



wwPDB X-ray Structure Validation Summary Report i

Jul 18, 2014 – 04:56 AM EDT

PDB ID : 4TNI
Title : RT XFEL structure of Photosystem II 500 ms after the third illumination at 4.6 Å resolution
Authors : Kern, J.; Tran, R.; Alonso-Mori, R.; Koroidov, S.; Echols, N.; Hattne, J.; Ibrahim, M.; Gul, S.; Laksmono, H.; Sierra, R.G.; Gildea, R.J.; Han, G.; Hellmich, J.; Lassalle-Kaiser, B.; Chatterjee, R.; Brewster, A.; Stan, C.A.; Gloeckner, C.; Lampe, A.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Seibert, M.M.; Koglin, J.E.; Gallo, E.; Uhlig, J.; Sokaras, D.; Weng, T.-C.; Zwart, P.H.; Skinner, D.E.; Bogan, M.J.; Messerschmidt, M.; Glatzel, P.; Williams, G.J.; Boutet, S.; Adams, P.D.; Zouni, A.; Messinger, J.; Sauter, N.K.; Bergmann, U.; Yano, J.; Yachandra, V.K.
Deposited on : 2014-06-04
Resolution : 4.60 Å (reported)

This is a wwPDB 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/ValidationPDFNotes.html>

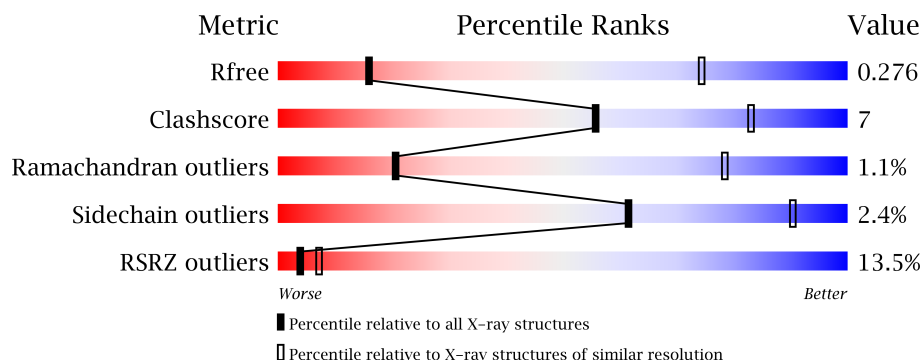
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23161
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23161

1 Overall quality at a glance

The reported resolution of this entry is 4.60 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}	66092	1032 (5.70-3.50)
Clashscore	79885	1304 (5.70-3.50)
Ramachandran outliers	78287	1225 (5.70-3.50)
Sidechain outliers	78261	1206 (5.70-3.50)
RSRZ outliers	66119	1031 (5.70-3.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	
2	B	510	
2	b	510	
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	

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Mol	Chain	Length	Quality of chain
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	
16	V	163	
16	v	163	
17	g	46	
17	y	46	
18	X	41	
18	x	41	
19	G	28	
19	Y	28	
20	Z	62	
20	z	62	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
22	CLA	A	405	-	X
22	CLA	B	601	-	X
22	CLA	B	603	-	X
22	CLA	B	604	-	X
22	CLA	B	605	-	X
22	CLA	B	608	-	X
22	CLA	B	614	-	X
22	CLA	B	615	-	X
22	CLA	C	501	-	X
22	CLA	C	502	-	X
22	CLA	C	506	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
22	CLA	C	508	-	X
22	CLA	C	510	-	X
22	CLA	C	511	-	X
22	CLA	C	512	-	X
22	CLA	D	406	-	X
22	CLA	a	404	-	X
22	CLA	a	405	-	X
22	CLA	a	407	-	X
22	CLA	b	605	-	X
22	CLA	b	606	-	X
22	CLA	b	607	-	X
22	CLA	b	609	-	X
22	CLA	b	612	-	X
22	CLA	b	613	-	X
22	CLA	b	618	-	X
22	CLA	b	619	-	X
22	CLA	c	501	-	X
22	CLA	c	502	-	X
22	CLA	c	503	-	X
22	CLA	c	505	-	X
22	CLA	c	506	-	X
22	CLA	c	511	-	X
22	CLA	c	512	-	X
22	CLA	d	406	-	X
23	PL9	J	101	-	X
23	PL9	d	407	-	X
23	PL9	j	101	-	X
24	BCR	A	407	-	X
24	BCR	B	619	-	X
24	BCR	C	513	-	X
24	BCR	C	514	-	X
24	BCR	H	102	-	X
24	BCR	J	102	-	X
24	BCR	K	102	-	X
24	BCR	a	409	-	X
24	BCR	b	623	-	X
24	BCR	c	513	-	X
24	BCR	c	514	-	X
24	BCR	c	521	-	X
24	BCR	g	101	-	X
24	BCR	x	101	-	X
24	BCR	y	101	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
25	DGD	B	625	-	X
25	DGD	D	410	-	X
25	DGD	b	601	-	X
25	DGD	d	410	-	X
27	LMG	C	518	-	X
27	LMG	E	101	-	X
27	LMG	I	101	-	X
27	LMG	M	101	-	X
27	LMG	c	518	-	X
27	LMG	i	101	-	X
29	SQD	B	622	-	X
29	SQD	B	626	-	X
29	SQD	F	103	-	X
29	SQD	a	401	-	X
29	SQD	d	403	-	X
29	SQD	f	103	-	X
30	LMT	B	623	-	X
30	LMT	B	624	-	X
30	LMT	B	627	-	X
30	LMT	D	411	-	X
30	LMT	I	102	-	X
30	LMT	b	603	-	X
30	LMT	b	626	-	X
30	LMT	b	627	-	X
30	LMT	d	411	-	X
30	LMT	i	102	-	X
34	HEM	v	201	-	X
35	CA	K	101	-	X
35	CA	O	301	-	X
35	CA	o	301	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50244 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			
1	a	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			
2	b	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			
3	c	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	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	82	Total	C	N	O	0	0	0
			666	434	108	124			
5	e	82	Total	C	N	O	0	0	0
			666	434	108	124			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			
6	f	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			
8	i	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			
9	j	34	Total	C	N	O	S	0	0	0
			249	170	38	40	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			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			
13	o	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			
14	t	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	0	0
			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
			1060	673	177	206	4			
16	v	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	y	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			
17	g	28	Total	C	N	O	S	0	0	0
			201	134	33	31	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		0	0	0
			270	182	41	47				
18	x	37	Total	C	N	O		0	0	0
			270	182	41	47				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Y	28	Total	C	N	O		0	0	0
			140	84	28	28				
19	G	28	Total	C	N	O		0	0	0
			140	84	28	28				

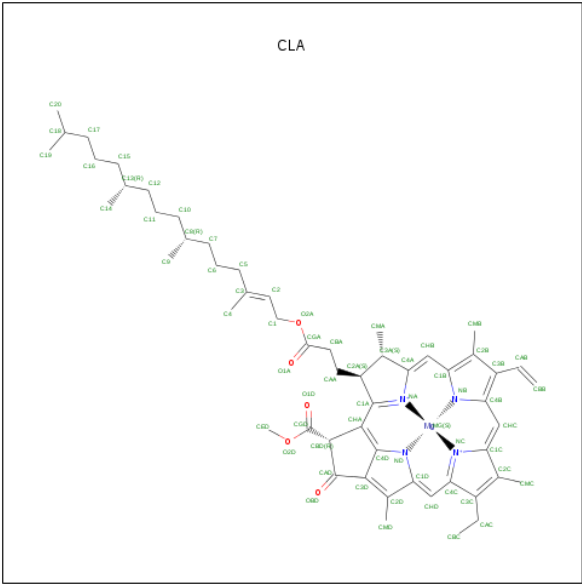
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

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

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

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



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

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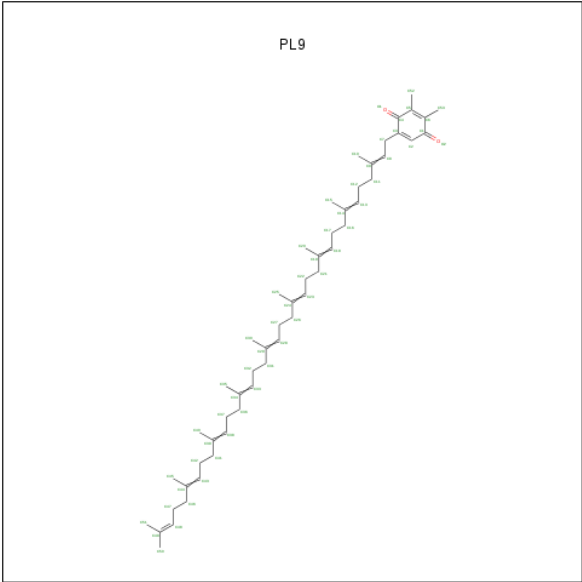
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N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

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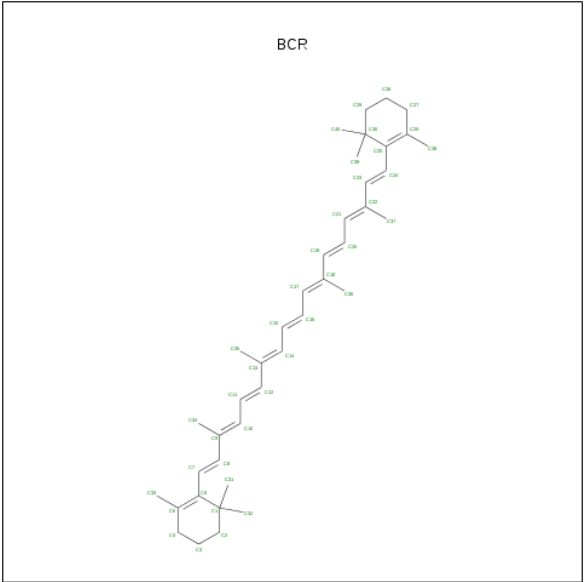
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 23 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
23	A	1	Total	C	O	0	0
			45	43	2		
23	D	1	Total	C	O	0	0
			55	53	2		
23	J	1	Total	C	O	0	0
			35	33	2		
23	a	1	Total	C	O	0	0
			45	43	2		
23	d	1	Total	C	O	0	0
			55	53	2		
23	j	1	Total	C	O	0	0
			35	33	2		

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



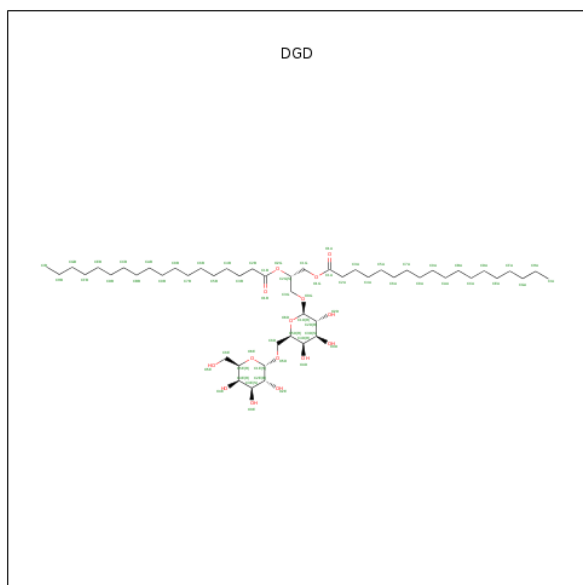
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	F	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	J	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	y	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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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	f	1	Total C 40 40	0	0
24	j	1	Total C 40 40	0	0
24	g	1	Total C 40 40	0	0
24	x	1	Total C 40 40	0	0

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



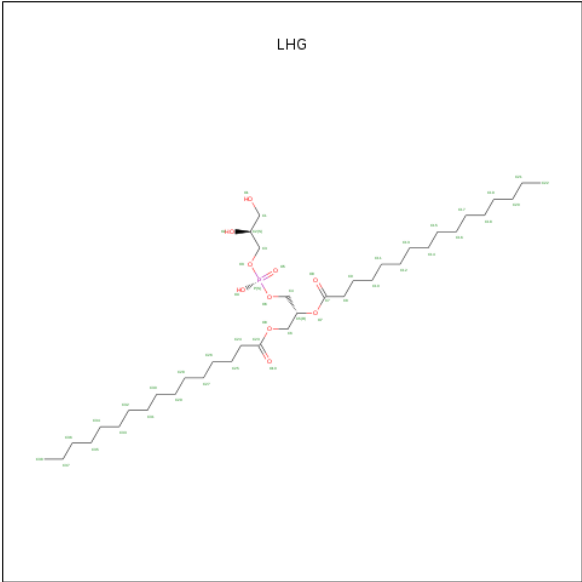
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 56 41 15	0	0

