



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 11:56 PM GMT

PDB ID : 5E7C  
Title : Macromolecular diffractive imaging using imperfect crystals - Bragg data  
Authors : Ayer, K.; Yefanov, O.; Oberthuer, D.; Roy-Chowdhury, S.; Galli, L.; Mariani, V.; Basu, S.; Coe, J.; Conrad, C.E.; Fromme, R.; Schaffner, A.; Doerner, K.; James, D.; Kupitz, C.; Metz, M.; Nelson, G.; Xavier, P.L.; Beyerlein, K.R.; Schmidt, M.; Sarrou, I.; Spence, J.C.H.; Weierstall, U.; White, T.A.; Yang, J.-H.; Zhao, Y.; Liang, M.; Aquila, A.; Hunter, M.S.; Robinson, J.S.; Koglin, J.E.; Boutet, S.; Fromme, P.; Barty, A.; Chapman, H.N.  
Deposited on : 2015-10-12  
Resolution : 4.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

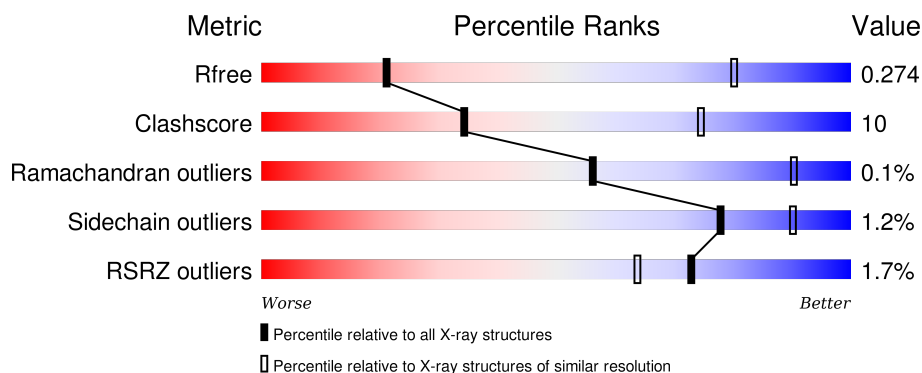
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



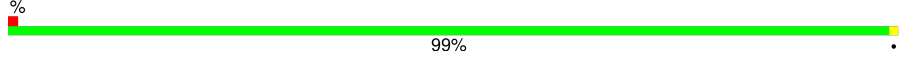

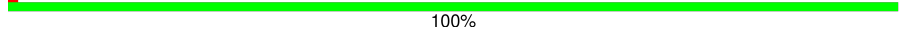

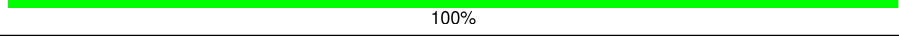
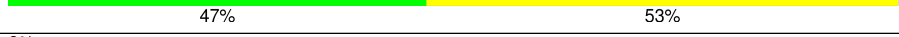
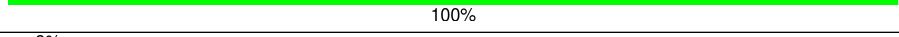
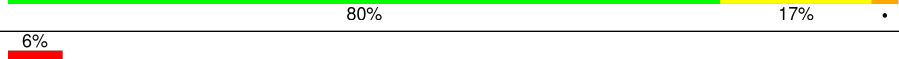
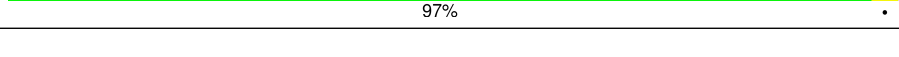




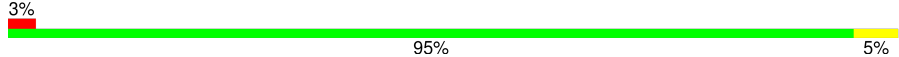

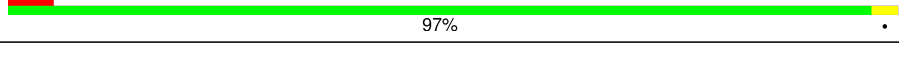

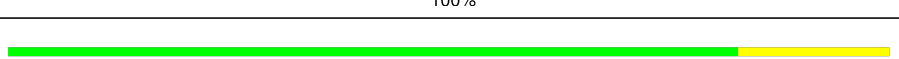
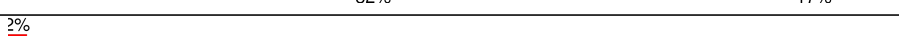
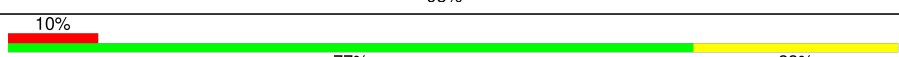
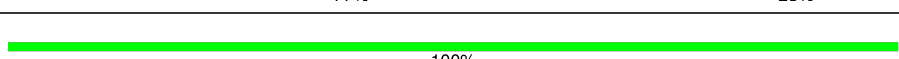

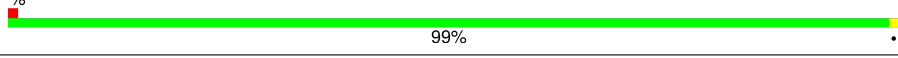


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1071 (5.40-3.60)
Clashscore	102246	1003 (5.30-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	334	<div> <div>73%</div> <div>27%</div> </div>
1	a	334	<div> <div>99%</div> <div>.</div> </div>
2	B	504	<div> <div>77%</div> <div>23%</div> </div>
2	b	504	<div> <div>99%</div> <div>.</div> </div>
3	C	451	<div> <div>79%</div> <div>20%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	c	451	
4	D	342	
4	d	342	
5	E	81	
5	e	81	
6	F	34	
6	f	34	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	38	
9	j	38	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	34	
12	m	34	
13	O	243	
13	o	243	
14	T	30	
14	t	30	
15	U	97	
15	u	97	

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Mol	Chain	Length	Quality of chain
16	V	137	
16	v	137	
17	Y	29	
17	y	29	
18	X	39	
18	x	39	
19	Z	62	
19	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	BCT	a	603	-	-	-	X
23	CLA	A	605	X	-	-	-
23	CLA	A	606	X	-	-	-
23	CLA	A	608	X	-	-	-
23	CLA	B	602	X	-	-	X
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607[A]	X	-	-	-
23	CLA	B	607[B]	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	B	617	X	-	-	X
23	CLA	C	501	X	-	-	-
23	CLA	C	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	X
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	X
23	CLA	C	513	X	-	-	X
23	CLA	D	402	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	a	604	X	-	-	-
23	CLA	a	605	X	-	-	-
23	CLA	a	607	X	-	-	X
23	CLA	a	613	X	-	-	-
23	CLA	b	604	X	-	-	X
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609[A]	X	-	-	X
23	CLA	b	609[B]	X	-	-	X
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	X
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	X
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	X
23	CLA	c	514	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
25	BCR	A	609	-	-	-	X
25	BCR	B	618	-	-	X	X
25	BCR	B	619	-	-	X	-
25	BCR	B	620	-	-	X	-
25	BCR	C	515	-	-	X	-
25	BCR	F	101	-	-	X	-
25	BCR	H	101	-	X	X	X
25	BCR	K	101	-	-	X	X
25	BCR	T	101	-	-	X	X
25	BCR	a	608	-	-	-	X
25	BCR	b	620	-	-	-	X
25	BCR	b	621	-	-	-	X
25	BCR	b	622	-	-	-	X
25	BCR	c	515	-	-	-	X
25	BCR	h	101	-	X	-	X
26	PL9	A	610	-	-	-	X
26	PL9	a	609	-	-	-	X
27	SQD	A	611	-	-	-	X
27	SQD	a	610	-	-	-	X
27	SQD	b	602	-	-	-	X
27	SQD	x	101	-	-	-	X
28	LMG	C	519	-	-	-	X
28	LMG	C	520	-	-	-	X
28	LMG	Z	101	-	-	-	X
28	LMG	c	520	-	-	-	X
28	LMG	c	521	-	-	-	X
28	LMG	z	101	-	-	-	X
31	LHG	e	101	-	-	-	X
32	DGD	D	406	-	-	-	X
32	DGD	c	519	-	-	-	X
32	DGD	d	405	-	-	-	X
33	HEM	e	102	-	-	-	X
34	MG	J	102	-	-	-	X

## 2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 49966 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	4	0
			2637	1730	432	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2637	1730	432	460	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	ALA	THR	conflict	UNP P0A444
a	286	ALA	THR	conflict	UNP P0A444

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4024	2641	668	702	13			
2	b	504	Total	C	N	O	S	6	10	0
			4024	2641	668	702	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	5	0
			3506	2296	584	613	13			
3	c	451	Total	C	N	O	S	0	5	0
			3506	2296	584	613	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O		0	2	0
			668	436	107	125				
5	e	81	Total	C	N	O		0	2	0
			668	436	107	125				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	2	0
			525	351	86	86	2			
7	h	65	Total	C	N	O	S	0	2	0
			525	351	86	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	1	0
			320	215	49	54	2			
8	i	38	Total	C	N	O	S	0	1	0
			320	215	49	54	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			



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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	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	1	0
			272	183	40	48	1			
12	m	34	Total	C	N	O	S	0	1	0
			272	183	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	4	0
			1883	1178	315	385	5			
13	o	243	Total	C	N	O	S	0	4	0
			1883	1178	315	385	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	2	0
			270	189	37	41	3			
14	t	30	Total	C	N	O	S	0	2	0
			270	189	37	41	3			

- 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	1	0
			1072	680	180	208	4			
16	v	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

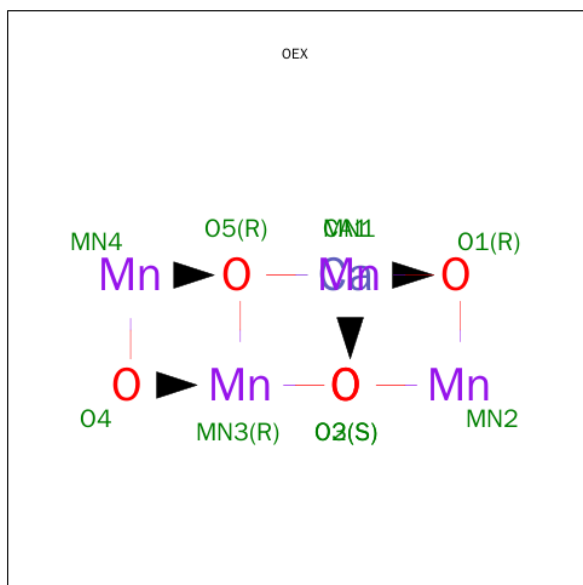
- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O	0	1	0
			292	196	46	50			
18	x	39	Total	C	N	O	0	1	0
			292	196	46	50			

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

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

- Molecule 20 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).

