



# wwPDB X-ray Structure Validation Summary Report i

Jul 18, 2014 – 01:58 AM EDT

PDB ID : 4TNK  
Title : RT XFEL structure of Photosystem II 250 microsec after the third illumination at 5.2 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 : 5.20 Å (reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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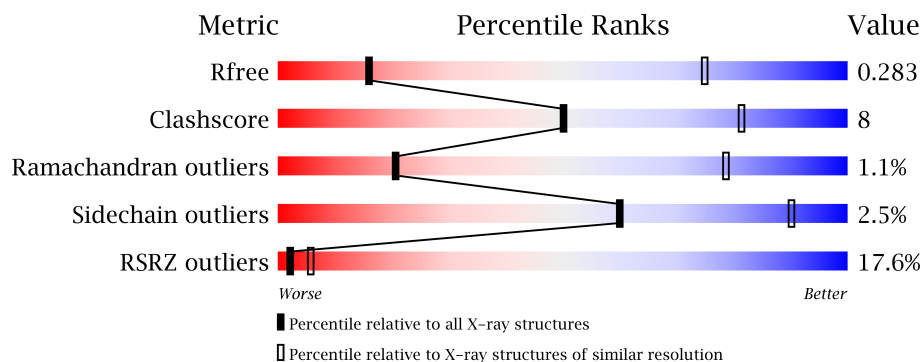
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 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 5.20 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))
$R_{free}$	66092	1060 (6.80-3.50)
Clashscore	79885	1336 (6.80-3.50)
Ramachandran outliers	78287	1250 (6.80-3.50)
Sidechain outliers	78261	1228 (6.80-3.50)
RSRZ outliers	66119	1059 (6.80-3.50)

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  $\geq 3$ , 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	406	-	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	609	-	X
22	CLA	B	614	-	X
22	CLA	B	615	-	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	a	403	-	X
22	CLA	a	404	-	X
22	CLA	a	406	-	X
22	CLA	b	605	-	X
22	CLA	b	607	-	X
22	CLA	b	613	-	X
22	CLA	b	614	-	X
22	CLA	b	619	-	X
22	CLA	b	620	-	X
22	CLA	c	501	-	X
22	CLA	c	502	-	X
22	CLA	c	505	-	X
22	CLA	c	506	-	X
22	CLA	c	510	-	X
22	CLA	c	511	-	X
22	CLA	c	512	-	X
24	PL9	j	101	-	X
25	BCR	B	619	-	X
25	BCR	C	513	-	X
25	BCR	C	520	-	X
25	BCR	H	102	-	X
25	BCR	K	101	-	X
25	BCR	b	624	-	X
25	BCR	c	513	-	X
25	BCR	c	514	-	X
25	BCR	c	521	-	X
25	BCR	f	102	-	X
25	BCR	g	101	-	X
25	BCR	i	101	-	X
25	BCR	x	101	-	X
25	BCR	y	101	-	X
26	DGD	B	626	-	X
26	DGD	D	407	-	X
26	DGD	b	601	-	X
26	DGD	d	410	-	X
30	SQD	B	622	-	X
30	SQD	B	627	-	X
30	SQD	F	103	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
30	SQD	a	401	-	X
30	SQD	d	403	-	X
30	SQD	f	103	-	X
31	LMG	C	517	-	X
31	LMG	I	101	-	X
31	LMG	b	627	-	X
31	LMG	c	518	-	X
31	LMG	i	102	-	X
31	LMG	m	101	-	X
32	LMT	B	623	-	X
32	LMT	B	628	-	X
32	LMT	D	408	-	X
32	LMT	I	102	-	X
32	LMT	b	628	-	X
32	LMT	b	629	-	X
32	LMT	d	411	-	X
32	LMT	i	103	-	X
34	HEM	v	201	-	X
35	CA	K	102	-	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				

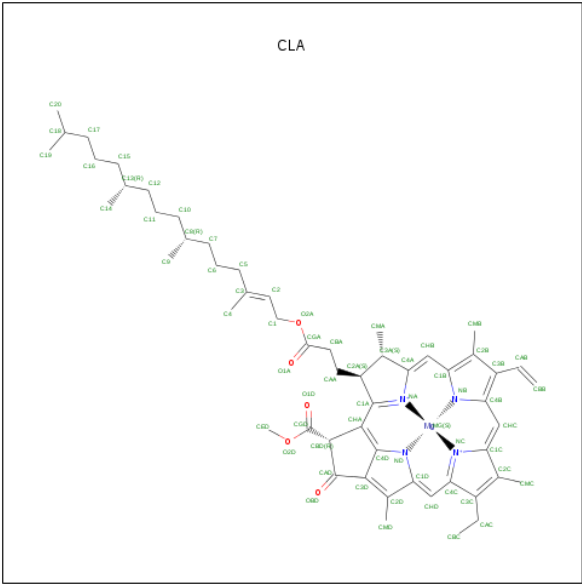
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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



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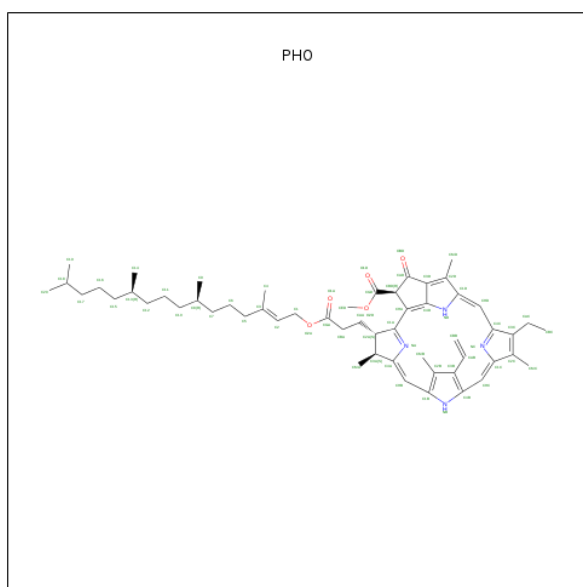
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N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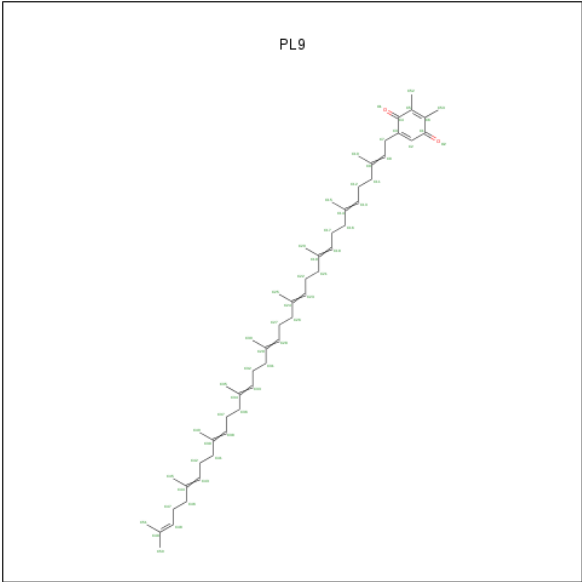
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N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

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



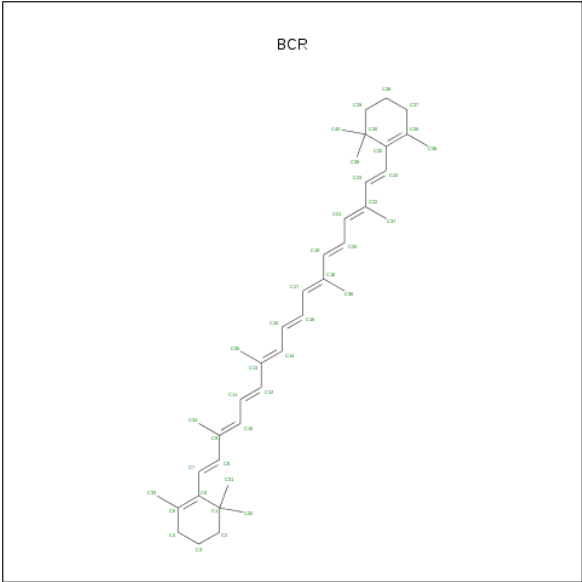
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	D	1	Total	C	N	O	0	0
			64	55	4	5		
23	d	1	Total	C	N	O	0	0
			64	55	4	5		
23	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 24 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
24	A	1	Total	C	O	0	0
			45	43	2		
24	D	1	Total	C	O	0	0
			55	53	2		
24	J	1	Total	C	O	0	0
			35	33	2		
24	a	1	Total	C	O	0	0
			45	43	2		
24	d	1	Total	C	O	0	0
			55	53	2		
24	j	1	Total	C	O	0	0
			35	33	2		

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



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

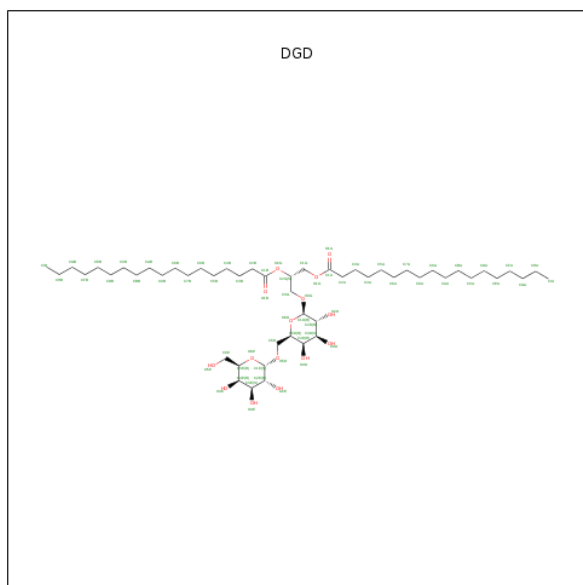
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	f	1	Total C 40 40	0	0
25	i	1	Total C 40 40	0	0
25	j	1	Total C 40 40	0	0
25	g	1	Total C 40 40	0	0
25	x	1	Total C 40 40	0	0

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



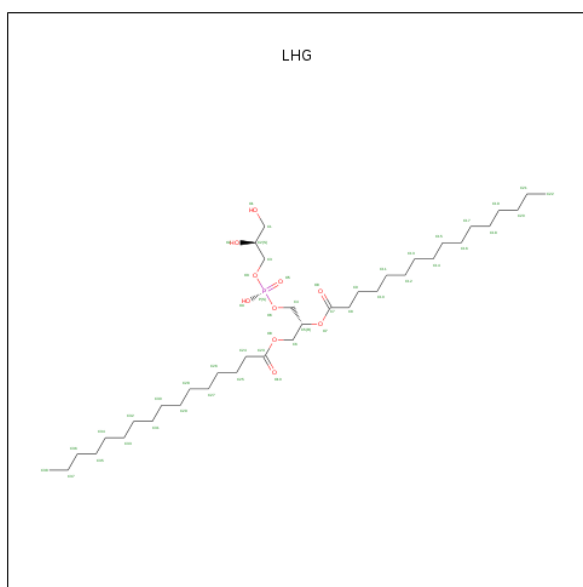
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O 56 41 15	0	0

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

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).

