



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:27 am GMT

PDB ID : 3A0H
Title : Crystal structure of I-substituted Photosystem II complex
Authors : Kawakami, K.; Umena, Y.; Kamiya, N.; Shen, J.-R.
Deposited on : 2009-03-17
Resolution : 4.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

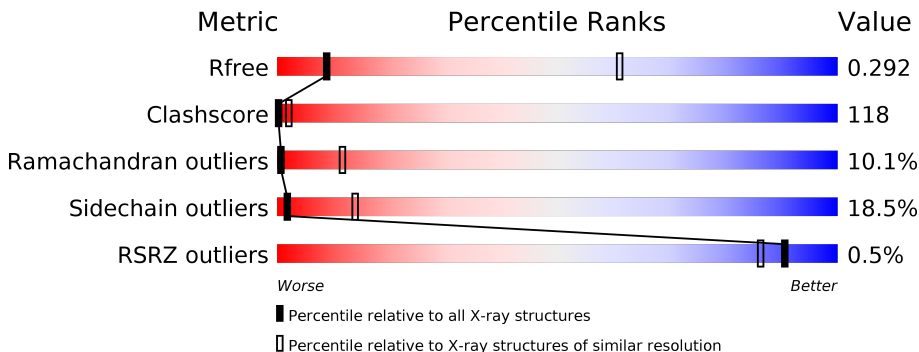
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

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X-RAY DIFFRACTION

A.

the following graphic. The table shows the number of entries on which the scores are based.



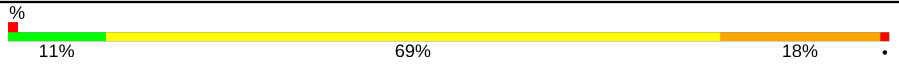

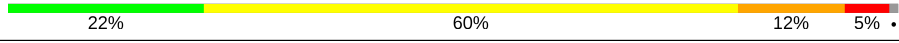

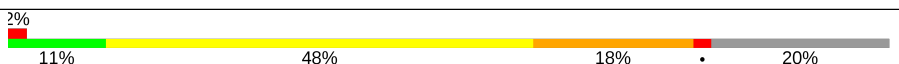
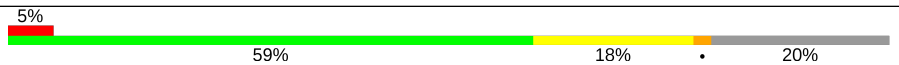
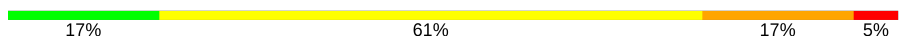

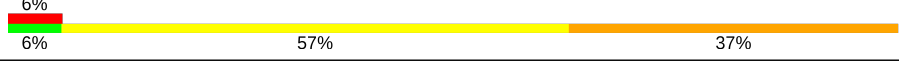
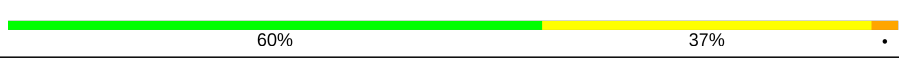

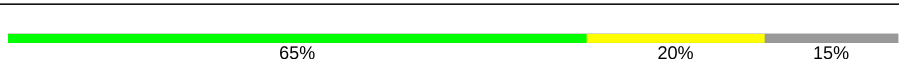
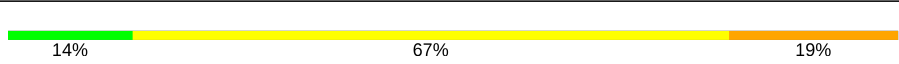

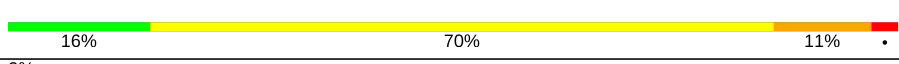
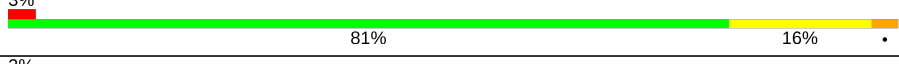

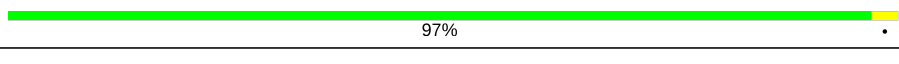
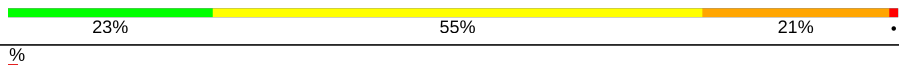

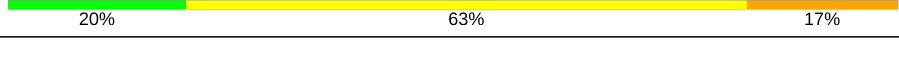
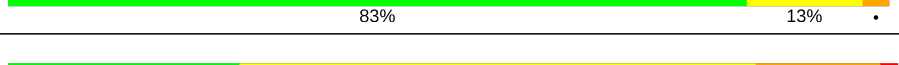
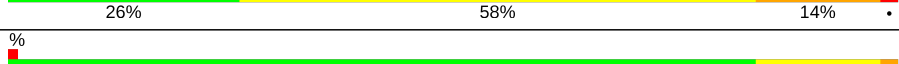
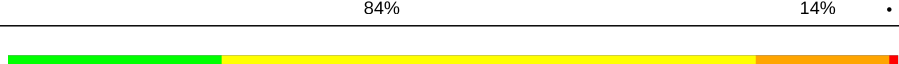
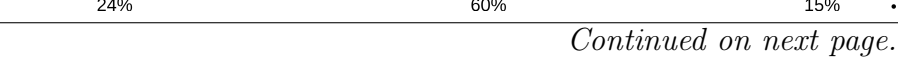
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	100719	1088 (4.40-3.60)
Clashscore	112137	1187 (4.40-3.60)
Ramachandran outliers	110173	1139 (4.40-3.60)
Sidechain outliers	110143	1126 (4.40-3.60)
RSRZ outliers	101464	1099 (4.40-3.60)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	<div><div style="width: 13%;">13%</div><div style="width: 62%;">62%</div><div style="width: 21%;">21%</div><div>• •</div></div>
1	a	344	<div><div style="width: 72%;">72%</div><div style="width: 24%;">24%</div><div>• •</div></div>
2	B	488	<div><div style="width: 20%;">20%</div><div style="width: 59%;">59%</div><div style="width: 19%;">19%</div><div>•</div></div>
2	b	488	<div><div style="width: 77%;">77%</div><div style="width: 22%;">22%</div><div>•</div></div>
3	C	447	<div><div style="width: 17%;">17%</div><div style="width: 64%;">64%</div><div style="width: 18%;">18%</div><div>•</div></div>
3	c	447	<div><div style="width: 77%;">77%</div><div style="width: 22%;">22%</div><div>•</div></div>


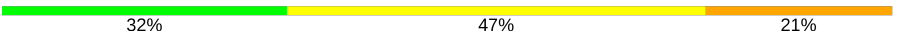







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Mol	Chain	Length	Quality of chain
4	D	340	
4	d	340	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	64	
7	h	64	
8	I	35	
8	i	35	
9	J	40	
9	j	40	
10	K	36	
10	k	36	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	242	
13	o	242	
14	T	30	
14	t	30	
15	U	98	
15	u	98	
16	V	137	

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Mol	Chain	Length	Quality of chain
16	v	137	
17	X	34	
17	x	34	
18	Y	28	
18	y	28	
19	N	23	
19	n	23	
20	Z	62	
20	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
23	CLA	A	1003	X	-	X	-
23	CLA	A	1006	X	-	X	X
23	CLA	A	1007	X	-	X	X
23	CLA	B	1009	X	-	X	-
23	CLA	B	1010	X	-	X	-
23	CLA	B	1011	X	-	X	-
23	CLA	B	1012	X	-	X	-
23	CLA	B	1013	X	-	X	-
23	CLA	B	1014	X	-	X	-
23	CLA	B	1015	X	-	X	-
23	CLA	B	1016	X	-	X	-
23	CLA	B	1018	X	-	X	X
23	CLA	B	1019	X	-	X	-
23	CLA	B	1020	X	-	X	-
23	CLA	B	1021	X	-	X	-
23	CLA	B	1022	X	-	X	-
23	CLA	B	1023	X	-	X	-
23	CLA	B	1024	X	-	X	X
23	CLA	C	1025	X	-	X	-
23	CLA	C	1026	X	-	X	X
23	CLA	C	1027	X	-	X	X
23	CLA	C	1028	X	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	1029	X	-	X	-
23	CLA	C	1030	X	-	X	-
23	CLA	C	1031	X	-	X	-
23	CLA	C	1032	X	-	X	-
23	CLA	C	1033	X	-	X	-
23	CLA	C	1035	X	-	X	-
23	CLA	C	1036	X	-	X	-
23	CLA	C	1037	X	-	X	X
23	CLA	D	1004	X	-	X	-
23	CLA	D	1005	X	-	X	X
23	CLA	D	1008	X	-	X	X
23	CLA	H	1017	X	-	X	X
23	CLA	K	1034	X	-	X	X
23	CLA	a	6003	X	-	-	-
23	CLA	a	6006	X	-	-	-
23	CLA	a	6007	X	-	-	X
23	CLA	b	6009	X	-	-	X
23	CLA	b	6010	X	-	-	-
23	CLA	b	6011	X	-	-	-
23	CLA	b	6012	X	-	-	X
23	CLA	b	6013	X	-	-	-
23	CLA	b	6014	X	-	-	X
23	CLA	b	6015	X	-	-	-
23	CLA	b	6016	X	-	-	-
23	CLA	b	6018	X	-	-	-
23	CLA	b	6019	X	-	-	-
23	CLA	b	6020	X	-	-	-
23	CLA	b	6021	X	-	-	X
23	CLA	b	6022	X	-	-	-
23	CLA	b	6023	X	-	-	-
23	CLA	b	6024	X	-	-	-
23	CLA	c	6025	X	-	-	-
23	CLA	c	6026	X	-	-	X
23	CLA	c	6027	X	-	-	X
23	CLA	c	6028	X	-	-	X
23	CLA	c	6029	X	-	-	X
23	CLA	c	6030	X	-	-	-
23	CLA	c	6031	X	-	-	X
23	CLA	c	6032	X	-	-	-
23	CLA	c	6033	X	-	-	-
23	CLA	c	6035	X	-	-	X
23	CLA	c	6036	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	6037	X	-	-	X
23	CLA	d	6004	X	-	-	-
23	CLA	d	6005	X	-	-	X
23	CLA	d	6008	X	-	-	X
23	CLA	h	6017	X	-	-	X
23	CLA	k	6034	X	-	-	X
24	PHO	A	1038	X	-	X	-
24	PHO	D	1039	X	-	X	X
24	PHO	a	6038	X	-	-	X
24	PHO	d	6039	X	-	-	-
25	PQ9	A	1043	-	-	X	X
25	PQ9	D	1042	-	-	X	X
25	PQ9	d	6042	-	-	-	X
26	BCR	A	1044	-	-	X	X
26	BCR	B	1045	-	-	X	X
26	BCR	B	1047	-	-	X	X
26	BCR	B	1048	-	-	X	X
26	BCR	C	1052	-	-	X	-
26	BCR	C	1054	-	-	X	X
26	BCR	D	1050	-	-	X	X
26	BCR	H	1049	-	-	X	X
26	BCR	K	1051	-	-	X	X
26	BCR	T	6046	-	-	X	X
26	BCR	T	6048	-	-	-	X
26	BCR	Z	1053	-	-	-	X
26	BCR	a	6044	-	-	-	X
26	BCR	b	6045	-	-	-	X
26	BCR	b	6047	-	-	-	X
26	BCR	c	6054	-	-	-	X
26	BCR	d	6050	-	-	-	X
26	BCR	h	6049	-	-	-	X
26	BCR	k	6051	-	-	-	X
26	BCR	k	6052	-	-	-	X
26	BCR	t	1046	-	-	-	X
26	BCR	z	6053	-	-	-	X
27	LHG	A	1063	-	-	X	X
27	LHG	a	6063	-	-	-	X
28	IOD	B	1067	-	-	X	-
28	IOD	D	1064	-	-	X	-
28	IOD	D	1068	-	-	X	X
28	IOD	T	1066	-	-	X	-
28	IOD	d	6068	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	DGD	B	1058	-	-	X	-
29	DGD	C	1055	-	-	X	X
29	DGD	C	1056	-	-	X	X
29	DGD	C	1057	-	-	X	-
29	DGD	b	6058	-	-	-	X
29	DGD	c	6055	-	-	-	X
29	DGD	c	6056	-	-	-	X
30	MGE	B	1060	-	-	X	X
30	MGE	D	1059	-	-	X	X
30	MGE	D	1062	-	-	X	X
30	MGE	L	1061	-	-	X	X
30	MGE	b	6060	-	-	-	X
30	MGE	d	6059	-	-	-	X
30	MGE	d	6062	-	-	-	X