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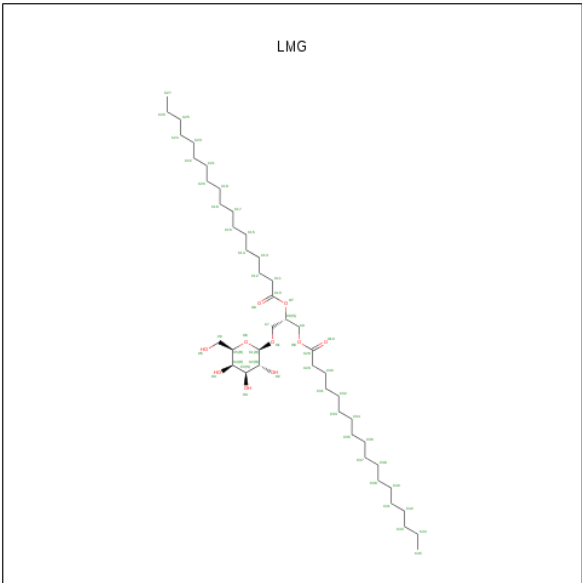
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			58	43	15		
25	B	1	Total	C	O	0	0
			52	37	15		
25	C	1	Total	C	O	0	0
			53	38	15		
25	C	1	Total	C	O	0	0
			62	47	15		
25	C	1	Total	C	O	0	0
			66	51	15		
25	D	1	Total	C	O	0	0
			63	48	15		
25	a	1	Total	C	O	0	0
			56	41	15		
25	b	1	Total	C	O	0	0
			52	37	15		
25	b	1	Total	C	O	0	0
			58	43	15		
25	c	1	Total	C	O	0	0
			53	38	15		
25	c	1	Total	C	O	0	0
			62	47	15		
25	c	1	Total	C	O	0	0
			66	51	15		
25	d	1	Total	C	O	0	0
			63	48	15		

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



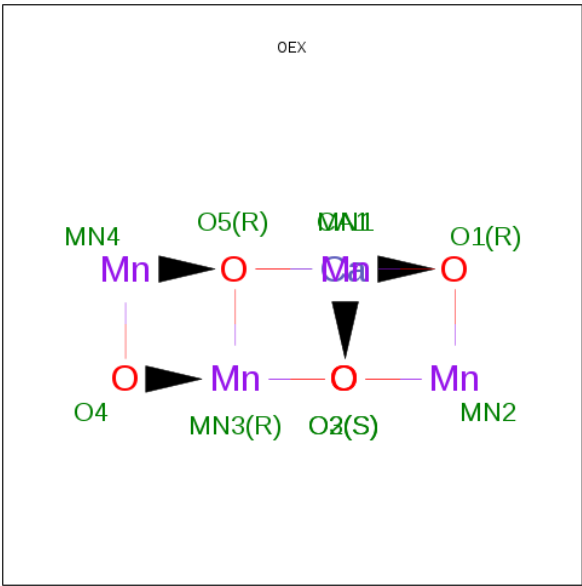
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	P	0	0
			39	28	10	1		
26	C	1	Total	C	O	P	0	0
			37	26	10	1		
26	a	1	Total	C	O	P	0	0
			39	28	10	1		
26	c	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



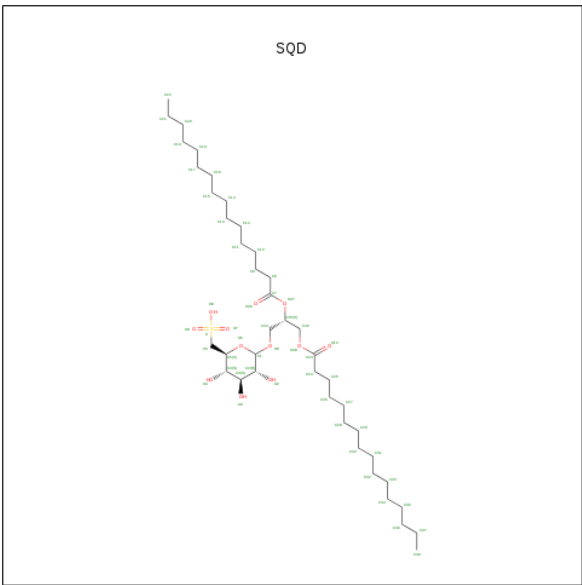
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			51	41	10		
27	A	1	Total	C	O	0	0
			42	32	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	C	1	Total	C	O	0	0
			45	35	10		
27	C	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			49	39	10		
27	D	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			46	36	10		
27	E	1	Total	C	O	0	0
			44	34	10		
27	I	1	Total	C	O	0	0
			43	33	10		
27	M	1	Total	C	O	0	0
			42	32	10		
27	a	1	Total	C	O	0	0
			42	32	10		
27	a	1	Total	C	O	0	0
			51	41	10		
27	b	1	Total	C	O	0	0
			49	39	10		
27	c	1	Total	C	O	0	0
			45	35	10		
27	c	1	Total	C	O	0	0
			48	38	10		
27	d	1	Total	C	O	0	0
			49	39	10		
27	d	1	Total	C	O	0	0
			48	38	10		
27	d	1	Total	C	O	0	0
			46	36	10		
27	e	1	Total	C	O	0	0
			44	34	10		
27	i	1	Total	C	O	0	0
			43	33	10		
27	m	1	Total	C	O	0	0
			42	32	10		

- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



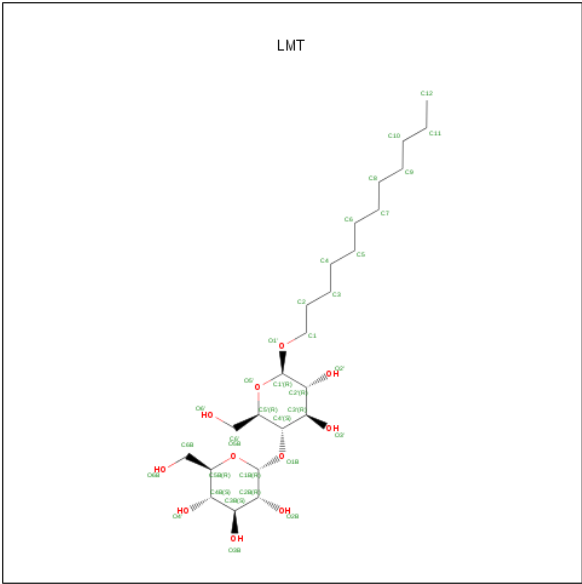
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
28	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	S	0	0
			51	38	12	1		
29	A	1	Total	C	O	S	0	0
			54	41	12	1		
29	B	1	Total	C	O	S	0	0
			43	30	12	1		
29	B	1	Total	C	O	S	0	0
			47	34	12	1		
29	F	1	Total	C	O	S	0	0
			45	32	12	1		
29	a	1	Total	C	O	S	0	0
			54	41	12	1		
29	a	1	Total	C	O	S	0	0
			51	38	12	1		
29	b	1	Total	C	O	S	0	0
			47	34	12	1		
29	d	1	Total	C	O	S	0	0
			43	30	12	1		
29	f	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 30 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



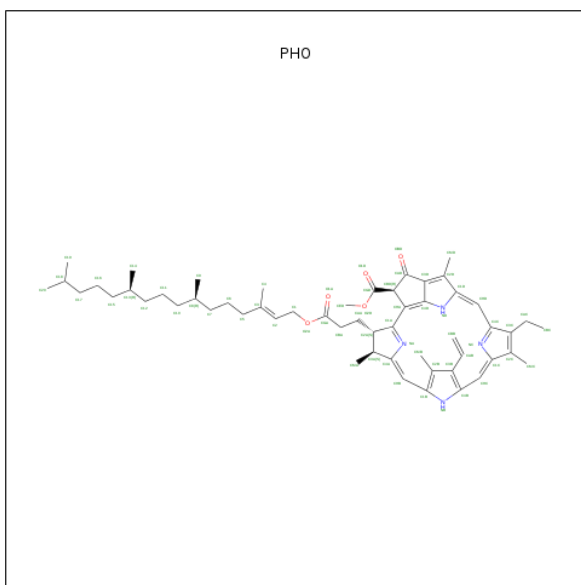
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	B	1	Total	C	O	0	0
			35	24	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	B	1	Total	C	O	0	0
			35	24	11		
30	B	1	Total	C	O	0	0
			35	24	11		
30	B	1	Total	C	O	0	0
			35	24	11		
30	D	1	Total	C	O	0	0
			31	20	11		
30	I	1	Total	C	O	0	0
			35	24	11		
30	M	1	Total	C	O	0	0
			35	24	11		
30	M	1	Total	C	O	0	0
			35	24	11		
30	b	1	Total	C	O	0	0
			35	24	11		
30	b	1	Total	C	O	0	0
			35	24	11		
30	b	1	Total	C	O	0	0
			35	24	11		
30	b	1	Total	C	O	0	0
			35	24	11		
30	d	1	Total	C	O	0	0
			31	20	11		
30	i	1	Total	C	O	0	0
			35	24	11		

- Molecule 31 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).

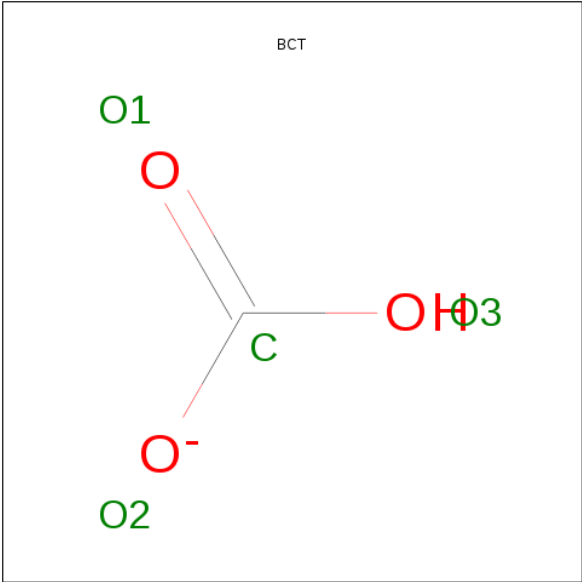


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	D	1	Total	C	N	O	0	0
			64	55	4	5		
31	D	1	Total	C	N	O	0	0
			64	55	4	5		
31	d	1	Total	C	N	O	0	0
			64	55	4	5		
31	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 32 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

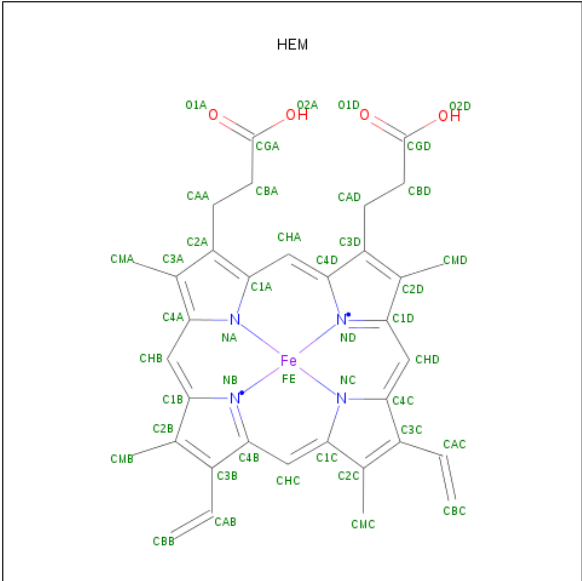
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	a	1	Total	Cl	0	0
			1	1		
32	D	1	Total	Cl	0	0
			1	1		

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	D	1	Total	C	O	0	0
			4	1	3		
33	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
34	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

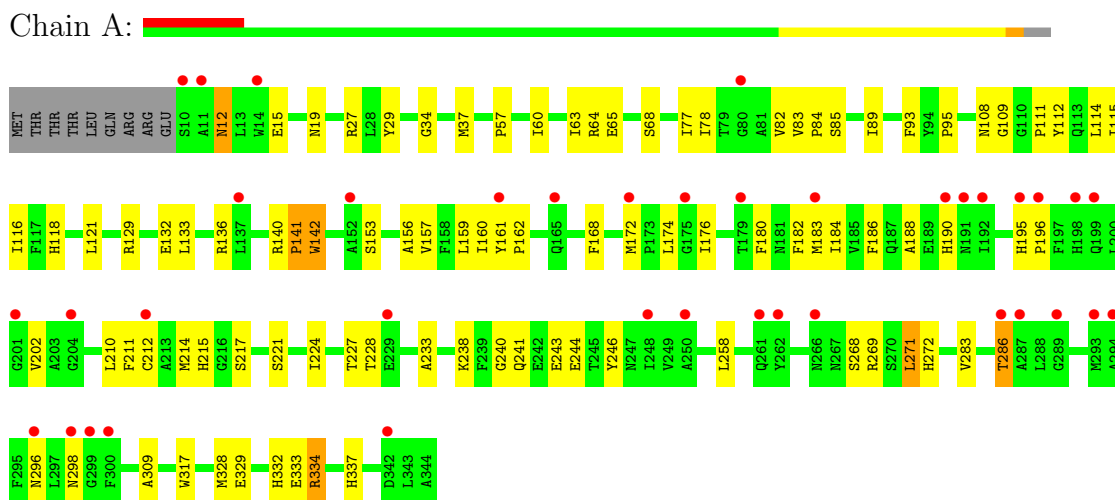
- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	o	1	Total 1	Ca 1	0	0
35	O	1	Total 1	Ca 1	0	0
35	K	1	Total 1	Ca 1	0	0
35	k	1	Total 1	Ca 1	0	0