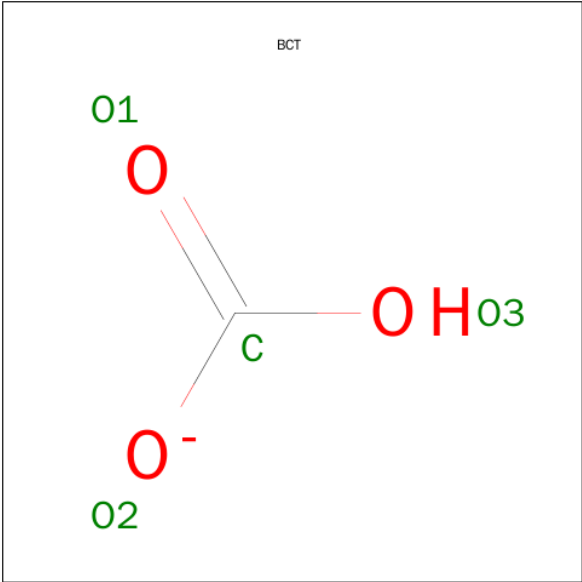


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
20	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

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

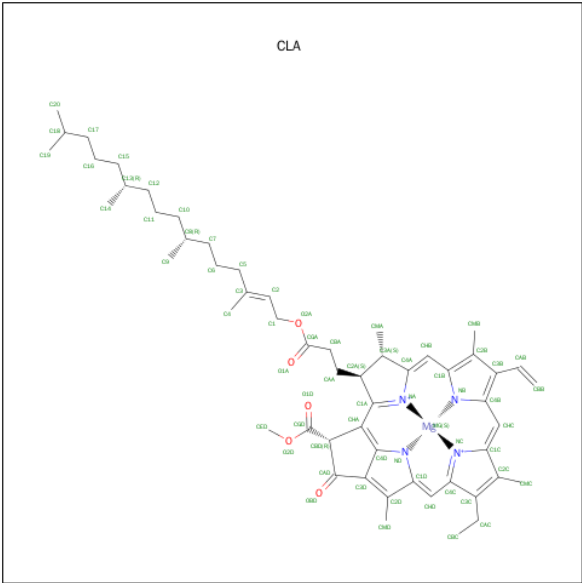
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Cl	0	0
			1	1		
21	A	2	Total	Cl	0	0
			2	2		
21	c	1	Total	Cl	0	0
			1	1		
21	V	1	Total	Cl	0	0
			1	1		
21	u	1	Total	Cl	0	0
			1	1		

- Molecule 22 is BICARBONATE ION (three-letter code: BCT) (formula: CHO<sub>3</sub>).



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

- Molecule 23 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
23	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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

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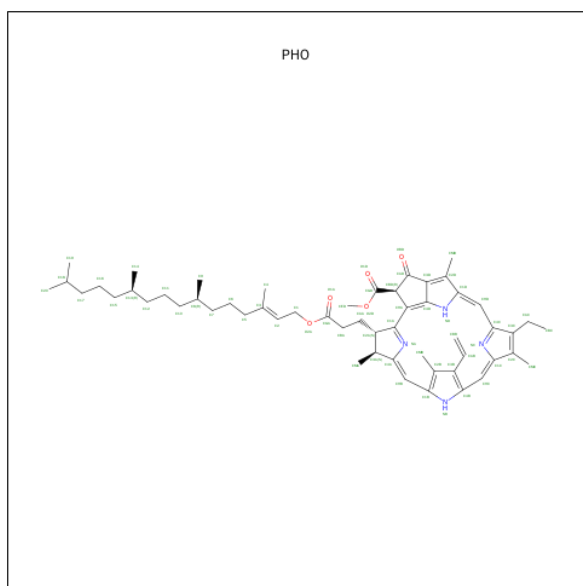
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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

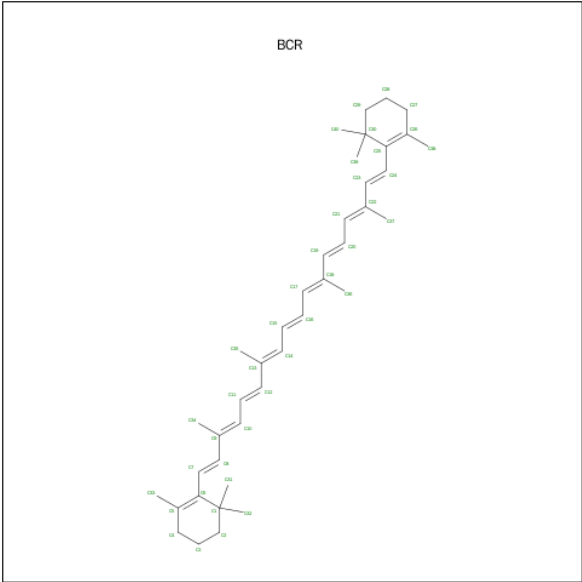
- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



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

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).





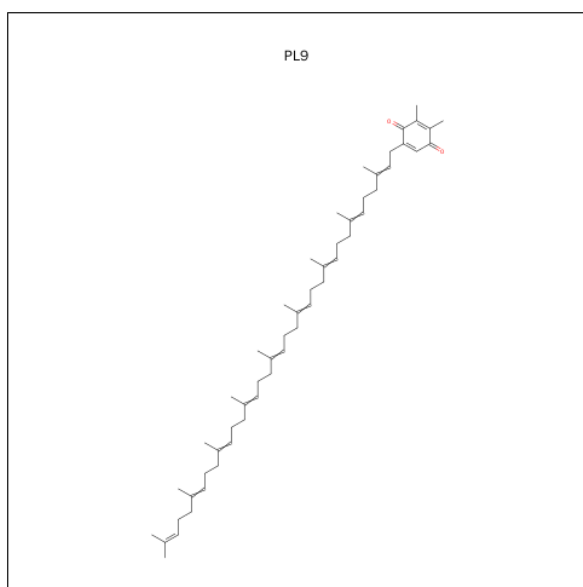
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	F	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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	h	1	Total C 40 40	0	0
25	k	1	Total C 40 40	0	0
25	t	1	Total C 40 40	0	0

- Molecule 26 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:  $C_{53}H_{80}O_2$ ).



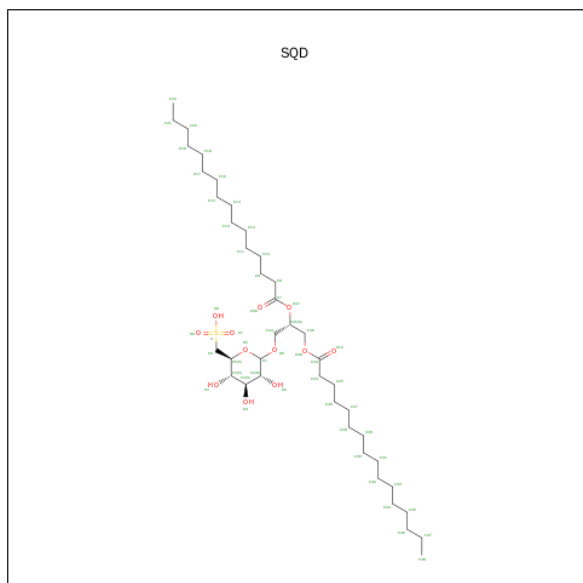
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O 55 53 2	0	0
26	D	1	Total C O 55 53 2	0	0

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

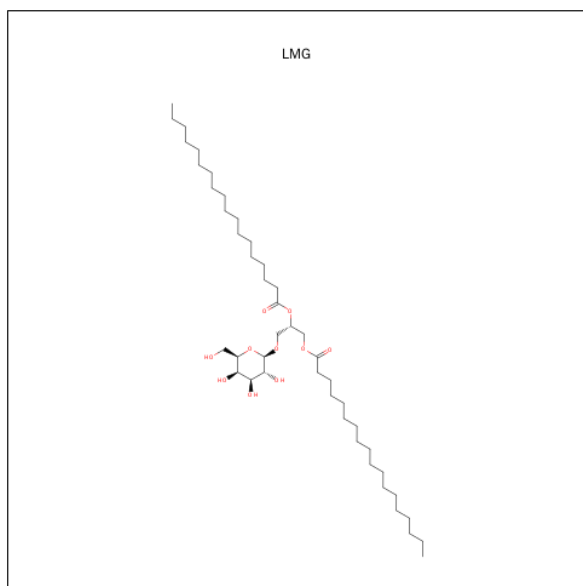
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	B	1	Total	C	O	S	0	0
			54	41	12	1		
27	X	1	Total	C	O	S	0	0
			43	30	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	b	1	Total	C	O	S	0	0
			54	41	12	1		
27	b	1	Total	C	O	S	0	0
			54	41	12	1		
27	x	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter

code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			51	41	10		
28	B	1	Total	C	O	0	0
			51	41	10		
28	C	1	Total	C	O	0	0
			51	41	10		
28	C	1	Total	C	O	0	0
			51	41	10		
28	J	1	Total	C	O	0	0
			51	41	10		
28	Z	1	Total	C	O	0	0
			37	27	10		
28	a	1	Total	C	O	0	0
			51	41	10		
28	b	1	Total	C	O	0	0
			51	41	10		
28	c	1	Total	C	O	0	0
			51	41	10		
28	c	1	Total	C	O	0	0
			51	41	10		
28	j	1	Total	C	O	0	0
			51	41	10		
28	z	1	Total	C	O	0	0
			37	27	10		

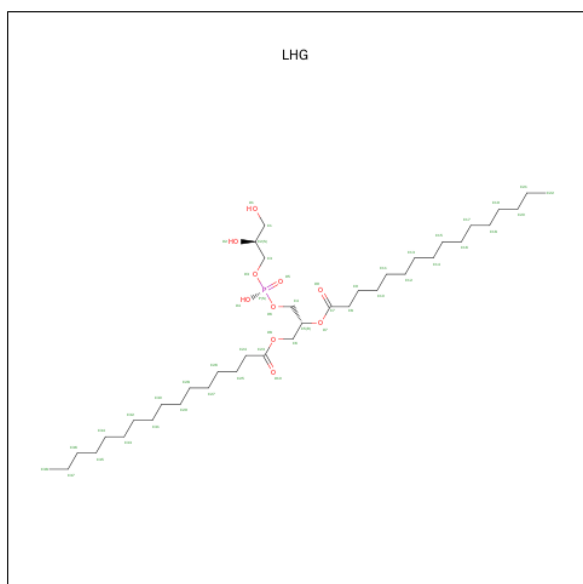
- Molecule 29 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 30 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	B	1	Total	Ca	0	0
			1	1		
30	F	1	Total	Ca	0	0
			1	1		
30	o	1	Total	Ca	0	0
			1	1		
30	O	1	Total	Ca	0	0
			1	1		
30	b	1	Total	Ca	0	0
			1	1		
30	f	1	Total	Ca	0	0
			1	1		

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



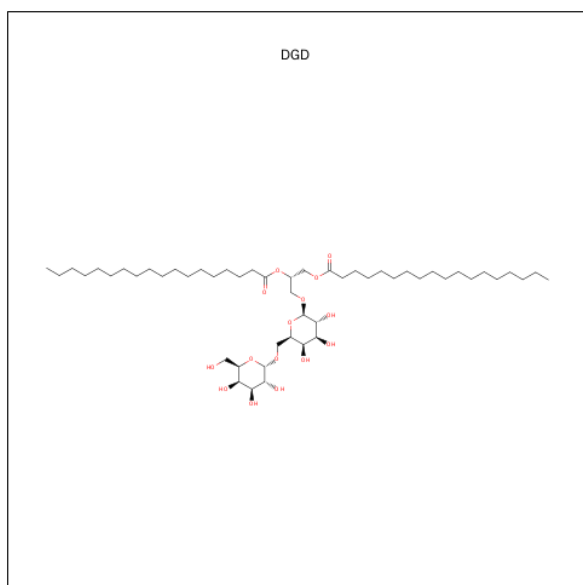
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total	C	O	P	0	0
			49	38	10	1		

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

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



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

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

- 
- Chemical structure of HEM (Heme) showing a central iron atom coordinated by four nitrogen atoms in a porphyrin-like ring, with various side chains and a central heme group.