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 48060 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 Q(B) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2630	1720	435	460	15			
1	a	335	Total	C	N	O	S	0	0	0
			2630	1720	435	460	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	488	Total	C	N	O	S	0	0	0
			3835	2518	638	666	13			
2	b	488	Total	C	N	O	S	0	0	0
			3835	2518	638	666	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
			3455	2264	576	602	13			
3	c	447	Total	C	N	O	S	0	0	0
			3455	2264	576	602	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	64	Total	C	N	O	S	0	0	0
			507	339	81	85	2			
7	h	64	Total	C	N	O	S	0	0	0
			507	339	81	85	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
			287	195	45	46	1			
8	i	35	Total	C	N	O	S	0	0	0
			287	195	45	46	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	36	Total	C	N	O	0	0	0
			278	195	38	45			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	36	Total	C	N	O	0	0	0
			278	195	38	45			

- 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	36	Total	C	N	O	S	0	0	0
			283	187	42	53	1			
12	m	36	Total	C	N	O	S	0	0	0
			283	187	42	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	242	Total	C	N	O	S	0	0	0
			1860	1162	314	380	4			
13	o	242	Total	C	N	O	S	0	0	0
			1860	1162	314	380	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			257	180	36	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			257	180	36	39	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	98	Total	C	N	O	0	0	0
			783	496	130	157			
15	u	98	Total	C	N	O	0	0	0
			783	496	130	157			

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	34	Total	C	N	O	0	0	0
			246	166	36	44			
17	x	34	Total	C	N	O	0	0	0
			246	166	36	44			

- Molecule 18 is a protein called Photosystem II reaction center protein ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Y	28	Total	C	N	O	S	0	0	0
			208	137	36	32	3			
18	y	28	Total	C	N	O	S	0	0	0
			208	137	36	32	3			

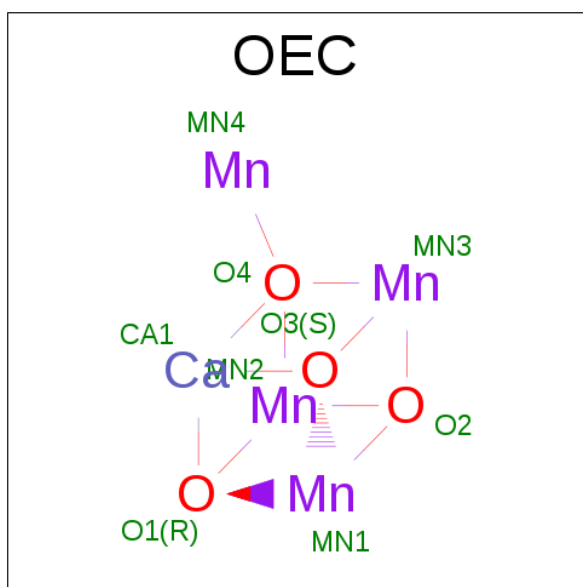
- Molecule 19 is a protein called Photosystem II reaction center protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	N	23	Total	C	N	O	0	0	0
			116	69	23	24			
19	n	23	Total	C	N	O	0	0	0
			116	69	23	24			

- 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 OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn_4O_4).

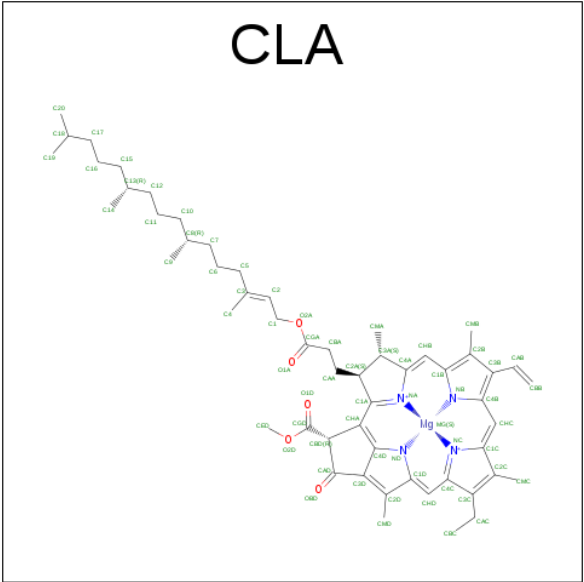


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	0	0
			5	1	4		
21	a	1	Total	Ca	Mn	0	0
			5	1	4		

- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	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	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		
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	H	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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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
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	K	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

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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	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	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	h	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

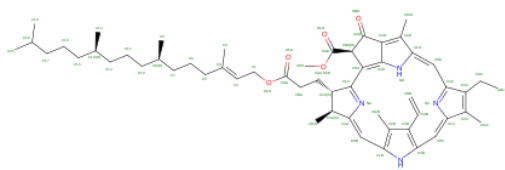
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	k	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	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: C₅₅H₇₄N₄O₅).

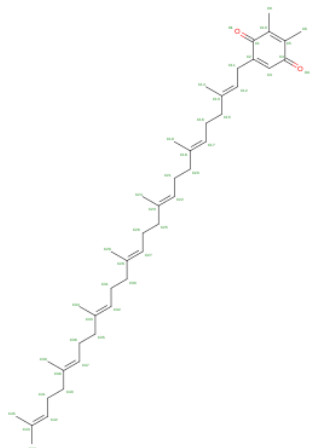
PHO



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		

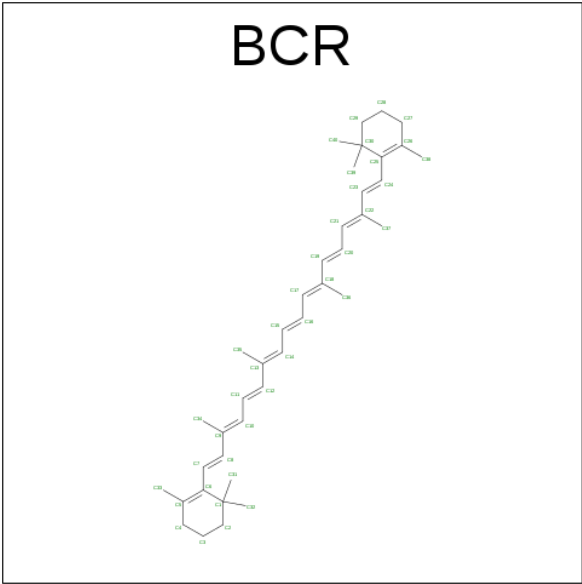
- Molecule 25 is 5-[(2E,6E,10E,14E,18E,22E)-3,7,11,15,19,23,27-HEPTAMETHYLOCTACOSA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (three-letter code: PQ9) (formula: $C_{43}H_{64}O_2$).

PQ9



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	O	0	0
			45	43	2		
25	D	1	Total	C	O	0	0
			45	43	2		
25	a	1	Total	C	O	0	0
			45	43	2		
25	d	1	Total	C	O	0	0
			45	43	2		

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



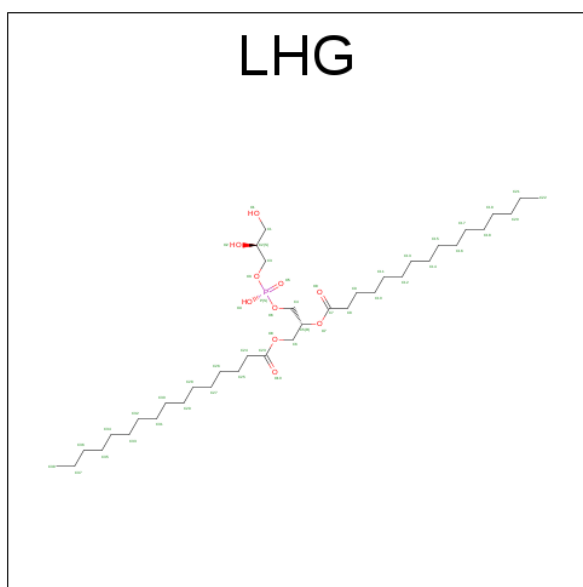
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	A	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	C	1	Total	C	0	0
			40	40		
26	Z	1	Total	C	0	0
			40	40		
26	C	1	Total	C	0	0
			40	40		
26	D	1	Total	C	0	0
			40	40		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	H	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	z	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	d	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).

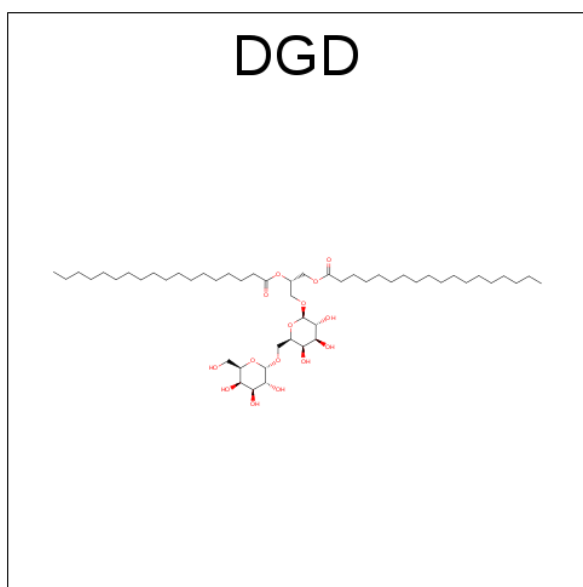


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	P	0	0
			49	38	10	1		
27	a	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 28 is IODIDE ION (three-letter code: IOD) (formula: I).

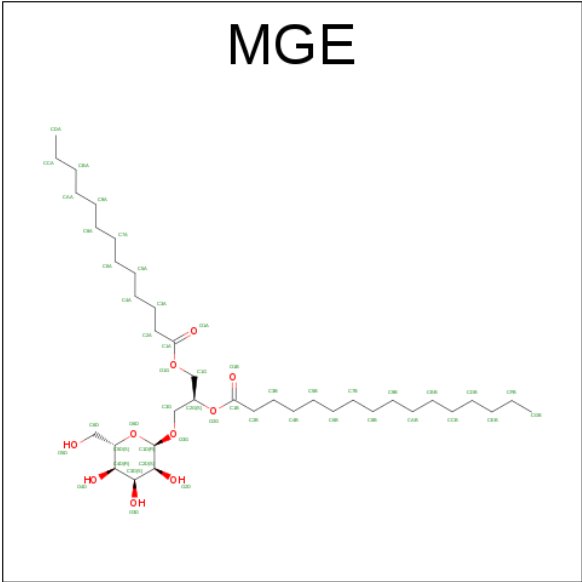
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	d	2	Total	I	0	0
			2	2		
28	B	1	Total	I	0	0
			1	1		
28	a	1	Total	I	0	0
			1	1		
28	A	1	Total	I	0	0
			1	1		
28	T	1	Total	I	0	0
			1	1		
28	D	2	Total	I	0	0
			2	2		
28	t	1	Total	I	0	0
			1	1		
28	b	1	Total	I	0	0
			1	1		

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



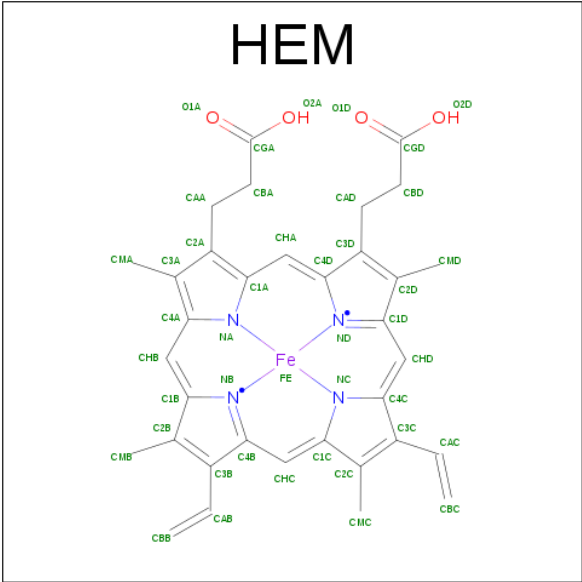
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	C	1	Total	C	O	0	0
			66	51	15		
29	C	1	Total	C	O	0	0
			66	51	15		
29	C	1	Total	C	O	0	0
			66	51	15		
29	B	1	Total	C	O	0	0
			66	51	15		
29	c	1	Total	C	O	0	0
			66	51	15		
29	c	1	Total	C	O	0	0
			66	51	15		
29	c	1	Total	C	O	0	0
			66	51	15		
29	b	1	Total	C	O	0	0
			66	51	15		

- Molecule 30 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (three-letter code: MGE) (formula: C₃₈H₇₂O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	D	1	Total	C	O	0	0
			48	38	10		
30	B	1	Total	C	O	0	0
			48	38	10		
30	D	1	Total	C	O	0	0
			48	38	10		
30	L	1	Total	C	O	0	0
			48	38	10		
30	d	1	Total	C	O	0	0
			48	38	10		
30	b	1	Total	C	O	0	0
			48	38	10		
30	d	1	Total	C	O	0	0
			48	38	10		
30	l	1	Total	C	O	0	0
			48	38	10		

- Molecule 31 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).