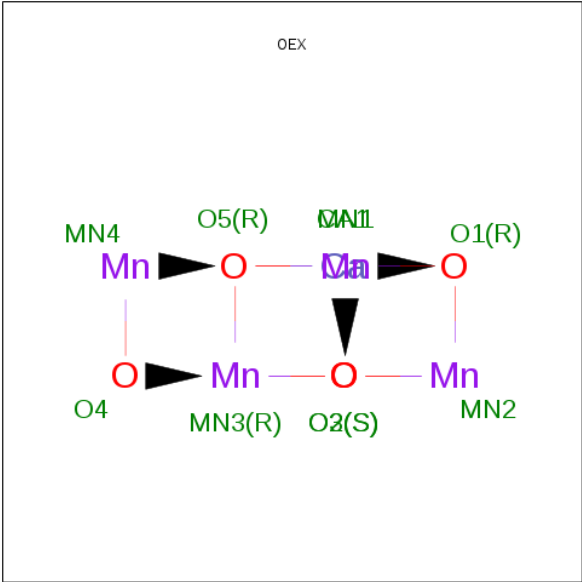


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	P	0	0
			39	28	10	1		
27	C	1	Total	C	O	P	0	0
			37	26	10	1		
27	a	1	Total	C	O	P	0	0
			39	28	10	1		
27	c	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 28 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

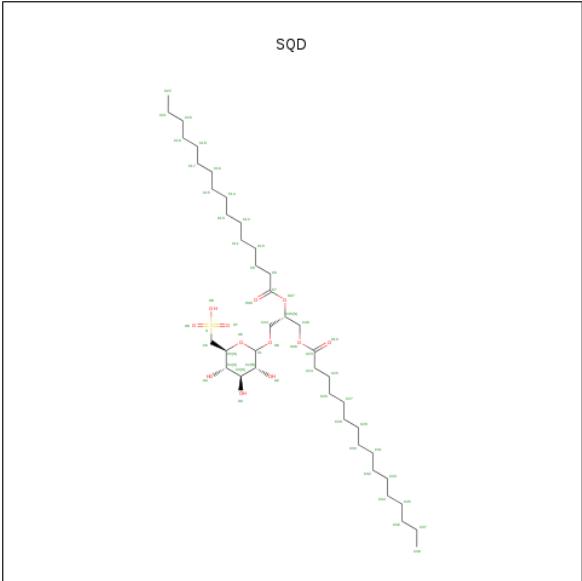
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	1	Total	Cl	0	0
			1	1		
28	a	1	Total	Cl	0	0
			1	1		

- Molecule 29 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



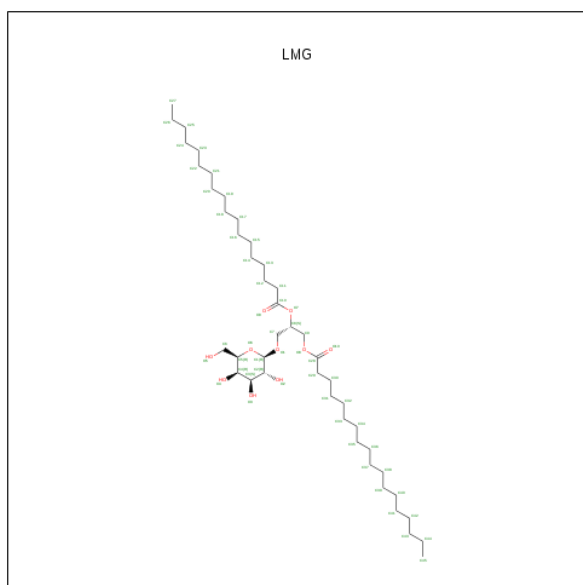
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			51	38	12	1		

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

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



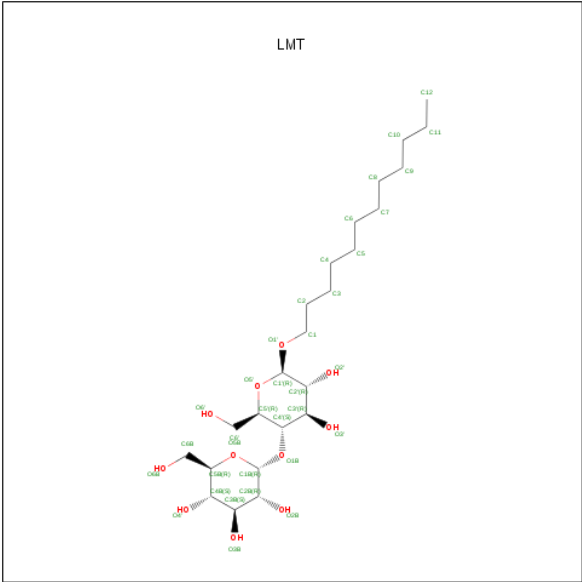
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			49	39	10		
31	B	1	Total	C	O	0	0
			49	39	10		

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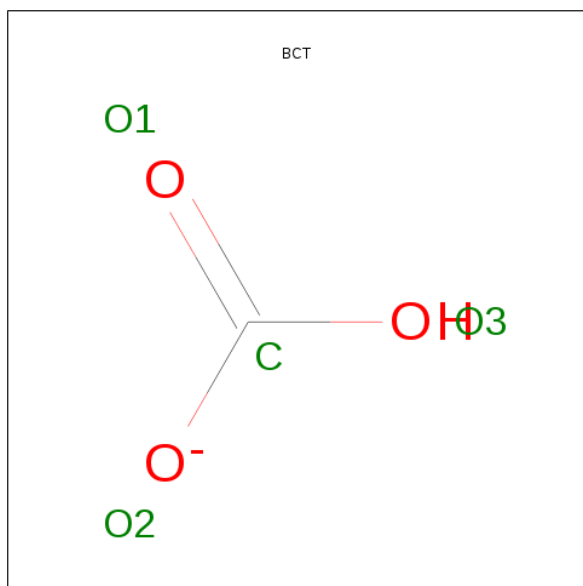
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	C	1	Total	C	O	0	0
			45	35	10		
31	C	1	Total	C	O	0	0
			48	38	10		
31	D	1	Total	C	O	0	0
			48	38	10		
31	D	1	Total	C	O	0	0
			46	36	10		
31	E	1	Total	C	O	0	0
			44	34	10		
31	I	1	Total	C	O	0	0
			43	33	10		
31	L	1	Total	C	O	0	0
			51	41	10		
31	M	1	Total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

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



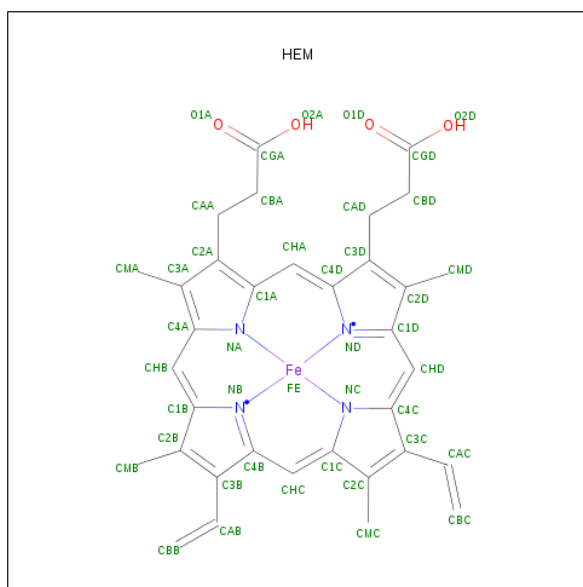
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	D	1	Total	C	O	0	0
			31	20	11		
32	I	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total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

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



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:  $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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
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

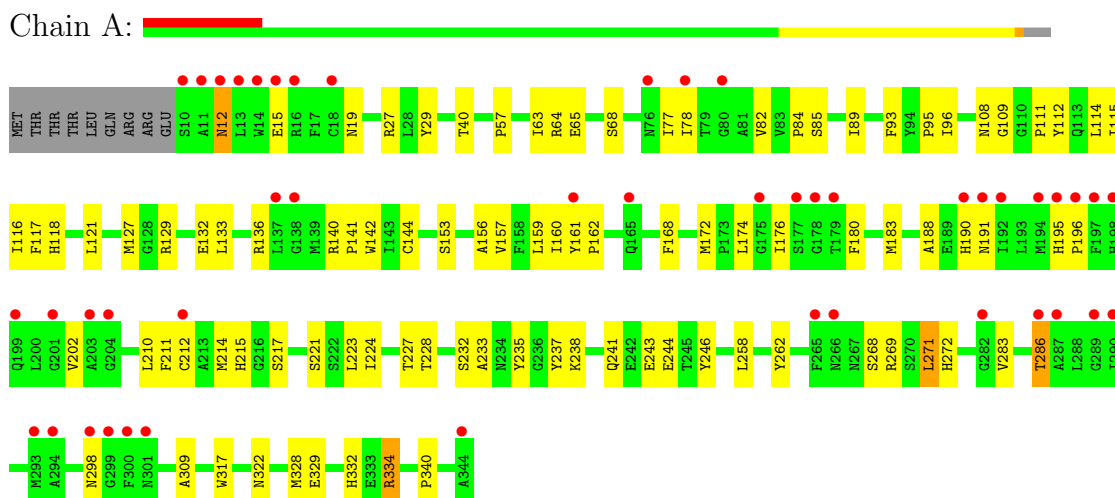
- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

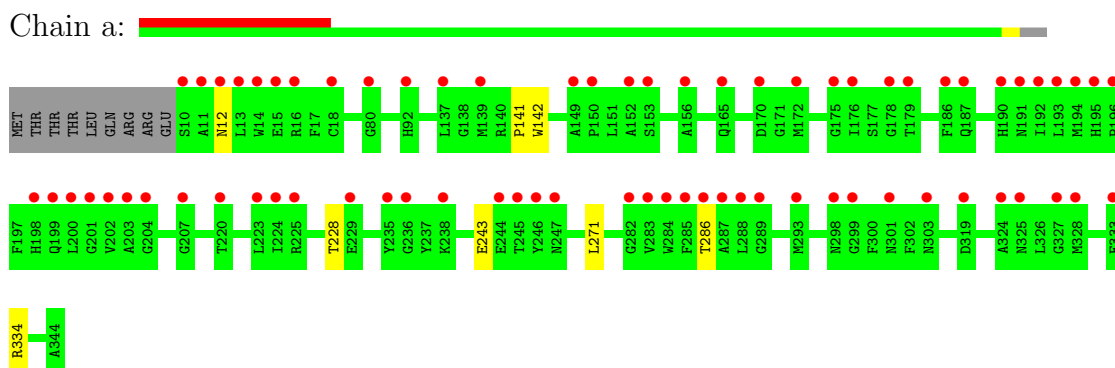
### 3 Residue-property plots

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.