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



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

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

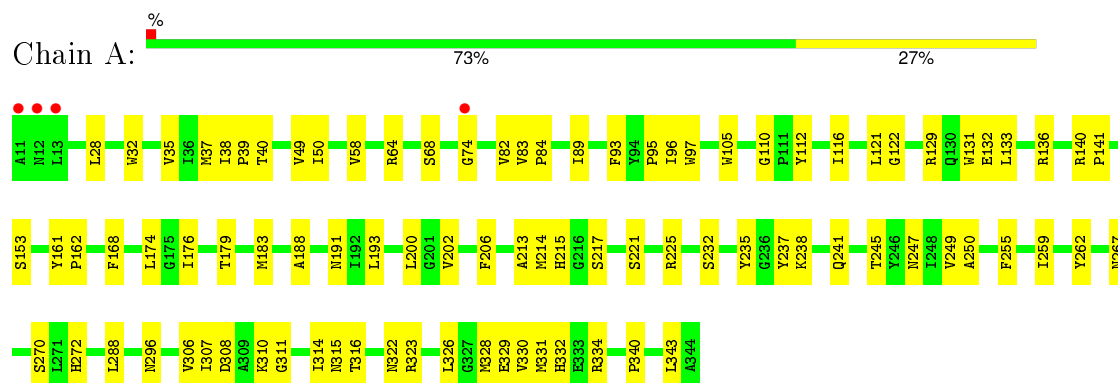
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	J	1	Total	Mg	0	0
			1	1		
34	j	1	Total	Mg	0	0
			1	1		



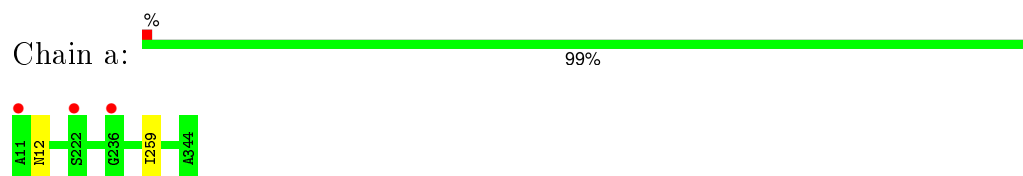
### 3 Residue-property plots

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.

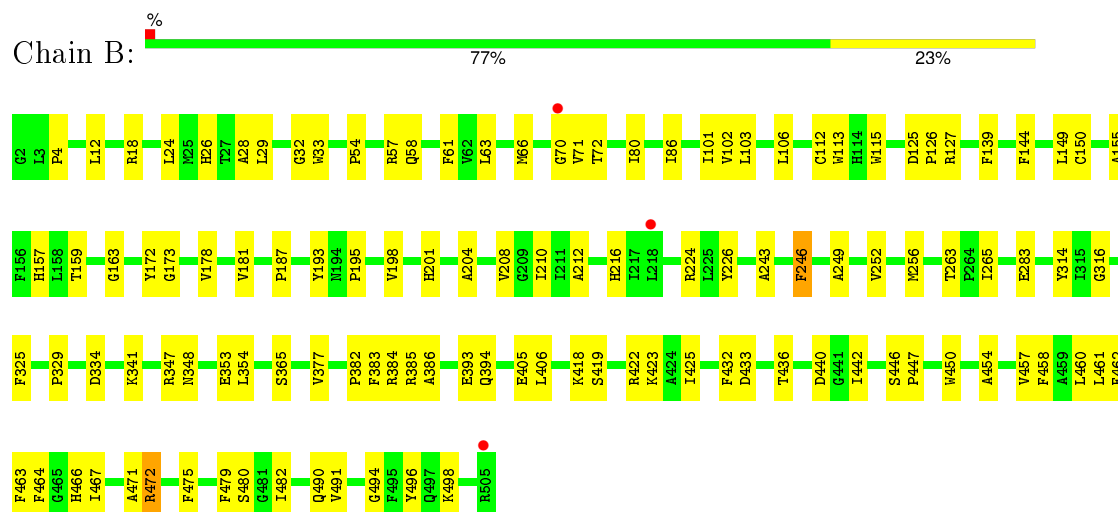
- Molecule 1: Photosystem II protein D1 1



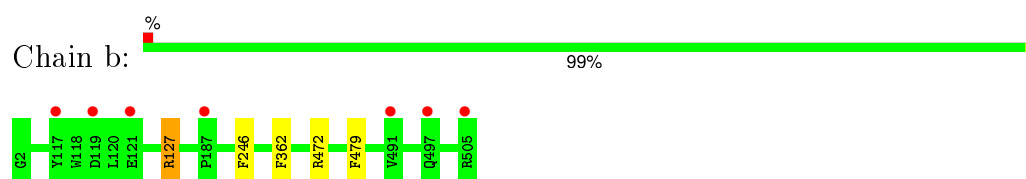
- Molecule 1: Photosystem II protein D1 1



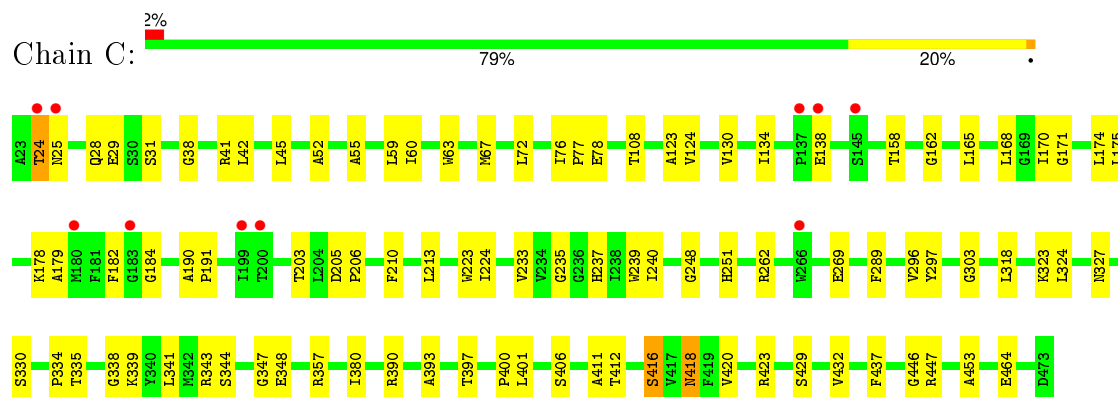
- Molecule 2: Photosystem II CP47 reaction center protein



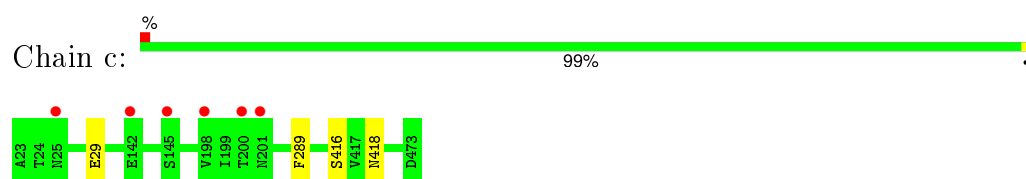
- Molecule 2: Photosystem II CP47 reaction center protein



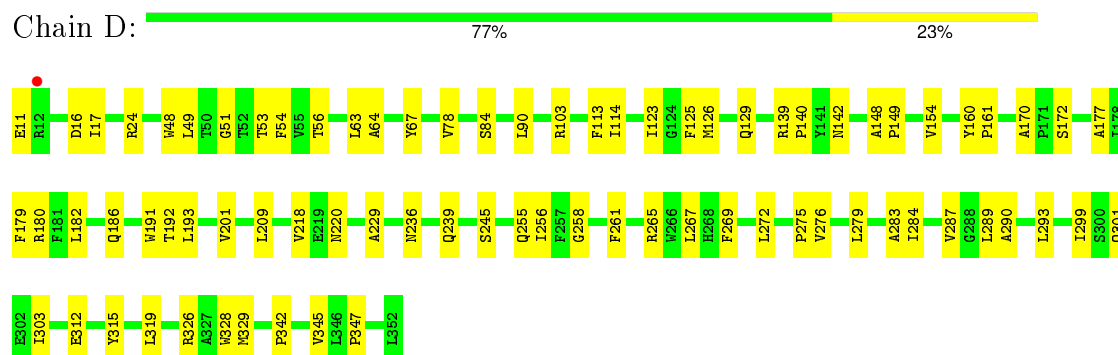
- Molecule 3: Photosystem II CP43 reaction center protein



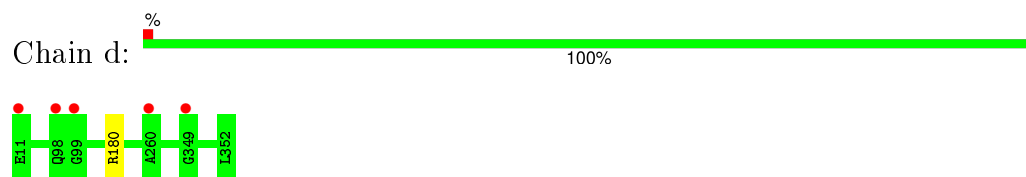
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 4: Photosystem II D2 protein

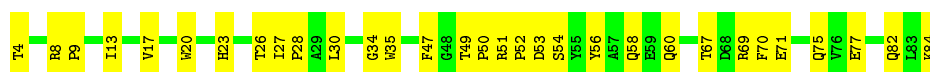


- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha

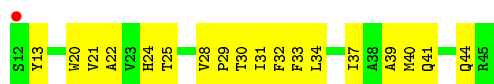




- Molecule 5: Cytochrome b559 subunit alpha



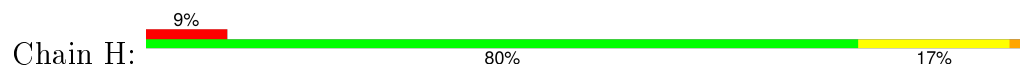
- Molecule 6: Cytochrome b559 subunit beta



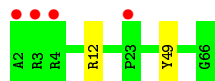
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I

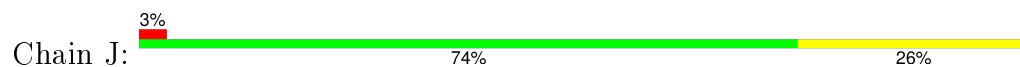


- Molecule 8: Photosystem II reaction center protein I





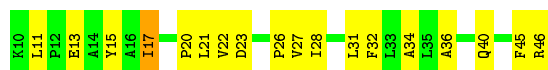
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



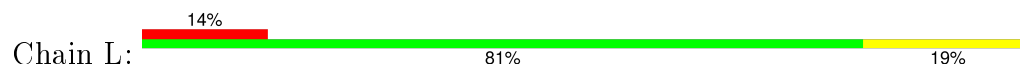
- Molecule 10: Photosystem II reaction center protein K



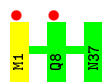
- Molecule 10: Photosystem II reaction center protein K



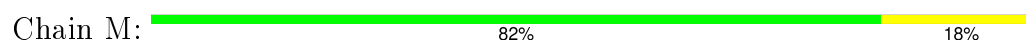
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M





- Molecule 12: Photosystem II reaction center protein M

Chain m: 100%

There are no outlier residues recorded for this chain.

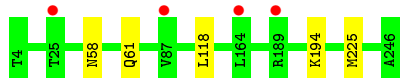
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 82% 17%



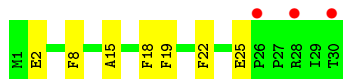
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 2% 98%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 10% 77% 23%



- Molecule 14: Photosystem II reaction center protein T

Chain t: 100%

There are no outlier residues recorded for this chain.

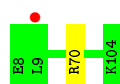
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 1% 81% 19%

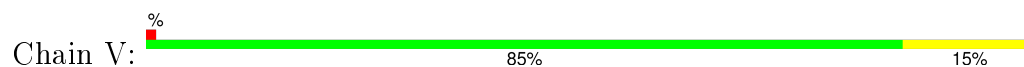


- Molecule 15: Photosystem II 12 kDa extrinsic protein

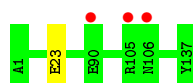
Chain u: 1% 99%



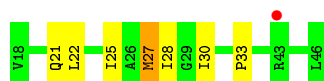
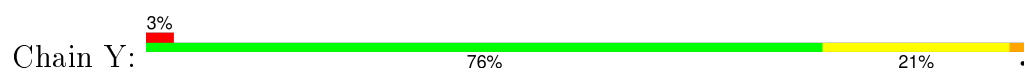
- Molecule 16: Cytochrome c-550



- Molecule 16: Cytochrome c-550



- Molecule 17: Photosystem II reaction center protein Ycf12

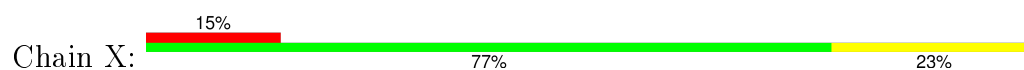


- Molecule 17: Photosystem II reaction center protein Ycf12



There are no outlier residues recorded for this chain.