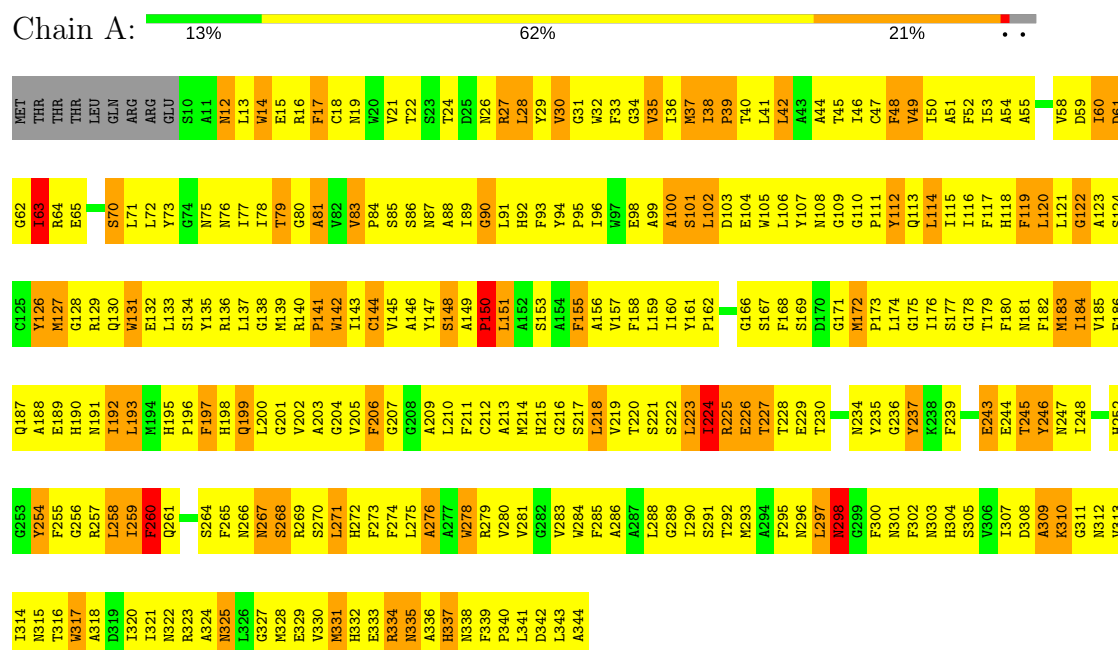


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
31	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
31	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
31	f	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
31	v	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

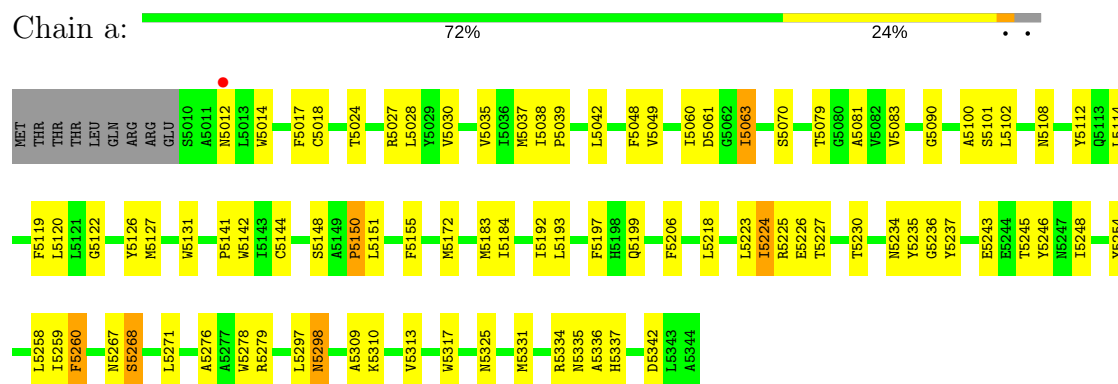
3 Residue-property plots

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

• Molecule 1: Photosystem Q(B) protein

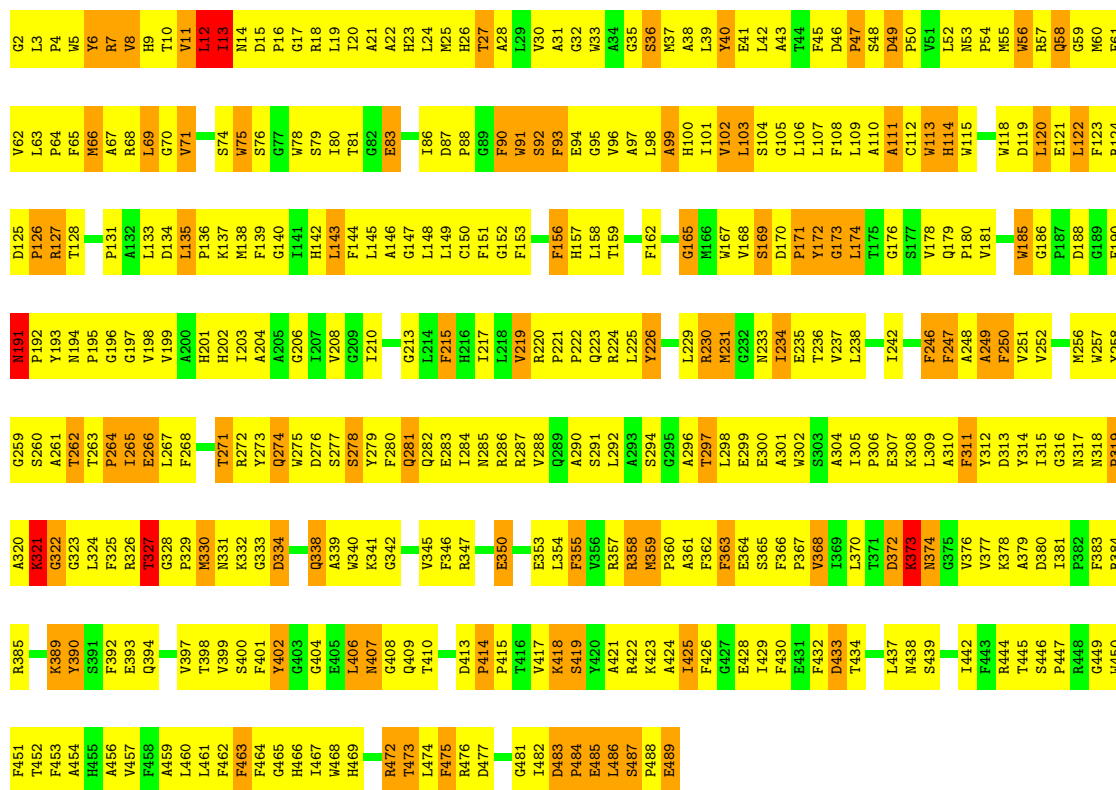


• Molecule 1: Photosystem Q(B) protein

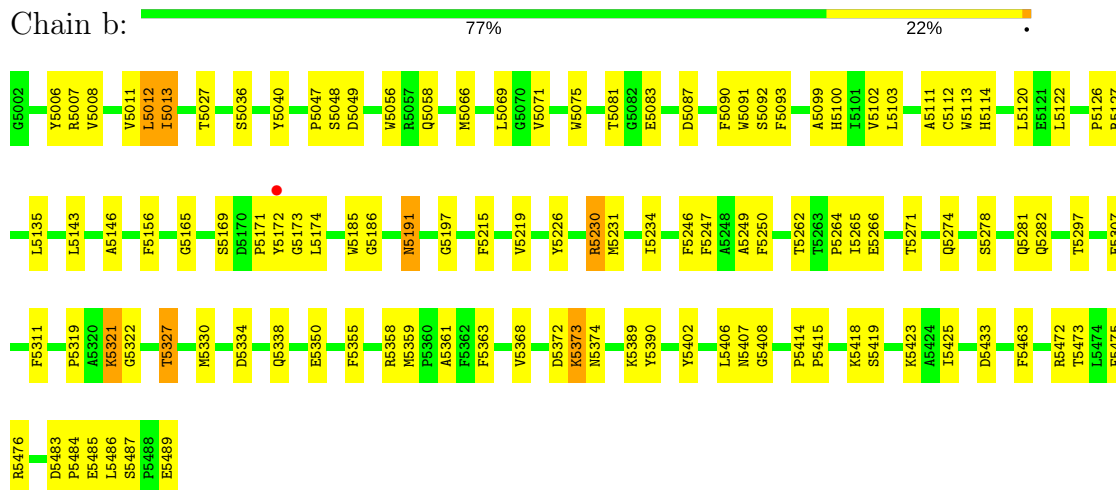


• Molecule 2: Photosystem II core light harvesting protein

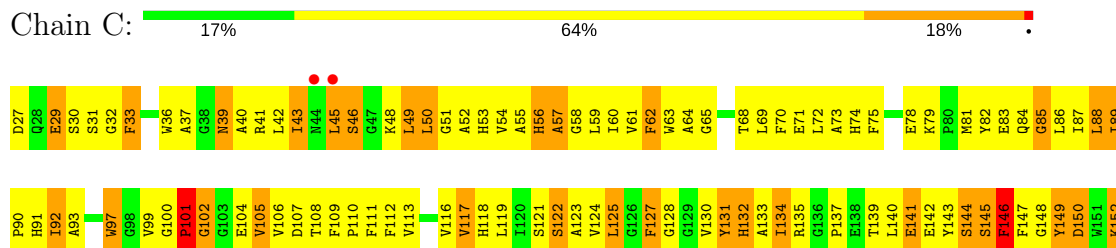




• Molecule 2: Photosystem II core light harvesting protein



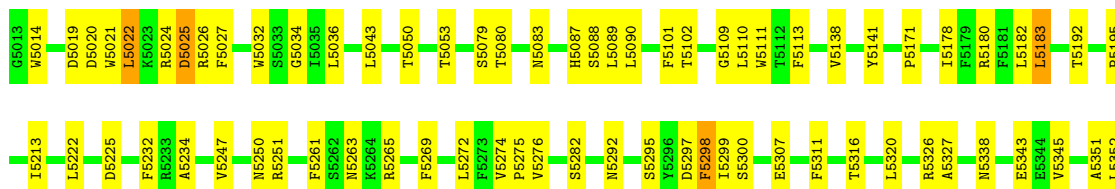
• Molecule 3: Photosystem II CP43 protein





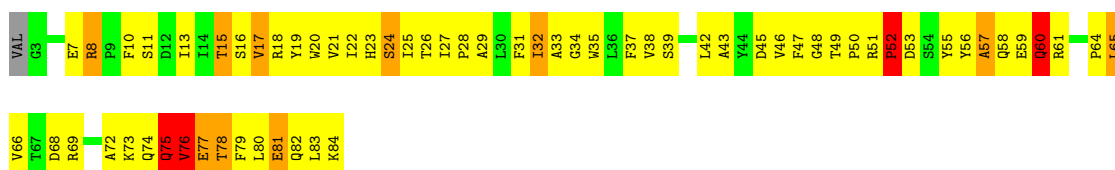
• Molecule 4: Photosystem II D2 protein

Chain d: 79% 20%



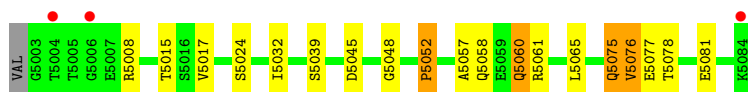
• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 22% 60% 12% 5%