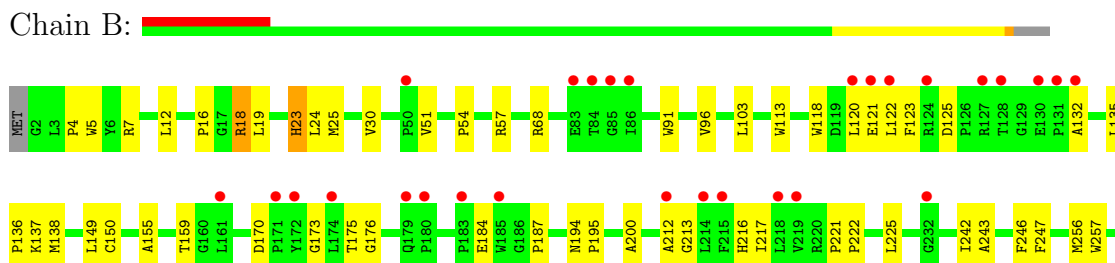
- Molecule 1: Photosystem Q(B) protein 1

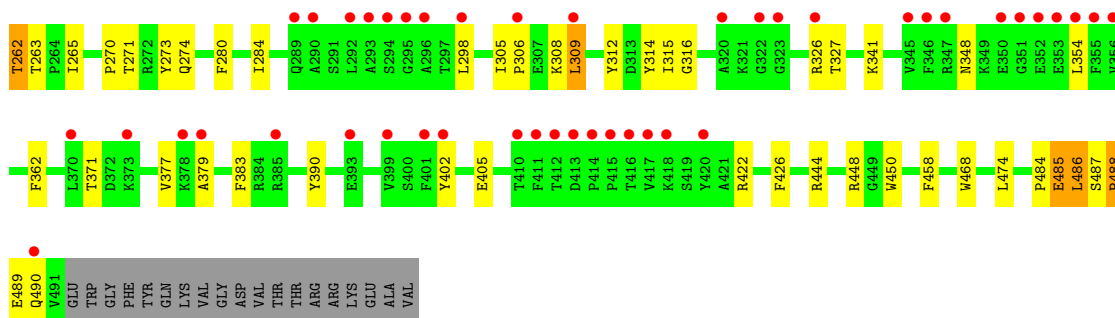


- Molecule 1: Photosystem Q(B) protein 1



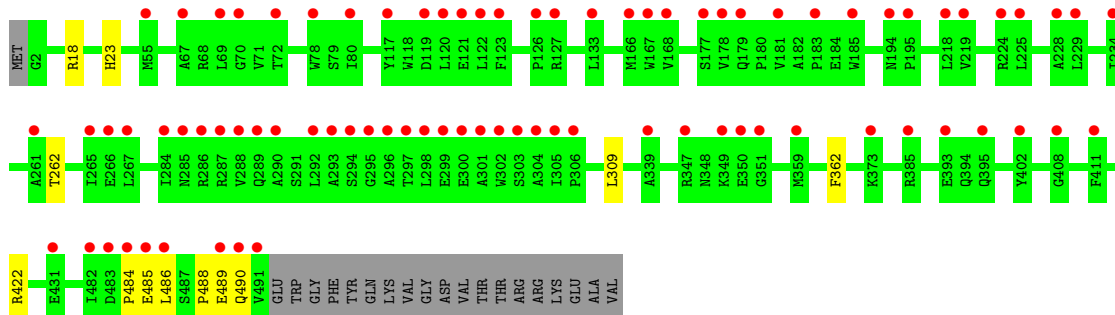
- Molecule 2: Photosystem II core light harvesting protein





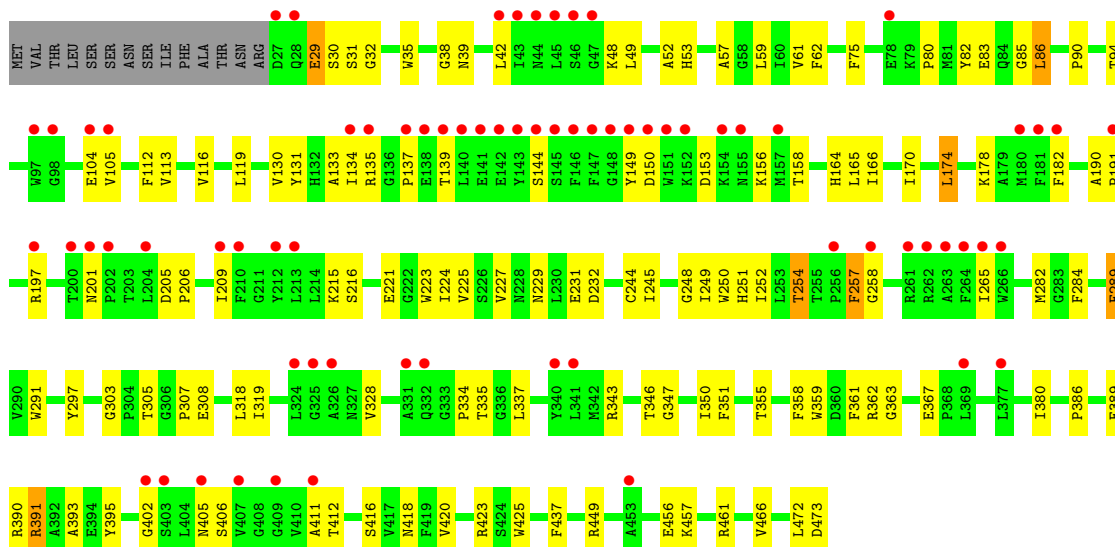
• Molecule 2: Photosystem II core light harvesting protein

Chain b:



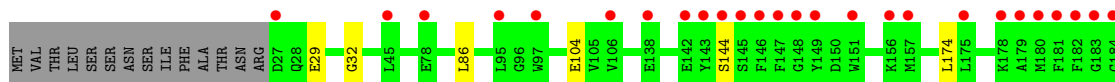
• Molecule 3: Photosystem II CP43 protein

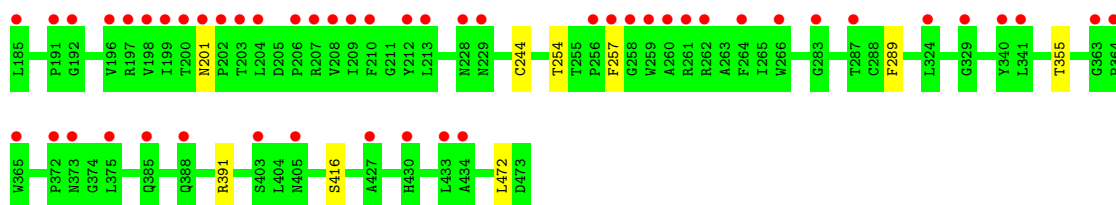
Chain C:



• Molecule 3: Photosystem II CP43 protein

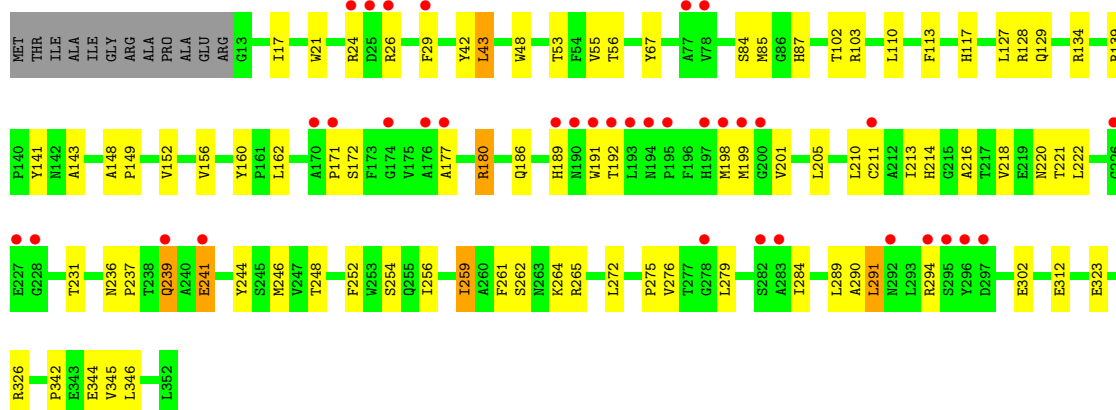
Chain c:





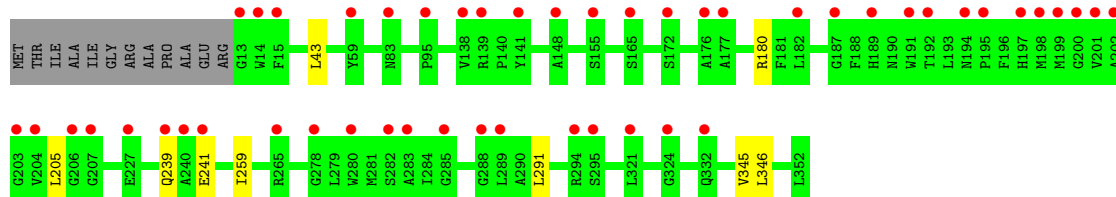
• Molecule 4: Photosystem II D2 protein

Chain D:



• Molecule 4: Photosystem II D2 protein

Chain d:



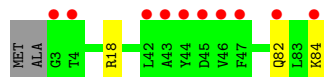
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



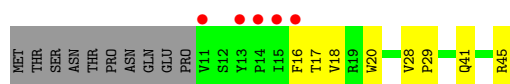
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



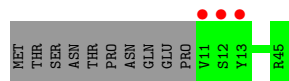
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



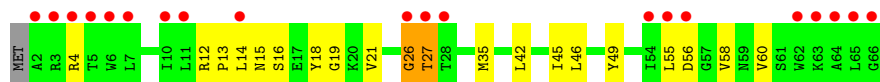
- Molecule 6: Cytochrome b559 subunit beta

Chain f:



- Molecule 7: Photosystem II reaction center protein H

Chain H:



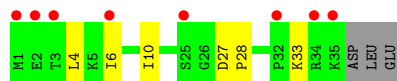
- Molecule 7: Photosystem II reaction center protein H

Chain h:



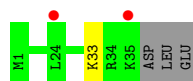
- Molecule 8: Photosystem II reaction center protein I

Chain I:



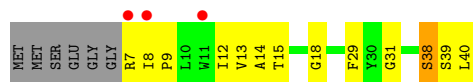
- Molecule 8: Photosystem II reaction center protein I

Chain i:



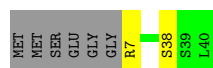
- Molecule 9: Photosystem II reaction center protein J

Chain J:



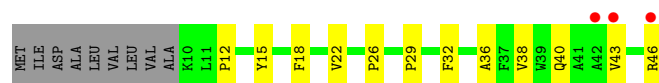
- Molecule 9: Photosystem II reaction center protein J

Chain j:



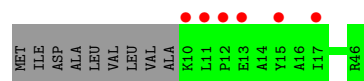
- Molecule 10: Photosystem II reaction center protein K

Chain K:



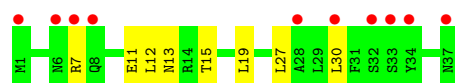
- Molecule 10: Photosystem II reaction center protein K

Chain k:



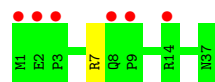
- Molecule 11: Photosystem II reaction center protein L

Chain L:



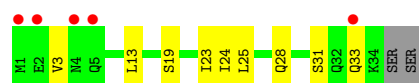
- Molecule 11: Photosystem II reaction center protein L

Chain l:



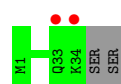
- Molecule 12: Photosystem II reaction center protein M

Chain M:



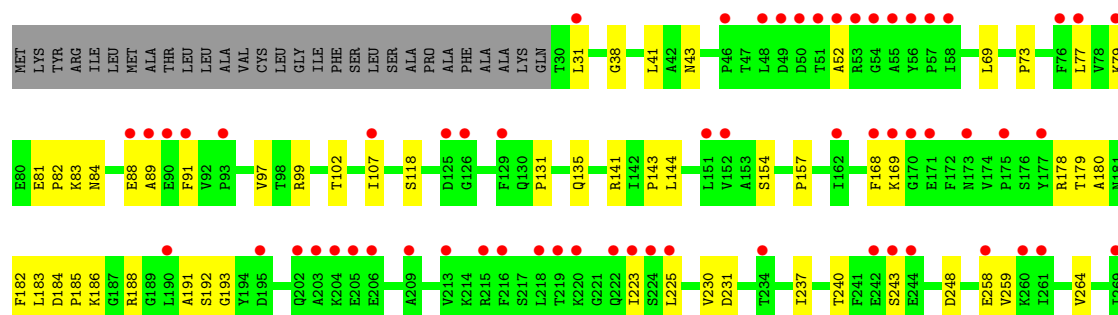
- Molecule 12: Photosystem II reaction center protein M

Chain m:



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

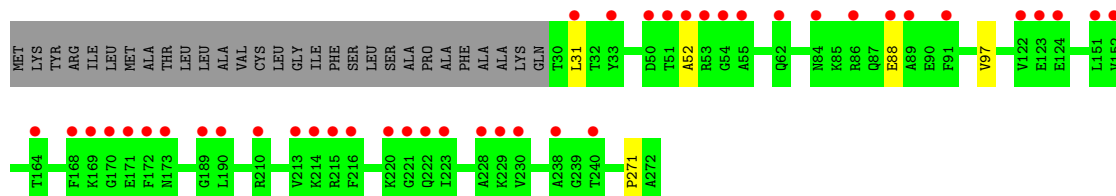
Chain O:





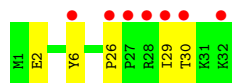
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



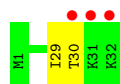
- Molecule 14: Photosystem II reaction center protein T

Chain T:



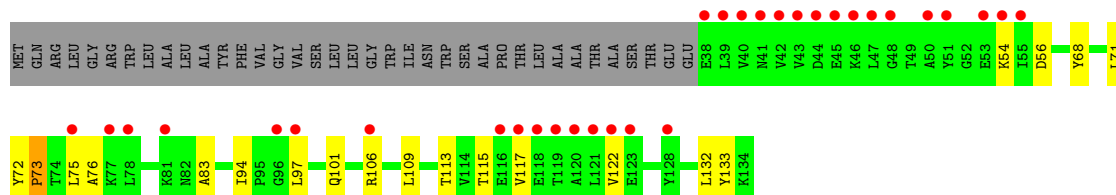
- Molecule 14: Photosystem II reaction center protein T

Chain t:



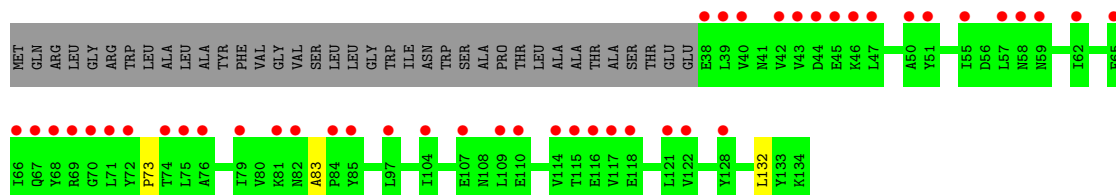
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



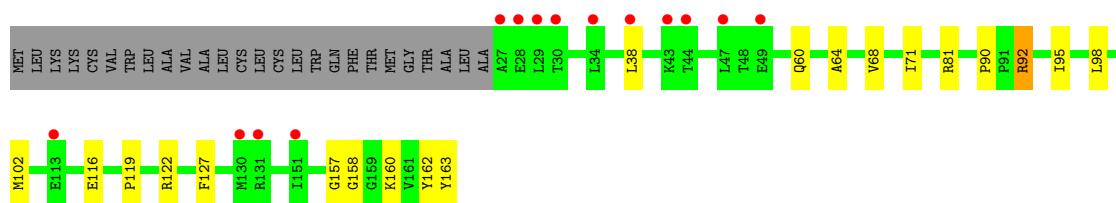
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



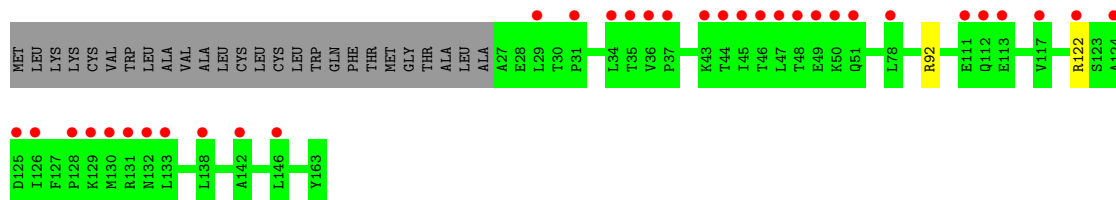
- Molecule 16: Cytochrome c-550

Chain V:



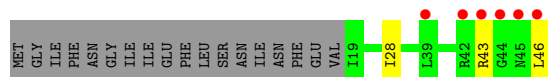
- Molecule 16: Cytochrome c-550

Chain v:



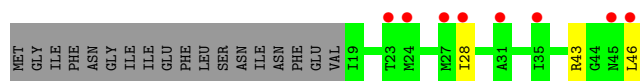
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain g:



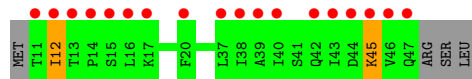
- Molecule 18: Photosystem II reaction center X protein

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

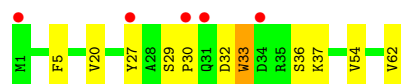
Chain G:



There are no outlier residues recorded for this chain.

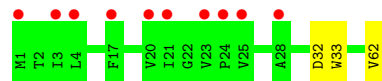
- Molecule 20: Photosystem II reaction center protein Z

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, $\alpha$ , $\beta$ , $\gamma$	132.62Å 229.30Å 306.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.41 – 5.20 68.41 – 5.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (68.41-5.20) 97.9 (68.41-5.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 5.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, $R_{free}$	0.271 , 0.289 0.267 , 0.283	Depositor DCC
$R_{free}$ test set	1751 reflections (4.87%)	DCC
Wilson B-factor (Å <sup>2</sup> )	176.5	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 152.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.33$ , $\langle L^2 \rangle = 0.15$	Xtriage
Outliers	0 of 35970 reflections	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	50244	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	207.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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, 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	0.25	0/2713	0.42	0/3700
1	a	0.24	0/2713	0.42	0/3700
2	B	0.24	0/3986	0.41	0/5433
2	b	0.24	0/3986	0.41	0/5433
3	C	0.23	0/3556	0.42	0/4842
3	c	0.23	0/3556	0.42	0/4842
4	D	0.24	0/2801	0.41	0/3818
4	d	0.24	0/2801	0.41	0/3818
5	E	0.23	0/685	0.44	0/933
5	e	0.23	0/685	0.43	0/933
6	F	0.23	0/291	0.40	0/397
6	f	0.23	0/291	0.41	0/397
7	H	0.24	0/520	0.46	0/709
7	h	0.23	0/520	0.46	0/709
8	I	0.25	0/293	0.44	0/395
8	i	0.26	0/293	0.44	0/395
9	J	0.21	0/255	0.41	0/346
9	j	0.22	0/255	0.40	0/346
10	K	0.27	0/303	0.49	0/416
10	k	0.27	0/303	0.49	0/416
11	L	0.23	0/311	0.40	0/422
11	l	0.22	0/311	0.40	0/422
12	M	0.24	0/270	0.44	0/367
12	m	0.24	0/270	0.44	0/367
13	O	0.23	0/1876	0.44	0/2548
13	o	0.23	0/1876	0.44	0/2548
14	T	0.25	0/284	0.41	0/381
14	t	0.25	0/284	0.40	0/381
15	U	0.23	0/785	0.43	0/1064
15	u	0.23	0/785	0.44	0/1064
16	V	0.22	0/1081	0.42	0/1468
16	v	0.22	0/1081	0.41	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	g	0.22	0/202	0.46	0/272
17	y	0.23	0/202	0.46	0/272
18	X	0.27	0/273	0.44	0/370
18	x	0.26	0/273	0.45	0/370
20	Z	0.25	0/490	0.45	0/669
20	z	0.24	0/490	0.45	0/669
All	All	0.24	0/41950	0.42	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	82	0
1	a	2628	0	2524	0	0
2	B	3850	0	3718	90	0
2	b	3850	0	3718	0	0
3	C	3444	0	3365	100	0
3	c	3444	0	3365	0	0
4	D	2706	0	2608	83	0
4	d	2706	0	2608	0	0
5	E	666	0	651	16	0
5	e	666	0	651	0	0
6	F	282	0	291	8	0
6	f	282	0	291	0	0
7	H	507	0	521	22	0
7	h	507	0	521	0	0
8	I	286	0	308	4	0
8	i	286	0	308	0	0
9	J	249	0	262	10	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	10	0
10	k	293	0	305	0	0
11	L	304	0	316	9	0
11	l	304	0	316	0	0
12	M	267	0	289	8	0
12	m	267	0	289	0	0
13	O	1845	0	1801	34	0
13	o	1845	0	1801	0	0
14	T	275	0	288	3	0
14	t	275	0	288	0	0
15	U	774	0	773	10	0
15	u	774	0	773	0	0
16	V	1060	0	1068	12	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	9	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	42	0
22	B	975	0	1080	103	0
22	C	845	0	936	45	0
22	D	130	0	144	13	0
22	H	65	0	72	11	0
22	a	260	0	288	0	0
22	b	1040	0	1152	0	0
22	c	845	0	936	0	0
22	d	130	0	144	0	0
23	A	64	0	74	6	0
23	D	64	0	74	12	0
23	d	128	0	148	0	0
24	A	45	0	61	6	0
24	D	55	0	80	10	0
24	J	35	0	45	0	0
24	a	45	0	61	0	0
24	d	55	0	80	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	j	35	0	45	0	0
25	A	40	0	56	3	0
25	B	160	0	224	13	0
25	C	80	0	112	15	0
25	F	40	0	56	3	0
25	H	40	0	56	2	0
25	J	40	0	56	3	0
25	K	40	0	56	3	0
25	b	160	0	224	0	0
25	c	120	0	168	0	0
25	f	40	0	56	0	0
25	g	40	0	56	0	0
25	i	40	0	56	0	0
25	j	40	0	56	0	0
25	x	40	0	56	0	0
25	y	40	0	56	0	0
26	A	56	0	70	1	0
26	B	110	0	136	4	0
26	C	181	0	245	18	0
26	D	63	0	87	2	0
26	a	56	0	70	0	0
26	b	110	0	136	0	0
26	c	181	0	245	0	0
26	d	63	0	87	0	0
27	A	39	0	51	2	0
27	C	37	0	44	3	0
27	a	39	0	51	0	0
27	c	37	0	44	0	0
28	A	1	0	0	0	0
28	a	1	0	0	0	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	105	0	147	6	0
30	B	90	0	111	3	0
30	F	45	0	54	3	0
30	a	105	0	147	0	0
30	b	47	0	61	0	0
30	d	43	0	50	0	0
30	f	45	0	54	0	0
31	B	98	0	136	6	0
31	C	93	0	126	3	0
31	D	94	0	128	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	E	44	0	58	2	0
31	I	43	0	56	1	0
31	L	51	0	72	2	0
31	M	42	0	54	3	0
31	a	42	0	54	0	0
31	b	91	0	122	0	0
31	c	93	0	126	0	0
31	d	143	0	196	0	0
31	e	44	0	58	0	0
31	i	43	0	56	0	0
31	l	51	0	72	0	0
31	m	42	0	54	0	0
32	B	140	0	184	5	0
32	D	31	0	35	0	0
32	I	35	0	46	1	0
32	M	70	0	92	0	0
32	b	140	0	184	0	0
32	d	31	0	35	0	0
32	i	35	0	46	0	0
33	D	4	0	1	0	0
33	d	4	0	1	0	0
34	F	43	0	30	5	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	51374	639	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 8.