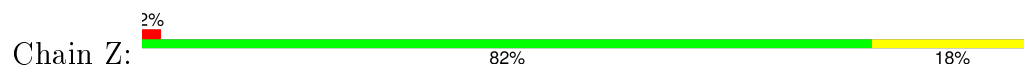
- Molecule 18: Photosystem II reaction center X protein



- Molecule 18: Photosystem II reaction center X protein

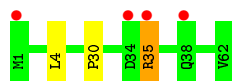


- Molecule 19: Photosystem II reaction center protein Z





- Molecule 19: Photosystem II reaction center protein Z



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.25Å 226.26Å 307.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.93 – 4.50 36.50 – 4.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.93-4.50) 99.9 (36.50-4.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 4.44Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.246 , 0.275 0.249 , 0.274	Depositor DCC
$R_{free}$ test set	2718 reflections (4.88%)	DCC
Wilson B-factor (Å <sup>2</sup> )	211.4	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 13.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 55740 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	49966	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, MG, OEX, PHO, DGD, CL, CA, 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	0.33	0/2734	0.53	0/3727
1	a	0.33	0/2734	0.53	0/3727
2	B	0.30	0/4194	0.51	0/5713
2	b	0.31	0/4194	0.52	1/5713 (0.0%)
3	C	0.31	0/3634	0.49	0/4947
3	c	0.32	0/3634	0.52	0/4947
4	D	0.31	0/2821	0.50	0/3844
4	d	0.30	0/2821	0.50	0/3844
5	E	0.30	0/693	0.49	0/944
5	e	0.31	0/693	0.55	0/944
6	F	0.34	0/284	0.49	0/387
6	f	0.40	0/284	0.74	0/387
7	H	0.29	0/544	0.52	0/739
7	h	0.28	0/544	0.52	0/739
8	I	0.31	0/327	0.54	0/439
8	i	0.31	0/327	0.60	0/439
9	J	0.27	0/278	0.44	0/376
9	j	0.31	0/278	0.50	0/376
10	K	0.31	0/303	0.57	0/416
10	k	0.34	0/303	0.55	0/416
11	L	0.28	0/319	0.44	0/433
11	l	0.28	0/319	0.45	0/433
12	M	0.33	0/278	0.56	0/378
12	m	0.34	0/278	0.57	0/378
13	O	0.29	0/1926	0.53	0/2611
13	o	0.32	0/1926	0.58	0/2611
14	T	0.34	0/282	0.52	0/382
14	t	0.34	0/282	0.51	0/382
15	U	0.28	0/785	0.51	0/1064
15	u	0.31	0/785	0.56	0/1064
16	V	0.29	0/1096	0.50	0/1487
16	v	0.29	0/1096	0.56	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	Y	0.33	0/216	0.49	0/289
17	y	0.36	0/216	0.59	0/289
18	X	0.29	0/298	0.42	0/403
18	x	0.32	0/298	0.54	0/403
19	Z	0.32	0/490	0.46	0/669
19	z	0.41	0/490	0.68	1/669 (0.1%)
All	All	0.31	0/43004	0.52	2/58496 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	z	35	ARG	CB-CG-CD	6.51	128.53	111.60
2	b	127	ARG	CG-CD-NE	5.53	123.42	111.80

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2637	0	2551	93	0
1	a	2637	0	2551	0	0
2	B	4024	0	3901	139	0
2	b	4024	0	3901	0	0
3	C	3506	0	3439	104	0
3	c	3506	0	3439	0	0
4	D	2726	0	2627	81	0
4	d	2726	0	2627	0	0
5	E	668	0	658	30	0
5	e	668	0	658	0	0
6	F	275	0	282	23	0
6	f	275	0	282	0	0
7	H	525	0	558	12	0
7	h	525	0	558	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	I	320	0	339	13	0
8	i	320	0	339	0	0
9	J	272	0	279	10	0
9	j	272	0	279	0	0
10	K	293	0	305	18	0
10	k	293	0	305	0	0
11	L	309	0	327	8	0
11	l	309	0	327	0	0
12	M	272	0	300	7	0
12	m	272	0	300	0	0
13	O	1883	0	1865	33	0
13	o	1883	0	1865	0	0
14	T	270	0	278	14	0
14	t	270	0	278	0	0
15	U	774	0	773	17	0
15	u	774	0	773	0	0
16	V	1072	0	1088	19	0
16	v	1072	0	1088	0	0
17	Y	215	0	246	12	0
17	y	215	0	246	0	0
18	X	292	0	328	13	0
18	x	292	0	328	0	0
19	Z	479	0	516	6	0
19	z	479	0	516	0	0
20	A	10	0	0	1	0
20	a	10	0	0	0	0
21	A	2	0	0	0	0
21	V	1	0	0	0	0
21	a	1	0	0	0	0
21	c	1	0	0	0	0
21	u	1	0	0	0	0
22	A	4	0	1	0	0
22	a	4	0	1	0	0
23	A	195	0	216	21	0
23	B	1105	0	1224	105	0
23	C	845	0	936	87	0
23	D	195	0	216	17	0
23	a	260	0	288	0	0
23	b	1105	0	1224	0	0
23	c	845	0	936	0	0
23	d	130	0	144	0	0
24	A	64	0	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	D	64	0	74	11	0
24	a	64	0	74	0	0
24	d	64	0	74	0	0
25	A	40	0	55	16	0
25	B	120	0	165	86	0
25	C	120	0	164	48	0
25	F	40	0	54	29	0
25	H	40	0	55	21	0
25	K	40	0	55	30	0
25	T	40	0	55	38	0
25	a	40	0	55	0	0
25	b	120	0	165	0	0
25	c	120	0	165	0	0
25	f	40	0	55	0	0
25	h	40	0	55	0	0
25	k	40	0	55	0	0
25	t	40	0	55	0	0
26	A	55	0	80	15	0
26	D	55	0	80	7	0
26	a	55	0	80	0	0
26	d	55	0	80	0	0
27	A	54	0	78	4	0
27	B	54	0	78	9	0
27	X	43	0	53	4	0
27	a	108	0	156	0	0
27	b	108	0	156	0	0
27	x	43	0	53	0	0
28	A	51	0	72	2	0
28	B	51	0	72	4	0
28	C	102	0	144	2	0
28	J	51	0	72	5	0
28	Z	37	0	44	2	0
28	a	51	0	72	0	0
28	b	51	0	72	0	0
28	c	102	0	144	0	0
28	j	51	0	72	0	0
28	z	37	0	44	0	0
29	A	1	0	0	0	0
29	a	1	0	0	0	0
30	B	1	0	0	0	0
30	F	1	0	0	0	0
30	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	b	1	0	0	0	0
30	f	1	0	0	0	0
30	o	1	0	0	0	0
31	B	49	0	74	3	0
31	D	98	0	148	11	0
31	E	42	0	57	4	0
31	L	49	0	74	4	0
31	a	49	0	74	0	0
31	b	49	0	74	0	0
31	d	49	0	74	0	0
31	e	42	0	57	0	0
31	l	49	0	74	0	0
32	C	186	0	246	11	0
32	D	62	0	82	1	0
32	H	62	0	82	5	0
32	c	186	0	246	0	0
32	d	62	0	82	0	0
32	h	62	0	82	0	0
33	E	43	0	30	5	0
33	V	43	0	30	3	0
33	e	43	0	30	0	0
33	v	43	0	30	0	0
34	J	1	0	0	0	0
34	j	1	0	0	0	0
All	All	49966	0	51358	844	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 844 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:620:BCR:C20	25:B:620:BCR:C19	1.74	1.66
25:T:101:BCR:C16	25:T:101:BCR:C17	1.75	1.64
25:K:101:BCR:C19	25:K:101:BCR:C20	1.75	1.64
25:K:101:BCR:C37	25:K:101:BCR:C22	1.75	1.63
25:A:609:BCR:C19	25:A:609:BCR:C20	1.74	1.63

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	336/334 (101%)	332 (99%)	3 (1%)	1 (0%)	46	83
1	a	336/334 (101%)	330 (98%)	5 (2%)	1 (0%)	46	83
2	B	512/504 (102%)	507 (99%)	5 (1%)	0	100	100
2	b	512/504 (102%)	503 (98%)	9 (2%)	0	100	100
3	C	454/451 (101%)	443 (98%)	9 (2%)	2 (0%)	39	80
3	c	454/451 (101%)	441 (97%)	11 (2%)	2 (0%)	39	80
4	D	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
4	d	340/342 (99%)	333 (98%)	7 (2%)	0	100	100
5	E	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
5	e	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	32/34 (94%)	32 (100%)	0	0	100	100
7	H	65/65 (100%)	60 (92%)	5 (8%)	0	100	100
7	h	65/65 (100%)	57 (88%)	8 (12%)	0	100	100
8	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
9	J	36/38 (95%)	36 (100%)	0	0	100	100
9	j	36/38 (95%)	36 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/34 (97%)	33 (100%)	0	0	100	100
12	m	33/34 (97%)	33 (100%)	0	0	100	100
13	O	245/243 (101%)	237 (97%)	7 (3%)	1 (0%)	39	80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	245/243 (101%)	235 (96%)	9 (4%)	1 (0%)	39	80
14	T	29/30 (97%)	28 (97%)	1 (3%)	0	100	100
14	t	29/30 (97%)	29 (100%)	0	0	100	100
15	U	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
15	u	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	136/137 (99%)	131 (96%)	5 (4%)	0	100	100
17	Y	27/29 (93%)	27 (100%)	0	0	100	100
17	y	27/29 (93%)	27 (100%)	0	0	100	100
18	X	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
18	x	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	5252/5264 (100%)	5134 (98%)	110 (2%)	8 (0%)	56	86

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	58	ASN
13	o	58	ASN
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER

### 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	273/269 (102%)	273 (100%)	0	100	100
1	a	273/269 (102%)	272 (100%)	1 (0%)	93	96
2	B	412/402 (102%)	410 (100%)	2 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	412/402 (102%)	407 (99%)	5 (1%)	78	90
3	C	357/352 (101%)	354 (99%)	3 (1%)	86	93
3	c	357/352 (101%)	354 (99%)	3 (1%)	86	93
4	D	277/277 (100%)	274 (99%)	3 (1%)	80	90
4	d	277/277 (100%)	276 (100%)	1 (0%)	93	96
5	E	74/72 (103%)	73 (99%)	1 (1%)	74	89
5	e	74/72 (103%)	74 (100%)	0	100	100
6	F	28/28 (100%)	27 (96%)	1 (4%)	42	75
6	f	28/28 (100%)	28 (100%)	0	100	100
7	H	56/54 (104%)	52 (93%)	4 (7%)	18	58
7	h	56/54 (104%)	53 (95%)	3 (5%)	27	66
8	I	36/35 (103%)	36 (100%)	0	100	100
8	i	36/35 (103%)	36 (100%)	0	100	100
9	J	26/26 (100%)	26 (100%)	0	100	100
9	j	26/26 (100%)	26 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	20	59
10	k	30/30 (100%)	28 (93%)	2 (7%)	20	59
11	L	36/35 (103%)	35 (97%)	1 (3%)	51	79
11	l	36/35 (103%)	35 (97%)	1 (3%)	51	79
12	M	32/31 (103%)	31 (97%)	1 (3%)	47	78
12	m	32/31 (103%)	32 (100%)	0	100	100
13	O	210/206 (102%)	206 (98%)	4 (2%)	65	86
13	o	210/206 (102%)	206 (98%)	4 (2%)	65	86
14	T	29/27 (107%)	29 (100%)	0	100	100
14	t	29/27 (107%)	29 (100%)	0	100	100
15	U	84/84 (100%)	83 (99%)	1 (1%)	78	90
15	u	84/84 (100%)	83 (99%)	1 (1%)	78	90
16	V	118/117 (101%)	117 (99%)	1 (1%)	86	93
16	v	118/117 (101%)	117 (99%)	1 (1%)	86	93
17	Y	22/22 (100%)	21 (96%)	1 (4%)	34	70
17	y	22/22 (100%)	22 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	X	33/32 (103%)	33 (100%)	0	100	100
18	x	33/32 (103%)	32 (97%)	1 (3%)	48	78
19	Z	52/52 (100%)	50 (96%)	2 (4%)	40	74
19	z	52/52 (100%)	49 (94%)	3 (6%)	25	64
All	All	4370/4302 (102%)	4317 (99%)	53 (1%)	78	90