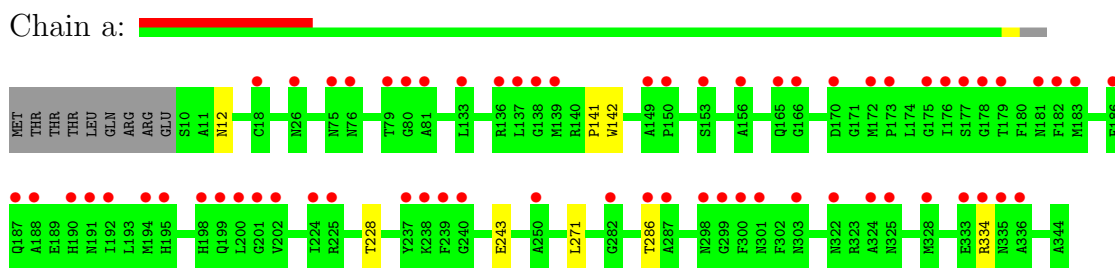
3 Residue-property plots

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

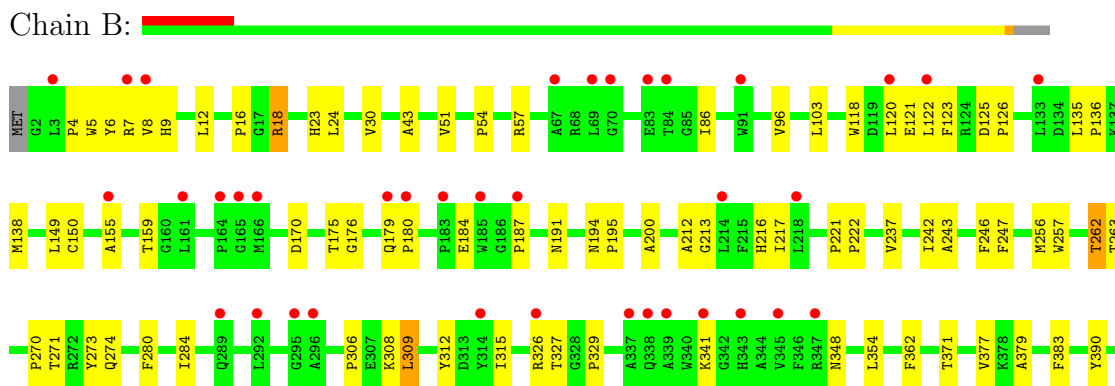
- Molecule 1: Photosystem Q(B) protein 1

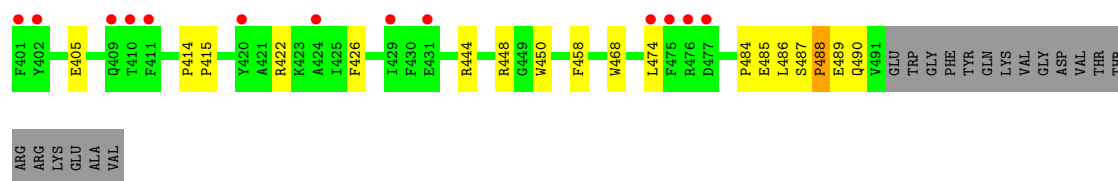


- Molecule 1: Photosystem Q(B) protein 1



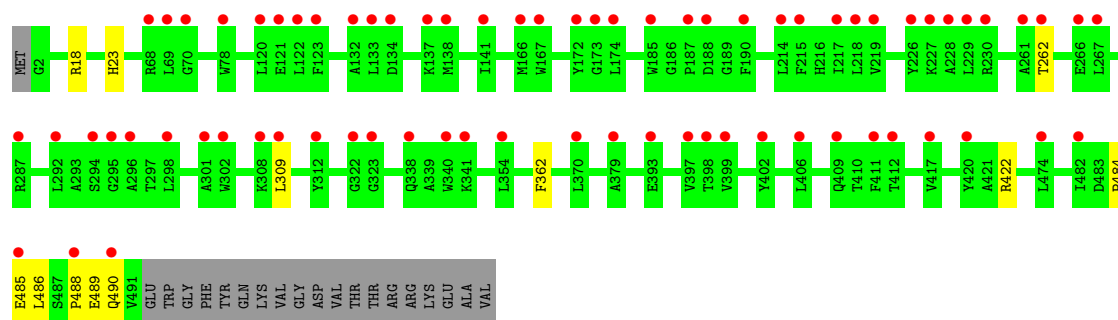
- Molecule 2: Photosystem II core light harvesting protein





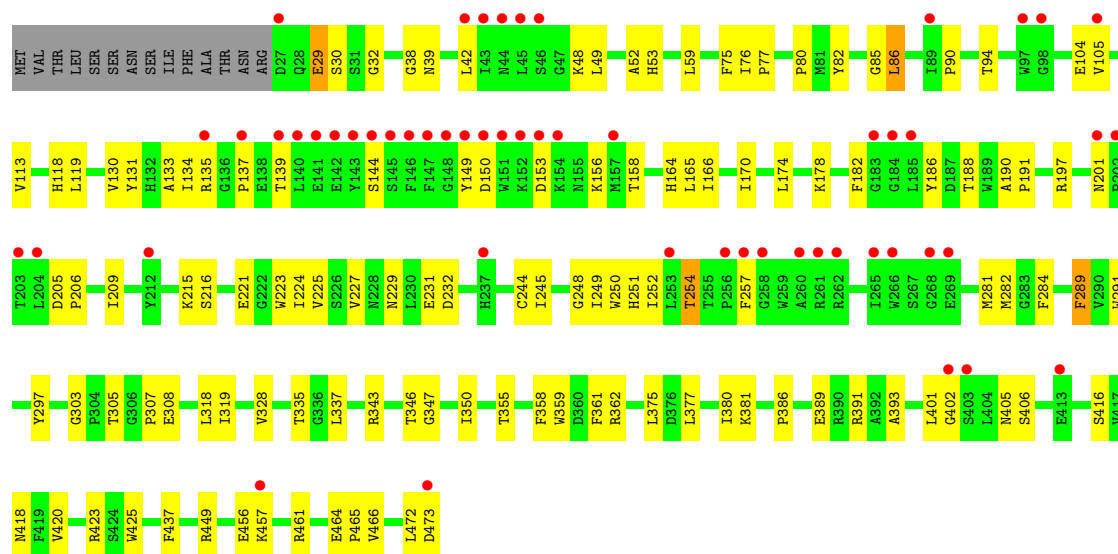
• Molecule 2: Photosystem II core light harvesting protein

Chain b:



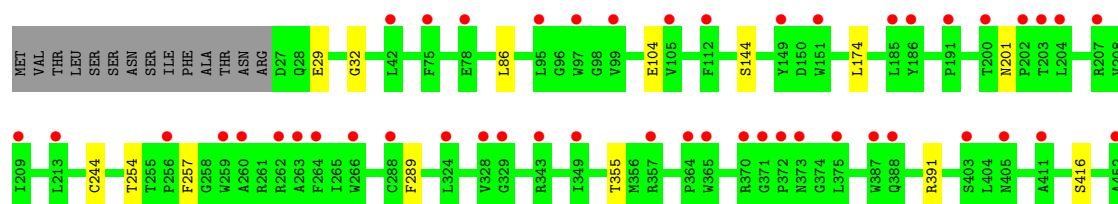
• Molecule 3: Photosystem II CP43 protein

Chain C:



• Molecule 3: Photosystem II CP43 protein

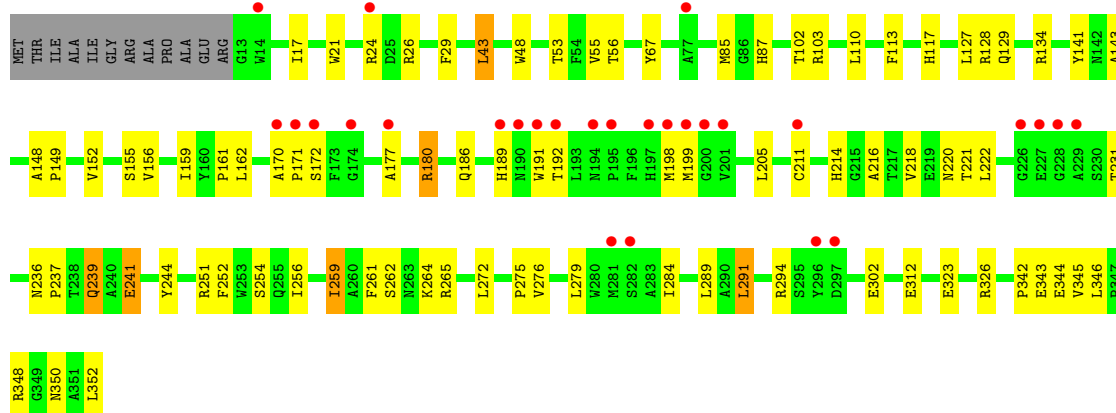
Chain c:





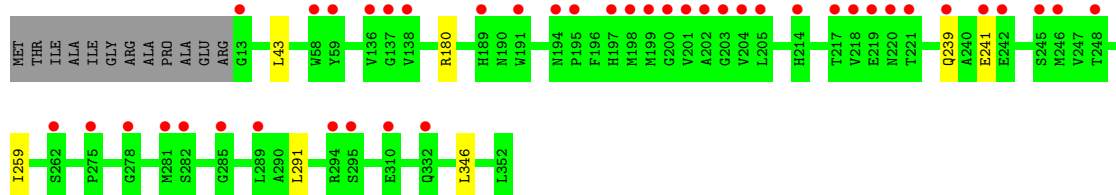
• Molecule 4: Photosystem II D2 protein

Chain D:



• Molecule 4: Photosystem II D2 protein

Chain d:



• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



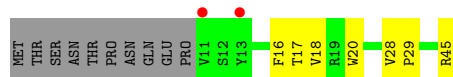
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



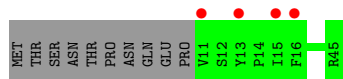
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



• Molecule 6: Cytochrome b559 subunit beta

Chain f:



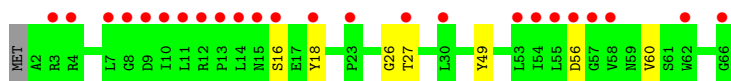
- Molecule 7: Photosystem II reaction center protein H

Chain H:



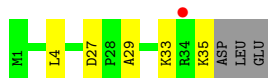
- Molecule 7: Photosystem II reaction center protein H

Chain h:



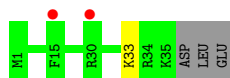
- Molecule 8: Photosystem II reaction center protein I

Chain I:



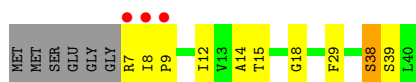
- Molecule 8: Photosystem II reaction center protein I

Chain i:



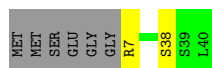
- Molecule 9: Photosystem II reaction center protein J

Chain J:



- Molecule 9: Photosystem II reaction center protein J

Chain j:



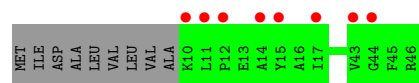
- Molecule 10: Photosystem II reaction center protein K

Chain K:



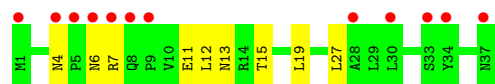
- Molecule 10: Photosystem II reaction center protein K

Chain k:



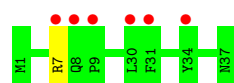
- Molecule 11: Photosystem II reaction center protein L

Chain L:



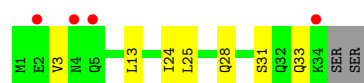
- Molecule 11: Photosystem II reaction center protein L

Chain l:



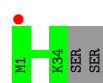
- Molecule 12: Photosystem II reaction center protein M

Chain M:



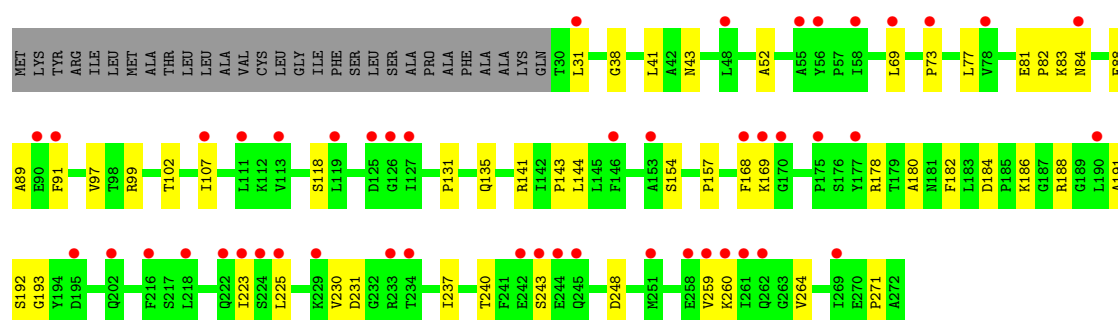
- Molecule 12: Photosystem II reaction center protein M

Chain m:



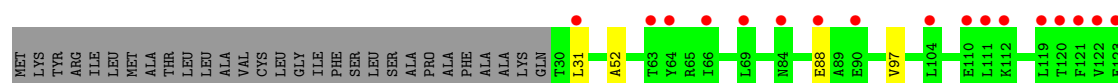
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

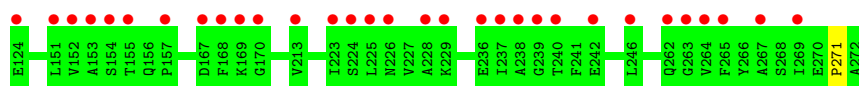
Chain O:



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

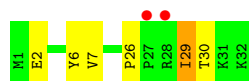
Chain o:





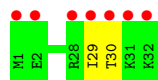
- Molecule 14: Photosystem II reaction center protein T

Chain T:



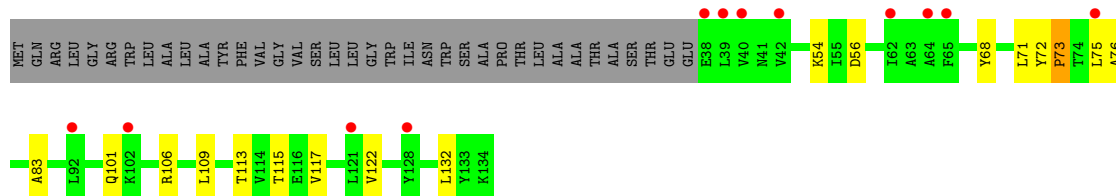
- Molecule 14: Photosystem II reaction center protein T

Chain t:



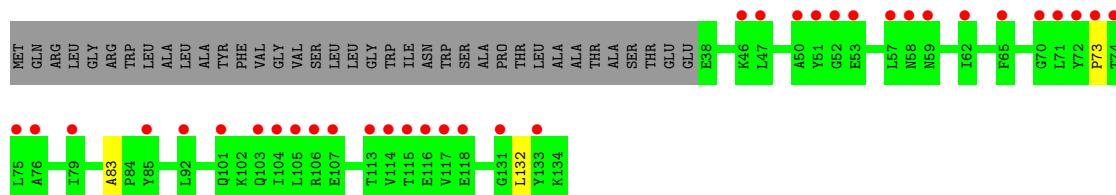
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



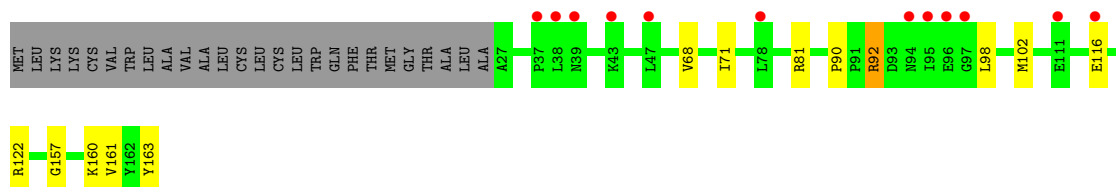
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



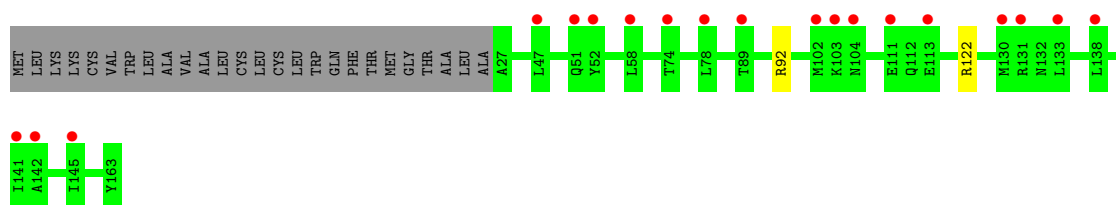
- Molecule 16: Cytochrome c-550

Chain V:



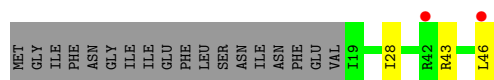
- Molecule 16: Cytochrome c-550

Chain v:



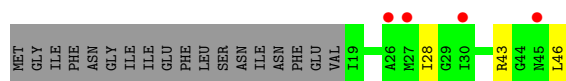
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain g:



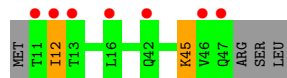
- Molecule 18: Photosystem II reaction center X protein

Chain X:



- Molecule 18: Photosystem II reaction center X protein

Chain x:



- Molecule 19: Photosystem II reaction center protein Y

Chain Y:

There are no outlier residues recorded for this chain.

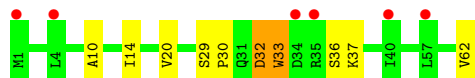
- Molecule 19: Photosystem II reaction center protein Y

Chain G:

There are no outlier residues recorded for this chain.

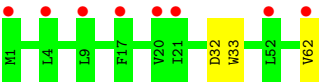
- Molecule 20: Photosystem II reaction center protein Z

Chain Z:



- Molecule 20: Photosystem II reaction center protein Z

Chain z: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.43Å 228.81Å 307.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.96 – 4.60 72.96 – 4.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (72.96-4.60) 97.7 (72.96-4.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 4.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, R_{free}	0.278 , 0.284 0.273 , 0.276	Depositor DCC
R_{free} test set	2524 reflections (4.90%)	DCC
Wilson B-factor (Å ²)	159.5	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 119.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	0 of 51515 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	50244	wwPDB-VP
Average B, all atoms (Å ²)	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, CA, LMT, CLA, PL9, FE2, BCT, HEM, LMG, BCR, SQD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.24	0/2713	0.41	0/3700
1	a	0.24	0/2713	0.41	0/3700
2	B	0.23	0/3986	0.40	0/5433
2	b	0.23	0/3986	0.40	0/5433
3	C	0.22	0/3556	0.41	0/4842
3	c	0.22	0/3556	0.41	0/4842
4	D	0.23	0/2801	0.40	0/3818
4	d	0.24	0/2801	0.40	0/3818
5	E	0.23	0/685	0.42	0/933
5	e	0.22	0/685	0.43	0/933
6	F	0.22	0/291	0.40	0/397
6	f	0.22	0/291	0.40	0/397
7	H	0.23	0/520	0.45	0/709
7	h	0.23	0/520	0.45	0/709
8	I	0.24	0/293	0.42	0/395
8	i	0.24	0/293	0.42	0/395
9	J	0.22	0/255	0.40	0/346
9	j	0.21	0/255	0.39	0/346
10	K	0.26	0/303	0.48	0/416
10	k	0.26	0/303	0.48	0/416
11	L	0.22	0/311	0.39	0/422
11	l	0.22	0/311	0.39	0/422
12	M	0.23	0/270	0.43	0/367
12	m	0.23	0/270	0.43	0/367
13	O	0.22	0/1876	0.43	0/2548
13	o	0.22	0/1876	0.43	0/2548
14	T	0.24	0/284	0.40	0/381
14	t	0.25	0/284	0.40	0/381
15	U	0.22	0/785	0.42	0/1064
15	u	0.22	0/785	0.43	0/1064
16	V	0.21	0/1081	0.41	0/1468
16	v	0.21	0/1081	0.40	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	g	0.21	0/202	0.45	0/272
17	y	0.22	0/202	0.45	0/272
18	X	0.26	0/273	0.43	0/370
18	x	0.25	0/273	0.43	0/370
20	Z	0.24	0/490	0.44	0/669
20	z	0.24	0/490	0.44	0/669
All	All	0.23	0/41950	0.41	0/57100

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2628	0	2524	78	0
1	a	2628	0	2524	0	0
2	B	3850	0	3718	85	0
2	b	3850	0	3718	0	0
3	C	3444	0	3365	83	0
3	c	3444	0	3365	0	0
4	D	2706	0	2608	74	0
4	d	2706	0	2608	0	0
5	E	666	0	651	13	0
5	e	666	0	651	0	0
6	F	282	0	291	6	0
6	f	282	0	291	0	0
7	H	507	0	521	17	0
7	h	507	0	521	0	0
8	I	286	0	308	3	0
8	i	286	0	308	0	0
9	J	249	0	262	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	249	0	262	0	0
10	K	293	0	305	8	0
10	k	293	0	305	0	0
11	L	304	0	316	7	0
11	l	304	0	316	0	0
12	M	267	0	289	7	0
12	m	267	0	289	0	0
13	O	1845	0	1801	31	0
13	o	1845	0	1801	0	0
14	T	275	0	288	5	0
14	t	275	0	288	0	0
15	U	774	0	773	8	0
15	u	774	0	773	0	0
16	V	1060	0	1068	7	0
16	v	1060	0	1068	0	0
17	g	201	0	226	0	0
17	y	201	0	226	0	0
18	X	270	0	299	10	0
18	x	270	0	299	0	0
19	G	140	0	31	0	0
19	Y	140	0	31	0	0
20	Z	479	0	516	8	0
20	z	479	0	516	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	260	0	288	44	0
22	B	975	0	1080	90	0
22	C	845	0	936	47	0
22	D	130	0	144	11	0
22	H	65	0	72	9	0
22	a	260	0	288	0	0
22	b	975	0	1080	0	0
22	c	845	0	936	0	0
22	d	130	0	144	0	0
22	h	65	0	72	0	0
23	A	45	0	61	4	0
23	D	55	0	80	12	0
23	J	35	0	45	0	0
23	a	45	0	61	0	0
23	d	55	0	80	0	0
23	j	35	0	45	0	0
24	A	40	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	B	160	0	224	10	0
24	C	80	0	112	14	0
24	F	40	0	56	4	0
24	H	40	0	56	2	0
24	J	40	0	56	1	0
24	K	40	0	56	3	0
24	a	40	0	56	0	0
24	b	160	0	224	0	0
24	c	120	0	168	0	0
24	f	40	0	56	0	0
24	g	40	0	56	0	0
24	j	40	0	56	0	0
24	x	40	0	56	0	0
24	y	40	0	56	0	0
25	A	56	0	70	1	0
25	B	110	0	136	4	0
25	C	181	0	245	11	0
25	D	63	0	87	2	0
25	a	56	0	70	0	0
25	b	110	0	136	0	0
25	c	181	0	245	0	0
25	d	63	0	87	0	0
26	A	39	0	51	3	0
26	C	37	0	44	2	0
26	a	39	0	51	0	0
26	c	37	0	44	0	0
27	A	93	0	126	3	0
27	B	49	0	68	3	0
27	C	93	0	126	4	0
27	D	143	0	196	11	0
27	E	44	0	58	1	0
27	I	43	0	56	1	0
27	M	42	0	54	2	0
27	a	93	0	126	0	0
27	b	49	0	68	0	0
27	c	93	0	126	0	0
27	d	143	0	196	0	0
27	e	44	0	58	0	0
27	i	43	0	56	0	0
27	m	42	0	54	0	0
28	A	10	0	0	0	0
28	a	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	A	105	0	147	6	0
29	B	90	0	111	4	0
29	F	45	0	54	3	0
29	a	105	0	147	0	0
29	b	47	0	61	0	0
29	d	43	0	50	0	0
29	f	45	0	54	0	0
30	B	140	0	184	6	0
30	D	31	0	35	0	0
30	I	35	0	46	1	0
30	M	70	0	91	0	0
30	b	140	0	183	0	0
30	d	31	0	35	0	0
30	i	35	0	46	0	0
31	D	128	0	148	15	0
31	d	128	0	148	0	0
32	D	1	0	0	0	0
32	a	1	0	0	0	0
33	D	4	0	1	0	0
33	d	4	0	1	0	0
34	F	43	0	30	4	0
34	V	43	0	30	3	0
34	f	43	0	30	0	0
34	v	43	0	30	0	0
35	K	1	0	0	0	0
35	O	1	0	0	0	0
35	k	1	0	0	0	0
35	o	1	0	0	0	0
All	All	50244	0	51372	579	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

The worst 5 of 579 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:39:ASN:HB2	22:C:507:CLA:HBA1	1.55	0.87
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.60	0.81
3:C:362:ARG:H	25:C:515:DGD:HE4	1.51	0.81
12:M:33:GLN:HB3	12:M:33:GLN:HB3	0.00	0.81
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.61	0.80

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	311 (93%)	18 (5%)	4 (1%)	19	77
1	a	333/344 (97%)	309 (93%)	20 (6%)	4 (1%)	19	77
2	B	488/510 (96%)	451 (92%)	33 (7%)	4 (1%)	27	82
2	b	488/510 (96%)	449 (92%)	36 (7%)	3 (1%)	33	86
3	C	445/461 (96%)	406 (91%)	35 (8%)	4 (1%)	25	81
3	c	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	25	81
4	D	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	50	91
4	d	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	50	91
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	18	75
5	e	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	18	75
6	F	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
6	f	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	4	44
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	4	44
8	I	33/38 (87%)	27 (82%)	6 (18%)	0	100	100
8	i	33/38 (87%)	26 (79%)	7 (21%)	0	100	100
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	7	57
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	7	57
10	K	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
10	k	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	l	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	M	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
12	m	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
13	O	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	19	77
13	o	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	19	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	6	55
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	6	55
15	U	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	11	66
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	11	66
16	V	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
16	v	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
17	g	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	5	51
17	y	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	5	51
18	X	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	3	39
18	x	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	3	39
20	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	14	70
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	14	70
All	All	5138/5618 (92%)	4675 (91%)	408 (8%)	55 (1%)	21	78

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
2	B	484	PRO
2	B	488	PRO
7	H	18	TYR
1	a	12	ASN