The worst 5 of 639 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	0.83
12:M:33:GLN:HB3	12:M:33:GLN:HB3	0.00	0.82
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.62	0.82
3:C:362:ARG:H	26:C:514:DGD:HE4	1.47	0.78

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%)	311 (93%)	18 (5%)	4 (1%)	19	77
2	B	488/510 (96%)	451 (92%)	33 (7%)	4 (1%)	27	83
2	b	488/510 (96%)	449 (92%)	36 (7%)	3 (1%)	33	86
3	C	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	25	81
3	c	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	25	81
4	D	338/352 (96%)	316 (94%)	21 (6%)	1 (0%)	50	91
4	d	338/352 (96%)	316 (94%)	21 (6%)	1 (0%)	50	91
5	E	80/84 (95%)	76 (95%)	3 (4%)	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%)	27 (82%)	6 (18%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	O	241/272 (89%)	207 (86%)	31 (13%)	3 (1%)	19	77
13	o	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	19	77
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	6	55
14	t	30/32 (94%)	26 (87%)	3 (10%)	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%)	19 (73%)	6 (23%)	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%)	4677 (91%)	406 (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
13	O	52	ALA

### 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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	390/407 (96%)	381 (98%)	9 (2%)	63	91
3	C	347/362 (96%)	336 (97%)	11 (3%)	51	87
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%)	267 (97%)	8 (3%)	55	88
5	E	72/73 (99%)	70 (97%)	2 (3%)	56	88
5	e	72/73 (99%)	70 (97%)	2 (3%)	56	88
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	50
17	y	20/37 (54%)	18 (90%)	2 (10%)	11	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	X	30/34 (88%)	28 (93%)	2 (7%)	23	70
18	x	30/34 (88%)	28 (93%)	2 (7%)	23	70
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%)	4140 (98%)	104 (2%)	60	90

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	X	12	ILE
2	b	309	LEU
16	v	92	ARG
18	X	45	LYS
1	a	243	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	117	HIS
4	d	117	HIS
4	D	332	GLN
1	A	266	ASN
1	a	241	GLN

### 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	1.64	10 (13%)	96,113,113	1.19	11 (11%)
22	CLA	A	403	-	73,73,73	1.61	11 (15%)	96,113,113	1.22	11 (11%)
22	CLA	A	404	-	73,73,73	1.59	10 (13%)	96,113,113	1.24	13 (13%)
23	PHO	A	405	-	69,69,69	1.24	11 (15%)	92,99,99	1.16	8 (8%)
22	CLA	A	406	-	73,73,73	1.59	10 (13%)	96,113,113	1.23	12 (12%)
24	PL9	A	407	-	45,45,55	1.09	3 (6%)	55,57,69	1.71	12 (21%)
25	BCR	A	408	-	41,41,41	1.06	2 (4%)	56,56,56	1.22	7 (12%)
26	DGD	A	409	-	57,57,67	2.23	2 (3%)	71,71,81	1.58	9 (12%)
27	LHG	A	410	-	38,38,48	2.38	2 (5%)	44,44,54	1.43	6 (13%)
29	OEX	A	412	1,3	8,15,15	10.59	8 (100%)	0,32,32	0.00	-
30	SQD	A	413	-	51,51,54	1.53	4 (7%)	62,62,65	2.01	11 (17%)
30	SQD	A	414	-	54,54,54	0.92	3 (5%)	65,65,65	1.74	12 (18%)
22	CLA	B	601	-	73,73,73	1.62	10 (13%)	96,113,113	1.24	11 (11%)
22	CLA	B	602	-	73,73,73	1.58	10 (13%)	96,113,113	1.26	14 (14%)
22	CLA	B	603	-	73,73,73	1.61	10 (13%)	96,113,113	1.30	14 (14%)
22	CLA	B	604	-	73,73,73	1.60	10 (13%)	96,113,113	1.27	13 (13%)
22	CLA	B	605	-	73,73,73	1.57	10 (13%)	96,113,113	1.27	13 (13%)
22	CLA	B	606	-	73,73,73	1.58	10 (13%)	96,113,113	1.23	13 (13%)
22	CLA	B	607	-	73,73,73	1.59	10 (13%)	96,113,113	1.25	14 (14%)
22	CLA	B	608	-	73,73,73	1.63	10 (13%)	96,113,113	1.23	13 (13%)
22	CLA	B	609	-	73,73,73	1.57	10 (13%)	96,113,113	1.26	12 (12%)
22	CLA	B	610	-	73,73,73	1.57	11 (15%)	96,113,113	1.45	14 (14%)
22	CLA	B	611	-	73,73,73	1.59	10 (13%)	96,113,113	1.26	14 (14%)
22	CLA	B	612	-	73,73,73	1.58	10 (13%)	96,113,113	1.30	14 (14%)
22	CLA	B	613	-	73,73,73	1.60	10 (13%)	96,113,113	1.27	13 (13%)
22	CLA	B	614	-	73,73,73	1.62	10 (13%)	96,113,113	1.24	13 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	615	-	73,73,73	1.61	11 (15%)	96,113,113	1.23	12 (12%)
25	BCR	B	616	-	41,41,41	1.09	2 (4%)	56,56,56	1.22	7 (12%)
25	BCR	B	617	-	41,41,41	1.02	2 (4%)	56,56,56	1.33	7 (12%)
25	BCR	B	618	-	41,41,41	1.08	2 (4%)	56,56,56	1.36	9 (16%)
25	BCR	B	619	-	41,41,41	1.06	2 (4%)	56,56,56	1.25	8 (14%)
26	DGD	B	620	-	59,59,67	2.24	2 (3%)	73,73,81	1.45	7 (9%)
31	LMG	B	621	-	49,49,55	2.34	4 (8%)	57,57,63	1.40	9 (15%)
30	SQD	B	622	-	43,43,54	1.25	4 (9%)	54,54,65	2.03	11 (20%)
32	LMT	B	623	-	36,36,36	1.09	4 (11%)	47,47,47	1.03	2 (4%)
32	LMT	B	624	-	36,36,36	1.06	3 (8%)	47,47,47	1.03	2 (4%)
31	LMG	B	625	-	49,49,55	2.52	2 (4%)	57,57,63	1.43	8 (14%)
26	DGD	B	626	-	53,53,67	2.29	6 (11%)	67,67,81	1.46	10 (14%)
30	SQD	B	627	-	47,47,54	1.08	4 (8%)	58,58,65	2.03	11 (18%)
32	LMT	B	628	-	36,36,36	1.08	5 (13%)	47,47,47	1.03	2 (4%)
32	LMT	B	629	-	36,36,36	1.10	4 (11%)	47,47,47	1.05	1 (2%)
22	CLA	C	501	-	73,73,73	1.61	11 (15%)	96,113,113	1.20	12 (12%)
22	CLA	C	502	-	73,73,73	1.60	11 (15%)	96,113,113	1.25	11 (11%)
22	CLA	C	503	-	73,73,73	1.60	10 (13%)	96,113,113	1.26	13 (13%)
22	CLA	C	504	-	73,73,73	1.58	11 (15%)	96,113,113	1.27	15 (15%)
22	CLA	C	505	-	73,73,73	1.59	10 (13%)	96,113,113	1.28	15 (15%)
22	CLA	C	506	-	73,73,73	1.59	10 (13%)	96,113,113	1.27	13 (13%)
22	CLA	C	507	-	73,73,73	1.61	10 (13%)	96,113,113	1.30	13 (13%)
22	CLA	C	508	-	73,73,73	1.60	10 (13%)	96,113,113	1.24	11 (11%)
22	CLA	C	509	-	73,73,73	1.60	10 (13%)	96,113,113	1.22	11 (11%)
22	CLA	C	510	3	73,73,73	1.60	10 (13%)	96,113,113	1.29	13 (13%)
22	CLA	C	511	-	73,73,73	1.62	10 (13%)	96,113,113	1.27	14 (14%)
22	CLA	C	512	-	73,73,73	1.60	10 (13%)	96,113,113	1.26	13 (13%)
25	BCR	C	513	-	41,41,41	1.07	2 (4%)	56,56,56	1.27	8 (14%)
26	DGD	C	514	-	54,54,67	2.40	4 (7%)	68,68,81	1.34	10 (14%)
26	DGD	C	515	-	63,63,67	1.49	2 (3%)	77,77,81	1.44	12 (15%)
26	DGD	C	516	-	67,67,67	0.86	2 (2%)	81,81,81	1.44	12 (14%)
31	LMG	C	517	-	45,45,55	2.64	2 (4%)	53,53,63	1.45	8 (15%)
27	LHG	C	518	-	36,36,48	2.39	2 (5%)	42,42,54	1.53	7 (16%)
22	CLA	C	519	-	73,73,73	1.59	10 (13%)	96,113,113	1.22	12 (12%)
25	BCR	C	520	-	41,41,41	1.04	2 (4%)	56,56,56	1.18	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LMG	C	521	-	48,48,55	2.37	2 (4%)	56,56,63	1.42	9 (16%)
23	PHO	D	401	-	69,69,69	1.23	10 (14%)	92,99,99	1.15	10 (10%)
33	BCT	D	402	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	D	403	-	73,73,73	1.60	10 (13%)	96,113,113	1.22	12 (12%)
22	CLA	D	404	-	73,73,73	1.59	10 (13%)	96,113,113	1.28	15 (15%)
24	PL9	D	405	-	55,55,55	1.22	3 (5%)	69,69,69	1.68	16 (23%)
31	LMG	D	406	-	48,48,55	2.41	3 (6%)	56,56,63	1.51	7 (12%)
26	DGD	D	407	-	64,64,67	1.41	3 (4%)	78,78,81	1.34	7 (8%)
32	LMT	D	408	-	32,32,36	2.79	6 (18%)	43,43,47	1.07	2 (4%)