• Molecule 5: Cytochrome b559 subunit alpha

Chain e: 4% 76% 18% 5%



• Molecule 6: Cytochrome b559 subunit beta

Chain F: 2% 11% 48% 18% 20%



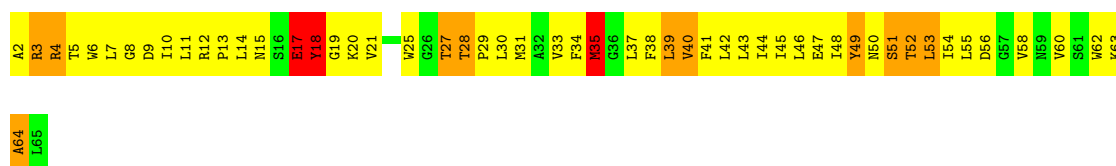
• Molecule 6: Cytochrome b559 subunit beta

Chain f: 5% 59% 18% 20%

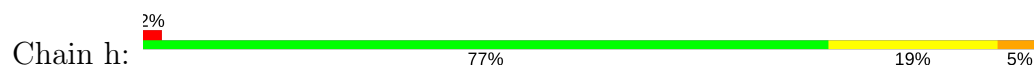


• Molecule 7: Photosystem II reaction center protein H

Chain H: 17% 61% 17% 5%



• Molecule 7: Photosystem II reaction center protein H



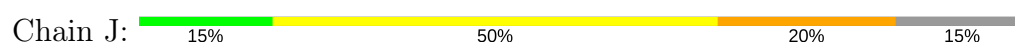
• Molecule 8: Photosystem II reaction center protein I



• Molecule 8: Photosystem II reaction center protein I



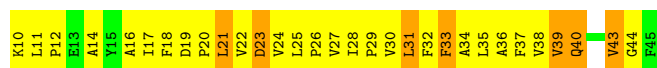
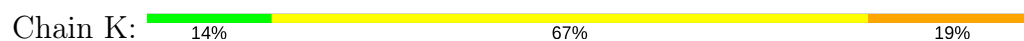
• Molecule 9: Photosystem II reaction center protein J



• Molecule 9: Photosystem II reaction center protein J



• Molecule 10: Photosystem II reaction center protein K



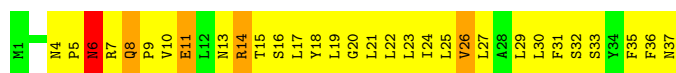
• Molecule 10: Photosystem II reaction center protein K

Chain k:  67% 31% .



- Molecule 11: Photosystem II reaction center protein L

Chain L:  16% 70% 11% .



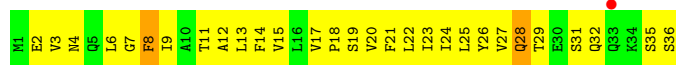
- Molecule 11: Photosystem II reaction center protein L

Chain I:  3% 81% 16% .



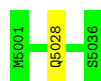
- Molecule 12: Photosystem II reaction center protein M

Chain M:  3% 19% 75% 6% .



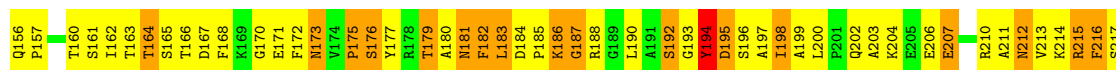
- Molecule 12: Photosystem II reaction center protein M

Chain m:  97% .

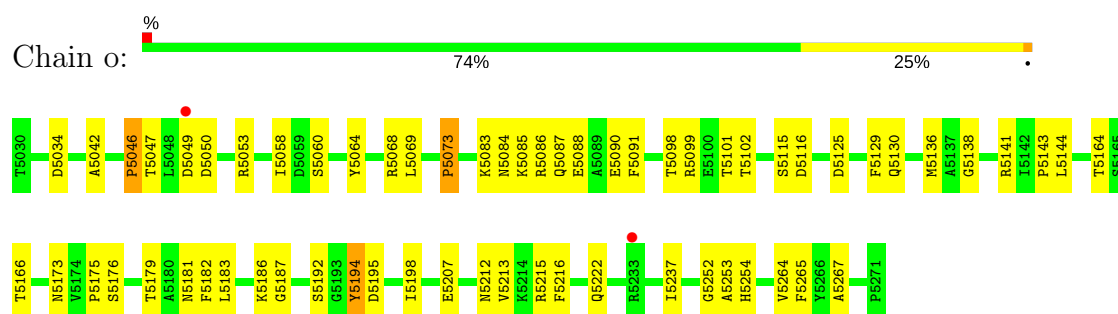


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

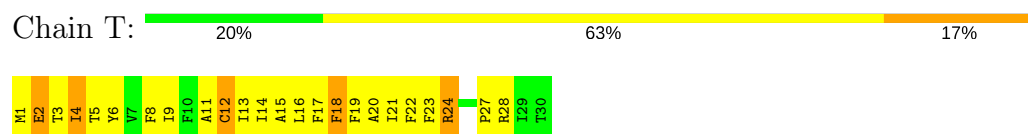
Chain O:  23% 55% 21% .



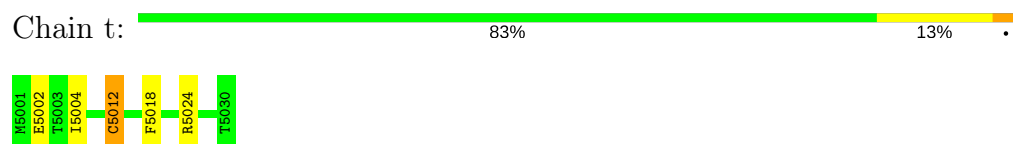
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



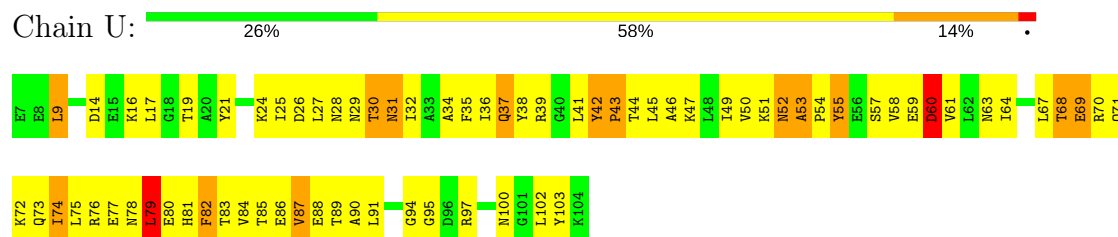
- Molecule 14: Photosystem II reaction center protein T



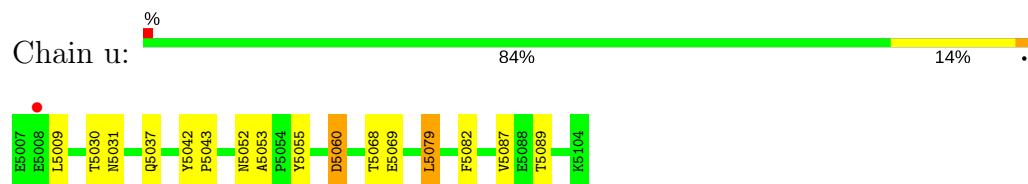
- Molecule 14: Photosystem II reaction center protein T



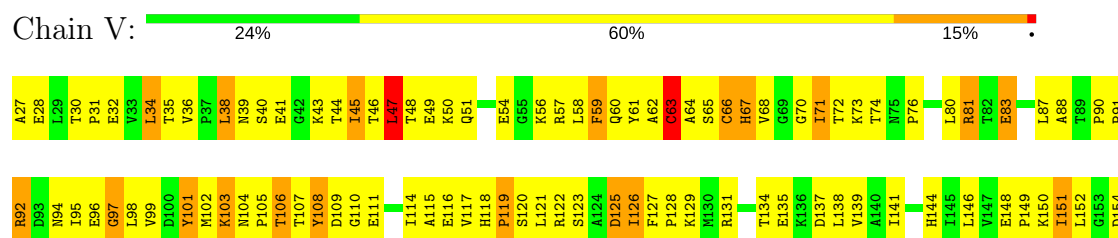
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Cytochrome c-550





• Molecule 16: Cytochrome c-550

Chain v: 79% 20%



• Molecule 17: Photosystem II reaction center protein X

Chain X: 32% 47% 21%



• Molecule 17: Photosystem II reaction center protein X

Chain x: 3% 71% 29%



• Molecule 18: Photosystem II reaction center protein ycf12

Chain Y: 29% 29% 36% 7%



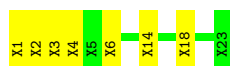
• Molecule 18: Photosystem II reaction center protein ycf12

Chain y: 57% 36% 7%



• Molecule 19: Photosystem II reaction center protein Y

Chain N: 70% 30%

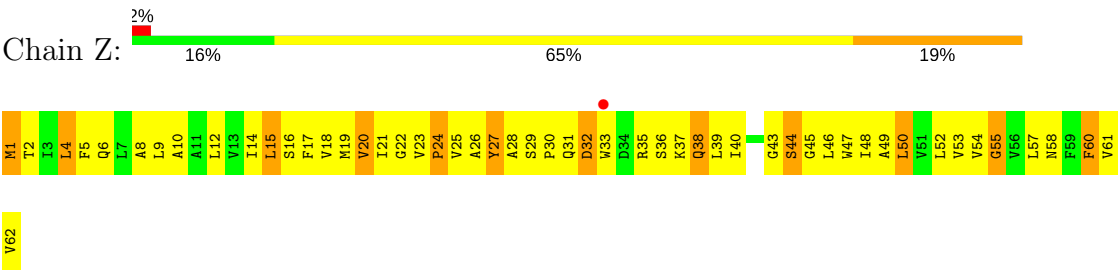


• Molecule 19: Photosystem II reaction center protein Y

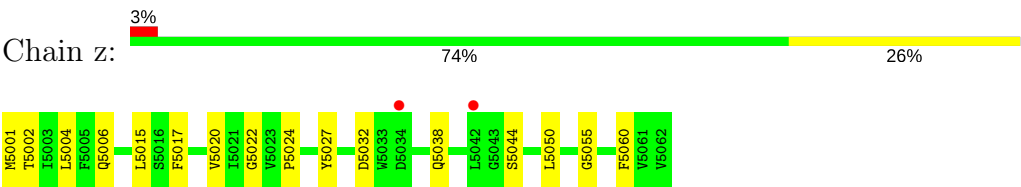
Chain n: 100%

There are no outlier residues recorded for this chain.