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	V	30	LYS
2	b	246	PHE
16	v	23	GLU
17	Y	27	MET
19	Z	31	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
12	M	33	GLN
1	a	198	HIS
3	c	25	ASN
12	m	33	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 166 ligands modelled in this entry, 16 are monoatomic - leaving 150 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$
20	OEX	A	601	1,3	0,15,15	0.00	-	0,32,32	0.00	-
22	BCT	A	604	29	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	A	605	-	57,73,73	2.58	22 (38%)	61,113,113	1.78	12 (19%)
23	CLA	A	606	-	57,73,73	2.55	22 (38%)	61,113,113	2.00	12 (19%)
24	PHO	A	607	-	67,69,69	1.25	8 (11%)	86,99,99	1.06	6 (6%)
23	CLA	A	608	-	57,73,73	2.53	23 (40%)	61,113,113	1.90	12 (19%)
25	BCR	A	609	-	41,41,41	9.45	30 (73%)	56,56,56	5.70	28 (50%)
26	PL9	A	610	-	54,55,55	4.01	16 (29%)	68,69,69	4.19	38 (55%)
27	SQD	A	611	-	53,54,54	1.49	3 (5%)	62,65,65	1.78	12 (19%)
28	LMG	A	612	-	51,51,55	1.28	5 (9%)	59,59,63	1.00	3 (5%)
23	CLA	B	602	-	57,73,73	2.56	22 (38%)	61,113,113	1.87	10 (16%)
23	CLA	B	603	-	57,73,73	2.54	22 (38%)	61,113,113	1.96	11 (18%)
23	CLA	B	604	-	57,73,73	2.55	22 (38%)	61,113,113	1.97	11 (18%)
23	CLA	B	605	-	57,73,73	2.52	21 (36%)	61,113,113	1.97	13 (21%)
23	CLA	B	606	-	57,73,73	2.56	22 (38%)	61,113,113	1.94	8 (13%)
23	CLA	B	607[A]	-	57,73,73	2.53	21 (36%)	61,113,113	2.02	14 (22%)
23	CLA	B	607[B]	-	57,73,73	2.53	22 (38%)	61,113,113	2.02	13 (21%)
23	CLA	B	608	-	57,73,73	2.55	22 (38%)	61,113,113	1.92	13 (21%)
23	CLA	B	609	-	57,73,73	2.56	22 (38%)	61,113,113	1.96	15 (24%)
23	CLA	B	610	-	57,73,73	2.53	22 (38%)	61,113,113	1.86	8 (13%)
23	CLA	B	611	-	57,73,73	2.54	21 (36%)	61,113,113	1.80	10 (16%)
23	CLA	B	612	-	57,73,73	2.53	22 (38%)	61,113,113	1.97	11 (18%)
23	CLA	B	613	-	57,73,73	2.56	22 (38%)	61,113,113	1.96	12 (19%)
23	CLA	B	614	-	57,73,73	2.56	22 (38%)	61,113,113	1.84	10 (16%)
23	CLA	B	615	-	57,73,73	2.55	22 (38%)	61,113,113	1.88	10 (16%)
23	CLA	B	616	-	57,73,73	2.54	20 (35%)	61,113,113	1.99	14 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	B	617	-	57,73,73	2.55	22 (38%)	61,113,113	1.93	13 (21%)
25	BCR	B	618	-	41,41,41	9.26	29 (70%)	56,56,56	6.15	30 (53%)
25	BCR	B	619	-	41,41,41	9.70	30 (73%)	56,56,56	5.31	27 (48%)
25	BCR	B	620	-	41,41,41	9.27	30 (73%)	56,56,56	6.13	32 (57%)
28	LMG	B	621	-	51,51,55	1.25	4 (7%)	59,59,63	0.91	2 (3%)
31	LHG	B	622	-	48,48,48	1.12	3 (6%)	49,54,54	0.98	3 (6%)
27	SQD	B	623	-	53,54,54	1.47	3 (5%)	62,65,65	1.73	9 (14%)
23	CLA	C	501	-	57,73,73	2.54	21 (36%)	61,113,113	1.98	12 (19%)
23	CLA	C	502	-	57,73,73	2.53	22 (38%)	61,113,113	1.87	12 (19%)
23	CLA	C	503	-	57,73,73	2.55	21 (36%)	61,113,113	1.84	11 (18%)
23	CLA	C	504	-	57,73,73	2.53	22 (38%)	61,113,113	1.99	11 (18%)
23	CLA	C	505	-	57,73,73	2.57	22 (38%)	61,113,113	1.88	9 (14%)
23	CLA	C	506	-	57,73,73	2.54	21 (36%)	61,113,113	1.92	9 (14%)
23	CLA	C	507	-	57,73,73	2.50	21 (36%)	61,113,113	2.11	13 (21%)
23	CLA	C	508	-	57,73,73	2.56	22 (38%)	61,113,113	1.95	10 (16%)
23	CLA	C	509	-	57,73,73	2.53	21 (36%)	61,113,113	1.94	13 (21%)
23	CLA	C	510	-	57,73,73	2.56	22 (38%)	61,113,113	1.79	12 (19%)
23	CLA	C	511	3	57,73,73	2.54	21 (36%)	61,113,113	1.83	11 (18%)
23	CLA	C	512	-	57,73,73	2.55	22 (38%)	61,113,113	1.89	12 (19%)
23	CLA	C	513	-	57,73,73	2.52	22 (38%)	61,113,113	1.92	11 (18%)
25	BCR	C	514	-	41,41,41	9.22	31 (75%)	56,56,56	6.19	30 (53%)
25	BCR	C	515	-	41,41,41	9.35	29 (70%)	56,56,56	6.09	29 (51%)
32	DGD	C	516	-	63,63,67	1.67	16 (25%)	77,77,81	0.93	2 (2%)
32	DGD	C	517	-	63,63,67	1.61	17 (26%)	77,77,81	1.03	5 (6%)
32	DGD	C	518	-	63,63,67	1.64	15 (23%)	77,77,81	1.04	5 (6%)
28	LMG	C	519	-	51,51,55	1.30	4 (7%)	59,59,63	1.07	2 (3%)
28	LMG	C	520	-	51,51,55	1.28	5 (9%)	59,59,63	1.03	4 (6%)
25	BCR	C	521	-	41,41,41	9.35	29 (70%)	56,56,56	5.96	27 (48%)
24	PHO	D	401	-	67,69,69	1.25	7 (10%)	86,99,99	1.07	5 (5%)
23	CLA	D	402	-	57,73,73	2.55	22 (38%)	61,113,113	1.98	13 (21%)
23	CLA	D	403	-	57,73,73	2.57	22 (38%)	61,113,113	1.80	13 (21%)
23	CLA	D	404	-	57,73,73	2.53	22 (38%)	61,113,113	1.94	12 (19%)
26	PL9	D	405	-	54,55,55	4.03	16 (29%)	68,69,69	4.16	35 (51%)
32	DGD	D	406	-	63,63,67	1.69	15 (23%)	77,77,81	1.14	7 (9%)
31	LHG	D	407	-	48,48,48	1.09	3 (6%)	49,54,54	0.91	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LHG	D	408	-	48,48,48	1.09	3 (6%)	49,54,54	0.99	2 (4%)
31	LHG	E	101	-	41,41,48	1.18	3 (7%)	42,47,54	0.93	2 (4%)
33	HEM	E	102	5,6	24,50,50	2.25	5 (20%)	16,82,82	1.61	2 (12%)
25	BCR	F	101	-	41,41,41	9.29	28 (68%)	56,56,56	6.12	29 (51%)
25	BCR	H	101	-	41,41,41	9.29	29 (70%)	56,56,56	5.90	36 (64%)
32	DGD	H	102	-	63,63,67	1.66	15 (23%)	77,77,81	0.93	2 (2%)
28	LMG	J	101	34	51,51,55	1.29	4 (7%)	59,59,63	0.99	4 (6%)
25	BCR	K	101	-	41,41,41	9.26	29 (70%)	56,56,56	5.96	27 (48%)
31	LHG	L	101	-	48,48,48	1.08	3 (6%)	49,54,54	0.88	2 (4%)
25	BCR	T	101	-	41,41,41	9.32	28 (68%)	56,56,56	6.10	29 (51%)
33	HEM	V	202	16	24,50,50	2.19	6 (25%)	16,82,82	1.54	3 (18%)
27	SQD	X	101	-	42,43,54	1.69	3 (7%)	51,54,65	1.78	8 (15%)
28	LMG	Z	101	-	37,37,55	1.40	5 (13%)	45,45,63	1.33	3 (6%)
20	OEX	a	601	1,3	0,15,15	0.00	-	0,32,32	0.00	-
22	BCT	a	603	29	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	a	604	-	57,73,73	2.58	22 (38%)	61,113,113	1.81	13 (21%)
23	CLA	a	605	-	57,73,73	2.56	22 (38%)	61,113,113	1.97	13 (21%)
24	PHO	a	606	-	67,69,69	1.24	9 (13%)	86,99,99	1.06	6 (6%)
23	CLA	a	607	-	57,73,73	2.55	21 (36%)	61,113,113	1.90	10 (16%)
25	BCR	a	608	-	41,41,41	9.36	30 (73%)	56,56,56	5.72	27 (48%)
26	PL9	a	609	-	54,55,55	3.99	16 (29%)	68,69,69	4.27	36 (52%)
27	SQD	a	610	-	53,54,54	1.49	3 (5%)	62,65,65	1.79	12 (19%)
28	LMG	a	611	-	51,51,55	1.28	5 (9%)	59,59,63	1.03	3 (5%)
27	SQD	a	612	-	53,54,54	1.50	3 (5%)	62,65,65	1.42	6 (9%)
23	CLA	a	613	-	57,73,73	2.55	22 (38%)	61,113,113	1.98	14 (22%)
31	LHG	a	614	-	48,48,48	1.07	3 (6%)	49,54,54	1.05	3 (6%)
27	SQD	b	601	-	53,54,54	1.51	3 (5%)	62,65,65	1.42	6 (9%)
27	SQD	b	602	-	53,54,54	1.49	4 (7%)	62,65,65	1.73	9 (14%)
23	CLA	b	604	-	57,73,73	2.54	21 (36%)	61,113,113	1.88	12 (19%)
23	CLA	b	605	-	57,73,73	2.57	22 (38%)	61,113,113	1.94	11 (18%)
23	CLA	b	606	-	57,73,73	2.57	22 (38%)	61,113,113	1.97	13 (21%)
23	CLA	b	607	-	57,73,73	2.52	21 (36%)	61,113,113	1.94	13 (21%)
23	CLA	b	608	-	57,73,73	2.56	22 (38%)	61,113,113	1.91	12 (19%)
23	CLA	b	609[A]	-	57,73,73	2.52	22 (38%)	61,113,113	2.02	13 (21%)
23	CLA	b	609[B]	-	57,73,73	2.54	22 (38%)	61,113,113	2.04	14 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	b	610	-	57,73,73	2.55	22 (38%)	61,113,113	1.95	12 (19%)
23	CLA	b	611	-	57,73,73	2.56	22 (38%)	61,113,113	1.93	14 (22%)
23	CLA	b	612	-	57,73,73	2.54	22 (38%)	61,113,113	1.84	9 (14%)
23	CLA	b	613	-	57,73,73	2.56	22 (38%)	61,113,113	1.79	12 (19%)
23	CLA	b	614	-	57,73,73	2.55	21 (36%)	61,113,113	1.95	11 (18%)
23	CLA	b	615	-	57,73,73	2.55	22 (38%)	61,113,113	2.00	14 (22%)
23	CLA	b	616	-	57,73,73	2.52	21 (36%)	61,113,113	1.86	12 (19%)
23	CLA	b	617	-	57,73,73	2.54	22 (38%)	61,113,113	1.87	10 (16%)
23	CLA	b	618	-	57,73,73	2.56	22 (38%)	61,113,113	1.99	12 (19%)
23	CLA	b	619	-	57,73,73	2.54	22 (38%)	61,113,113	1.93	12 (19%)
25	BCR	b	620	-	41,41,41	9.17	29 (70%)	56,56,56	5.95	29 (51%)
25	BCR	b	621	-	41,41,41	9.24	29 (70%)	56,56,56	5.63	28 (50%)
25	BCR	b	622	-	41,41,41	9.40	31 (75%)	56,56,56	5.88	32 (57%)
28	LMG	b	623	-	51,51,55	1.27	4 (7%)	59,59,63	0.95	2 (3%)
31	LHG	b	624	-	48,48,48	1.08	3 (6%)	49,54,54	0.97	3 (6%)
23	CLA	c	502	-	57,73,73	2.52	22 (38%)	61,113,113	1.90	11 (18%)
23	CLA	c	503	-	57,73,73	2.54	22 (38%)	61,113,113	1.95	12 (19%)
23	CLA	c	504	-	57,73,73	2.55	22 (38%)	61,113,113	1.83	10 (16%)
23	CLA	c	505	-	57,73,73	2.54	22 (38%)	61,113,113	1.96	12 (19%)
23	CLA	c	506	-	57,73,73	2.56	23 (40%)	61,113,113	1.87	9 (14%)
23	CLA	c	507	-	57,73,73	2.55	22 (38%)	61,113,113	1.96	10 (16%)
23	CLA	c	508	-	57,73,73	2.50	21 (36%)	61,113,113	2.14	13 (21%)