31	LMG	D	409	-	46,46,55	2.57	4 (8%)	54,54,63	1.43	6 (11%)
31	LMG	E	101	-	44,44,55	2.64	3 (6%)	52,52,63	1.41	6 (11%)
34	HEM	F	101	5,6	42,50,50	3.65	13 (30%)	27,82,82	1.14	1 (3%)
25	BCR	F	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	6 (10%)
30	SQD	F	103	-	45,45,54	1.39	5 (11%)	56,56,65	1.92	12 (21%)
22	CLA	H	101	-	73,73,73	1.62	10 (13%)	96,113,113	1.21	13 (13%)
25	BCR	H	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.20	4 (7%)
31	LMG	I	101	-	43,43,55	2.37	3 (6%)	51,51,63	1.35	7 (13%)
32	LMT	I	102	-	36,36,36	1.07	5 (13%)	47,47,47	1.10	2 (4%)
24	PL9	J	101	-	35,35,55	1.16	1 (2%)	43,45,69	1.85	8 (18%)
25	BCR	J	102	-	41,41,41	1.03	2 (4%)	56,56,56	1.59	13 (23%)
25	BCR	K	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.31	8 (14%)
31	LMG	L	101	-	51,51,55	2.34	3 (5%)	59,59,63	1.43	8 (13%)
31	LMG	M	101	-	42,42,55	2.38	3 (7%)	50,50,63	1.33	5 (10%)
32	LMT	M	102	-	36,36,36	1.10	4 (11%)	47,47,47	1.04	2 (4%)
32	LMT	M	103	-	36,36,36	1.09	5 (13%)	47,47,47	1.03	3 (6%)
34	HEM	V	201	16	42,50,50	3.69	12 (28%)	27,82,82	1.14	2 (7%)
30	SQD	a	401	-	54,54,54	0.92	3 (5%)	65,65,65	1.74	10 (15%)
31	LMG	a	402	-	42,42,55	2.53	4 (9%)	50,50,63	1.33	5 (10%)
22	CLA	a	403	-	73,73,73	1.64	10 (13%)	96,113,113	1.21	11 (11%)
22	CLA	a	404	-	73,73,73	1.58	10 (13%)	96,113,113	1.22	11 (11%)
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	1.59	10 (13%)	96,113,113	1.25	13 (13%)
24	PL9	a	407	-	45,45,55	1.13	3 (6%)	55,57,69	1.74	13 (23%)
26	DGD	a	408	-	57,57,67	2.29	2 (3%)	71,71,81	1.54	9 (12%)
27	LHG	a	409	-	38,38,48	2.34	2 (5%)	44,44,54	1.43	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	OEX	a	411	1,3	8,15,15	10.48	8 (100%)	0,32,32	0.00	-
30	SQD	a	412	-	51,51,54	1.55	4 (7%)	62,62,65	2.00	12 (19%)
26	DGD	b	601	-	53,53,67	2.29	6 (11%)	67,67,81	1.47	10 (14%)
30	SQD	b	602	-	47,47,54	1.10	4 (8%)	58,58,65	2.05	10 (17%)
32	LMT	b	603	-	36,36,36	1.09	5 (13%)	47,47,47	0.99	1 (2%)
32	LMT	b	604	-	36,36,36	1.09	5 (13%)	47,47,47	1.06	1 (2%)
22	CLA	b	605	-	73,73,73	1.63	11 (15%)	96,113,113	1.24	11 (11%)
22	CLA	b	606	-	73,73,73	1.59	11 (15%)	96,113,113	1.24	12 (12%)
22	CLA	b	607	-	73,73,73	1.59	10 (13%)	96,113,113	1.23	12 (12%)
22	CLA	b	608	-	73,73,73	1.60	10 (13%)	96,113,113	1.29	15 (15%)
22	CLA	b	609	-	73,73,73	1.59	10 (13%)	96,113,113	1.26	12 (12%)
22	CLA	b	610	-	73,73,73	1.60	10 (13%)	96,113,113	1.24	13 (13%)
22	CLA	b	611	-	73,73,73	1.59	10 (13%)	96,113,113	1.20	11 (11%)
22	CLA	b	612	-	73,73,73	1.60	10 (13%)	96,113,113	1.23	12 (12%)
22	CLA	b	613	-	73,73,73	1.61	10 (13%)	96,113,113	1.23	13 (13%)
22	CLA	b	614	-	73,73,73	1.58	10 (13%)	96,113,113	1.26	12 (12%)
22	CLA	b	615	-	73,73,73	1.57	11 (15%)	96,113,113	1.43	16 (16%)
22	CLA	b	616	-	73,73,73	1.61	10 (13%)	96,113,113	1.23	13 (13%)
22	CLA	b	617	-	73,73,73	1.59	10 (13%)	96,113,113	1.28	14 (14%)
22	CLA	b	618	-	73,73,73	1.60	10 (13%)	96,113,113	1.25	12 (12%)
22	CLA	b	619	-	73,73,73	1.61	10 (13%)	96,113,113	1.24	14 (14%)
22	CLA	b	620	-	73,73,73	1.62	11 (15%)	96,113,113	1.21	11 (11%)
25	BCR	b	621	-	41,41,41	1.07	2 (4%)	56,56,56	1.20	6 (10%)
25	BCR	b	622	-	41,41,41	1.04	2 (4%)	56,56,56	1.32	8 (14%)
25	BCR	b	623	-	41,41,41	1.08	2 (4%)	56,56,56	1.36	10 (17%)
25	BCR	b	624	-	41,41,41	1.08	2 (4%)	56,56,56	1.29	9 (16%)
26	DGD	b	625	-	59,59,67	2.24	2 (3%)	73,73,81	1.48	7 (9%)
31	LMG	b	626	-	49,49,55	2.36	3 (6%)	57,57,63	1.42	10 (17%)
31	LMG	b	627	-	42,42,55	2.45	3 (7%)	50,50,63	1.34	5 (10%)
32	LMT	b	628	-	36,36,36	1.09	4 (11%)	47,47,47	1.03	2 (4%)
32	LMT	b	629	-	36,36,36	1.07	5 (13%)	47,47,47	1.06	3 (6%)
22	CLA	c	501	-	73,73,73	1.62	11 (15%)	96,113,113	1.19	13 (13%)
22	CLA	c	502	-	73,73,73	1.61	10 (13%)	96,113,113	1.26	12 (12%)
22	CLA	c	503	-	73,73,73	1.62	10 (13%)	96,113,113	1.25	13 (13%)
22	CLA	c	504	-	73,73,73	1.60	10 (13%)	96,113,113	1.25	13 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	c	505	-	73,73,73	1.60	10 (13%)	96,113,113	1.30	13 (13%)
22	CLA	c	506	-	73,73,73	1.59	10 (13%)	96,113,113	1.28	13 (13%)
22	CLA	c	507	-	73,73,73	1.59	10 (13%)	96,113,113	1.32	14 (14%)
22	CLA	c	508	-	73,73,73	1.61	10 (13%)	96,113,113	1.25	13 (13%)
22	CLA	c	509	-	73,73,73	1.62	10 (13%)	96,113,113	1.24	12 (12%)
22	CLA	c	510	3	73,73,73	1.63	11 (15%)	96,113,113	1.25	13 (13%)
22	CLA	c	511	-	73,73,73	1.63	10 (13%)	96,113,113	1.24	14 (14%)
22	CLA	c	512	-	73,73,73	1.63	10 (13%)	96,113,113	1.23	13 (13%)
25	BCR	c	513	-	41,41,41	1.07	2 (4%)	56,56,56	1.31	9 (16%)
25	BCR	c	514	-	41,41,41	1.06	2 (4%)	56,56,56	1.28	8 (14%)
26	DGD	c	515	-	54,54,67	2.45	3 (5%)	68,68,81	1.38	10 (14%)
26	DGD	c	516	-	63,63,67	1.46	2 (3%)	77,77,81	1.46	12 (15%)
26	DGD	c	517	-	67,67,67	0.88	2 (2%)	81,81,81	1.40	9 (11%)
31	LMG	c	518	-	45,45,55	2.53	2 (4%)	53,53,63	1.43	8 (15%)
27	LHG	c	519	-	36,36,48	2.33	3 (8%)	42,42,54	1.53	8 (19%)
22	CLA	c	520	-	73,73,73	1.60	10 (13%)	96,113,113	1.22	12 (12%)
25	BCR	c	521	-	41,41,41	1.04	2 (4%)	56,56,56	1.21	7 (12%)
31	LMG	c	522	-	48,48,55	2.36	3 (6%)	56,56,63	1.41	9 (16%)
23	PHO	d	401	-	69,69,69	1.22	10 (14%)	92,99,99	1.19	9 (9%)
23	PHO	d	402	-	69,69,69	1.26	11 (15%)	92,99,99	1.17	10 (10%)
30	SQD	d	403	-	43,43,54	1.23	4 (9%)	54,54,65	1.97	11 (20%)
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	13 (13%)
22	CLA	d	406	-	73,73,73	1.61	10 (13%)	96,113,113	1.25	13 (13%)
24	PL9	d	407	-	55,55,55	1.15	3 (5%)	69,69,69	1.68	15 (21%)
31	LMG	d	408	-	49,49,55	2.51	2 (4%)	57,57,63	1.44	8 (14%)
31	LMG	d	409	-	48,48,55	2.39	3 (6%)	56,56,63	1.52	6 (10%)
26	DGD	d	410	-	64,64,67	1.48	2 (3%)	78,78,81	1.37	9 (11%)
32	LMT	d	411	-	32,32,36	2.81	6 (18%)	43,43,47	1.07	2 (4%)
31	LMG	d	412	-	46,46,55	2.61	4 (8%)	54,54,63	1.41	7 (12%)
31	LMG	e	101	-	44,44,55	2.69	3 (6%)	52,52,63	1.41	7 (13%)
34	HEM	f	101	5,6	42,50,50	3.62	13 (30%)	27,82,82	1.27	3 (11%)
25	BCR	f	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.19	6 (10%)
30	SQD	f	103	-	45,45,54	1.40	4 (8%)	56,56,65	1.92	12 (21%)
25	BCR	g	101	-	41,41,41	1.10	3 (7%)	56,56,56	1.28	8 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	i	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.19	6 (10%)
31	LMG	i	102	-	43,43,55	2.33	2 (4%)	51,51,63	1.34	6 (11%)
32	LMT	i	103	-	36,36,36	1.06	4 (11%)	47,47,47	1.08	2 (4%)
24	PL9	j	101	-	35,35,55	1.24	2 (5%)	43,45,69	1.81	8 (18%)
25	BCR	j	102	-	41,41,41	1.02	2 (4%)	56,56,56	1.52	12 (21%)
31	LMG	l	101	-	51,51,55	2.34	3 (5%)	59,59,63	1.41	8 (13%)
31	LMG	m	101	-	42,42,55	2.47	4 (9%)	50,50,63	1.35	5 (10%)
34	HEM	v	201	16	42,50,50	3.70	14 (33%)	27,82,82	1.12	1 (3%)
25	BCR	x	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.16	4 (7%)
25	BCR	y	101	-	41,41,41	1.09	3 (7%)	56,56,56	1.23	5 (8%)

