR	D	404	40/40	0.91	0.13	0.76	23,33,49,50	0
22	CLA	B	610	65/65	0.94	0.17	0.76	12,18,24,29	0
22	CLA	c	511	65/65	0.94	0.21	0.75	27,32,38,44	0
22	CLA	H	101	65/65	0.89	0.15	0.75	30,45,64,72	0
32	LHG	l	101	49/49	0.93	0.13	0.75	17,25,34,39	0
26	SQD	a	410	54/54	0.92	0.15	0.74	30,48,58,62	0
22	CLA	B	609	65/65	0.95	0.15	0.70	15,20,27,29	0
30	LMG	f	101	51/55	0.93	0.13	0.68	31,38,55,61	0
32	LHG	D	406	49/49	0.93	0.14	0.68	17,24,30,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	PHO	a	406	64/64	0.93	0.14	0.68	13,17,25,27	0
22	CLA	B	606	65/65	0.95	0.15	0.68	10,18,33,37	0
22	CLA	C	509	65/65	0.92	0.16	0.68	22,31,62,66	0
33	HEM	V	201	43/43	0.95	0.12	0.67	28,36,41,45	0
23	PHO	A	405	64/64	0.95	0.17	0.67	15,21,28,31	0
24	BCR	C	516	40/40	0.92	0.12	0.65	21,30,37,38	0
22	CLA	b	605	65/65	0.95	0.17	0.64	18,22,37,49	0
30	LMG	c	519	51/55	0.86	0.20	0.63	38,52,64,67	0
24	BCR	k	101	40/40	0.91	0.16	0.61	29,43,51,54	0
22	CLA	B	613	65/65	0.93	0.14	0.60	18,25,46,57	0
24	BCR	B	618	40/40	0.92	0.12	0.59	18,26,34,36	0
31	DGD	C	517	62/66	0.92	0.17	0.59	20,26,49,52	0
30	LMG	m	103	51/55	0.86	0.18	0.58	17,30,41,45	0
22	CLA	B	607	65/65	0.94	0.17	0.57	13,19,26,34	0
22	CLA	b	609	65/65	0.95	0.16	0.56	11,21,29,32	0
31	DGD	c	516	62/66	0.92	0.15	0.55	23,28,49,52	0
22	CLA	C	511	65/65	0.90	0.18	0.54	25,34,41,49	0
27	LFA	c	521	15/20	0.92	0.11	0.52	31,35,41,41	0
22	CLA	B	602	65/65	0.94	0.15	0.52	18,21,35,38	0
23	PHO	D	401	64/64	0.95	0.15	0.48	14,18,25,28	0
22	CLA	c	508	65/65	0.92	0.15	0.46	22,30,34,37	0
30	LMG	D	409	51/55	0.94	0.13	0.45	25,36,51,54	0
22	CLA	C	507	65/65	0.93	0.12	0.44	22,30,55,57	0
22	CLA	B	611	65/65	0.93	0.16	0.43	14,19,25,28	0
22	CLA	C	514	65/65	0.92	0.14	0.43	37,49,63,67	0
22	CLA	C	505	65/65	0.92	0.19	0.42	28,35,48,61	0
22	CLA	c	503	65/65	0.91	0.20	0.42	23,30,38,39	0
22	CLA	b	614	65/65	0.94	0.17	0.42	16,23,28,32	0
25	PL9	d	405	55/55	0.94	0.12	0.40	16,23,27,30	0
24	BCR	c	524	40/40	0.90	0.18	0.38	36,43,53,53	0
23	PHO	a	414	64/64	0.94	0.14	0.35	21,28,33,39	0
22	CLA	c	504	65/65	0.90	0.16	0.35	26,34,39,40	0
22	CLA	B	605	65/65	0.91	0.12	0.34	17,25,38,44	0
27	LFA	J	101	11/20	0.91	0.15	0.33	38,43,49,49	0
24	BCR	K	102	40/40	0.91	0.14	0.32	39,44,47,48	0
22	CLA	b	606	65/65	0.90	0.20	0.28	16,23,38,45	0
31	DGD	c	517	55/66	0.92	0.18	0.26	25,34,50,63	0
22	CLA	b	616	65/65	0.93	0.13	0.26	20,26,39,42	0
22	CLA	c	502	65/65	0.92	0.14	0.25	17,28,35,38	0
31	DGD	C	519	62/66	0.91	0.15	0.23	27,33,46,60	0
22	CLA	b	612	65/65	0.95	0.14	0.22	16,25,31,33	0
22	CLA	C	508	65/65	0.93	0.13	0.22	21,26,35,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
27	LFA	T	102	12/20	0.89	0.13	0.22	22,28,32,32	0
22	CLA	b	610	65/65	0.93	0.17	0.20	22,28,37,45	0
32	LHG	L	102	49/49	0.94	0.13	0.19	18,24,31,34	0
22	CLA	b	611	65/65	0.93	0.12	0.18	23,30,40,52	0
24	BCR	h	101	40/40	0.85	0.17	0.17	28,40,45,49	0
22	CLA	c	510	65/65	0.93	0.15	0.16	22,31,38,40	0
22	CLA	C	510	65/65	0.93	0.14	0.13	25,31,39,40	0
24	BCR	b	620	40/40	0.92	0.15	0.13	18,25,30,32	0
22	CLA	B	601	65/65	0.94	0.15	0.12	17,26,32,36	0
22	CLA	b	615	65/65	0.94	0.20	0.11	16,21,36,39	0