23	CLA	c	509	-	57,73,73	2.53	22 (38%)	61,113,113	1.98	11 (18%)
23	CLA	c	510	-	57,73,73	2.53	20 (35%)	61,113,113	1.94	12 (19%)
23	CLA	c	511	-	57,73,73	2.56	22 (38%)	61,113,113	1.76	11 (18%)
23	CLA	c	512	3	57,73,73	2.55	20 (35%)	61,113,113	1.81	10 (16%)
23	CLA	c	513	-	57,73,73	2.55	21 (36%)	61,113,113	1.90	12 (19%)
23	CLA	c	514	-	57,73,73	2.52	22 (38%)	61,113,113	1.84	10 (16%)
25	BCR	c	515	-	41,41,41	9.21	30 (73%)	56,56,56	6.31	32 (57%)
25	BCR	c	516	-	41,41,41	9.41	30 (73%)	56,56,56	5.93	27 (48%)
32	DGD	c	517	-	63,63,67	1.67	16 (25%)	77,77,81	0.93	4 (5%)
32	DGD	c	518	-	63,63,67	1.62	15 (23%)	77,77,81	1.00	4 (5%)
32	DGD	c	519	-	63,63,67	1.63	16 (25%)	77,77,81	1.09	4 (5%)
28	LMG	c	520	-	51,51,55	1.30	4 (7%)	59,59,63	1.03	2 (3%)
28	LMG	c	521	-	51,51,55	1.29	5 (9%)	59,59,63	1.03	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	c	522	-	41,41,41	9.29	29 (70%)	56,56,56	5.92	28 (50%)
24	PHO	d	401	-	67,69,69	1.25	8 (11%)	86,99,99	1.03	5 (5%)
23	CLA	d	402	-	57,73,73	2.56	22 (38%)	61,113,113	1.80	11 (18%)
23	CLA	d	403	-	57,73,73	2.52	21 (36%)	61,113,113	1.88	12 (19%)
26	PL9	d	404	-	54,55,55	4.04	16 (29%)	68,69,69	4.13	35 (51%)
32	DGD	d	405	-	63,63,67	1.67	16 (25%)	77,77,81	1.04	6 (7%)
31	LHG	d	406	-	48,48,48	1.10	3 (6%)	49,54,54	0.91	3 (6%)
31	LHG	e	101	-	41,41,48	1.18	3 (7%)	42,47,54	0.98	2 (4%)
33	HEM	e	102	5,6	24,50,50	2.21	5 (20%)	16,82,82	1.68	2 (12%)
25	BCR	f	101	-	41,41,41	9.30	30 (73%)	56,56,56	5.87	28 (50%)
25	BCR	h	101	-	41,41,41	9.29	29 (70%)	56,56,56	5.92	36 (64%)
32	DGD	h	102	-	63,63,67	1.65	15 (23%)	77,77,81	0.99	4 (5%)
28	LMG	j	101	34	51,51,55	1.28	4 (7%)	59,59,63	0.93	3 (5%)
25	BCR	k	101	-	41,41,41	9.36	30 (73%)	56,56,56	5.76	26 (46%)
31	LHG	l	101	-	48,48,48	1.10	2 (4%)	49,54,54	0.90	2 (4%)
25	BCR	t	101	-	41,41,41	9.37	29 (70%)	56,56,56	5.84	27 (48%)
33	HEM	v	201	16	24,50,50	2.26	6 (25%)	16,82,82	1.61	3 (18%)
27	SQD	x	101	-	42,43,54	1.69	3 (7%)	51,54,65	1.78	8 (15%)
28	LMG	z	101	-	37,37,55	1.40	5 (13%)	45,45,63	1.27	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	OEX	A	601	1,3	-	0/0/68/68	0/0/6/6
22	BCT	A	604	29	-	0/0/0/0	0/0/0/0
23	CLA	A	605	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	A	606	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	A	607	-	-	0/53/103/103	0/1/6/6
23	CLA	A	608	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	A	609	-	-	1/29/63/63	0/2/2/2
26	PL9	A	610	-	-	0/53/73/73	0/1/1/1
27	SQD	A	611	-	-	0/49/69/69	0/1/1/1
28	LMG	A	612	-	-	0/46/66/70	0/1/1/1
23	CLA	B	602	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	607[A]	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	607[B]	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	609	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	610	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	613	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	617	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	B	618	-	-	1/29/63/63	0/2/2/2
25	BCR	B	619	-	-	1/29/63/63	0/2/2/2
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
28	LMG	B	621	-	-	0/46/66/70	0/1/1/1
31	LHG	B	622	-	-	0/53/53/53	0/0/0/0
27	SQD	B	623	-	-	0/49/69/69	0/1/1/1
23	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	502	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	C	503	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	505	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	508	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	511	3	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	C	512	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	C	513	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	C	514	-	-	0/29/63/63	0/2/2/2
25	BCR	C	515	-	-	2/29/63/63	0/2/2/2
32	DGD	C	516	-	-	0/51/91/95	0/2/2/2
32	DGD	C	517	-	-	0/51/91/95	0/2/2/2
32	DGD	C	518	-	-	0/51/91/95	0/2/2/2
28	LMG	C	519	-	-	0/46/66/70	0/1/1/1
28	LMG	C	520	-	-	0/46/66/70	0/1/1/1
25	BCR	C	521	-	-	0/29/63/63	0/2/2/2
24	PHO	D	401	-	-	0/53/103/103	0/1/6/6
23	CLA	D	402	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	D	403	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	D	404	-	3/3/20/25	0/37/135/135	0/0/9/9
26	PL9	D	405	-	-	0/53/73/73	0/1/1/1
32	DGD	D	406	-	-	0/51/91/95	0/2/2/2
31	LHG	D	407	-	-	0/53/53/53	0/0/0/0
31	LHG	D	408	-	-	0/53/53/53	0/0/0/0
31	LHG	E	101	-	-	0/46/46/53	0/0/0/0
33	HEM	E	102	5,6	-	0/6/54/54	0/0/8/8
25	BCR	F	101	-	-	0/29/63/63	0/2/2/2
25	BCR	H	101	-	-	0/29/63/63	0/2/2/2
32	DGD	H	102	-	-	0/51/91/95	0/2/2/2
28	LMG	J	101	34	-	0/46/66/70	0/1/1/1
25	BCR	K	101	-	-	1/29/63/63	0/2/2/2
31	LHG	L	101	-	-	0/53/53/53	0/0/0/0
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
33	HEM	V	202	16	-	0/6/54/54	0/0/8/8
27	SQD	X	101	-	-	0/38/58/69	0/1/1/1
28	LMG	Z	101	-	-	1/31/51/70	0/1/1/1
20	OEX	a	601	1,3	-	0/0/68/68	0/0/6/6
22	BCT	a	603	29	-	0/0/0/0	0/0/0/0
23	CLA	a	604	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	a	605	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	a	606	-	-	0/53/103/103	0/1/6/6
23	CLA	a	607	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	a	608	-	-	1/29/63/63	0/2/2/2
26	PL9	a	609	-	-	0/53/73/73	0/1/1/1
27	SQD	a	610	-	-	0/49/69/69	0/1/1/1
28	LMG	a	611	-	-	0/46/66/70	0/1/1/1
27	SQD	a	612	-	-	0/49/69/69	0/1/1/1
23	CLA	a	613	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LHG	a	614	-	-	0/53/53/53	0/0/0/0
27	SQD	b	601	-	-	0/49/69/69	0/1/1/1
27	SQD	b	602	-	-	0/49/69/69	0/1/1/1
23	CLA	b	604	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	609[A]	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	609[B]	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	610	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	612	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	614	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	615	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	616	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	618	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	619	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	b	620	-	-	0/29/63/63	0/2/2/2
25	BCR	b	621	-	-	4/29/63/63	0/2/2/2
25	BCR	b	622	-	-	0/29/63/63	0/2/2/2
28	LMG	b	623	-	-	0/46/66/70	0/1/1/1
31	LHG	b	624	-	-	0/53/53/53	0/0/0/0
23	CLA	c	502	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	504	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	505	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	506	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	507	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	508	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	510	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	511	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	512	3	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	c	513	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	514	-	2/2/20/25	0/37/135/135	0/0/9/9
25	BCR	c	515	-	-	0/29/63/63	0/2/2/2
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
32	DGD	c	517	-	-	0/51/91/95	0/2/2/2
32	DGD	c	518	-	-	0/51/91/95	0/2/2/2
32	DGD	c	519	-	-	0/51/91/95	0/2/2/2
28	LMG	c	520	-	-	0/46/66/70	0/1/1/1
28	LMG	c	521	-	-	0/46/66/70	0/1/1/1
25	BCR	c	522	-	-	1/29/63/63	0/2/2/2
24	PHO	d	401	-	-	0/53/103/103	0/1/6/6
23	CLA	d	402	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	d	403	-	3/3/20/25	0/37/135/135	0/0/9/9
26	PL9	d	404	-	-	0/53/73/73	0/1/1/1
32	DGD	d	405	-	-	0/51/91/95	0/2/2/2
31	LHG	d	406	-	-	0/53/53/53	0/0/0/0
31	LHG	e	101	-	-	0/46/46/53	0/0/0/0
33	HEM	e	102	5,6	-	0/6/54/54	0/0/8/8
25	BCR	f	101	-	-	0/29/63/63	0/2/2/2
25	BCR	h	101	-	-	1/29/63/63	0/2/2/2
32	DGD	h	102	-	-	0/51/91/95	0/2/2/2
28	LMG	j	101	34	-	0/46/66/70	0/1/1/1
25	BCR	k	101	-	-	2/29/63/63	0/2/2/2
31	LHG	l	101	-	-	0/53/53/53	0/0/0/0
25	BCR	t	101	-	-	1/29/63/63	0/2/2/2
33	HEM	v	201	16	-	0/6/54/54	0/0/8/8
27	SQD	x	101	-	-	0/38/58/69	0/1/1/1
28	LMG	z	101	-	-	1/31/51/70	0/1/1/1