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	271/280 (97%)	267 (98%)	4 (2%)	76	94
1	a	271/280 (97%)	267 (98%)	4 (2%)	76	94
2	B	390/407 (96%)	381 (98%)	9 (2%)	63	91
2	b	390/407 (96%)	381 (98%)	9 (2%)	63	91
3	C	347/362 (96%)	336 (97%)	11 (3%)	51	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	c	347/362 (96%)	336 (97%)	11 (3%)	51	87
4	D	275/283 (97%)	269 (98%)	6 (2%)	64	91
4	d	275/283 (97%)	269 (98%)	6 (2%)	64	91
5	E	72/73 (99%)	70 (97%)	2 (3%)	56	89
5	e	72/73 (99%)	70 (97%)	2 (3%)	56	89
6	F	29/39 (74%)	29 (100%)	0	100	100
6	f	29/39 (74%)	29 (100%)	0	100	100
7	H	53/55 (96%)	49 (92%)	4 (8%)	19	65
7	h	53/55 (96%)	49 (92%)	4 (8%)	19	65
8	I	32/35 (91%)	31 (97%)	1 (3%)	52	88
8	i	32/35 (91%)	31 (97%)	1 (3%)	52	88
9	J	24/28 (86%)	23 (96%)	1 (4%)	40	82
9	j	24/28 (86%)	23 (96%)	1 (4%)	40	82
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	34 (97%)	1 (3%)	55	88
11	l	35/35 (100%)	34 (97%)	1 (3%)	55	88
12	M	31/33 (94%)	31 (100%)	0	100	100
12	m	31/33 (94%)	31 (100%)	0	100	100
13	O	202/228 (89%)	200 (99%)	2 (1%)	85	96
13	o	202/228 (89%)	200 (99%)	2 (1%)	85	96
14	T	29/29 (100%)	28 (97%)	1 (3%)	49	87
14	t	29/29 (100%)	28 (97%)	1 (3%)	49	87
15	U	84/112 (75%)	83 (99%)	1 (1%)	82	95
15	u	84/112 (75%)	83 (99%)	1 (1%)	82	95
16	V	116/138 (84%)	114 (98%)	2 (2%)	73	93
16	v	116/138 (84%)	114 (98%)	2 (2%)	73	93
17	g	20/37 (54%)	18 (90%)	2 (10%)	11	51
17	y	20/37 (54%)	18 (90%)	2 (10%)	11	51
18	X	30/34 (88%)	28 (93%)	2 (7%)	23	70
18	x	30/34 (88%)	28 (93%)	2 (7%)	23	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	Z	52/52 (100%)	50 (96%)	2 (4%)	44	85
20	z	52/52 (100%)	50 (96%)	2 (4%)	44	85
All	All	4244/4594 (92%)	4142 (98%)	102 (2%)	61	90

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	y	46	LEU
2	b	262	THR
16	v	92	ARG
18	X	12	ILE
1	a	228	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	118	HIS
4	D	117	HIS
4	d	117	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 184 ligands modelled in this entry, 8 are monoatomic - leaving 176 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	402	-	73,73,73	1.63	10 (13%)	96,113,113	1.21	11 (11%)
22	CLA	A	403	-	73,73,73	1.60	10 (13%)	96,113,113	1.23	11 (11%)
22	CLA	A	404	-	73,73,73	1.59	10 (13%)	96,113,113	1.23	12 (12%)
22	CLA	A	405	-	73,73,73	1.59	10 (13%)	96,113,113	1.24	13 (13%)
23	PL9	A	406	-	45,45,55	1.11	3 (6%)	55,57,69	1.72	12 (21%)
24	BCR	A	407	-	41,41,41	1.05	2 (4%)	56,56,56	1.20	6 (10%)
25	DGD	A	408	-	57,57,67	2.14	2 (3%)	71,71,81	1.56	9 (12%)
26	LHG	A	409	-	38,38,48	2.28	1 (2%)	44,44,54	1.40	6 (13%)
27	LMG	A	410	-	51,51,55	2.32	3 (5%)	59,59,63	1.44	8 (13%)
28	OEX	A	411	1,3	8,15,15	10.57	8 (100%)	0,32,32	0.00	-
29	SQD	A	412	-	51,51,54	1.54	4 (7%)	62,62,65	1.96	11 (17%)
29	SQD	A	413	-	54,54,54	0.92	3 (5%)	65,65,65	1.71	12 (18%)
27	LMG	A	414	-	42,42,55	2.46	2 (4%)	50,50,63	1.35	6 (12%)
22	CLA	B	601	-	73,73,73	1.62	10 (13%)	96,113,113	1.22	12 (12%)
22	CLA	B	602	-	73,73,73	1.58	10 (13%)	96,113,113	1.25	12 (12%)
22	CLA	B	603	-	73,73,73	1.60	10 (13%)	96,113,113	1.30	15 (15%)
22	CLA	B	604	-	73,73,73	1.59	10 (13%)	96,113,113	1.23	11 (11%)
22	CLA	B	605	-	73,73,73	1.58	10 (13%)	96,113,113	1.24	14 (14%)
22	CLA	B	606	-	73,73,73	1.60	10 (13%)	96,113,113	1.22	13 (13%)
22	CLA	B	607	-	73,73,73	1.59	10 (13%)	96,113,113	1.23	13 (13%)
22	CLA	B	608	-	73,73,73	1.61	10 (13%)	96,113,113	1.22	14 (14%)
22	CLA	B	609	-	73,73,73	1.60	10 (13%)	96,113,113	1.24	12 (12%)
22	CLA	B	610	-	73,73,73	1.57	11 (15%)	96,113,113	1.39	12 (12%)
22	CLA	B	611	-	73,73,73	1.60	10 (13%)	96,113,113	1.26	14 (14%)
22	CLA	B	612	-	73,73,73	1.59	10 (13%)	96,113,113	1.29	14 (14%)
22	CLA	B	613	-	73,73,73	1.61	10 (13%)	96,113,113	1.23	12 (12%)
22	CLA	B	614	-	73,73,73	1.61	10 (13%)	96,113,113	1.23	13 (13%)
22	CLA	B	615	-	73,73,73	1.60	11 (15%)	96,113,113	1.22	12 (12%)
24	BCR	B	616	-	41,41,41	1.07	2 (4%)	56,56,56	1.20	7 (12%)
24	BCR	B	617	-	41,41,41	1.04	2 (4%)	56,56,56	1.30	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	B	618	-	41,41,41	1.06	2 (4%)	56,56,56	1.32	8 (14%)
24	BCR	B	619	-	41,41,41	1.05	2 (4%)	56,56,56	1.24	8 (14%)
25	DGD	B	620	-	59,59,67	2.25	3 (5%)	73,73,81	1.45	7 (9%)
27	LMG	B	621	-	49,49,55	2.34	3 (6%)	57,57,63	1.41	9 (15%)
29	SQD	B	622	-	43,43,54	1.23	4 (9%)	54,54,65	1.96	13 (24%)
30	LMT	B	623	-	36,36,36	1.09	4 (11%)	47,47,47	0.99	2 (4%)
30	LMT	B	624	-	36,36,36	1.06	4 (11%)	47,47,47	1.04	3 (6%)
25	DGD	B	625	-	53,53,67	2.30	5 (9%)	67,67,81	1.46	9 (13%)
29	SQD	B	626	-	47,47,54	1.09	4 (8%)	58,58,65	1.96	10 (17%)
30	LMT	B	627	-	36,36,36	1.08	4 (11%)	47,47,47	0.98	1 (2%)
30	LMT	B	628	-	36,36,36	1.10	5 (13%)	47,47,47	1.06	1 (2%)
22	CLA	C	501	-	73,73,73	1.60	11 (15%)	96,113,113	1.20	13 (13%)
22	CLA	C	502	-	73,73,73	1.60	11 (15%)	96,113,113	1.25	13 (13%)
22	CLA	C	503	-	73,73,73	1.59	10 (13%)	96,113,113	1.24	13 (13%)
22	CLA	C	504	-	73,73,73	1.60	10 (13%)	96,113,113	1.25	14 (14%)
22	CLA	C	505	-	73,73,73	1.61	10 (13%)	96,113,113	1.28	13 (13%)
22	CLA	C	506	-	73,73,73	1.58	10 (13%)	96,113,113	1.28	13 (13%)
22	CLA	C	507	-	73,73,73	1.60	10 (13%)	96,113,113	1.29	13 (13%)
22	CLA	C	508	-	73,73,73	1.61	10 (13%)	96,113,113	1.21	11 (11%)
22	CLA	C	509	-	73,73,73	1.61	10 (13%)	96,113,113	1.22	11 (11%)
22	CLA	C	510	3	73,73,73	1.60	10 (13%)	96,113,113	1.27	13 (13%)
22	CLA	C	511	-	73,73,73	1.61	10 (13%)	96,113,113	1.25	14 (14%)
22	CLA	C	512	-	73,73,73	1.60	10 (13%)	96,113,113	1.24	13 (13%)
24	BCR	C	513	-	41,41,41	1.07	2 (4%)	56,56,56	1.30	8 (14%)
24	BCR	C	514	-	41,41,41	1.07	2 (4%)	56,56,56	1.26	9 (16%)
25	DGD	C	515	-	54,54,67	2.39	4 (7%)	68,68,81	1.34	10 (14%)
25	DGD	C	516	-	63,63,67	1.48	2 (3%)	77,77,81	1.45	13 (16%)
25	DGD	C	517	-	67,67,67	0.86	2 (2%)	81,81,81	1.42	10 (12%)
27	LMG	C	518	-	45,45,55	2.56	2 (4%)	53,53,63	1.42	6 (11%)
26	LHG	C	519	-	36,36,48	2.36	3 (8%)	42,42,54	1.50	8 (19%)
22	CLA	C	520	-	73,73,73	1.60	10 (13%)	96,113,113	1.22	12 (12%)
27	LMG	C	521	-	48,48,55	2.34	2 (4%)	56,56,63	1.42	9 (16%)
31	PHO	D	401	-	69,69,69	1.24	9 (13%)	92,99,99	1.18	10 (10%)
31	PHO	D	402	-	69,69,69	1.26	11 (15%)	92,99,99	1.17	9 (9%)
33	BCT	D	404	21	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	D	405	-	73,73,73	1.62	10 (13%)	96,113,113	1.21	11 (11%)
22	CLA	D	406	-	73,73,73	1.59	10 (13%)	96,113,113	1.26	14 (14%)
23	PL9	D	407	-	55,55,55	1.12	3 (5%)	69,69,69	1.66	15 (21%)
27	LMG	D	408	-	49,49,55	2.48	3 (6%)	57,57,63	1.40	8 (14%)
27	LMG	D	409	-	48,48,55	2.37	2 (4%)	56,56,63	1.49	7 (12%)
25	DGD	D	410	-	64,64,67	1.40	1 (1%)	78,78,81	1.33	9 (11%)
30	LMT	D	411	-	32,32,36	2.83	5 (15%)	43,43,47	1.07	2 (4%)
27	LMG	D	412	-	46,46,55	2.58	3 (6%)	54,54,63	1.41	7 (12%)
27	LMG	E	101	-	44,44,55	2.57	2 (4%)	52,52,63	1.40	7 (13%)
34	HEM	F	101	5,6	42,50,50	3.64	13 (30%)	27,82,82	1.20	2 (7%)
24	BCR	F	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	6 (10%)
29	SQD	F	103	-	45,45,54	1.39	5 (11%)	56,56,65	1.85	11 (19%)
22	CLA	H	101	-	73,73,73	1.61	10 (13%)	96,113,113	1.22	13 (13%)
24	BCR	H	102	-	41,41,41	1.08	2 (4%)	56,56,56	1.17	5 (8%)
27	LMG	I	101	-	43,43,55	2.30	2 (4%)	51,51,63	1.36	7 (13%)
30	LMT	I	102	-	36,36,36	1.07	4 (11%)	47,47,47	1.06	2 (4%)
23	PL9	J	101	-	35,35,55	1.13	1 (2%)	43,45,69	1.79	8 (18%)
24	BCR	J	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.59	12 (21%)
24	BCR	K	102	-	41,41,41	1.05	2 (4%)	56,56,56	1.21	8 (14%)
27	LMG	M	101	-	42,42,55	2.44	3 (7%)	50,50,63	1.33	5 (10%)
30	LMT	M	102	-	36,36,36	1.11	4 (11%)	47,47,47	1.02	2 (4%)
30	LMT	M	103	-	36,36,36	1.11	5 (13%)	47,47,47	1.01	3 (6%)
34	HEM	V	201	16	42,50,50	3.68	13 (30%)	27,82,82	1.13	1 (3%)
29	SQD	a	401	-	54,54,54	0.92	3 (5%)	65,65,65	1.71	11 (16%)
27	LMG	a	402	-	42,42,55	2.49	2 (4%)	50,50,63	1.36	5 (10%)
22	CLA	a	404	-	73,73,73	1.63	10 (13%)	96,113,113	1.21	10 (10%)
22	CLA	a	405	-	73,73,73	1.61	10 (13%)	96,113,113	1.22	11 (11%)
22	CLA	a	406	-	73,73,73	1.60	10 (13%)	96,113,113	1.23	11 (11%)
22	CLA	a	407	-	73,73,73	1.59	10 (13%)	96,113,113	1.25	13 (13%)
23	PL9	a	408	-	45,45,55	1.16	3 (6%)	55,57,69	1.71	11 (20%)
24	BCR	a	409	-	41,41,41	1.05	2 (4%)	56,56,56	1.20	7 (12%)
25	DGD	a	410	-	57,57,67	2.15	3 (5%)	71,71,81	1.54	9 (12%)
26	LHG	a	411	-	38,38,48	2.29	2 (5%)	44,44,54	1.41	6 (13%)
27	LMG	a	412	-	51,51,55	2.30	3 (5%)	59,59,63	1.42	9 (15%)
28	OEX	a	414	1,3	8,15,15	10.50	8 (100%)	0,32,32	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	SQD	a	415	-	51,51,54	1.55	4 (7%)	62,62,65	1.98	11 (17%)
25	DGD	b	601	-	53,53,67	2.26	6 (11%)	67,67,81	1.46	10 (14%)
29	SQD	b	602	-	47,47,54	1.09	5 (10%)	58,58,65	1.97	10 (17%)
30	LMT	b	603	-	36,36,36	1.09	4 (11%)	47,47,47	0.96	1 (2%)
30	LMT	b	604	-	36,36,36	1.09	4 (11%)	47,47,47	1.06	1 (2%)
22	CLA	b	605	-	73,73,73	1.62	10 (13%)	96,113,113	1.23	12 (12%)
22	CLA	b	606	-	73,73,73	1.59	10 (13%)	96,113,113	1.24	11 (11%)
22	CLA	b	607	-	73,73,73	1.60	10 (13%)	96,113,113	1.29	14 (14%)
22	CLA	b	608	-	73,73,73	1.59	10 (13%)	96,113,113	1.24	13 (13%)
22	CLA	b	609	-	73,73,73	1.59	10 (13%)	96,113,113	1.25	13 (13%)
22	CLA	b	610	-	73,73,73	1.59	10 (13%)	96,113,113	1.22	11 (11%)
22	CLA	b	611	-	73,73,73	1.60	10 (13%)	96,113,113	1.23	13 (13%)
22	CLA	b	612	-	73,73,73	1.62	10 (13%)	96,113,113	1.21	13 (13%)
22	CLA	b	613	-	73,73,73	1.59	10 (13%)	96,113,113	1.24	13 (13%)
22	CLA	b	614	-	73,73,73	1.58	11 (15%)	96,113,113	1.38	12 (12%)
22	CLA	b	615	-	73,73,73	1.60	11 (15%)	96,113,113	1.26	14 (14%)
22	CLA	b	616	-	73,73,73	1.59	10 (13%)	96,113,113	1.29	15 (15%)
22	CLA	b	617	-	73,73,73	1.59	10 (13%)	96,113,113	1.24	12 (12%)
22	CLA	b	618	-	73,73,73	1.61	10 (13%)	96,113,113	1.24	14 (14%)
22	CLA	b	619	-	73,73,73	1.61	11 (15%)	96,113,113	1.20	12 (12%)
24	BCR	b	620	-	41,41,41	1.06	2 (4%)	56,56,56	1.19	5 (8%)
24	BCR	b	621	-	41,41,41	1.04	2 (4%)	56,56,56	1.31	9 (16%)
24	BCR	b	622	-	41,41,41	1.06	2 (4%)	56,56,56	1.33	9 (16%)
24	BCR	b	623	-	41,41,41	1.05	2 (4%)	56,56,56	1.26	8 (14%)
25	DGD	b	624	-	59,59,67	2.23	3 (5%)	73,73,81	1.44	6 (8%)
27	LMG	b	625	-	49,49,55	2.35	3 (6%)	57,57,63	1.40	9 (15%)
30	LMT	b	626	-	36,36,36	1.09	4 (11%)	47,47,47	0.98	1 (2%)
30	LMT	b	627	-	36,36,36	1.06	4 (11%)	47,47,47	1.01	3 (6%)
22	CLA	c	501	-	73,73,73	1.59	11 (15%)	96,113,113	1.21	13 (13%)
22	CLA	c	502	-	73,73,73	1.60	10 (13%)	96,113,113	1.25	13 (13%)
22	CLA	c	503	-	73,73,73	1.61	10 (13%)	96,113,113	1.23	13 (13%)
22	CLA	c	504	-	73,73,73	1.62	10 (13%)	96,113,113	1.23	14 (14%)
22	CLA	c	505	-	73,73,73	1.60	10 (13%)	96,113,113	1.27	13 (13%)
22	CLA	c	506	-	73,73,73	1.59	10 (13%)	96,113,113	1.28	14 (14%)
22	CLA	c	507	-	73,73,73	1.59	10 (13%)	96,113,113	1.31	14 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	508	-	73,73,73	1.63	10 (13%)	96,113,113	1.20	11 (11%)
22	CLA	c	509	-	73,73,73	1.61	10 (13%)	96,113,113	1.22	13 (13%)
22	CLA	c	510	3	73,73,73	1.61	10 (13%)	96,113,113	1.27	14 (14%)
22	CLA	c	511	-	73,73,73	1.61	10 (13%)	96,113,113	1.25	14 (14%)
22	CLA	c	512	-	73,73,73	1.60	10 (13%)	96,113,113	1.24	13 (13%)
24	BCR	c	513	-	41,41,41	1.05	2 (4%)	56,56,56	1.31	8 (14%)
24	BCR	c	514	-	41,41,41	1.06	2 (4%)	56,56,56	1.25	8 (14%)
25	DGD	c	515	-	54,54,67	2.43	3 (5%)	68,68,81	1.34	9 (13%)
25	DGD	c	516	-	63,63,67	1.47	2 (3%)	77,77,81	1.45	12 (15%)
25	DGD	c	517	-	67,67,67	0.86	2 (2%)	81,81,81	1.41	8 (9%)
27	LMG	c	518	-	45,45,55	2.54	2 (4%)	53,53,63	1.42	7 (13%)
26	LHG	c	519	-	36,36,48	2.31	2 (5%)	42,42,54	1.51	8 (19%)
22	CLA	c	520	-	73,73,73	1.60	10 (13%)	96,113,113	1.22	12 (12%)
24	BCR	c	521	-	41,41,41	1.03	2 (4%)	56,56,56	1.21	7 (12%)
27	LMG	c	522	-	48,48,55	2.32	2 (4%)	56,56,63	1.41	8 (14%)
31	PHO	d	401	-	69,69,69	1.24	9 (13%)	92,99,99	1.18	10 (10%)
31	PHO	d	402	-	69,69,69	1.26	11 (15%)	92,99,99	1.15	10 (10%)
29	SQD	d	403	-	43,43,54	1.23	4 (9%)	54,54,65	1.97	12 (22%)
33	BCT	d	404	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	d	405	-	73,73,73	1.62	10 (13%)	96,113,113	1.19	12 (12%)
22	CLA	d	406	-	73,73,73	1.60	10 (13%)	96,113,113	1.26	14 (14%)
23	PL9	d	407	-	55,55,55	1.13	2 (3%)	69,69,69	1.66	15 (21%)
27	LMG	d	408	-	49,49,55	2.41	2 (4%)	57,57,63	1.40	7 (12%)
27	LMG	d	409	-	48,48,55	2.37	2 (4%)	56,56,63	1.49	6 (10%)
25	DGD	d	410	-	64,64,67	1.41	2 (3%)	78,78,81	1.35	8 (10%)
30	LMT	d	411	-	32,32,36	2.83	5 (15%)	43,43,47	1.04	2 (4%)
27	LMG	d	412	-	46,46,55	2.59	3 (6%)	54,54,63	1.41	7 (12%)
27	LMG	e	101	-	44,44,55	2.61	2 (4%)	52,52,63	1.40	7 (13%)
34	HEM	f	101	5,6	42,50,50	3.64	13 (30%)	27,82,82	1.23	2 (7%)
24	BCR	f	102	-	41,41,41	1.08	2 (4%)	56,56,56	1.19	5 (8%)
29	SQD	f	103	-	45,45,54	1.39	6 (13%)	56,56,65	1.85	11 (19%)
24	BCR	g	101	-	41,41,41	1.10	3 (7%)	56,56,56	1.25	7 (12%)
22	CLA	h	101	-	73,73,73	1.61	10 (13%)	96,113,113	1.22	12 (12%)
27	LMG	i	101	-	43,43,55	2.35	2 (4%)	51,51,63	1.37	7 (13%)
30	LMT	i	102	-	36,36,36	1.06	4 (11%)	47,47,47	1.04	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PL9	j	101	-	35,35,55	1.11	1 (2%)	43,45,69	1.80	8 (18%)
24	BCR	j	102	-	41,41,41	1.03	2 (4%)	56,56,56	1.57	12 (21%)
27	LMG	m	101	-	42,42,55	2.44	3 (7%)	50,50,63	1.33	5 (10%)
34	HEM	v	201	16	42,50,50	3.70	14 (33%)	27,82,82	1.13	1 (3%)
24	BCR	x	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.15	2 (3%)
24	BCR	y	101	-	41,41,41	1.10	3 (7%)	56,56,56	1.23	6 (10%)