31	DGD	c	518	62/66	0.92	0.15	0.10	26,32,52,58	0
26	SQD	A	409	54/54	0.90	0.15	0.08	24,42,54,56	0
24	BCR	b	621	40/40	0.92	0.12	0.07	23,34,42,47	0
24	BCR	C	515	40/40	0.91	0.14	0.06	36,45,52,55	0
32	LHG	b	628	49/49	0.94	0.13	0.05	22,27,35,49	0
27	LFA	b	630	15/20	0.86	0.13	0.04	31,39,42,42	0
22	CLA	d	401	65/65	0.94	0.15	0.03	18,27,63,69	0
27	LFA	b	602	15/20	0.92	0.12	0.03	29,33,42,42	0
22	CLA	C	512	65/65	0.91	0.13	0.02	35,44,52,56	0
22	CLA	c	506	65/65	0.93	0.12	-0.00	21,26,37,40	0
31	DGD	C	518	56/66	0.88	0.17	0.00	29,38,48,53	0
22	CLA	C	504	65/65	0.90	0.14	-0.03	20,35,38,42	0
22	CLA	B	612	65/65	0.94	0.17	-0.04	13,18,40,43	0
22	CLA	A	404	65/65	0.94	0.15	-0.06	15,23,61,72	0
27	LFA	M	102	16/20	0.90	0.13	-0.06	25,27,46,47	0
22	CLA	C	502	65/65	0.94	0.13	-0.06	18,24,33,35	0
21	CL	a	402	1/1	0.94	0.15	-0.07	52,52,52,52	0
22	CLA	a	404	65/65	0.93	0.15	-0.08	14,20,27,36	0
22	CLA	C	506	65/65	0.94	0.12	-0.09	17,27,32,40	0
22	CLA	a	405	65/65	0.93	0.13	-0.09	14,19,25,31	0
22	CLA	B	603	65/65	0.90	0.17	-0.10	14,21,35,44	0
22	CLA	b	604	65/65	0.93	0.15	-0.10	25,30,41,46	0
22	CLA	b	613	65/65	0.94	0.15	-0.13	18,23,29,31	0
22	CLA	B	608	65/65	0.94	0.11	-0.14	15,24,33,36	0
22	CLA	C	503	65/65	0.91	0.16	-0.15	24,32,36,38	0
24	BCR	a	408	40/40	0.94	0.10	-0.15	18,22,29,31	0
29	BCT	a	413	4/4	0.96	0.11	-0.16	31,33,34,40	0
24	BCR	H	102	40/40	0.90	0.13	-0.17	22,28,42,43	0
33	HEM	e	102	43/43	0.94	0.13	-0.22	37,48,57,60	0
24	BCR	B	617	40/40	0.92	0.15	-0.29	15,24,30,30	0
24	BCR	A	407	40/40	0.94	0.10	-0.31	14,23,30,31	0
22	CLA	c	512	65/65	0.92	0.11	-0.39	28,39,47,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	CLA	d	402	65/65	0.94	0.13	-0.42	17,20,37,40	0
22	CLA	D	402	65/65	0.95	0.14	-0.45	13,18,26,35	0
33	HEM	E	102	43/43	0.94	0.12	-0.51	34,43,52,54	0
22	CLA	b	617	65/65	0.94	0.11	-0.52	21,27,39,50	0
22	CLA	A	403	65/65	0.95	0.14	-0.55	12,18,23,30	0
28	FE	a	401	1/1	0.99	0.10	-0.55	39,39,39,39	0
22	CLA	A	412	65/65	0.94	0.12	-0.58	16,20,25,27	0
22	CLA	B	614	65/65	0.94	0.10	-0.62	15,22,32,47	0
21	CL	A	401	1/1	0.91	0.13	-0.98	57,57,57,57	0
33	HEM	v	201	43/43	0.97	0.09	-1.00	28,34,38,41	0
29	BCT	A	415	4/4	0.97	0.09	-1.09	25,29,31,32	0
21	CL	A	402	1/1	0.96	0.12	-1.17	57,57,57,57	0
21	CL	a	403	1/1	0.92	0.10	-1.30	40,40,40,40	0
28	FE	A	414	1/1	0.98	0.04	-6.20	26,26,26,26	0
27	LFA	b	629	9/20	0.82	0.26	-	29,31,33,39	0
27	LFA	D	412	8/20	0.91	0.15	-	25,30,37,40	0
27	LFA	i	102	7/20	0.74	0.17	-	26,32,34,39	0
27	LFA	B	622	16/20	0.87	0.14	-	27,32,36,37	0
27	LFA	A	410	14/20	0.73	0.20	-	37,39,43,45	0
27	LFA	b	625	16/20	0.82	0.17	-	27,32,41,45	0
27	LFA	d	409	9/20	0.86	0.19	-	24,35,40,46	0
27	LFA	a	411	7/20	0.93	0.09	-	26,32,35,35	0
27	LFA	c	520	9/20	0.92	0.17	-	31,39,46,47	0
27	LFA	B	625	9/20	0.92	0.17	-	20,25,27,33	0
27	LFA	M	101	10/20	0.94	0.17	-	26,31,41,42	0
27	LFA	b	627	11/20	0.81	0.19	-	36,46,49,53	0
27	LFA	m	101	10/20	0.78	0.17	-	28,36,44,50	0
27	LFA	I	101	14/20	0.91	0.10	-	21,29,32,32	0
27	LFA	i	101	16/20	0.88	0.16	-	23,32,40,41	0

6.5 Other polymers ⓘ

There are no such residues in this entry.