The worst 5 of 2593 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	619	BCR	C21-C22	-25.81	1.00	1.35
25	H	101	BCR	C21-C22	-23.42	1.04	1.35
25	F	101	BCR	C21-C22	-22.64	1.05	1.35
25	C	514	BCR	C21-C22	-22.64	1.05	1.35
25	c	516	BCR	C21-C22	-22.57	1.05	1.35

The worst 5 of 1830 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	622	BCR	C38-C26-C25	-15.64	107.96	124.62
25	T	101	BCR	C33-C5-C6	-15.52	108.08	124.62
25	B	620	BCR	C38-C26-C25	-15.34	108.27	124.62
25	c	515	BCR	C38-C26-C25	-14.98	108.66	124.62
25	C	514	BCR	C38-C26-C25	-14.58	109.09	124.62

5 of 200 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	b	609[B]	CLA	NA
23	b	609[B]	CLA	NC
23	b	609[B]	CLA	ND
23	c	514	CLA	NC
23	c	514	CLA	ND

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	k	101	BCR	C10-C11-C12-C13
25	t	101	BCR	C21-C20-C19-C18
25	b	621	BCR	C16-C17-C18-C19
25	c	522	BCR	C21-C20-C19-C18
25	B	618	BCR	C21-C20-C19-C18

There are no ring outliers.

73 monomers are involved in 543 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	601	OEX	1	0
23	A	605	CLA	8	0
23	A	606	CLA	6	0
24	A	607	PHO	1	0
23	A	608	CLA	7	0
25	A	609	BCR	16	0
26	A	610	PL9	15	0
27	A	611	SQD	4	0
28	A	612	LMG	2	0
23	B	602	CLA	5	0
23	B	603	CLA	2	0
23	B	604	CLA	15	0
23	B	605	CLA	10	0
23	B	606	CLA	16	0
23	B	607[A]	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	607[B]	CLA	4	0
23	B	608	CLA	12	0
23	B	609	CLA	1	0
23	B	610	CLA	5	0
23	B	611	CLA	3	0
23	B	612	CLA	8	0
23	B	613	CLA	9	0
23	B	614	CLA	6	0
23	B	615	CLA	8	0
23	B	616	CLA	5	0
23	B	617	CLA	14	0
25	B	618	BCR	27	0
25	B	619	BCR	28	0
25	B	620	BCR	36	0
28	B	621	LMG	4	0
31	B	622	LHG	3	0
27	B	623	SQD	9	0
23	C	501	CLA	8	0
23	C	502	CLA	12	0
23	C	503	CLA	12	0
23	C	504	CLA	10	0
23	C	505	CLA	8	0
23	C	506	CLA	11	0
23	C	507	CLA	12	0
23	C	508	CLA	7	0
23	C	509	CLA	6	0
23	C	510	CLA	9	0
23	C	511	CLA	10	0
23	C	512	CLA	6	0
23	C	513	CLA	4	0
25	C	514	BCR	11	0
25	C	515	BCR	22	0
32	C	516	DGD	2	0
32	C	517	DGD	2	0
32	C	518	DGD	7	0
28	C	519	LMG	1	0
28	C	520	LMG	1	0
25	C	521	BCR	15	0
24	D	401	PHO	11	0
23	D	402	CLA	9	0
23	D	403	CLA	6	0
23	D	404	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	D	405	PL9	7	0
32	D	406	DGD	1	0
31	D	407	LHG	1	0
31	D	408	LHG	10	0
31	E	101	LHG	4	0
33	E	102	HEM	5	0
25	F	101	BCR	29	0
25	H	101	BCR	21	0
32	H	102	DGD	5	0
28	J	101	LMG	5	0
25	K	101	BCR	30	0
31	L	101	LHG	4	0
25	T	101	BCR	38	0
33	V	202	HEM	3	0
27	X	101	SQD	4	0
28	Z	101	LMG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	334/334 (100%)	-0.30	4 (1%) 81 73	57, 63, 84, 93	0
1	a	334/334 (100%)	-0.22	3 (0%) 85 80	78, 84, 104, 114	0
2	B	504/504 (100%)	-0.18	3 (0%) 90 86	59, 68, 89, 111	0
2	b	504/504 (100%)	-0.10	7 (1%) 78 69	80, 88, 110, 131	0
3	C	451/451 (100%)	-0.05	10 (2%) 65 56	61, 72, 85, 97	0
3	c	451/451 (100%)	-0.18	6 (1%) 79 71	82, 93, 105, 118	0
4	D	342/342 (100%)	-0.28	1 (0%) 94 92	57, 64, 80, 102	0
4	d	342/342 (100%)	-0.21	5 (1%) 76 67	78, 85, 101, 123	0
5	E	81/81 (100%)	-0.12	0 100 100	68, 81, 98, 104	0
5	e	81/81 (100%)	0.11	1 (1%) 81 73	89, 102, 119, 125	0
6	F	34/34 (100%)	-0.31	1 (2%) 55 44	68, 74, 99, 102	0
6	f	34/34 (100%)	-0.22	1 (2%) 55 44	89, 95, 120, 122	0
7	H	65/65 (100%)	0.26	6 (9%) 11 9	64, 74, 81, 99	0
7	h	65/65 (100%)	0.40	4 (6%) 24 17	85, 95, 102, 120	0
8	I	38/38 (100%)	-0.23	0 100 100	70, 74, 105, 109	0
8	i	38/38 (100%)	-0.11	1 (2%) 59 49	90, 95, 126, 130	0
9	J	38/38 (100%)	-0.16	1 (2%) 59 49	66, 78, 109, 112	0
9	j	38/38 (100%)	-0.19	1 (2%) 59 49	87, 99, 129, 133	0
10	K	37/37 (100%)	-0.55	0 100 100	74, 79, 86, 88	0
10	k	37/37 (100%)	-0.03	1 (2%) 58 48	94, 100, 107, 108	0
11	L	37/37 (100%)	0.06	5 (13%) 4 5	58, 62, 90, 99	0
11	l	37/37 (100%)	-0.05	2 (5%) 29 23	79, 83, 111, 120	0
12	M	34/34 (100%)	-0.63	0 100 100	62, 64, 77, 93	0
12	m	34/34 (100%)	-0.44	0 100 100	83, 84, 98, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/243 (100%)	-0.24	0 100 100	59, 73, 95, 111	0
13	o	243/243 (100%)	0.04	4 (1%) 74 65	79, 94, 116, 132	0
14	T	30/30 (100%)	-0.11	3 (10%) 9 8	60, 64, 85, 93	0
14	t	30/30 (100%)	-0.42	0 100 100	80, 85, 105, 114	0
15	U	97/97 (100%)	-0.10	1 (1%) 84 78	64, 71, 89, 90	0
15	u	97/97 (100%)	-0.18	1 (1%) 84 78	84, 92, 110, 111	0
16	V	137/137 (100%)	-0.30	1 (0%) 89 84	64, 69, 80, 88	0
16	v	137/137 (100%)	-0.23	3 (2%) 65 56	84, 89, 101, 109	0
17	Y	29/29 (100%)	-0.14	1 (3%) 49 39	82, 89, 115, 118	0
17	y	29/29 (100%)	-0.30	0 100 100	103, 110, 136, 138	0
18	X	39/39 (100%)	0.08	6 (15%) 3 4	74, 80, 107, 108	0
18	x	39/39 (100%)	-0.10	3 (7%) 16 12	95, 101, 127, 129	0
19	Z	62/62 (100%)	-0.30	1 (1%) 74 65	80, 89, 109, 112	0
19	z	62/62 (100%)	-0.13	4 (6%) 22 16	101, 110, 129, 133	0
All	All	5264/5264 (100%)	-0.16	91 (1%) 73 64	57, 83, 107, 138	0

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	L	2	GLU	4.9
11	L	3	PRO	4.3
7	H	2	ALA	4.3
7	h	2	ALA	4.1
18	X	2	THR	3.9