● Molecule 20: Photosystem II reaction center protein Z



● Molecule 20: 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, α , β , γ	128.50Å 224.70Å 304.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.00 20.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	94.7 (20.00-4.00) 94.8 (20.00-4.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 4.07Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.290 , 0.326 0.290 , 0.292	Depositor DCC
R_{free} test set	3592 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	148.7	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 71.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	48060	wwPDB-VP
Average B, all atoms (Å ²)	165.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, PHO, MGE, DGD, CLA, FE2, PQ9, OEC, HEM, IOD, BCR

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	0.53	0/2714	0.74	0/3699
1	a	0.53	0/2714	0.74	0/3699
2	B	0.55	0/3971	0.80	2/5411 (0.0%)
2	b	0.55	0/3971	0.80	2/5411 (0.0%)
3	C	0.50	0/3568	0.80	2/4858 (0.0%)
3	c	0.50	0/3568	0.80	2/4858 (0.0%)
4	D	0.52	0/2801	0.78	0/3818
4	d	0.52	0/2801	0.78	0/3818
5	E	0.58	0/685	0.79	0/933
5	e	0.58	0/685	0.79	0/933
6	F	0.62	0/291	0.72	0/397
6	f	0.62	0/291	0.72	0/397
7	H	0.54	0/520	0.88	0/708
7	h	0.53	0/520	0.88	0/708
8	I	0.67	0/294	0.75	0/395
8	i	0.67	0/294	0.75	0/395
9	J	0.57	0/255	0.72	0/346
9	j	0.57	0/255	0.71	0/346
10	K	0.52	0/287	0.82	0/394
10	k	0.51	0/287	0.84	0/394
11	L	0.50	0/311	0.76	0/422
11	l	0.50	0/311	0.76	0/422
12	M	0.57	0/287	0.73	0/388
12	m	0.57	0/287	0.73	0/388
13	O	0.51	0/1891	0.83	1/2564 (0.0%)
13	o	0.51	0/1891	0.83	1/2564 (0.0%)
14	T	0.69	0/266	0.83	0/359
14	t	0.66	0/266	0.81	0/359
15	U	0.50	0/794	0.81	0/1076
15	u	0.50	0/794	0.80	0/1076
16	V	0.45	0/1085	0.77	1/1473 (0.1%)
16	v	0.45	0/1085	0.77	1/1473 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	X	0.49	0/249	0.73	0/337
17	x	0.50	0/249	0.73	0/337
18	Y	0.63	0/209	0.94	0/279
18	y	0.63	0/209	0.94	0/279
20	Z	0.61	0/490	0.78	0/669
20	z	0.61	0/490	0.78	0/669
All	All	0.53	0/41936	0.79	12/57052 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	5327	THR	N-CA-C	5.91	126.96	111.00
2	B	327	THR	N-CA-C	5.89	126.91	111.00
3	c	5341	LEU	CA-CB-CG	-5.60	102.43	115.30
3	C	341	LEU	CA-CB-CG	-5.59	102.44	115.30
16	V	110	GLY	N-CA-C	-5.46	99.44	113.10

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	2630	0	2528	733	0
1	a	2630	0	2528	0	0
2	B	3835	0	3700	797	0
2	b	3835	0	3700	0	0
3	C	3455	0	3376	844	0
3	c	3455	0	3376	0	0
4	D	2706	0	2607	750	0
4	d	2706	0	2608	0	0
5	E	666	0	651	109	0
5	e	666	0	651	0	0
6	F	282	0	291	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	f	282	0	291	0	0
7	H	507	0	529	142	0
7	h	507	0	529	0	0
8	I	287	0	308	65	0
8	i	287	0	305	0	0
9	J	249	0	262	62	0
9	j	249	0	262	0	0
10	K	278	0	289	84	0
10	k	278	0	289	0	0
11	L	304	0	316	76	0
11	l	304	0	313	0	0
12	M	283	0	297	50	0
12	m	283	0	294	0	0
13	O	1860	0	1833	305	0
13	o	1860	0	1833	0	0
14	T	257	0	261	55	0
14	t	257	0	259	0	0
15	U	783	0	779	137	0
15	u	783	0	779	0	0
16	V	1064	0	1072	206	0
16	v	1064	0	1072	0	0
17	X	246	0	269	39	0
17	x	246	0	269	0	0
18	Y	208	0	237	77	0
18	y	208	0	237	0	0
19	N	116	0	26	6	0
19	n	116	0	26	0	0
20	Z	479	0	516	73	0
20	z	479	0	513	0	0
21	A	5	0	0	0	0
21	a	5	0	0	0	0
22	D	1	0	0	0	0
22	a	1	0	0	0	0
23	A	195	0	216	139	0
23	B	975	0	1080	668	0
23	C	780	0	864	488	0
23	D	195	0	216	157	0
23	H	65	0	72	45	0
23	K	65	0	72	87	0
23	a	195	0	216	0	0
23	b	975	0	1080	0	0
23	c	780	0	864	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	d	195	0	216	0	0
23	h	65	0	72	0	0
23	k	65	0	72	0	0
24	A	64	0	74	63	0
24	D	64	0	74	53	0
24	a	64	0	74	0	0
24	d	64	0	74	0	0
25	A	45	0	64	39	0
25	D	45	0	64	52	0
25	a	45	0	64	0	0
25	d	45	0	64	0	0
26	A	40	0	47	25	0
26	B	120	0	142	74	0
26	C	80	0	96	81	0
26	D	40	0	48	40	0
26	H	40	0	48	36	0
26	K	40	0	47	27	0
26	T	80	0	95	40	0
26	Z	40	0	47	18	0
26	a	40	0	47	0	0
26	b	80	0	95	0	0
26	c	40	0	48	0	0
26	d	40	0	48	0	0
26	h	40	0	48	0	0
26	k	80	0	95	0	0
26	t	40	0	48	0	0
26	z	40	0	47	0	0
27	A	49	0	74	36	0
27	a	49	0	74	0	0
28	A	1	0	0	1	0
28	B	1	0	0	3	0
28	D	2	0	0	10	0
28	T	1	0	0	2	0
28	a	1	0	0	0	0
28	b	1	0	0	0	0
28	d	2	0	0	0	0
28	t	1	0	0	0	0
29	B	66	0	96	32	0
29	C	198	0	288	118	0
29	b	66	0	96	0	0
29	c	198	0	288	0	0
30	B	48	0	72	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	D	96	0	144	66	0
30	L	48	0	72	29	0
30	b	48	0	72	0	0
30	d	96	0	144	0	0
30	l	48	0	72	0	0
31	F	43	0	30	17	0
31	V	43	0	30	12	0
31	f	43	0	30	0	0
31	v	43	0	30	0	0
All	All	48060	0	48531	5652	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 118.

The worst 5 of 5652 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:PHE:CE2	23:B:1012:CLA:HMA2	1.39	1.55
23:B:1011:CLA:HED2	23:B:1012:CLA:CED	1.31	1.53
26:C:1052:BCR:H371	26:C:1052:BCR:C26	1.34	1.50
23:B:1016:CLA:H162	23:D:1008:CLA:CMA	1.38	1.49
23:A:1003:CLA:CAA	23:A:1003:CLA:HED2	1.44	1.47

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	333/344 (97%)	219 (66%)	75 (22%)	39 (12%)	0 8
1	a	333/344 (97%)	216 (65%)	76 (23%)	41 (12%)	0 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	486/488 (100%)	350 (72%)	86 (18%)	50 (10%)	0	11
2	b	486/488 (100%)	350 (72%)	86 (18%)	50 (10%)	0	11
3	C	445/447 (100%)	330 (74%)	80 (18%)	35 (8%)	1	17
3	c	445/447 (100%)	330 (74%)	80 (18%)	35 (8%)	1	17
4	D	338/340 (99%)	222 (66%)	78 (23%)	38 (11%)	0	9
4	d	338/340 (99%)	224 (66%)	77 (23%)	37 (11%)	0	9
5	E	80/83 (96%)	54 (68%)	17 (21%)	9 (11%)	0	8
5	e	80/83 (96%)	54 (68%)	17 (21%)	9 (11%)	0	8
6	F	33/44 (75%)	20 (61%)	9 (27%)	4 (12%)	0	7
6	f	33/44 (75%)	20 (61%)	9 (27%)	4 (12%)	0	7
7	H	62/64 (97%)	42 (68%)	12 (19%)	8 (13%)	0	6
7	h	62/64 (97%)	42 (68%)	12 (19%)	8 (13%)	0	6
8	I	33/35 (94%)	21 (64%)	6 (18%)	6 (18%)	0	3
8	i	33/35 (94%)	21 (64%)	6 (18%)	6 (18%)	0	3
9	J	32/40 (80%)	29 (91%)	0	3 (9%)	1	14
9	j	32/40 (80%)	29 (91%)	0	3 (9%)	1	14
10	K	34/36 (94%)	23 (68%)	5 (15%)	6 (18%)	0	3
10	k	34/36 (94%)	17 (50%)	8 (24%)	9 (26%)	0	1
11	L	35/37 (95%)	25 (71%)	8 (23%)	2 (6%)	2	26
11	l	35/37 (95%)	25 (71%)	8 (23%)	2 (6%)	2	26
12	M	34/36 (94%)	23 (68%)	11 (32%)	0	100	100
12	m	34/36 (94%)	23 (68%)	11 (32%)	0	100	100
13	O	240/242 (99%)	172 (72%)	41 (17%)	27 (11%)	0	8
13	o	240/242 (99%)	172 (72%)	41 (17%)	27 (11%)	0	8
14	T	28/30 (93%)	22 (79%)	5 (18%)	1 (4%)	4	37
14	t	28/30 (93%)	22 (79%)	4 (14%)	2 (7%)	1	20
15	U	96/98 (98%)	70 (73%)	17 (18%)	9 (9%)	1	14
15	u	96/98 (98%)	70 (73%)	18 (19%)	8 (8%)	1	16
16	V	135/137 (98%)	100 (74%)	25 (18%)	10 (7%)	1	19
16	v	135/137 (98%)	99 (73%)	26 (19%)	10 (7%)	1	19
17	X	32/34 (94%)	29 (91%)	3 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	x	32/34 (94%)	29 (91%)	3 (9%)	0	100	100
18	Y	26/28 (93%)	20 (77%)	1 (4%)	5 (19%)	0	2
18	y	26/28 (93%)	20 (77%)	1 (4%)	5 (19%)	0	2
20	Z	60/62 (97%)	44 (73%)	12 (20%)	4 (7%)	1	22
20	z	60/62 (97%)	44 (73%)	12 (20%)	4 (7%)	1	22
All	All	5124/5250 (98%)	3622 (71%)	986 (19%)	516 (10%)	1	12

5 of 516 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ILE
1	A	61	ASP
1	A	100	ALA
1	A	224	ILE
1	A	226	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/279 (97%)	218 (81%)	52 (19%)	1	13
1	a	270/279 (97%)	217 (80%)	53 (20%)	1	12
2	B	388/388 (100%)	319 (82%)	69 (18%)	2	16
2	b	388/388 (100%)	319 (82%)	69 (18%)	2	16
3	C	349/349 (100%)	277 (79%)	72 (21%)	1	10
3	c	349/349 (100%)	276 (79%)	73 (21%)	1	10
4	D	275/275 (100%)	236 (86%)	39 (14%)	4	26
4	d	275/275 (100%)	237 (86%)	38 (14%)	4	27
5	E	72/73 (99%)	58 (81%)	14 (19%)	1	12
5	e	72/73 (99%)	58 (81%)	14 (19%)	1	12
6	F	29/38 (76%)	23 (79%)	6 (21%)	1	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	f	29/38 (76%)	23 (79%)	6 (21%)	1	10
7	H	54/54 (100%)	44 (82%)	10 (18%)	2	14
7	h	54/54 (100%)	44 (82%)	10 (18%)	2	14
8	I	32/32 (100%)	23 (72%)	9 (28%)	0	3
8	i	32/32 (100%)	23 (72%)	9 (28%)	0	3
9	J	24/28 (86%)	19 (79%)	5 (21%)	1	10
9	j	24/28 (86%)	19 (79%)	5 (21%)	1	10
10	K	29/29 (100%)	24 (83%)	5 (17%)	2	17
10	k	29/29 (100%)	25 (86%)	4 (14%)	4	27
11	L	35/35 (100%)	29 (83%)	6 (17%)	2	17
11	l	35/35 (100%)	29 (83%)	6 (17%)	2	17
12	M	33/33 (100%)	31 (94%)	2 (6%)	22	58
12	m	33/33 (100%)	32 (97%)	1 (3%)	46	75
13	O	206/206 (100%)	168 (82%)	38 (18%)	2	14
13	o	206/206 (100%)	168 (82%)	38 (18%)	2	14
14	T	27/27 (100%)	23 (85%)	4 (15%)	3	23
14	t	27/27 (100%)	23 (85%)	4 (15%)	3	23
15	U	85/85 (100%)	74 (87%)	11 (13%)	5	28
15	u	85/85 (100%)	75 (88%)	10 (12%)	6	32
16	V	117/117 (100%)	96 (82%)	21 (18%)	2	15
16	v	117/117 (100%)	97 (83%)	20 (17%)	2	17
17	X	27/27 (100%)	17 (63%)	10 (37%)	0	1
17	x	27/27 (100%)	17 (63%)	10 (37%)	0	1
18	Y	21/21 (100%)	12 (57%)	9 (43%)	0	0
18	y	21/21 (100%)	12 (57%)	9 (43%)	0	0
20	Z	52/52 (100%)	40 (77%)	12 (23%)	1	7
20	z	52/52 (100%)	40 (77%)	12 (23%)	1	7
All	All	4250/4296 (99%)	3465 (82%)	785 (18%)	2	14

5 of 785 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	V	101	TYR

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Mol	Chain	Res	Type
1	a	5279	ARG
15	u	5031	ASN
17	X	15	SER
1	a	5024	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 169 such sidechains are listed below:

Mol	Chain	Res	Type
15	U	99	ASN
1	a	5241	GLN
15	u	5028	ASN
16	V	60	GLN
20	Z	38	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 136 ligands modelled in this entry, 12 are monoatomic - leaving 124 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	OEC	A	1001	1,3	0,0,13	0.00	-	0,0,27	0.00	-
23	CLA	A	1003	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	A	1006	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	19 (29%)
23	CLA	A	1007	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
24	PHO	A	1038	-	67,69,69	2.87	23 (34%)	87,99,99	2.86	23 (26%)
25	PQ9	A	1043	-	45,45,45	0.64	1 (2%)	57,57,57	1.71	17 (29%)
26	BCR	A	1044	-	41,41,41	4.14	16 (39%)	56,56,56	7.03	29 (51%)
27	LHG	A	1063	-	48,48,48	0.93	2 (4%)	49,54,54	1.08	3 (6%)
23	CLA	B	1009	-	56,73,73	1.78	12 (21%)	65,113,113	2.39	20 (30%)
23	CLA	B	1010	2	56,73,73	1.75	12 (21%)	65,113,113	2.40	19 (29%)
23	CLA	B	1011	-	56,73,73	1.76	12 (21%)	65,113,113	2.39	20 (30%)
23	CLA	B	1012	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	19 (29%)
23	CLA	B	1013	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	B	1014	-	56,73,73	1.81	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	B	1015	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	B	1016	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	19 (29%)
23	CLA	B	1018	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	B	1019	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	19 (29%)
23	CLA	B	1020	-	56,73,73	1.81	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	B	1021	2	56,73,73	1.76	12 (21%)	65,113,113	2.38	21 (32%)
23	CLA	B	1022	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	B	1023	-	56,73,73	1.75	12 (21%)	65,113,113	2.37	21 (32%)
23	CLA	B	1024	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
26	BCR	B	1045	-	41,41,41	4.25	17 (41%)	56,56,56	6.01	24 (42%)
26	BCR	B	1047	-	41,41,41	4.24	16 (39%)	56,56,56	5.34	28 (50%)
26	BCR	B	1048	-	41,41,41	4.24	16 (39%)	56,56,56	6.09	28 (50%)
29	DGD	B	1058	-	67,67,67	0.84	2 (2%)	81,81,81	0.93	3 (3%)
30	MGE	B	1060	-	48,48,48	0.95	2 (4%)	56,56,56	1.04	3 (5%)
23	CLA	C	1025	-	56,73,73	1.81	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	C	1026	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	C	1027	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	C	1028	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	19 (29%)
23	CLA	C	1029	-	56,73,73	1.75	12 (21%)	65,113,113	2.39	21 (32%)
23	CLA	C	1030	-	56,73,73	1.76	11 (19%)	65,113,113	2.35	20 (30%)
23	CLA	C	1031	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	1032	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	19 (29%)
23	CLA	C	1033	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	C	1035	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	C	1036	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	19 (29%)
23	CLA	C	1037	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	19 (29%)
26	BCR	C	1052	-	41,41,41	4.25	16 (39%)	56,56,56	6.73	27 (48%)
26	BCR	C	1054	-	41,41,41	4.25	15 (36%)	56,56,56	5.26	24 (42%)
29	DGD	C	1055	-	67,67,67	0.84	2 (2%)	81,81,81	0.93	3 (3%)
29	DGD	C	1056	-	67,67,67	0.84	2 (2%)	81,81,81	0.93	3 (3%)
29	DGD	C	1057	-	67,67,67	0.84	2 (2%)	81,81,81	0.93	3 (3%)
23	CLA	D	1004	-	56,73,73	1.81	12 (21%)	65,113,113	2.37	19 (29%)
23	CLA	D	1005	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	D	1008	-	56,73,73	1.75	12 (21%)	65,113,113	2.38	21 (32%)
24	PHO	D	1039	-	67,69,69	2.87	23 (34%)	87,99,99	2.86	23 (26%)
25	PQ9	D	1042	-	45,45,45	0.64	1 (2%)	57,57,57	1.71	17 (29%)
26	BCR	D	1050	-	41,41,41	4.25	15 (36%)	56,56,56	5.03	24 (42%)
30	MGE	D	1059	-	48,48,48	0.95	2 (4%)	56,56,56	1.04	3 (5%)
30	MGE	D	1062	-	48,48,48	0.95	2 (4%)	56,56,56	1.04	3 (5%)
31	HEM	F	1040	5	28,50,50	2.26	6 (21%)	17,82,82	1.39	1 (5%)
23	CLA	H	1017	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
26	BCR	H	1049	-	41,41,41	4.25	16 (39%)	56,56,56	5.13	24 (42%)
23	CLA	K	1034	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
26	BCR	K	1051	-	41,41,41	4.25	15 (36%)	56,56,56	4.83	24 (42%)
30	MGE	L	1061	-	48,48,48	0.94	2 (4%)	56,56,56	1.04	3 (5%)
26	BCR	T	6046	-	41,41,41	4.17	17 (41%)	56,56,56	5.87	27 (48%)
26	BCR	T	6048	-	41,41,41	4.24	16 (39%)	56,56,56	6.09	28 (50%)
31	HEM	V	1041	16	28,50,50	2.27	6 (21%)	17,82,82	1.41	1 (5%)
26	BCR	Z	1053	-	41,41,41	4.25	16 (39%)	56,56,56	5.83	24 (42%)
21	OEC	a	6001	1,3	0,0,13	0.00	-	0,0,27	0.00	-
23	CLA	a	6003	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	a	6006	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	a	6007	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	19 (29%)
24	PHO	a	6038	-	67,69,69	2.87	23 (34%)	87,99,99	2.86	23 (26%)
25	PQ9	a	6043	-	45,45,45	0.65	1 (2%)	57,57,57	1.71	17 (29%)
26	BCR	a	6044	-	41,41,41	4.14	16 (39%)	56,56,56	7.04	30 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LHG	a	6063	-	48,48,48	0.93	2 (4%)	49,54,54	1.08	3 (6%)
23	CLA	b	6009	-	56,73,73	1.78	12 (21%)	65,113,113	2.39	21 (32%)
23	CLA	b	6010	2	56,73,73	1.75	12 (21%)	65,113,113	2.39	20 (30%)
23	CLA	b	6011	-	56,73,73	1.76	12 (21%)	65,113,113	2.39	20 (30%)
23	CLA	b	6012	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	b	6013	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	19 (29%)
23	CLA	b	6014	-	56,73,73	1.81	12 (21%)	65,113,113	2.38	19 (29%)
23	CLA	b	6015	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	b	6016	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	19 (29%)
23	CLA	b	6018	-	56,73,73	1.80	12 (21%)	65,113,113	2.36	20 (30%)
23	CLA	b	6019	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	b	6020	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	b	6021	2	56,73,73	1.76	12 (21%)	65,113,113	2.38	21 (32%)
23	CLA	b	6022	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	b	6023	-	56,73,73	1.75	12 (21%)	65,113,113	2.38	21 (32%)
23	CLA	b	6024	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)
26	BCR	b	6045	-	41,41,41	4.25	16 (39%)	56,56,56	6.01	24 (42%)
26	BCR	b	6047	-	41,41,41	4.24	16 (39%)	56,56,56	5.34	28 (50%)
29	DGD	b	6058	-	67,67,67	0.84	2 (2%)	81,81,81	0.93	3 (3%)
30	MGE	b	6060	-	48,48,48	0.95	2 (4%)	56,56,56	1.04	3 (5%)
23	CLA	c	6025	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	c	6026	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	c	6027	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	c	6028	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	19 (29%)
23	CLA	c	6029	-	56,73,73	1.75	12 (21%)	65,113,113	2.40	21 (32%)
23	CLA	c	6030	-	56,73,73	1.76	11 (19%)	65,113,113	2.35	20 (30%)
23	CLA	c	6031	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	c	6032	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	20 (30%)
23	CLA	c	6033	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	c	6035	-	56,73,73	1.81	12 (21%)	65,113,113	2.39	20 (30%)
23	CLA	c	6036	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	19 (29%)
23	CLA	c	6037	-	56,73,73	1.81	12 (21%)	65,113,113	2.36	19 (29%)
26	BCR	c	6054	-	41,41,41	4.25	15 (36%)	56,56,56	5.26	24 (42%)
29	DGD	c	6055	-	67,67,67	0.84	2 (2%)	81,81,81	0.93	3 (3%)
29	DGD	c	6056	-	67,67,67	0.84	2 (2%)	81,81,81	0.93	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	DGD	c	6057	-	67,67,67	0.84	2 (2%)	81,81,81	0.93	3 (3%)
23	CLA	d	6004	-	56,73,73	1.80	12 (21%)	65,113,113	2.36	19 (29%)
23	CLA	d	6005	-	56,73,73	1.80	12 (21%)	65,113,113	2.38	20 (30%)
23	CLA	d	6008	-	56,73,73	1.76	12 (21%)	65,113,113	2.38	21 (32%)
24	PHO	d	6039	-	67,69,69	2.87	23 (34%)	87,99,99	2.86	23 (26%)
25	PQ9	d	6042	-	45,45,45	0.64	1 (2%)	57,57,57	1.72	17 (29%)
26	BCR	d	6050	-	41,41,41	4.25	15 (36%)	56,56,56	5.03	24 (42%)
30	MGE	d	6059	-	48,48,48	0.95	2 (4%)	56,56,56	1.03	3 (5%)
30	MGE	d	6062	-	48,48,48	0.95	2 (4%)	56,56,56	1.04	3 (5%)
31	HEM	f	6040	5	28,50,50	2.25	6 (21%)	17,82,82	1.39	1 (5%)
23	CLA	h	6017	-	56,73,73	1.80	12 (21%)	65,113,113	2.37	19 (29%)
26	BCR	h	6049	-	41,41,41	4.25	15 (36%)	56,56,56	5.13	24 (42%)
23	CLA	k	6034	-	56,73,73	1.81	12 (21%)	65,113,113	2.38	20 (30%)
26	BCR	k	6051	-	41,41,41	4.25	16 (39%)	56,56,56	4.83	24 (42%)
26	BCR	k	6052	-	41,41,41	4.25	16 (39%)	56,56,56	6.73	27 (48%)
30	MGE	l	6061	-	48,48,48	0.94	2 (4%)	56,56,56	1.04	3 (5%)
26	BCR	t	1046	-	41,41,41	4.17	17 (41%)	56,56,56	5.87	26 (46%)
31	HEM	v	6041	16	28,50,50	2.27	6 (21%)	17,82,82	1.41	1 (5%)
26	BCR	z	6053	-	41,41,41	4.26	17 (41%)	56,56,56	5.82	24 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	OEC	A	1001	1,3	-	0/0/0/54	0/0/0/5
23	CLA	A	1003	-	4/4/20/25	1/37/135/135	0/0/9/9
23	CLA	A	1006	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	A	1007	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	A	1038	-	1/1/17/22	0/53/103/103	0/1/6/6
25	PQ9	A	1043	-	-	0/41/61/61	0/1/1/1
26	BCR	A	1044	-	-	0/29/63/63	0/2/2/2
27	LHG	A	1063	-	-	0/53/53/53	0/0/0/0
23	CLA	B	1009	-	4/4/20/25	1/37/135/135	0/0/9/9
23	CLA	B	1010	2	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1011	-	5/5/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	1012	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1013	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1014	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1015	-	4/4/20/25	1/37/135/135	0/0/9/9
23	CLA	B	1016	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1018	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1019	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1020	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1021	2	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1022	-	5/5/20/25	1/37/135/135	0/0/9/9
23	CLA	B	1023	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1024	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	B	1045	-	-	0/29/63/63	0/2/2/2
26	BCR	B	1047	-	-	1/29/63/63	0/2/2/2
26	BCR	B	1048	-	-	1/29/63/63	0/2/2/2
29	DGD	B	1058	-	-	0/55/95/95	0/2/2/2
30	MGE	B	1060	-	-	0/43/63/63	0/1/1/1
23	CLA	C	1025	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1026	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1027	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1028	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1029	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1030	-	4/4/20/25	1/37/135/135	0/0/9/9
23	CLA	C	1031	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1032	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1033	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1035	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1036	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1037	-	4/4/20/25	0/37/135/135	0/0/9/9
26	BCR	C	1052	-	-	0/29/63/63	0/2/2/2
26	BCR	C	1054	-	-	1/29/63/63	0/2/2/2
29	DGD	C	1055	-	-	1/55/95/95	0/2/2/2
29	DGD	C	1056	-	-	0/55/95/95	0/2/2/2
29	DGD	C	1057	-	-	0/55/95/95	0/2/2/2
23	CLA	D	1004	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	D	1005	-	4/4/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	D	1008	-	5/5/20/25	1/37/135/135	0/0/9/9
24	PHO	D	1039	-	3/3/17/22	0/53/103/103	0/1/6/6
25	PQ9	D	1042	-	-	0/41/61/61	0/1/1/1
26	BCR	D	1050	-	-	2/29/63/63	0/2/2/2
30	MGE	D	1059	-	-	0/43/63/63	0/1/1/1
30	MGE	D	1062	-	-	1/43/63/63	0/1/1/1
31	HEM	F	1040	5	-	2/6/54/54	0/0/8/8
23	CLA	H	1017	-	4/4/20/25	0/37/135/135	0/0/9/9
26	BCR	H	1049	-	-	1/29/63/63	0/2/2/2
23	CLA	K	1034	-	7/7/20/25	0/37/135/135	0/0/9/9
26	BCR	K	1051	-	-	0/29/63/63	0/2/2/2
30	MGE	L	1061	-	-	0/43/63/63	0/1/1/1
26	BCR	T	6046	-	-	1/29/63/63	0/2/2/2
26	BCR	T	6048	-	-	1/29/63/63	0/2/2/2
31	HEM	V	1041	16	-	0/6/54/54	0/0/8/8
26	BCR	Z	1053	-	-	0/29/63/63	0/2/2/2
21	OEC	a	6001	1,3	-	0/0/0/54	0/0/0/5
23	CLA	a	6003	-	4/4/20/25	1/37/135/135	0/0/9/9
23	CLA	a	6006	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	a	6007	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	a	6038	-	1/1/17/22	0/53/103/103	0/1/6/6
25	PQ9	a	6043	-	-	0/41/61/61	0/1/1/1
26	BCR	a	6044	-	-	0/29/63/63	0/2/2/2
27	LHG	a	6063	-	-	0/53/53/53	0/0/0/0
23	CLA	b	6009	-	4/4/20/25	1/37/135/135	0/0/9/9
23	CLA	b	6010	2	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6011	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6012	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6013	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6014	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6015	-	4/4/20/25	1/37/135/135	0/0/9/9
23	CLA	b	6016	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6018	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6019	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6020	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6021	2	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6022	-	5/5/20/25	1/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	6023	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6024	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	b	6045	-	-	0/29/63/63	0/2/2/2
26	BCR	b	6047	-	-	1/29/63/63	0/2/2/2
29	DGD	b	6058	-	-	0/55/95/95	0/2/2/2
30	MGE	b	6060	-	-	0/43/63/63	0/1/1/1
23	CLA	c	6025	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6026	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6027	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6028	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6029	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6030	-	4/4/20/25	1/37/135/135	0/0/9/9
23	CLA	c	6031	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6032	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6033	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6035	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6036	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6037	-	4/4/20/25	0/37/135/135	0/0/9/9
26	BCR	c	6054	-	-	1/29/63/63	0/2/2/2
29	DGD	c	6055	-	-	1/55/95/95	0/2/2/2
29	DGD	c	6056	-	-	0/55/95/95	0/2/2/2
29	DGD	c	6057	-	-	0/55/95/95	0/2/2/2
23	CLA	d	6004	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	d	6005	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	d	6008	-	5/5/20/25	1/37/135/135	0/0/9/9
24	PHO	d	6039	-	3/3/17/22	0/53/103/103	0/1/6/6
25	PQ9	d	6042	-	-	0/41/61/61	0/1/1/1
26	BCR	d	6050	-	-	2/29/63/63	0/2/2/2
30	MGE	d	6059	-	-	0/43/63/63	0/1/1/1
30	MGE	d	6062	-	-	1/43/63/63	0/1/1/1
31	HEM	f	6040	5	-	2/6/54/54	0/0/8/8
23	CLA	h	6017	-	4/4/20/25	0/37/135/135	0/0/9/9
26	BCR	h	6049	-	-	1/29/63/63	0/2/2/2
23	CLA	k	6034	-	7/7/20/25	0/37/135/135	0/0/9/9
26	BCR	k	6051	-	-	0/29/63/63	0/2/2/2
26	BCR	k	6052	-	-	0/29/63/63	0/2/2/2
30	MGE	l	6061	-	-	0/43/63/63	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	t	1046	-	-	1/29/63/63	0/2/2/2
31	HEM	v	6041	16	-	0/6/54/54	0/0/8/8
26	BCR	z	6053	-	-	0/29/63/63	0/2/2/2