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
23	PHO	A	405	-	-	0/49/103/103	0/1/6/6
22	CLA	A	406	-	-	0/37/135/135	0/0/9/9
24	PL9	A	407	-	-	0/41/61/73	0/1/1/1
25	BCR	A	408	-	-	0/29/63/63	0/2/2/2
26	DGD	A	409	-	-	0/45/85/95	0/2/2/2
27	LHG	A	410	-	-	0/43/43/53	0/0/0/0
29	OEX	A	412	1,3	-	0/0/68/68	0/0/6/6
30	SQD	A	413	-	-	0/46/66/69	0/1/1/1
30	SQD	A	414	-	-	0/49/69/69	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

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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
25	BCR	B	616	-	-	0/29/63/63	0/2/2/2
25	BCR	B	617	-	-	0/29/63/63	0/2/2/2
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
26	DGD	B	620	-	-	0/47/87/95	0/2/2/2
31	LMG	B	621	-	-	0/44/64/70	0/1/1/1
30	SQD	B	622	-	-	1/38/58/69	0/1/1/1
32	LMT	B	623	-	-	0/21/61/61	0/2/2/2
32	LMT	B	624	-	-	0/21/61/61	0/2/2/2
31	LMG	B	625	-	-	0/44/64/70	0/1/1/1
26	DGD	B	626	-	-	0/41/81/95	0/2/2/2
30	SQD	B	627	-	-	0/42/62/69	0/1/1/1
32	LMT	B	628	-	-	0/21/61/61	0/2/2/2
32	LMT	B	629	-	-	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
25	BCR	C	513	-	-	0/29/63/63	0/2/2/2
26	DGD	C	514	-	-	0/42/82/95	0/2/2/2
26	DGD	C	515	-	-	1/51/91/95	0/2/2/2
26	DGD	C	516	-	-	0/55/95/95	0/2/2/2
31	LMG	C	517	-	-	0/40/60/70	0/1/1/1
27	LHG	C	518	-	-	0/41/41/53	0/0/0/0
22	CLA	C	519	-	-	0/37/135/135	0/0/9/9
25	BCR	C	520	-	-	0/29/63/63	0/2/2/2
31	LMG	C	521	-	-	0/43/63/70	0/1/1/1
23	PHO	D	401	-	-	0/49/103/103	0/1/6/6
33	BCT	D	402	21	-	0/0/0/0	0/0/0/0
22	CLA	D	403	-	-	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	D	404	-	-	0/37/135/135	0/0/9/9
24	PL9	D	405	-	-	0/53/73/73	0/1/1/1
31	LMG	D	406	-	-	0/43/63/70	0/1/1/1
26	DGD	D	407	-	-	0/52/92/95	0/2/2/2
32	LMT	D	408	-	-	0/17/57/61	0/2/2/2
31	LMG	D	409	-	-	0/41/61/70	0/1/1/1
31	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
25	BCR	F	102	-	-	0/29/63/63	0/2/2/2
30	SQD	F	103	-	-	0/40/60/69	0/1/1/1
22	CLA	H	101	-	-	0/37/135/135	0/0/9/9
25	BCR	H	102	-	-	0/29/63/63	0/2/2/2
31	LMG	I	101	-	-	0/38/58/70	0/1/1/1
32	LMT	I	102	-	-	0/21/61/61	0/2/2/2
24	PL9	J	101	-	-	0/29/49/73	0/1/1/1
25	BCR	J	102	-	-	0/29/63/63	0/2/2/2
25	BCR	K	101	-	-	0/29/63/63	0/2/2/2
31	LMG	L	101	-	-	0/46/66/70	0/1/1/1
31	LMG	M	101	-	-	0/37/57/70	0/1/1/1
32	LMT	M	102	-	-	0/21/61/61	0/2/2/2
32	LMT	M	103	-	-	0/21/61/61	0/2/2/2
34	HEM	V	201	16	-	0/14/114/114	0/0/8/8
30	SQD	a	401	-	-	0/49/69/69	0/1/1/1
31	LMG	a	402	-	-	0/37/57/70	0/1/1/1
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
22	CLA	a	406	-	-	0/37/135/135	0/0/9/9
24	PL9	a	407	-	-	0/41/61/73	0/1/1/1
26	DGD	a	408	-	-	0/45/85/95	0/2/2/2
27	LHG	a	409	-	-	0/43/43/53	0/0/0/0
29	OEX	a	411	1,3	-	0/0/68/68	0/0/6/6
30	SQD	a	412	-	-	0/46/66/69	0/1/1/1
26	DGD	b	601	-	-	0/41/81/95	0/2/2/2
30	SQD	b	602	-	-	0/42/62/69	0/1/1/1
32	LMT	b	603	-	-	0/21/61/61	0/2/2/2
32	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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
22	CLA	b	620	-	-	0/37/135/135	0/0/9/9
25	BCR	b	621	-	-	0/29/63/63	0/2/2/2
25	BCR	b	622	-	-	0/29/63/63	0/2/2/2
25	BCR	b	623	-	-	0/29/63/63	0/2/2/2
25	BCR	b	624	-	-	0/29/63/63	0/2/2/2
26	DGD	b	625	-	-	0/47/87/95	0/2/2/2
31	LMG	b	626	-	-	0/44/64/70	0/1/1/1
31	LMG	b	627	-	-	0/37/57/70	0/1/1/1
32	LMT	b	628	-	-	0/21/61/61	0/2/2/2
32	LMT	b	629	-	-	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
25	BCR	c	513	-	-	0/29/63/63	0/2/2/2
25	BCR	c	514	-	-	0/29/63/63	0/2/2/2
26	DGD	c	515	-	-	0/42/82/95	0/2/2/2
26	DGD	c	516	-	-	1/51/91/95	0/2/2/2
26	DGD	c	517	-	-	0/55/95/95	0/2/2/2
31	LMG	c	518	-	-	0/40/60/70	0/1/1/1
27	LHG	c	519	-	-	0/41/41/53	0/0/0/0
22	CLA	c	520	-	-	0/37/135/135	0/0/9/9
25	BCR	c	521	-	-	0/29/63/63	0/2/2/2
31	LMG	c	522	-	-	0/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PHO	d	401	-	-	0/49/103/103	0/1/6/6
23	PHO	d	402	-	-	0/49/103/103	0/1/6/6
30	SQD	d	403	-	-	1/38/58/69	0/1/1/1
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
24	PL9	d	407	-	-	0/53/73/73	0/1/1/1
31	LMG	d	408	-	-	0/44/64/70	0/1/1/1
31	LMG	d	409	-	-	0/43/63/70	0/1/1/1
26	DGD	d	410	-	-	0/52/92/95	0/2/2/2
32	LMT	d	411	-	-	0/17/57/61	0/2/2/2
31	LMG	d	412	-	-	0/41/61/70	0/1/1/1
31	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
25	BCR	f	102	-	-	0/29/63/63	0/2/2/2
30	SQD	f	103	-	-	0/40/60/69	0/1/1/1
25	BCR	g	101	-	-	0/29/63/63	0/2/2/2
25	BCR	i	101	-	-	0/29/63/63	0/2/2/2
31	LMG	i	102	-	-	0/38/58/70	0/1/1/1
32	LMT	i	103	-	-	0/21/61/61	0/2/2/2
24	PL9	j	101	-	-	0/29/49/73	0/1/1/1
25	BCR	j	102	-	-	0/29/63/63	0/2/2/2
31	LMG	l	101	-	-	0/46/66/70	0/1/1/1
31	LMG	m	101	-	-	0/37/57/70	0/1/1/1
34	HEM	v	201	16	-	0/14/114/114	0/0/8/8
25	BCR	x	101	-	-	0/29/63/63	0/2/2/2
25	BCR	y	101	-	-	0/29/63/63	0/2/2/2

The worst 5 of 1105 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	V	201	HEM	C3C-C2C	-14.70	1.33	1.45
32	d	411	LMT	C8-C7	-14.56	1.49	1.55
29	A	412	OEX	O1-MN1	-14.52	1.88	2.02
34	v	201	HEM	C3C-C2C	-14.52	1.34	1.45
29	A	412	OEX	O3-MN1	-14.45	1.88	2.02

The worst 5 of 1649 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	602	SQD	O6-C1-C2	7.58	117.87	108.15
30	B	627	SQD	O6-C1-C2	7.26	117.45	108.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	413	SQD	O9-S-C6	7.14	113.14	106.83
30	A	413	SQD	O6-C1-C2	6.80	116.86	108.15
30	a	412	SQD	O6-C1-C2	6.80	116.86	108.15

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	d	403	SQD	C45-O47-C7-C8
30	B	622	SQD	C45-O47-C7-C8
26	C	515	DGD	C2G-O2G-C1B-C2B
26	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	335/344 (97%)	1.00	46 (13%) 4 8	206, 208, 208, 209	0
1	a	335/344 (97%)	1.07	72 (21%) 1 4	206, 208, 209, 209	0
2	B	490/510 (96%)	0.81	72 (14%) 3 7	206, 207, 209, 210	0
2	b	490/510 (96%)	0.95	82 (16%) 2 6	206, 208, 209, 210	0
3	C	447/461 (96%)	0.98	71 (15%) 3 7	206, 208, 209, 209	0
3	c	447/461 (96%)	0.89	76 (17%) 2 6	205, 208, 209, 210	0
4	D	340/352 (96%)	0.79	36 (10%) 7 13	205, 207, 208, 210	0
4	d	340/352 (96%)	0.85	49 (14%) 3 8	206, 208, 209, 209	0
5	E	82/84 (97%)	0.95	15 (18%) 2 5	206, 208, 209, 209	0
5	e	82/84 (97%)	0.67	10 (12%) 5 10	207, 208, 209, 209	0
6	F	35/45 (77%)	0.53	5 (14%) 3 8	207, 207, 208, 209	0
6	f	35/45 (77%)	0.47	3 (8%) 11 17	207, 208, 209, 209	0
7	H	65/66 (98%)	1.35	20 (30%) 1 3	206, 208, 209, 209	0
7	h	65/66 (98%)	1.66	26 (40%) 1 3	207, 208, 209, 209	0
8	I	35/38 (92%)	1.18	8 (22%) 1 4	207, 208, 209, 209	0
8	i	35/38 (92%)	0.55	2 (5%) 23 25	206, 207, 209, 210	0
9	J	34/40 (85%)	0.84	3 (8%) 10 16	207, 208, 208, 209	0
9	j	34/40 (85%)	0.10	0 100 100	206, 208, 209, 209	0
10	K	37/46 (80%)	0.65	3 (8%) 12 18	207, 208, 209, 209	0
10	k	37/46 (80%)	0.61	6 (16%) 2 6	207, 208, 209, 209	0
11	L	37/37 (100%)	1.13	10 (27%) 1 4	207, 208, 209, 209	0
11	l	37/37 (100%)	0.98	6 (16%) 2 6	206, 208, 209, 210	0
12	M	34/36 (94%)	0.97	5 (14%) 3 7	206, 207, 208, 209	0
12	m	34/36 (94%)	0.63	2 (5%) 22 24	207, 207, 208, 209	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/272 (89%)	1.28	62 (25%) 1 4	205, 208, 209, 210	0
13	o	243/272 (89%)	1.09	42 (17%) 2 6	206, 208, 209, 210	0
14	T	32/32 (100%)	0.86	7 (21%) 1 4	206, 208, 208, 209	0
14	t	32/32 (100%)	0.99	3 (9%) 9 15	206, 207, 209, 209	0
15	U	97/134 (72%)	1.71	32 (32%) 1 3	206, 207, 208, 209	0
15	u	97/134 (72%)	1.91	45 (46%) 1 3	206, 207, 208, 209	0
16	V	137/163 (84%)	0.62	14 (10%) 7 14	206, 207, 208, 209	0
16	v	137/163 (84%)	1.16	33 (24%) 1 4	206, 208, 209, 209	0
17	g	28/46 (60%)	1.37	8 (28%) 1 3	207, 208, 209, 209	0
17	y	28/46 (60%)	0.82	6 (21%) 1 4	206, 208, 209, 209	0
18	X	37/41 (90%)	1.24	8 (21%) 1 4	206, 208, 209, 210	0
18	x	37/41 (90%)	1.70	18 (48%) 1 3	207, 208, 208, 209	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	0.55	5 (8%) 12 18	206, 207, 208, 209	0
20	z	62/62 (100%)	1.01	10 (16%) 2 7	207, 208, 209, 210	0
All	All	5214/5674 (91%)	0.98	921 (17%) 2 6	205, 208, 209, 210	0

The worst 5 of 921 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	84	LYS	10.6
15	U	38	GLU	8.5
3	C	149	TYR	8.0
1	A	11	ALA	7.8
7	h	66	GLY	7.4