## 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
25	BCR	b	620	40/40	0.78	0.60	5.78	84,88,90,90	0
25	BCR	b	621	40/40	0.76	0.40	4.94	83,89,101,101	0
27	SQD	a	610	54/54	0.69	0.50	4.07	110,119,128,128	0
25	BCR	A	609	40/40	0.77	0.55	4.05	63,68,73,73	0
25	BCR	a	608	40/40	0.62	0.65	3.97	83,89,93,94	0
32	DGD	D	406	62/66	0.69	0.44	3.36	118,130,143,144	0
25	BCR	K	101	40/40	0.79	0.39	3.07	75,78,79,80	0
25	BCR	T	101	40/40	0.69	0.41	2.81	65,78,85,86	0
23	CLA	B	602	65/65	0.80	0.41	2.46	73,82,107,107	0
26	PL9	a	609	55/55	0.59	0.45	2.32	113,130,139,140	0
23	CLA	a	607	65/65	0.85	0.41	2.27	83,85,133,133	0
28	LMG	c	520	51/55	0.77	0.39	2.25	92,118,134,135	0
25	BCR	B	618	40/40	0.82	0.38	2.05	63,68,69,70	0
26	PL9	A	610	55/55	0.46	0.37	2.04	93,109,118,119	0
28	LMG	b	623	51/55	0.81	0.38	2.00	91,100,112,116	0
23	CLA	b	604	65/65	0.76	0.73	1.96	94,102,127,128	0
23	CLA	b	616	65/65	0.88	0.31	1.93	80,84,106,108	0
25	BCR	t	101	40/40	0.77	0.37	1.92	86,99,106,106	0
28	LMG	z	101	37/55	0.77	0.50	1.88	117,145,149,150	0
22	BCT	a	603	4/4	0.89	0.48	1.88	100,101,101,103	0
27	SQD	x	101	43/54	0.73	0.49	1.84	128,136,140,140	0
23	CLA	d	403	65/65	0.83	0.34	1.83	86,89,126,128	0
25	BCR	B	619	40/40	0.87	0.30	1.78	62,69,81,81	0
27	SQD	b	602	54/54	0.76	0.42	1.59	99,107,121,121	0
23	CLA	D	404	65/65	0.87	0.34	1.54	65,68,106,107	0
32	DGD	c	519	62/66	0.83	0.47	1.54	83,93,113,117	0
28	LMG	c	521	51/55	0.74	0.50	1.53	104,137,142,143	0
23	CLA	A	608	65/65	0.89	0.35	1.52	62,65,112,113	0
23	CLA	a	605	65/65	0.83	0.33	1.43	80,83,124,126	0
25	BCR	F	101	40/40	0.77	0.33	1.41	66,71,88,90	0
23	CLA	C	501	65/65	0.88	0.35	1.40	69,73,85,87	0
28	LMG	C	520	51/55	0.64	0.55	1.34	83,117,122,123	0
23	CLA	c	502	65/65	0.76	0.35	1.32	90,93,106,108	0
32	DGD	d	405	62/66	0.57	0.49	1.29	138,151,164,165	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
28	LMG	B	621	51/55	0.85	0.35	1.23	70,80,92,95	0
34	MG	J	102	1/1	0.91	0.46	1.21	68,68,68,68	0
23	CLA	B	608	65/65	0.85	0.35	1.19	58,61,73,74	0
23	CLA	D	402	65/65	0.92	0.29	1.18	54,59,70,76	0
27	SQD	A	611	54/54	0.75	0.41	1.17	90,98,107,108	0
25	BCR	f	101	40/40	0.76	0.35	1.16	87,91,109,110	0
28	LMG	C	519	51/55	0.79	0.41	1.15	72,98,113,114	0
31	LHG	a	614	49/49	0.87	0.35	1.14	87,94,124,125	0
25	BCR	H	101	40/40	0.62	0.56	1.12	67,74,83,83	0
25	BCR	h	101	40/40	0.51	0.61	1.11	87,94,103,104	0
25	BCR	c	516	40/40	0.82	0.27	1.08	92,98,102,102	0
28	LMG	Z	101	37/55	0.80	0.41	1.07	96,124,129,129	0
25	BCR	C	515	40/40	0.75	0.34	1.01	71,78,81,82	0
23	CLA	b	615	65/65	0.87	0.35	0.99	81,85,91,92	0
32	DGD	c	518	62/66	0.88	0.31	0.97	84,96,124,124	0
23	CLA	b	613	65/65	0.86	0.44	0.97	82,86,94,98	0
25	BCR	B	620	40/40	0.81	0.40	0.97	68,74,80,80	0
28	LMG	A	612	51/55	0.85	0.30	0.95	94,100,105,105	0
25	BCR	b	622	40/40	0.71	0.55	0.94	89,94,100,101	0
31	LHG	E	101	42/49	0.72	0.39	0.92	110,124,127,127	0
23	CLA	a	613	65/65	0.90	0.35	0.91	75,79,91,96	0
31	LHG	e	101	42/49	0.72	0.41	0.90	131,145,147,148	0
23	CLA	b	609[A]	65/65	0.75	0.46	0.90	85,90,102,103	65
23	CLA	b	609[B]	65/65	0.75	0.46	0.90	83,87,93,95	65
33	HEM	e	102	43/43	0.89	0.45	0.90	101,103,107,108	0
23	CLA	b	618	65/65	0.78	0.39	0.81	86,89,107,108	0
24	PHO	a	606	64/64	0.88	0.33	0.81	78,83,86,87	0
25	BCR	c	515	40/40	0.79	0.45	0.79	99,105,108,108	0
23	CLA	b	614	65/65	0.92	0.29	0.73	80,83,94,96	0
32	DGD	C	517	62/66	0.88	0.32	0.71	63,75,103,104	0
23	CLA	b	610	65/65	0.90	0.31	0.69	79,82,94,95	0
24	PHO	D	401	64/64	0.85	0.31	0.67	59,63,69,73	0
27	SQD	X	101	43/54	0.80	0.39	0.66	108,115,119,119	0
32	DGD	C	518	62/66	0.85	0.36	0.65	62,72,93,97	0
23	CLA	A	606	65/65	0.89	0.31	0.62	60,62,104,106	0
24	PHO	d	401	64/64	0.87	0.29	0.61	80,84,90,94	0
23	CLA	c	503	65/65	0.81	0.36	0.58	85,87,101,103	0
31	LHG	B	622	49/49	0.88	0.25	0.57	70,75,81,82	0
23	CLA	C	507	65/65	0.77	0.41	0.56	70,74,92,94	0
25	BCR	k	101	40/40	0.86	0.32	0.53	95,99,100,100	0
28	LMG	J	101	51/55	0.80	0.33	0.49	66,76,106,108	0
23	CLA	b	611	65/65	0.90	0.26	0.47	82,86,92,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	C	502	65/65	0.91	0.34	0.47	65,67,80,83	0
23	CLA	C	505	65/65	0.85	0.30	0.46	69,71,85,85	0
23	CLA	c	513	65/65	0.77	0.40	0.46	99,102,124,124	0
23	CLA	c	507	65/65	0.85	0.30	0.46	93,100,136,136	0
31	LHG	L	101	49/49	0.92	0.23	0.45	63,72,83,85	0
23	CLA	B	617	65/65	0.74	0.45	0.43	63,69,118,119	0
31	LHG	d	406	49/49	0.88	0.35	0.42	85,89,98,102	0
23	CLA	b	619	65/65	0.81	0.44	0.42	83,90,139,139	0
20	OEX	A	601	10/10	0.94	0.31	0.40	63,64,67,67	0
25	BCR	c	522	40/40	0.58	0.39	0.40	91,95,98,99	0
23	CLA	a	604	65/65	0.84	0.31	0.37	77,80,87,95	0
33	HEM	v	201	43/43	0.91	0.30	0.36	84,86,88,90	0
29	FE2	A	613	1/1	0.85	0.29	0.36	67,67,67,67	0
23	CLA	D	403	65/65	0.91	0.28	0.36	54,59,75,76	0
27	SQD	b	601	54/54	0.81	0.32	0.35	91,103,109,109	0
23	CLA	b	617	65/65	0.82	0.37	0.34	82,86,121,122	0
31	LHG	l	101	49/49	0.81	0.30	0.32	84,92,104,106	0
25	BCR	C	514	40/40	0.76	0.38	0.32	78,84,87,88	0
23	CLA	C	512	65/65	0.75	0.42	0.31	78,82,103,104	0
27	SQD	a	612	54/54	0.85	0.31	0.29	111,124,129,130	0
31	LHG	D	408	49/49	0.87	0.35	0.29	67,74,103,104	0
23	CLA	B	616	65/65	0.84	0.35	0.22	65,68,86,87	0
23	CLA	C	506	65/65	0.82	0.30	0.22	72,79,115,115	0
23	CLA	B	607[B]	65/65	0.80	0.39	0.20	63,67,72,75	65
28	LMG	a	611	51/55	0.87	0.26	0.20	114,121,126,126	0
25	BCR	C	521	40/40	0.71	0.30	0.19	70,74,78,78	0
32	DGD	h	102	62/66	0.89	0.26	0.19	87,93,99,101	0
28	LMG	j	101	51/55	0.88	0.24	0.19	87,96,126,129	0
27	SQD	B	623	54/54	0.78	0.30	0.19	119,127,141,142	0
23	CLA	b	606	65/65	0.88	0.28	0.18	79,84,92,96	0
23	CLA	B	607[A]	65/65	0.80	0.39	0.18	65,69,81,82	65
23	CLA	c	508	65/65	0.81	0.31	0.17	91,94,113,115	0
23	CLA	C	503	65/65	0.91	0.34	0.17	68,72,76,77	0
23	CLA	c	505	65/65	0.93	0.26	0.16	86,89,115,116	0
24	PHO	A	607	64/64	0.93	0.26	0.10	57,62,65,67	0
26	PL9	d	404	55/55	0.67	0.31	0.08	80,84,91,93	0
23	CLA	A	605	65/65	0.92	0.25	0.08	56,59,66,75	0
33	HEM	E	102	43/43	0.90	0.28	0.03	80,82,86,87	0
23	CLA	B	603	65/65	0.91	0.23	0.02	64,67,72,73	0
23	CLA	C	513	65/65	0.71	0.47	-0.00	80,85,105,105	0
32	DGD	c	517	62/66	0.87	0.25	0.00	84,94,122,124	0
23	CLA	C	511	65/65	0.81	0.33	-0.04	70,75,78,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
20	OEX	a	601	10/10	0.95	0.32	-0.06	83,84,87,88	0
23	CLA	C	504	65/65	0.89	0.29	-0.08	66,68,95,95	0
23	CLA	B	610	65/65	0.88	0.30	-0.09	64,69,72,73	0
23	CLA	B	615	65/65	0.88	0.27	-0.11	61,65,101,102	0
23	CLA	B	613	65/65	0.91	0.29	-0.12	61,64,71,72	0
23	CLA	B	612	65/65	0.94	0.24	-0.16	60,62,73,75	0
32	DGD	C	516	62/66	0.89	0.22	-0.18	64,73,102,103	0
23	CLA	b	608	65/65	0.89	0.28	-0.20	80,84,95,97	0
23	CLA	B	604	65/65	0.90	0.25	-0.20	58,63,72,76	0
23	CLA	c	509	65/65	0.91	0.27	-0.21	87,90,115,119	0
23	CLA	c	504	65/65	0.80	0.29	-0.22	89,93,96,97	0
31	LHG	b	624	49/49	0.88	0.25	-0.22	91,96,102,102	0
23	CLA	B	611	65/65	0.89	0.27	-0.22	62,65,73,77	0
33	HEM	V	202	43/43	0.94	0.25	-0.25	63,65,68,69	0
23	CLA	c	512	65/65	0.88	0.25	-0.28	90,95,99,99	0
23	CLA	C	508	65/65	0.88	0.30	-0.31	66,70,95,99	0
23	CLA	b	605	65/65	0.89	0.24	-0.34	85,88,93,94	0
23	CLA	c	506	65/65	0.90	0.23	-0.35	89,92,106,106	0
32	DGD	H	102	62/66	0.89	0.23	-0.37	66,72,79,81	0
23	CLA	b	607	65/65	0.92	0.24	-0.41	81,84,111,112	0
23	CLA	B	606	65/65	0.90	0.23	-0.41	59,64,75,76	0
23	CLA	c	510	65/65	0.87	0.26	-0.42	91,93,108,108	0
31	LHG	D	407	49/49	0.91	0.21	-0.42	64,69,78,81	0
23	CLA	b	612	65/65	0.86	0.28	-0.44	85,90,92,93	0
23	CLA	B	609	65/65	0.92	0.24	-0.45	61,65,71,72	0
23	CLA	B	605	65/65	0.91	0.25	-0.45	60,63,91,91	0
23	CLA	c	514	65/65	0.87	0.29	-0.50	101,106,125,126	0
26	PL9	D	405	55/55	0.87	0.21	-0.52	60,64,70,72	0
23	CLA	B	614	65/65	0.91	0.26	-0.53	60,63,85,87	0
21	CL	A	602	1/1	0.80	0.23	-0.54	65,65,65,65	0
23	CLA	d	402	65/65	0.94	0.26	-0.59	75,80,95,96	0
23	CLA	c	511	65/65	0.93	0.24	-0.60	86,90,96,99	0
34	MG	j	102	1/1	0.85	0.19	-0.69	89,89,89,89	0
23	CLA	C	510	65/65	0.95	0.24	-0.84	65,69,76,78	0
23	CLA	C	509	65/65	0.88	0.23	-1.01	70,72,87,88	0
22	BCT	A	604	4/4	0.97	0.21	-1.04	79,80,81,82	0
29	FE2	a	615	1/1	0.81	0.17	-1.39	88,88,88,88	0
30	CA	o	301	1/1	0.96	0.26	-1.56	110,110,110,110	0
21	CL	a	602	1/1	0.63	0.16	-1.56	86,86,86,86	0
21	CL	A	603	1/1	0.92	0.20	-2.21	62,62,62,62	0
21	CL	c	501	1/1	0.95	0.16	-2.65	83,83,83,83	0
30	CA	b	603	1/1	0.19	0.58	-	137,137,137,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
30	CA	F	102	1/1	0.81	0.61	-	97,97,97,97	0
30	CA	B	601	1/1	0.21	1.08	-	117,117,117,117	0
21	CL	V	201	1/1	0.23	0.31	-	91,91,91,91	0
21	CL	u	201	1/1	0.06	0.16	-	112,112,112,112	0
30	CA	f	102	1/1	0.79	0.40	-	118,118,118,118	0
30	CA	O	301	1/1	0.97	0.17	-	90,90,90,90	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.