The worst 5 of 1344 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	6047	BCR	C19-C18	-9.23	1.25	1.45
26	z	6053	BCR	C8-C9	-9.23	1.25	1.45
26	b	6047	BCR	C8-C9	-9.23	1.25	1.45
26	k	6051	BCR	C12-C13	-9.22	1.25	1.45
26	B	1047	BCR	C8-C9	-9.22	1.25	1.45

The worst 5 of 2174 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	1039	PHO	CAC-C3C-C4C	-13.38	109.49	125.21
24	a	6038	PHO	CAC-C3C-C4C	-13.38	109.49	125.21
24	A	1038	PHO	CAC-C3C-C4C	-13.38	109.49	125.21
24	d	6039	PHO	CAC-C3C-C4C	-13.38	109.50	125.21
24	D	1039	PHO	CMC-C2C-C1C	-9.99	109.47	125.04

5 of 302 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	b	6013	CLA	C8
23	b	6013	CLA	NC
23	b	6013	CLA	ND
23	b	6013	CLA	NA
23	C	1026	CLA	NC

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	H	1049	BCR	C10-C11-C12-C13
26	h	6049	BCR	C10-C11-C12-C13
31	f	6040	HEM	C1A-C2A-CAA-CBA
31	F	1040	HEM	C1A-C2A-CAA-CBA
31	f	6040	HEM	C3A-C2A-CAA-CBA

There are no ring outliers.