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	402	-	-	0/37/135/135	0/0/9/9
22	CLA	A	403	-	-	0/37/135/135	0/0/9/9
22	CLA	A	404	-	-	0/37/135/135	0/0/9/9
22	CLA	A	405	-	-	0/37/135/135	0/0/9/9
23	PL9	A	406	-	-	0/41/61/73	0/1/1/1
24	BCR	A	407	-	-	0/29/63/63	0/2/2/2
25	DGD	A	408	-	-	0/45/85/95	0/2/2/2
26	LHG	A	409	-	-	0/43/43/53	0/0/0/0
27	LMG	A	410	-	-	0/46/66/70	0/1/1/1
28	OEX	A	411	1,3	-	0/0/68/68	0/0/6/6
29	SQD	A	412	-	-	0/46/66/69	0/1/1/1
29	SQD	A	413	-	-	0/49/69/69	0/1/1/1
27	LMG	A	414	-	-	0/37/57/70	0/1/1/1
22	CLA	B	601	-	-	0/37/135/135	0/0/9/9
22	CLA	B	602	-	-	0/37/135/135	0/0/9/9
22	CLA	B	603	-	-	0/37/135/135	0/0/9/9
22	CLA	B	604	-	-	0/37/135/135	0/0/9/9
22	CLA	B	605	-	-	0/37/135/135	0/0/9/9
22	CLA	B	606	-	-	0/37/135/135	0/0/9/9
22	CLA	B	607	-	-	0/37/135/135	0/0/9/9
22	CLA	B	608	-	-	0/37/135/135	0/0/9/9
22	CLA	B	609	-	-	0/37/135/135	0/0/9/9
22	CLA	B	610	-	-	0/37/135/135	0/0/9/9
22	CLA	B	611	-	-	0/37/135/135	0/0/9/9
22	CLA	B	612	-	-	0/37/135/135	0/0/9/9
22	CLA	B	613	-	-	0/37/135/135	0/0/9/9
22	CLA	B	614	-	-	0/37/135/135	0/0/9/9
22	CLA	B	615	-	-	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
24	BCR	B	619	-	-	0/29/63/63	0/2/2/2
25	DGD	B	620	-	-	0/47/87/95	0/2/2/2
27	LMG	B	621	-	-	0/44/64/70	0/1/1/1
29	SQD	B	622	-	-	1/38/58/69	0/1/1/1
30	LMT	B	623	-	-	0/21/61/61	0/2/2/2
30	LMT	B	624	-	-	0/21/61/61	0/2/2/2
25	DGD	B	625	-	-	0/41/81/95	0/2/2/2
29	SQD	B	626	-	-	0/42/62/69	0/1/1/1
30	LMT	B	627	-	-	0/21/61/61	0/2/2/2
30	LMT	B	628	-	-	0/21/61/61	0/2/2/2
22	CLA	C	501	-	-	0/37/135/135	0/0/9/9
22	CLA	C	502	-	-	0/37/135/135	0/0/9/9
22	CLA	C	503	-	-	0/37/135/135	0/0/9/9
22	CLA	C	504	-	-	0/37/135/135	0/0/9/9
22	CLA	C	505	-	-	0/37/135/135	0/0/9/9
22	CLA	C	506	-	-	0/37/135/135	0/0/9/9
22	CLA	C	507	-	-	0/37/135/135	0/0/9/9
22	CLA	C	508	-	-	0/37/135/135	0/0/9/9
22	CLA	C	509	-	-	0/37/135/135	0/0/9/9
22	CLA	C	510	3	-	0/37/135/135	0/0/9/9
22	CLA	C	511	-	-	0/37/135/135	0/0/9/9
22	CLA	C	512	-	-	0/37/135/135	0/0/9/9
24	BCR	C	513	-	-	0/29/63/63	0/2/2/2
24	BCR	C	514	-	-	0/29/63/63	0/2/2/2
25	DGD	C	515	-	-	0/42/82/95	0/2/2/2
25	DGD	C	516	-	-	1/51/91/95	0/2/2/2
25	DGD	C	517	-	-	0/55/95/95	0/2/2/2
27	LMG	C	518	-	-	0/40/60/70	0/1/1/1
26	LHG	C	519	-	-	0/41/41/53	0/0/0/0
22	CLA	C	520	-	-	0/37/135/135	0/0/9/9
27	LMG	C	521	-	-	0/43/63/70	0/1/1/1
31	PHO	D	401	-	-	0/49/103/103	0/1/6/6
31	PHO	D	402	-	-	0/49/103/103	0/1/6/6
33	BCT	D	404	21	-	0/0/0/0	0/0/0/0
22	CLA	D	405	-	-	0/37/135/135	0/0/9/9
22	CLA	D	406	-	-	0/37/135/135	0/0/9/9
23	PL9	D	407	-	-	0/53/73/73	0/1/1/1
27	LMG	D	408	-	-	0/44/64/70	0/1/1/1
27	LMG	D	409	-	-	0/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	DGD	D	410	-	-	0/52/92/95	0/2/2/2
30	LMT	D	411	-	-	0/17/57/61	0/2/2/2
27	LMG	D	412	-	-	0/41/61/70	0/1/1/1
27	LMG	E	101	-	-	0/39/59/70	0/1/1/1
34	HEM	F	101	5,6	-	0/14/114/114	0/0/8/8
24	BCR	F	102	-	-	0/29/63/63	0/2/2/2
29	SQD	F	103	-	-	0/40/60/69	0/1/1/1
22	CLA	H	101	-	-	0/37/135/135	0/0/9/9
24	BCR	H	102	-	-	0/29/63/63	0/2/2/2
27	LMG	I	101	-	-	0/38/58/70	0/1/1/1
30	LMT	I	102	-	-	0/21/61/61	0/2/2/2
23	PL9	J	101	-	-	0/29/49/73	0/1/1/1
24	BCR	J	102	-	-	0/29/63/63	0/2/2/2
24	BCR	K	102	-	-	0/29/63/63	0/2/2/2
27	LMG	M	101	-	-	0/37/57/70	0/1/1/1
30	LMT	M	102	-	-	0/21/61/61	0/2/2/2
30	LMT	M	103	-	-	0/21/61/61	0/2/2/2
34	HEM	V	201	16	-	0/14/114/114	0/0/8/8
29	SQD	a	401	-	-	0/49/69/69	0/1/1/1
27	LMG	a	402	-	-	0/37/57/70	0/1/1/1
22	CLA	a	404	-	-	0/37/135/135	0/0/9/9
22	CLA	a	405	-	-	0/37/135/135	0/0/9/9
22	CLA	a	406	-	-	0/37/135/135	0/0/9/9
22	CLA	a	407	-	-	0/37/135/135	0/0/9/9
23	PL9	a	408	-	-	0/41/61/73	0/1/1/1
24	BCR	a	409	-	-	0/29/63/63	0/2/2/2
25	DGD	a	410	-	-	0/45/85/95	0/2/2/2
26	LHG	a	411	-	-	0/43/43/53	0/0/0/0
27	LMG	a	412	-	-	0/46/66/70	0/1/1/1
28	OEX	a	414	1,3	-	0/0/68/68	0/0/6/6
29	SQD	a	415	-	-	0/46/66/69	0/1/1/1
25	DGD	b	601	-	-	0/41/81/95	0/2/2/2
29	SQD	b	602	-	-	0/42/62/69	0/1/1/1
30	LMT	b	603	-	-	0/21/61/61	0/2/2/2
30	LMT	b	604	-	-	0/21/61/61	0/2/2/2
22	CLA	b	605	-	-	0/37/135/135	0/0/9/9
22	CLA	b	606	-	-	0/37/135/135	0/0/9/9
22	CLA	b	607	-	-	0/37/135/135	0/0/9/9
22	CLA	b	608	-	-	0/37/135/135	0/0/9/9
22	CLA	b	609	-	-	0/37/135/135	0/0/9/9
22	CLA	b	610	-	-	0/37/135/135	0/0/9/9
22	CLA	b	611	-	-	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	612	-	-	0/37/135/135	0/0/9/9
22	CLA	b	613	-	-	0/37/135/135	0/0/9/9
22	CLA	b	614	-	-	0/37/135/135	0/0/9/9
22	CLA	b	615	-	-	0/37/135/135	0/0/9/9
22	CLA	b	616	-	-	0/37/135/135	0/0/9/9
22	CLA	b	617	-	-	0/37/135/135	0/0/9/9
22	CLA	b	618	-	-	0/37/135/135	0/0/9/9
22	CLA	b	619	-	-	0/37/135/135	0/0/9/9
24	BCR	b	620	-	-	0/29/63/63	0/2/2/2
24	BCR	b	621	-	-	0/29/63/63	0/2/2/2
24	BCR	b	622	-	-	0/29/63/63	0/2/2/2
24	BCR	b	623	-	-	0/29/63/63	0/2/2/2
25	DGD	b	624	-	-	0/47/87/95	0/2/2/2
27	LMG	b	625	-	-	0/44/64/70	0/1/1/1
30	LMT	b	626	-	-	0/21/61/61	0/2/2/2
30	LMT	b	627	-	-	0/21/61/61	0/2/2/2
22	CLA	c	501	-	-	0/37/135/135	0/0/9/9
22	CLA	c	502	-	-	0/37/135/135	0/0/9/9
22	CLA	c	503	-	-	0/37/135/135	0/0/9/9
22	CLA	c	504	-	-	0/37/135/135	0/0/9/9
22	CLA	c	505	-	-	0/37/135/135	0/0/9/9
22	CLA	c	506	-	-	0/37/135/135	0/0/9/9
22	CLA	c	507	-	-	0/37/135/135	0/0/9/9
22	CLA	c	508	-	-	0/37/135/135	0/0/9/9
22	CLA	c	509	-	-	0/37/135/135	0/0/9/9
22	CLA	c	510	3	-	0/37/135/135	0/0/9/9
22	CLA	c	511	-	-	0/37/135/135	0/0/9/9
22	CLA	c	512	-	-	0/37/135/135	0/0/9/9
24	BCR	c	513	-	-	0/29/63/63	0/2/2/2
24	BCR	c	514	-	-	0/29/63/63	0/2/2/2
25	DGD	c	515	-	-	0/42/82/95	0/2/2/2
25	DGD	c	516	-	-	1/51/91/95	0/2/2/2
25	DGD	c	517	-	-	0/55/95/95	0/2/2/2
27	LMG	c	518	-	-	0/40/60/70	0/1/1/1
26	LHG	c	519	-	-	0/41/41/53	0/0/0/0
22	CLA	c	520	-	-	0/37/135/135	0/0/9/9
24	BCR	c	521	-	-	0/29/63/63	0/2/2/2
27	LMG	c	522	-	-	0/43/63/70	0/1/1/1
31	PHO	d	401	-	-	0/49/103/103	0/1/6/6
31	PHO	d	402	-	-	0/49/103/103	0/1/6/6
29	SQD	d	403	-	-	1/38/58/69	0/1/1/1
33	BCT	d	404	21	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	d	405	-	-	0/37/135/135	0/0/9/9
22	CLA	d	406	-	-	0/37/135/135	0/0/9/9
23	PL9	d	407	-	-	0/53/73/73	0/1/1/1
27	LMG	d	408	-	-	0/44/64/70	0/1/1/1
27	LMG	d	409	-	-	0/43/63/70	0/1/1/1
25	DGD	d	410	-	-	0/52/92/95	0/2/2/2
30	LMT	d	411	-	-	0/17/57/61	0/2/2/2
27	LMG	d	412	-	-	0/41/61/70	0/1/1/1
27	LMG	e	101	-	-	0/39/59/70	0/1/1/1
34	HEM	f	101	5,6	-	0/14/114/114	0/0/8/8
24	BCR	f	102	-	-	0/29/63/63	0/2/2/2
29	SQD	f	103	-	-	0/40/60/69	0/1/1/1
24	BCR	g	101	-	-	0/29/63/63	0/2/2/2
22	CLA	h	101	-	-	0/37/135/135	0/0/9/9
27	LMG	i	101	-	-	0/38/58/70	0/1/1/1
30	LMT	i	102	-	-	0/21/61/61	0/2/2/2
23	PL9	j	101	-	-	0/29/49/73	0/1/1/1
24	BCR	j	102	-	-	0/29/63/63	0/2/2/2
27	LMG	m	101	-	-	0/37/57/70	0/1/1/1
34	HEM	v	201	16	-	0/14/114/114	0/0/8/8
24	BCR	x	101	-	-	0/29/63/63	0/2/2/2
24	BCR	y	101	-	-	0/29/63/63	0/2/2/2