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
35	CA	o	301	1/1	0.66	13.65	209,209,209,209	0
32	LMT	i	103	35/35	1.26	8.11	206,209,210,210	0
35	CA	K	102	1/1	0.67	6.01	210,210,210,210	0
22	CLA	a	406	65/65	0.69	5.67	206,208,208,209	0
25	BCR	i	101	40/40	0.74	5.64	206,207,208,208	0
25	BCR	B	619	40/40	1.05	5.29	205,207,208,208	0
31	LMG	i	102	43/55	0.77	4.97	205,207,209,210	0
30	SQD	a	401	54/54	0.70	4.87	205,208,210,213	0
25	BCR	c	521	40/40	1.56	4.69	206,208,209,209	0
31	LMG	C	517	45/55	1.13	4.44	206,207,209,210	0
32	LMT	I	102	35/35	1.26	4.32	206,208,210,210	0
25	BCR	b	624	40/40	0.74	4.06	205,206,207,208	0
26	DGD	D	407	63/66	0.66	4.01	206,208,209,210	0
24	PL9	j	101	35/55	0.39	3.95	205,208,209,210	0
26	DGD	B	626	52/66	0.56	3.61	206,208,210,211	0
22	CLA	b	605	65/65	1.41	3.50	206,208,210,210	0
25	BCR	c	513	40/40	0.76	3.20	206,207,208,209	0
25	BCR	y	101	40/40	0.77	3.13	206,207,208,208	0
25	BCR	K	101	40/40	0.54	2.98	206,207,208,209	0
22	CLA	A	406	65/65	0.64	2.96	206,208,209,209	0
22	CLA	B	604	65/65	0.54	2.84	206,207,208,209	0
31	LMG	c	518	45/55	0.80	2.82	206,208,209,210	0
31	LMG	I	101	43/55	0.96	2.80	205,208,210,211	0
22	CLA	B	603	65/65	0.53	2.46	205,207,208,208	0
25	BCR	g	101	40/40	0.76	2.38	205,207,208,209	0
22	CLA	c	512	65/65	1.05	2.37	206,207,209,210	0
25	BCR	f	102	40/40	0.34	2.33	206,207,208,209	0
25	BCR	C	520	40/40	1.05	2.24	206,207,209,210	0
26	DGD	b	601	52/66	0.44	2.21	204,208,209,210	0
30	SQD	B	627	47/54	0.78	2.21	206,208,210,212	0
32	LMT	B	623	35/35	0.66	2.13	206,208,210,210	0
32	LMT	D	408	31/35	0.45	2.10	207,208,210,210	0
22	CLA	B	609	65/65	0.63	2.08	206,207,209,210	0
25	BCR	c	514	40/40	1.18	2.06	206,208,208,209	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
25	BCR	H	102	40/40	1.22	2.04	206,207,209,210	0
32	LMT	d	411	31/35	0.63	2.02	206,209,210,211	0
22	CLA	B	601	65/65	1.05	2.02	205,208,209,209	0
32	LMT	b	629	35/35	0.96	2.00	206,208,209,210	0
22	CLA	B	605	65/65	0.53	1.96	206,207,208,209	0
22	CLA	B	614	65/65	0.86	1.93	205,207,208,209	0
22	CLA	D	404	65/65	0.48	1.93	205,207,208,208	0
31	LMG	e	101	44/55	0.48	1.89	205,208,209,211	0
22	CLA	d	406	65/65	0.47	1.89	206,207,209,209	0
24	PL9	J	101	35/55	0.44	1.89	206,207,210,210	0
22	CLA	c	501	65/65	0.67	1.86	206,207,209,209	0
26	DGD	d	410	63/66	0.81	1.85	206,208,210,211	0
31	LMG	b	627	42/55	0.53	1.83	204,207,211,211	0
30	SQD	d	403	43/54	0.76	1.77	205,208,209,209	0
22	CLA	B	608	65/65	0.80	1.75	205,207,209,210	0
25	BCR	C	513	40/40	0.91	1.74	205,207,208,208	0
22	CLA	B	602	65/65	0.48	1.69	205,207,208,209	0
25	BCR	A	408	40/40	0.48	1.61	206,207,208,208	0
30	SQD	f	103	45/54	0.69	1.59	205,208,210,210	0
22	CLA	B	615	65/65	0.86	1.56	206,207,209,209	0
35	CA	k	101	1/1	0.27	1.54	208,208,208,208	0
32	LMT	b	628	35/35	0.50	1.49	206,208,210,210	0
25	BCR	B	617	40/40	0.42	1.49	205,207,208,209	0
22	CLA	C	511	65/65	1.15	1.37	206,207,208,209	0
22	CLA	B	611	65/65	0.39	1.34	205,207,208,208	0
22	CLA	b	620	65/65	0.95	1.29	206,208,209,210	0
22	CLA	b	614	65/65	0.62	1.27	206,207,209,210	0
22	CLA	c	511	65/65	0.94	1.23	206,208,209,209	0
25	BCR	F	102	40/40	0.42	1.21	205,207,208,208	0
32	LMT	B	628	35/35	0.62	1.21	206,208,210,211	0
22	CLA	C	501	65/65	0.43	1.19	206,208,209,209	0
30	SQD	B	622	43/54	0.52	1.09	205,208,209,212	0
22	CLA	c	506	65/65	0.68	1.08	206,208,209,209	0
30	SQD	F	103	45/54	0.71	1.06	205,208,209,210	0
22	CLA	c	510	65/65	0.62	1.06	206,208,209,211	0
22	CLA	b	607	65/65	0.53	1.06	205,207,208,208	0
22	CLA	C	512	65/65	1.00	1.05	205,207,209,211	0
22	CLA	b	608	65/65	0.45	1.05	205,207,208,209	0
30	SQD	A	414	54/54	0.46	1.04	205,207,209,210	0
22	CLA	b	619	65/65	0.86	1.04	206,208,209,209	0
22	CLA	b	609	65/65	0.46	1.03	206,207,208,209	0
22	CLA	B	607	65/65	0.42	1.01	206,207,208,209	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	LMT	B	624	35/35	0.45	1.00	206,207,211,212	0
26	DGD	a	408	56/66	0.44	0.92	206,208,210,211	0
31	LMG	a	402	42/55	0.39	0.92	204,207,209,210	0
30	SQD	b	602	47/54	0.44	0.92	205,208,209,212	0
22	CLA	C	508	65/65	0.79	0.91	205,207,208,209	0
22	CLA	C	502	65/65	0.54	0.89	206,207,208,208	0
34	HEM	v	201	43/43	0.56	0.88	206,207,208,209	0
31	LMG	m	101	42/55	0.53	0.85	205,207,209,210	0
26	DGD	A	409	56/66	0.45	0.82	206,208,210,211	0
25	BCR	x	101	40/40	0.76	0.78	206,207,209,209	0
22	CLA	C	506	65/65	0.56	0.72	206,207,208,209	0
31	LMG	M	101	42/55	0.44	0.68	205,208,209,210	0
22	CLA	c	503	65/65	0.45	0.68	206,207,208,209	0
22	CLA	C	510	65/65	0.61	0.64	206,207,209,209	0
32	LMT	b	603	35/35	0.46	0.62	206,208,210,210	0
22	CLA	b	610	65/65	0.46	0.62	206,207,209,209	0
34	HEM	F	101	43/43	0.47	0.61	206,207,208,210	0
22	CLA	B	613	65/65	0.44	0.58	206,207,208,209	0
22	CLA	c	505	65/65	0.59	0.57	205,207,208,209	0
22	CLA	c	502	65/65	0.64	0.55	206,207,208,209	0
25	BCR	b	623	40/40	0.35	0.54	205,206,207,207	0
22	CLA	b	612	65/65	0.37	0.54	205,207,209,209	0
22	CLA	b	613	65/65	0.55	0.52	205,207,208,209	0
25	BCR	j	102	40/40	0.27	0.49	206,208,209,210	0
24	PL9	a	407	45/55	0.33	0.46	205,207,208,209	0
31	LMG	E	101	44/55	0.42	0.44	204,208,209,210	0
33	BCT	d	404	4/4	0.47	0.42	206,207,208,208	0
22	CLA	b	616	65/65	0.36	0.42	206,207,208,209	0
22	CLA	c	508	65/65	0.48	0.41	205,208,209,209	0
32	LMT	b	604	35/35	0.37	0.38	207,208,210,210	0
22	CLA	b	606	65/65	0.39	0.38	205,207,209,210	0
34	HEM	V	201	43/43	0.33	0.35	201,207,208,209	0
24	PL9	A	407	45/55	0.46	0.34	206,207,208,210	0
25	BCR	b	621	40/40	0.32	0.33	206,207,208,208	0
22	CLA	H	101	65/65	0.36	0.28	206,207,208,209	0
22	CLA	C	507	65/65	0.37	0.27	206,207,208,208	0
22	CLA	c	504	65/65	0.34	0.27	205,207,208,209	0
32	LMT	B	629	35/35	0.36	0.24	206,208,209,210	0
22	CLA	B	610	65/65	0.34	0.18	205,207,208,208	0
25	BCR	B	616	40/40	0.35	0.16	205,207,208,209	0
21	FE2	A	401	1/1	0.28	0.16	209,209,209,209	0
22	CLA	C	505	65/65	0.39	0.11	206,207,209,210	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
34	HEM	f	101	43/43	0.25	0.11	206,207,209,209	0
22	CLA	b	618	65/65	0.37	0.11	206,207,209,210	0
26	DGD	B	620	58/66	0.35	0.11	205,207,209,209	0
31	LMG	c	522	48/55	0.28	0.10	205,207,209,210	0
22	CLA	C	504	65/65	0.33	0.07	205,207,208,209	0
22	CLA	C	503	65/65	0.37	0.05	206,207,208,209	0
35	CA	O	301	1/1	0.36	0.05	208,208,208,208	0
25	BCR	B	618	40/40	0.28	0.05	205,206,208,208	0
22	CLA	b	617	65/65	0.32	0.04	206,207,208,209	0
22	CLA	C	509	65/65	0.37	0.01	205,207,208,208	0
23	PHO	d	401	64/64	0.43	0.01	206,207,208,208	0
30	SQD	a	412	51/54	0.23	-0.00	205,207,208,209	0
27	LHG	c	519	37/49	0.30	-0.03	204,207,210,213	0
25	BCR	b	622	40/40	0.33	-0.03	205,207,208,208	0
22	CLA	a	404	65/65	0.51	-0.05	204,207,208,208	0
31	LMG	C	521	48/55	0.29	-0.06	206,207,208,209	0
26	DGD	b	625	58/66	0.34	-0.08	206,207,208,209	0
29	OEX	a	411	10/10	0.49	-0.14	200,204,205,206	0
28	CL	A	411	1/1	0.36	-0.18	204,204,204,204	0
33	BCT	D	402	4/4	0.27	-0.23	208,208,208,208	0
22	CLA	B	612	65/65	0.30	-0.29	203,207,208,209	0
31	LMG	l	101	51/55	0.27	-0.29	206,207,209,209	0
22	CLA	c	507	65/65	0.27	-0.31	206,207,209,209	0
31	LMG	d	409	48/55	0.26	-0.32	206,207,209,210	0
31	LMG	D	406	48/55	0.26	-0.33	204,207,208,209	0
25	BCR	J	102	40/40	0.29	-0.34	205,207,209,209	0
27	LHG	A	410	39/49	0.28	-0.39	206,207,209,210	0
24	PL9	d	407	55/55	0.29	-0.42	205,207,208,208	0
29	OEX	A	412	10/10	0.45	-0.42	197,202,205,206	0
22	CLA	c	509	65/65	0.26	-0.43	206,207,209,209	0
27	LHG	a	409	39/49	0.26	-0.49	206,207,209,209	0
23	PHO	D	401	64/64	0.34	-0.51	205,207,208,209	0
22	CLA	a	403	65/65	0.51	-0.51	205,207,208,210	0
22	CLA	b	615	65/65	0.25	-0.56	205,207,208,209	0
30	SQD	A	413	51/54	0.22	-0.57	204,207,209,209	0
22	CLA	d	405	65/65	0.44	-0.58	205,207,208,208	0
31	LMG	D	409	46/55	0.29	-0.58	205,207,208,209	0
31	LMG	d	412	46/55	0.19	-0.59	205,207,208,209	0
26	DGD	C	514	53/66	0.28	-0.65	205,206,208,209	0
23	PHO	A	405	64/64	0.29	-0.68	205,207,208,209	0
31	LMG	B	625	49/55	0.28	-0.69	205,207,208,208	0
26	DGD	c	515	53/66	0.30	-0.71	205,207,209,210	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	LMT	M	102	35/35	0.36	-0.71	205,208,209,209	0
22	CLA	A	402	65/65	0.32	-0.73	206,207,208,209	0
22	CLA	c	520	65/65	0.26	-0.78	206,207,208,209	0
22	CLA	a	405	65/65	0.32	-0.79	205,207,209,209	0
22	CLA	A	403	65/65	0.31	-0.80	205,207,208,208	0
26	DGD	C	516	66/66	0.31	-0.80	205,207,208,208	0
23	PHO	d	402	64/64	0.24	-0.82	206,207,209,209	0
24	PL9	D	405	55/55	0.25	-0.83	205,207,208,208	0
31	LMG	d	408	49/55	0.23	-0.83	205,207,208,209	0
28	CL	a	410	1/1	0.40	-0.90	205,205,205,205	0
22	CLA	b	611	65/65	0.25	-0.93	206,207,208,209	0
26	DGD	C	515	62/66	0.24	-1.00	205,207,209,210	0
26	DGD	c	517	66/66	0.22	-1.02	206,207,209,209	0
22	CLA	C	519	65/65	0.24	-1.04	205,207,209,209	0
22	CLA	B	606	65/65	0.29	-1.07	205,207,208,209	0
22	CLA	D	403	65/65	0.31	-1.10	205,207,208,208	0
31	LMG	L	101	51/55	0.22	-1.12	205,207,208,209	0
32	LMT	M	103	35/35	0.28	-1.13	206,208,209,209	0
31	LMG	b	626	49/55	0.27	-1.19	205,207,209,209	0
27	LHG	C	518	37/49	0.29	-1.19	205,208,210,211	0
22	CLA	A	404	65/65	0.26	-1.37	204,207,208,209	0
26	DGD	c	516	62/66	0.21	-1.45	206,208,208,209	0
31	LMG	B	621	49/55	0.24	-1.47	206,207,208,209	0
21	FE2	a	413	1/1	0.12	-2.88	206,206,206,206	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.