62 monomers are involved in 2123 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	1003	CLA	55	0
23	A	1006	CLA	45	0
23	A	1007	CLA	40	0
24	A	1038	PHO	63	0
25	A	1043	PQ9	39	0
26	A	1044	BCR	25	0
27	A	1063	LHG	36	0
23	B	1009	CLA	63	0
23	B	1010	CLA	38	0
23	B	1011	CLA	89	0
23	B	1012	CLA	61	0
23	B	1013	CLA	67	0
23	B	1014	CLA	49	0
23	B	1015	CLA	45	0
23	B	1016	CLA	49	0
23	B	1018	CLA	34	0
23	B	1019	CLA	40	0
23	B	1020	CLA	54	0
23	B	1021	CLA	63	0
23	B	1022	CLA	75	0
23	B	1023	CLA	70	0
23	B	1024	CLA	45	0
26	B	1045	BCR	21	0
26	B	1047	BCR	31	0
26	B	1048	BCR	23	0
29	B	1058	DGD	32	0
30	B	1060	MGE	39	0
23	C	1025	CLA	67	0
23	C	1026	CLA	29	0
23	C	1027	CLA	37	0
23	C	1028	CLA	34	0
23	C	1029	CLA	62	0
23	C	1030	CLA	38	0
23	C	1031	CLA	63	0
23	C	1032	CLA	43	0
23	C	1033	CLA	65	0
23	C	1035	CLA	56	0
23	C	1036	CLA	24	0
23	C	1037	CLA	23	0
26	C	1052	BCR	40	0
26	C	1054	BCR	41	0
29	C	1055	DGD	26	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	C	1056	DGD	55	0
29	C	1057	DGD	41	0
23	D	1004	CLA	57	0
23	D	1005	CLA	58	0
23	D	1008	CLA	48	0
24	D	1039	PHO	53	0
25	D	1042	PQ9	52	0
26	D	1050	BCR	40	0
30	D	1059	MGE	45	0
30	D	1062	MGE	21	0
31	F	1040	HEM	17	0
23	H	1017	CLA	45	0
26	H	1049	BCR	36	0
23	K	1034	CLA	87	0
26	K	1051	BCR	27	0
30	L	1061	MGE	29	0
26	T	6046	BCR	25	0
26	T	6048	BCR	15	0
31	V	1041	HEM	12	0
26	Z	1053	BCR	18	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/344 (97%)	-0.57	0 100 100	135, 156, 186, 200	0
1	a	335/344 (97%)	-0.62	1 (0%) 93 91	135, 156, 186, 200	0
2	B	488/488 (100%)	-0.56	0 100 100	133, 156, 180, 191	0
2	b	488/488 (100%)	-0.54	1 (0%) 94 93	133, 156, 180, 191	0
3	C	447/447 (100%)	-0.55	2 (0%) 92 88	138, 165, 181, 193	0
3	c	447/447 (100%)	-0.43	1 (0%) 94 93	138, 165, 181, 193	0
4	D	340/340 (100%)	-0.59	3 (0%) 84 77	134, 156, 179, 192	0
4	d	340/340 (100%)	-0.60	0 100 100	134, 156, 179, 192	0
5	E	82/83 (98%)	-0.48	0 100 100	153, 172, 191, 198	0
5	e	82/83 (98%)	-0.32	3 (3%) 42 33	153, 172, 191, 198	0
6	F	35/44 (79%)	-0.42	1 (2%) 52 42	153, 167, 187, 191	0
6	f	35/44 (79%)	-0.39	2 (5%) 24 19	153, 167, 187, 191	0
7	H	64/64 (100%)	-0.48	0 100 100	154, 163, 175, 185	0
7	h	64/64 (100%)	-0.33	1 (1%) 72 63	154, 163, 175, 185	0
8	I	35/35 (100%)	-0.12	2 (5%) 24 19	152, 169, 196, 201	0
8	i	35/35 (100%)	-0.08	0 100 100	152, 169, 196, 201	0
9	J	34/40 (85%)	-0.65	0 100 100	155, 162, 184, 192	0
9	j	34/40 (85%)	-0.65	0 100 100	155, 162, 184, 192	0
10	K	36/36 (100%)	-0.66	0 100 100	144, 168, 182, 185	0
10	k	36/36 (100%)	-0.52	0 100 100	156, 170, 182, 192	0
11	L	37/37 (100%)	-0.42	0 100 100	138, 160, 191, 197	0
11	l	37/37 (100%)	-0.31	1 (2%) 55 44	138, 160, 191, 197	0
12	M	36/36 (100%)	-0.35	1 (2%) 53 43	131, 146, 188, 194	0
12	m	36/36 (100%)	-0.56	0 100 100	131, 146, 188, 194	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	242/242 (100%)	-0.45	1 (0%) 92 88	139, 160, 181, 187	0
13	o	242/242 (100%)	-0.46	2 (0%) 86 79	139, 160, 181, 187	0
14	T	30/30 (100%)	-0.68	0 100 100	124, 143, 186, 191	0
14	t	30/30 (100%)	-0.78	0 100 100	131, 143, 186, 191	0
15	U	98/98 (100%)	-0.57	0 100 100	139, 155, 165, 173	0
15	u	98/98 (100%)	-0.63	1 (1%) 82 74	139, 155, 165, 173	0
16	V	137/137 (100%)	-0.54	0 100 100	144, 162, 173, 178	0
16	v	137/137 (100%)	-0.56	0 100 100	144, 162, 173, 178	0
17	X	34/34 (100%)	-0.76	0 100 100	173, 181, 198, 201	0
17	x	34/34 (100%)	-0.47	1 (2%) 52 42	173, 181, 198, 201	0
18	Y	28/28 (100%)	0.08	0 100 100	187, 199, 208, 210	0
18	y	28/28 (100%)	-0.29	0 100 100	187, 199, 208, 210	0
19	N	0/23	-	-	-	-
19	n	0/23	-	-	-	-
20	Z	62/62 (100%)	-0.55	1 (1%) 72 63	159, 173, 188, 196	0
20	z	62/62 (100%)	-0.36	2 (3%) 48 38	159, 173, 188, 196	0
All	All	5200/5296 (98%)	-0.52	27 (0%) 90 86	124, 161, 185, 210	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	45	LEU	6.7
3	C	44	ASN	5.3
4	D	228	GLY	3.6
5	e	5006	GLY	3.2
5	e	5084	LYS	3.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
28	IOD	D	1068	1/1	0.69	1.30	14.01	198,198,198,198	0
26	BCR	h	6049	40/40	0.71	0.44	9.17	177,182,188,189	0
26	BCR	a	6044	40/40	0.71	0.52	6.32	155,177,185,185	0
30	MGE	d	6059	48/48	0.67	0.47	6.17	179,190,215,216	0
26	BCR	B	1045	40/40	0.77	0.51	6.15	163,196,216,216	0
26	BCR	T	6046	40/40	0.70	0.51	5.98	179,185,188,189	0
23	CLA	C	1027	65/65	0.65	0.51	5.87	192,198,204,216	0
28	IOD	d	6068	1/1	0.76	0.63	5.61	199,199,199,199	0
26	BCR	A	1044	40/40	0.73	0.61	5.54	155,177,185,185	0
26	BCR	z	6053	40/40	0.64	0.53	5.16	190,214,216,216	0
26	BCR	D	1050	40/40	0.79	0.49	5.09	184,193,198,199	0
26	BCR	T	6048	40/40	0.74	0.65	4.89	179,184,203,204	0
26	BCR	H	1049	40/40	0.72	0.40	4.87	177,182,188,189	0
26	BCR	d	6050	40/40	0.79	0.47	4.82	184,193,198,199	0
26	BCR	b	6047	40/40	0.77	0.43	4.48	155,171,200,202	0
30	MGE	D	1059	48/48	0.71	0.41	4.36	179,190,215,216	0
23	CLA	K	1034	65/65	0.64	0.48	4.22	138,189,216,216	0
26	BCR	b	6045	40/40	0.74	0.50	4.19	163,196,216,216	0
26	BCR	Z	1053	40/40	0.60	0.59	4.11	190,214,216,216	0
23	CLA	d	6008	65/65	0.72	0.47	4.07	184,188,216,216	0
23	CLA	k	6034	65/65	0.69	0.43	4.05	138,189,216,216	0
26	BCR	B	1048	40/40	0.75	0.58	4.00	179,184,203,204	0
26	BCR	k	6052	40/40	0.59	0.41	3.95	191,195,202,203	0
26	BCR	t	1046	40/40	0.75	0.40	3.91	179,185,188,189	0
23	CLA	A	1007	65/65	0.73	0.45	3.89	129,174,204,205	0
23	CLA	a	6007	65/65	0.66	0.50	3.83	129,174,204,205	0
26	BCR	k	6051	40/40	0.72	0.42	3.76	192,202,210,210	0
23	CLA	D	1008	65/65	0.73	0.45	3.67	184,188,216,216	0
29	DGD	c	6056	66/66	0.75	0.43	3.42	190,201,216,216	0
25	PQ9	d	6042	45/45	0.68	0.43	3.37	171,173,185,187	0
23	CLA	D	1005	65/65	0.83	0.35	3.35	135,162,169,173	0
23	CLA	C	1037	65/65	0.71	0.49	3.19	201,211,214,216	0
23	CLA	C	1028	65/65	0.88	0.29	3.19	178,182,201,202	0
23	CLA	c	6029	65/65	0.87	0.36	3.17	177,187,190,201	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
29	DGD	C	1056	66/66	0.73	0.38	2.91	190,201,216,216	0
23	CLA	H	1017	65/65	0.79	0.35	2.89	169,197,201,208	0
30	MGE	B	1060	48/48	0.69	0.50	2.88	186,199,213,216	0
30	MGE	D	1062	48/48	0.74	0.37	2.82	187,202,208,210	0
26	BCR	K	1051	40/40	0.67	0.46	2.77	192,202,210,210	0
23	CLA	c	6027	65/65	0.66	0.51	2.77	192,198,204,216	0
23	CLA	b	6021	65/65	0.85	0.30	2.66	154,164,172,176	0
24	PHO	D	1039	64/64	0.80	0.34	2.66	184,187,196,198	0
29	DGD	c	6055	66/66	0.73	0.41	2.61	184,192,202,203	0
23	CLA	c	6026	65/65	0.85	0.34	2.54	138,171,178,183	0
26	BCR	B	1047	40/40	0.80	0.35	2.50	155,171,200,202	0
29	DGD	b	6058	66/66	0.82	0.32	2.50	175,188,196,203	0
30	MGE	b	6060	48/48	0.76	0.41	2.37	186,199,213,216	0
23	CLA	h	6017	65/65	0.72	0.42	2.35	169,197,201,208	0
23	CLA	C	1026	65/65	0.86	0.29	2.35	138,171,178,183	0
23	CLA	B	1018	65/65	0.86	0.30	2.33	172,186,191,192	0
30	MGE	L	1061	48/48	0.74	0.45	2.29	177,191,195,199	0
23	CLA	b	6012	65/65	0.84	0.34	2.27	160,167,172,174	0
24	PHO	a	6038	64/64	0.85	0.34	2.26	166,176,178,181	0
23	CLA	d	6005	65/65	0.83	0.33	2.23	135,162,169,173	0
29	DGD	C	1055	66/66	0.80	0.36	2.22	184,192,202,203	0
23	CLA	A	1006	65/65	0.84	0.33	2.18	166,181,211,213	0
30	MGE	d	6062	48/48	0.67	0.42	2.17	187,202,208,210	0
23	CLA	B	1024	65/65	0.74	0.39	2.09	165,193,197,198	0
23	CLA	c	6028	65/65	0.88	0.28	2.06	178,182,201,202	0
23	CLA	c	6037	65/65	0.63	0.56	2.04	201,211,214,216	0
25	PQ9	D	1042	45/45	0.82	0.32	2.02	171,173,185,187	0
23	CLA	b	6016	65/65	0.89	0.29	1.91	130,172,175,180	0
23	CLA	b	6013	65/65	0.89	0.29	1.90	146,173,183,184	0
23	CLA	d	6004	65/65	0.92	0.24	1.88	130,168,179,181	0
26	BCR	C	1052	40/40	0.78	0.28	1.87	191,195,202,203	0
26	BCR	C	1054	40/40	0.68	0.43	1.80	197,201,216,216	0
23	CLA	D	1004	65/65	0.91	0.27	1.79	130,168,179,181	0
25	PQ9	A	1043	45/45	0.71	0.42	1.77	171,172,193,197	30
23	CLA	C	1029	65/65	0.89	0.31	1.68	177,187,190,201	0
23	CLA	a	6003	65/65	0.89	0.29	1.64	160,169,175,212	0
25	PQ9	a	6043	45/45	0.75	0.39	1.64	171,172,193,197	30
29	DGD	C	1057	66/66	0.82	0.33	1.62	177,190,206,207	0
27	LHG	a	6063	49/49	0.58	0.53	1.61	199,213,216,216	0
30	MGE	l	6061	48/48	0.77	0.39	1.59	177,191,195,199	0
23	CLA	B	1010	65/65	0.85	0.29	1.57	160,183,186,189	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	c	6031	65/65	0.79	0.41	1.56	181,185,202,216	0
26	BCR	c	6054	40/40	0.70	0.42	1.53	197,201,216,216	0
23	CLA	C	1036	65/65	0.73	0.38	1.52	186,190,203,216	0
23	CLA	C	1033	65/65	0.89	0.32	1.51	138,185,199,200	0
24	PHO	A	1038	64/64	0.87	0.30	1.50	166,176,178,181	0
23	CLA	b	6015	65/65	0.82	0.31	1.49	177,182,185,216	0
23	CLA	b	6014	65/65	0.72	0.40	1.48	178,187,197,216	0
23	CLA	a	6006	65/65	0.89	0.24	1.45	166,181,211,213	0
31	HEM	f	6040	43/43	0.85	0.37	1.44	186,215,216,216	0
23	CLA	C	1025	65/65	0.89	0.27	1.43	156,187,191,194	0
23	CLA	B	1019	65/65	0.89	0.30	1.43	167,172,175,180	0
23	CLA	b	6018	65/65	0.88	0.27	1.42	172,186,191,192	0
24	PHO	d	6039	64/64	0.87	0.24	1.41	184,187,196,198	0
27	LHG	A	1063	49/49	0.52	0.59	1.41	199,213,216,216	0
23	CLA	b	6011	65/65	0.86	0.31	1.36	168,178,184,188	0
23	CLA	C	1032	65/65	0.81	0.37	1.31	184,188,192,216	0
23	CLA	c	6035	65/65	0.77	0.42	1.26	189,202,210,216	0
23	CLA	b	6009	65/65	0.74	0.43	1.26	143,192,213,213	0
23	CLA	B	1009	65/65	0.80	0.35	1.25	143,192,213,213	0
23	CLA	B	1014	65/65	0.76	0.37	1.21	178,187,197,216	0
29	DGD	c	6057	66/66	0.77	0.36	1.13	177,190,206,207	0
29	DGD	B	1058	66/66	0.86	0.29	1.10	175,188,196,203	0
31	HEM	F	1040	43/43	0.83	0.37	1.09	186,215,216,216	0
23	CLA	C	1031	65/65	0.83	0.33	1.09	181,185,202,216	0
23	CLA	B	1015	65/65	0.89	0.27	1.05	177,182,185,216	0
23	CLA	B	1020	65/65	0.94	0.24	1.04	167,175,180,197	0
23	CLA	c	6033	65/65	0.85	0.33	0.99	138,185,199,200	0
23	CLA	C	1035	65/65	0.82	0.36	0.98	189,202,210,216	0
23	CLA	C	1030	65/65	0.79	0.34	0.96	185,197,216,216	0
23	CLA	b	6010	65/65	0.89	0.26	0.94	160,183,186,189	0
23	CLA	B	1012	65/65	0.86	0.29	0.82	160,167,172,174	0
23	CLA	A	1003	65/65	0.90	0.25	0.81	160,169,175,212	0
23	CLA	c	6032	65/65	0.82	0.34	0.79	186,189,200,216	0
23	CLA	b	6024	65/65	0.73	0.37	0.78	165,193,197,198	0
23	CLA	c	6025	65/65	0.87	0.26	0.77	156,187,191,194	0
23	CLA	B	1011	65/65	0.89	0.25	0.75	168,178,184,188	0
23	CLA	B	1016	65/65	0.93	0.21	0.75	130,172,175,180	0
23	CLA	c	6036	65/65	0.78	0.36	0.75	186,190,203,216	0
31	HEM	V	1041	43/43	0.94	0.28	0.72	131,181,185,187	0
23	CLA	b	6019	65/65	0.89	0.25	0.69	167,172,175,180	0
23	CLA	B	1021	65/65	0.87	0.25	0.67	154,164,172,176	0
23	CLA	b	6020	65/65	0.92	0.24	0.62	167,175,180,197	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	B	1013	65/65	0.92	0.22	0.61	146,173,183,184	0
31	HEM	v	6041	43/43	0.93	0.25	0.60	131,181,185,187	0
23	CLA	B	1023	65/65	0.88	0.25	0.53	174,179,181,191	0
23	CLA	b	6023	65/65	0.87	0.27	0.51	174,179,181,191	0
23	CLA	c	6030	65/65	0.81	0.28	0.06	185,197,216,216	0
23	CLA	b	6022	65/65	0.90	0.25	0.03	138,180,198,200	0
23	CLA	B	1022	65/65	0.91	0.23	-0.26	138,180,198,200	0
22	FE2	D	1002	1/1	0.93	0.17	-1.03	148,148,148,148	0
21	OEC	A	1001	5/9	0.97	0.14	-1.42	132,148,162,172	0
21	OEC	a	6001	5/9	0.98	0.17	-1.58	132,148,162,172	0
28	IOD	A	1065	1/1	0.98	0.13	-1.99	158,158,158,158	0
22	FE2	a	6002	1/1	0.80	0.24	-2.10	148,148,148,148	0
28	IOD	a	6065	1/1	0.99	0.13	-2.54	158,158,158,158	0
28	IOD	T	1066	1/1	0.65	0.23	-	199,199,199,199	0
28	IOD	t	6066	1/1	0.99	0.08	-	199,199,199,199	0
28	IOD	b	6067	1/1	0.84	0.51	-	199,199,199,199	0
28	IOD	D	1064	1/1	0.98	0.04	-	160,160,160,160	0
28	IOD	d	6064	1/1	0.98	0.12	-	160,160,160,160	0
28	IOD	B	1067	1/1	0.59	0.51	-	198,198,198,198	0

6.5 Other polymers [i](#)

There are no such residues in this entry.