The worst 5 of 1083 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	411	OEX	O3-MN1	-15.24	1.87	2.02
28	a	414	OEX	O3-MN1	-15.06	1.87	2.02
30	D	411	LMT	C8-C7	-14.66	1.49	1.55
30	d	411	LMT	C8-C7	-14.62	1.49	1.55
34	v	201	HEM	C3C-C2C	-14.56	1.34	1.45

The worst 5 of 1633 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	415	SQD	O6-C1-C2	7.00	117.13	108.15
29	A	412	SQD	O9-S-C6	6.90	112.92	106.83
29	A	412	SQD	O6-C1-C2	6.83	116.91	108.15
29	a	415	SQD	O9-S-C6	6.76	112.81	106.83
29	b	602	SQD	O6-C1-C2	6.70	116.74	108.15

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	B	622	SQD	C45-O47-C7-C8
29	d	403	SQD	C45-O47-C7-C8
25	C	516	DGD	C2G-O2G-C1B-C2B
25	c	516	DGD	C2G-O2G-C1B-C2B

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	335/344 (97%)	0.95	38 (11%) 6 10	178, 179, 180, 181	0
1	a	335/344 (97%)	1.11	65 (19%) 2 4	178, 179, 180, 181	0
2	B	490/510 (96%)	0.78	50 (10%) 7 12	178, 179, 180, 181	0
2	b	490/510 (96%)	0.92	72 (14%) 3 6	178, 179, 180, 181	0
3	C	447/461 (96%)	0.84	54 (12%) 5 9	178, 179, 180, 181	0
3	c	447/461 (96%)	0.79	47 (10%) 7 11	178, 180, 180, 181	0
4	D	340/352 (96%)	0.74	28 (8%) 12 16	177, 179, 180, 181	0
4	d	340/352 (96%)	0.80	42 (12%) 5 9	177, 179, 180, 181	0
5	E	82/84 (97%)	0.70	7 (8%) 11 15	178, 180, 180, 181	0
5	e	82/84 (97%)	0.66	6 (7%) 15 18	178, 180, 181, 181	0
6	F	35/45 (77%)	0.33	2 (5%) 23 23	179, 179, 180, 180	0
6	f	35/45 (77%)	0.31	4 (11%) 6 10	179, 180, 181, 181	0
7	H	65/66 (98%)	1.17	17 (26%) 1 3	179, 180, 180, 181	0
7	h	65/66 (98%)	1.42	24 (36%) 1 2	179, 180, 181, 181	0
8	I	35/38 (92%)	0.62	1 (2%) 49 41	178, 179, 180, 181	0
8	i	35/38 (92%)	0.66	2 (5%) 23 23	179, 179, 181, 181	0
9	J	34/40 (85%)	0.55	3 (8%) 10 15	178, 179, 180, 180	0
9	j	34/40 (85%)	0.04	0 100 100	179, 180, 181, 181	0
10	K	37/46 (80%)	0.23	0 100 100	179, 180, 180, 180	0
10	k	37/46 (80%)	0.95	8 (21%) 1 3	179, 180, 181, 181	0
11	L	37/37 (100%)	1.50	12 (32%) 1 3	178, 179, 180, 181	0
11	l	37/37 (100%)	1.00	6 (16%) 2 5	178, 179, 180, 181	0
12	M	34/36 (94%)	0.97	4 (11%) 5 10	178, 179, 180, 181	0
12	m	34/36 (94%)	0.63	1 (2%) 49 41	178, 179, 180, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/272 (89%)	1.12	48 (19%) 2 4	177, 179, 180, 181	0
13	o	243/272 (89%)	1.13	48 (19%) 2 4	177, 179, 181, 181	0
14	T	32/32 (100%)	0.88	2 (6%) 19 21	178, 179, 181, 181	0
14	t	32/32 (100%)	1.36	7 (21%) 1 3	178, 179, 180, 181	0
15	U	97/134 (72%)	1.10	12 (12%) 5 9	178, 179, 180, 181	0
15	u	97/134 (72%)	1.54	35 (36%) 1 2	178, 179, 180, 181	0
16	V	137/163 (84%)	0.68	12 (8%) 10 15	178, 179, 180, 181	0
16	v	137/163 (84%)	0.82	19 (13%) 4 7	178, 180, 181, 181	0
17	g	28/46 (60%)	1.40	4 (14%) 3 6	179, 180, 181, 182	0
17	y	28/46 (60%)	0.59	2 (7%) 16 19	178, 180, 181, 181	0
18	X	37/41 (90%)	0.77	2 (5%) 25 24	179, 179, 181, 181	0
18	x	37/41 (90%)	1.13	7 (18%) 2 4	179, 180, 180, 181	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	0.80	6 (9%) 8 13	179, 180, 181, 181	0
20	z	62/62 (100%)	1.12	8 (12%) 4 8	179, 180, 181, 181	0
All	All	5214/5674 (91%)	0.89	705 (13%) 4 7	177, 179, 180, 182	0

The worst 5 of 705 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	169	LYS	9.1
5	e	84	LYS	9.0
7	H	66	GLY	7.3
15	U	38	GLU	6.5
5	E	84	LYS	6.2

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

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

6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
27	LMG	i	101	43/55	0.65	8.15	177,180,182,184	0
24	BCR	c	521	40/40	1.73	6.78	178,179,181,181	0
35	CA	K	101	1/1	0.47	6.38	184,184,184,184	0
25	DGD	D	410	63/66	0.88	5.89	178,181,182,183	0
27	LMG	C	518	45/55	1.19	5.57	178,179,180,181	0
24	BCR	y	101	40/40	0.90	5.47	177,179,180,180	0
30	LMT	i	102	35/35	0.78	5.44	178,181,183,183	0
23	PL9	J	101	35/55	0.52	5.25	177,180,181,181	0
25	DGD	d	410	63/66	0.88	5.23	178,180,183,183	0
30	LMT	I	102	35/35	0.89	5.20	178,180,182,183	0
23	PL9	j	101	35/55	0.39	5.04	179,180,181,181	0
22	CLA	c	512	65/65	0.97	4.70	178,180,181,182	0
30	LMT	D	411	31/35	0.92	4.54	179,180,182,182	0
22	CLA	A	405	65/65	0.70	4.45	177,179,180,181	0
24	BCR	H	102	40/40	1.03	4.26	178,180,181,182	0
24	BCR	C	513	40/40	0.67	4.25	177,179,180,180	0
24	BCR	b	623	40/40	0.71	4.08	177,178,180,180	0
22	CLA	b	605	65/65	1.26	3.46	179,180,182,183	0
30	LMT	B	627	35/35	0.62	3.39	178,180,182,182	0
35	CA	o	301	1/1	0.67	3.27	184,184,184,184	0
22	CLA	c	511	65/65	0.91	3.24	178,180,181,182	0
27	LMG	I	101	43/55	0.74	3.21	178,180,181,182	0
24	BCR	B	619	40/40	0.67	3.07	178,179,180,180	0
24	BCR	C	514	40/40	0.93	3.05	178,179,180,181	0
24	BCR	g	101	40/40	0.89	3.00	178,179,180,180	0
27	LMG	c	518	45/55	1.11	3.00	178,180,181,181	0
25	DGD	b	601	52/66	0.59	2.90	178,180,181,182	0
22	CLA	B	601	65/65	0.99	2.78	177,180,181,182	0
24	BCR	J	102	40/40	0.40	2.78	178,180,181,181	0
24	BCR	c	514	40/40	1.00	2.76	177,179,180,180	0
24	BCR	K	102	40/40	1.06	2.72	178,180,181,182	0
24	BCR	A	407	40/40	0.57	2.61	177,179,180,180	0
30	LMT	b	603	35/35	0.57	2.55	178,179,181,182	0
24	BCR	a	409	40/40	0.66	2.52	177,178,180,180	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	CLA	D	406	65/65	0.51	2.51	177,179,180,181	0
35	CA	O	301	1/1	0.59	2.49	182,182,182,182	0
30	LMT	b	626	35/35	0.60	2.39	178,180,182,183	0
30	LMT	d	411	31/35	0.70	2.39	178,181,182,183	0
22	CLA	a	407	65/65	0.63	2.34	178,179,180,181	0
30	LMT	B	623	35/35	0.82	2.28	177,181,182,183	0
22	CLA	d	406	65/65	0.60	2.23	177,179,180,181	0
30	LMT	b	627	35/35	0.83	2.10	178,180,182,182	0
29	SQD	a	401	54/54	0.74	2.07	178,180,181,183	0
29	SQD	f	103	45/54	0.68	1.90	177,179,181,182	0
24	BCR	x	101	40/40	1.01	1.86	178,179,180,181	0
24	BCR	F	102	40/40	0.41	1.86	177,179,180,180	0
27	LMG	e	101	44/55	0.40	1.85	177,179,181,181	0
22	CLA	B	603	65/65	0.51	1.83	176,179,180,180	0
30	LMT	B	624	35/35	0.56	1.78	178,180,182,183	0
22	CLA	C	501	65/65	0.63	1.76	178,179,180,180	0
22	CLA	C	502	65/65	0.62	1.73	178,179,180,180	0
27	LMG	M	101	42/55	0.58	1.73	178,180,181,182	0
24	BCR	c	513	40/40	0.69	1.73	178,179,180,180	0
22	CLA	c	501	65/65	0.65	1.67	177,179,180,181	0
29	SQD	d	403	43/54	0.94	1.64	178,180,182,186	0
25	DGD	B	625	52/66	0.61	1.62	177,180,182,182	0
24	BCR	f	102	40/40	0.30	1.61	177,179,181,181	0
22	CLA	b	606	65/65	0.67	1.55	177,179,180,181	0
22	CLA	b	607	65/65	0.52	1.52	177,179,180,181	0
22	CLA	b	613	65/65	0.70	1.46	178,179,180,181	0
22	CLA	b	609	65/65	0.61	1.39	178,179,180,181	0
27	LMG	a	402	42/55	0.43	1.37	177,180,181,182	0
30	LMT	b	604	35/35	0.46	1.30	177,179,181,182	0
29	SQD	B	626	47/54	0.56	1.27	175,179,181,183	0
29	SQD	F	103	45/54	0.64	1.25	178,180,182,182	0
22	CLA	B	611	65/65	0.39	1.24	177,179,180,180	0
24	BCR	B	618	40/40	0.29	1.21	177,178,179,179	0
22	CLA	C	511	65/65	0.95	1.19	178,179,180,181	0
27	LMG	E	101	44/55	0.61	1.16	176,179,181,182	0
22	CLA	c	506	65/65	0.69	1.13	178,179,180,181	0
22	CLA	C	512	65/65	0.94	1.10	177,180,181,182	0
24	BCR	B	616	40/40	0.43	1.06	176,178,180,180	0
22	CLA	B	609	65/65	0.47	1.06	178,179,180,181	0
22	CLA	c	502	65/65	0.62	1.02	178,179,180,181	0
35	CA	k	101	1/1	0.29	1.00	180,180,180,180	0
24	BCR	B	617	40/40	0.44	1.00	177,179,180,180	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
27	LMG	A	414	42/55	0.48	0.99	177,179,182,182	0
22	CLA	B	614	65/65	0.69	0.97	177,179,180,181	0
22	CLA	C	510	65/65	0.54	0.94	177,179,180,181	0
22	CLA	C	503	65/65	0.49	0.93	177,179,180,180	0
22	CLA	B	604	65/65	0.57	0.91	177,179,180,180	0
22	CLA	b	608	65/65	0.49	0.86	178,179,180,181	0
22	CLA	c	510	65/65	0.50	0.86	178,179,181,181	0
22	CLA	b	618	65/65	0.88	0.85	177,179,180,180	0
25	DGD	A	408	56/66	0.44	0.83	178,179,181,182	0
29	SQD	B	622	43/54	0.55	0.82	177,180,182,185	0
22	CLA	b	615	65/65	0.38	0.79	177,179,180,180	0
34	HEM	V	201	43/43	0.43	0.78	176,178,180,180	0
22	CLA	B	608	65/65	0.51	0.77	177,179,180,180	0
22	CLA	c	505	65/65	0.64	0.75	177,179,180,181	0
22	CLA	c	508	65/65	0.48	0.72	177,179,180,181	0
22	CLA	C	508	65/65	0.68	0.71	177,179,180,180	0
22	CLA	b	611	65/65	0.45	0.71	177,179,180,180	0
22	CLA	c	503	65/65	0.52	0.69	177,179,180,181	0
34	HEM	v	201	43/43	0.54	0.67	177,179,180,180	0
22	CLA	B	615	65/65	0.66	0.63	176,179,180,181	0
22	CLA	h	101	65/65	0.45	0.60	176,179,180,181	0
29	SQD	A	413	54/54	0.35	0.60	178,180,182,184	0
22	CLA	C	506	65/65	0.58	0.59	177,179,180,180	0
22	CLA	B	605	65/65	0.66	0.56	178,179,180,180	0
25	DGD	b	624	58/66	0.38	0.53	177,178,180,180	0
24	BCR	b	621	40/40	0.38	0.52	178,178,179,179	0
24	BCR	j	102	40/40	0.33	0.49	179,180,182,183	0
22	CLA	b	612	65/65	0.56	0.47	176,179,181,181	0
25	DGD	a	410	56/66	0.37	0.47	178,180,181,182	0
29	SQD	b	602	47/54	0.44	0.44	176,179,182,185	0
23	PL9	A	406	45/55	0.44	0.43	177,179,180,180	0
22	CLA	b	619	65/65	0.69	0.39	177,179,180,181	0
24	BCR	b	620	40/40	0.37	0.39	177,179,179,180	0
23	PL9	a	408	45/55	0.30	0.39	176,179,180,180	0
30	LMT	B	628	35/35	0.45	0.38	177,180,182,183	0
27	LMG	m	101	42/55	0.45	0.38	175,179,181,181	0
27	LMG	a	412	51/55	0.34	0.33	177,179,180,180	0
22	CLA	C	504	65/65	0.37	0.33	177,179,180,180	0
22	CLA	B	602	65/65	0.49	0.33	176,178,180,180	0
22	CLA	a	404	65/65	0.68	0.32	177,178,180,180	0
34	HEM	f	101	43/43	0.35	0.25	178,180,180,181	0
22	CLA	C	509	65/65	0.39	0.23	177,179,180,180	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	CLA	H	101	65/65	0.36	0.23	177,179,180,181	0
22	CLA	B	607	65/65	0.36	0.22	178,179,180,181	0
22	CLA	a	405	65/65	0.67	0.21	174,178,179,180	0
27	LMG	d	412	46/55	0.26	0.17	177,178,180,180	0
24	BCR	b	622	40/40	0.37	0.16	176,178,179,179	0
27	LMG	C	521	48/55	0.31	0.15	177,179,180,181	0
22	CLA	B	613	65/65	0.46	0.10	177,179,180,180	0
23	PL9	d	407	55/55	0.50	0.08	177,179,180,181	0
22	CLA	b	617	65/65	0.43	0.06	178,179,180,182	0
31	PHO	d	401	64/64	0.49	-0.00	178,179,180,180	0
22	CLA	b	616	65/65	0.34	-0.01	177,179,180,180	0
22	CLA	C	505	65/65	0.38	-0.03	177,179,180,181	0
34	HEM	F	101	43/43	0.32	-0.05	178,180,181,182	0
22	CLA	c	509	65/65	0.32	-0.08	177,179,180,180	0
22	CLA	c	504	65/65	0.30	-0.09	177,179,180,180	0
22	CLA	C	507	65/65	0.37	-0.12	178,179,180,181	0
27	LMG	c	522	48/55	0.30	-0.14	178,180,180,181	0
22	CLA	b	614	65/65	0.30	-0.15	178,179,180,180	0
26	LHG	c	519	37/49	0.34	-0.17	178,180,183,187	0
23	PL9	D	407	55/55	0.35	-0.18	177,178,179,180	0
26	LHG	A	409	39/49	0.35	-0.22	178,179,181,181	0
22	CLA	A	402	65/65	0.45	-0.24	178,179,180,181	0
22	CLA	d	405	65/65	0.49	-0.24	177,178,179,180	0
27	LMG	D	409	48/55	0.27	-0.24	175,178,180,181	0
27	LMG	d	409	48/55	0.29	-0.30	177,179,180,180	0
22	CLA	B	610	65/65	0.37	-0.31	177,179,180,180	0
29	SQD	a	415	51/54	0.26	-0.31	178,179,181,182	0
25	DGD	B	620	58/66	0.28	-0.35	176,179,181,182	0
25	DGD	c	515	53/66	0.33	-0.39	176,179,181,182	0
31	PHO	D	401	64/64	0.34	-0.41	177,179,180,180	0
27	LMG	A	410	51/55	0.28	-0.48	177,178,180,181	0
30	LMT	M	103	35/35	0.47	-0.50	177,179,180,180	0
22	CLA	B	612	65/65	0.31	-0.54	176,178,180,181	0
28	OEX	A	411	10/10	0.43	-0.58	172,175,178,178	0
22	CLA	D	405	65/65	0.38	-0.60	177,179,180,180	0
25	DGD	c	517	66/66	0.34	-0.61	177,179,181,181	0
22	CLA	a	406	65/65	0.30	-0.62	177,179,180,181	0
25	DGD	C	515	53/66	0.30	-0.65	177,178,179,180	0
22	CLA	c	520	65/65	0.26	-0.67	177,179,180,181	0
22	CLA	A	403	65/65	0.39	-0.67	177,179,179,180	0
29	SQD	A	412	51/54	0.25	-0.70	178,179,180,181	0
27	LMG	D	408	49/55	0.29	-0.71	177,178,180,180	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	PHO	d	402	64/64	0.24	-0.72	178,179,180,181	0
22	CLA	c	507	65/65	0.26	-0.74	177,179,180,181	0
26	LHG	C	519	37/49	0.34	-0.74	176,180,184,188	0
31	PHO	D	402	64/64	0.30	-0.77	177,179,180,181	0
22	CLA	B	606	65/65	0.28	-0.79	177,179,180,180	0
26	LHG	a	411	39/49	0.28	-0.84	177,179,180,181	0
27	LMG	D	412	46/55	0.25	-0.95	178,179,180,181	0
22	CLA	C	520	65/65	0.31	-0.98	178,179,180,181	0
25	DGD	c	516	62/66	0.26	-1.02	178,179,180,181	0
27	LMG	d	408	49/55	0.20	-1.02	178,179,180,180	0
22	CLA	A	404	65/65	0.28	-1.06	176,178,180,181	0
22	CLA	b	610	65/65	0.25	-1.06	177,179,180,180	0
25	DGD	C	517	66/66	0.26	-1.19	177,179,180,181	0
25	DGD	C	516	62/66	0.26	-1.20	177,179,180,181	0
33	BCT	D	404	4/4	0.20	-1.27	178,179,179,179	0
27	LMG	B	621	49/55	0.23	-1.33	177,179,180,180	0
28	OEX	a	414	10/10	0.42	-1.43	174,177,179,182	0
27	LMG	b	625	49/55	0.24	-1.46	178,179,180,180	0
30	LMT	M	102	35/35	0.31	-1.50	178,179,181,182	0
33	BCT	d	404	4/4	0.13	-1.52	178,180,180,180	0
21	FE2	a	403	1/1	0.06	-1.85	182,182,182,182	0
32	CL	a	413	1/1	0.24	-1.94	177,177,177,177	0
21	FE2	A	401	1/1	0.18	-3.53	176,176,176,176	0
32	CL	D	403	1/1	0.16	-3.53	180,180,180,180	0

6.5 Other polymers ⓘ

There are no such residues in this entry.