



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 01:56 am GMT

PDB ID : 3A0B  
Title : Crystal structure of Br-substituted Photosystem II complex  
Authors : Kawakami, K.; Umena, Y.; Kamiya, N.; Shen, J.-R.  
Deposited on : 2009-03-16  
Resolution : 3.70 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

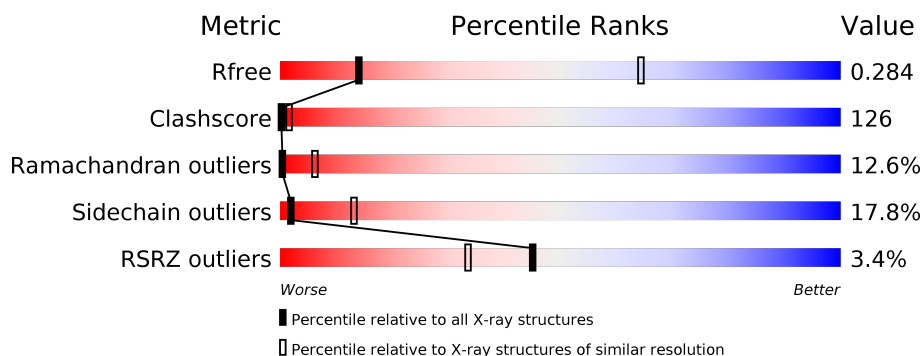
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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))
$R_{free}$	111664	1413 (3.90-3.50)
Clashscore	122126	1524 (3.90-3.50)
Ramachandran outliers	120053	1470 (3.90-3.50)
Sidechain outliers	120020	1467 (3.90-3.50)
RSRZ outliers	108989	1298 (3.90-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>9%</div> <div>66%</div> <div>22%</div> <div>• •</div> </div>
1	a	344	<div> <div>71%</div> <div>24%</div> <div>• •</div> </div>
2	B	488	<div> <div>2%</div> <div>16%</div> <div>64%</div> <div>18%</div> <div>• •</div> </div>
2	b	488	<div> <div>3%</div> <div>77%</div> <div>20%</div> <div>• •</div> </div>
3	C	447	<div> <div>2%</div> <div>16%</div> <div>62%</div> <div>21%</div> <div>•</div> </div>
3	c	447	<div> <div>5%</div> <div>78%</div> <div>21%</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	24	
19	n	24	
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	-
23	CLA	A	1007	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	-
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	-
23	CLA	C	1027	X	-	X	X
23	CLA	C	1028	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	X
23	CLA	C	1033	X	-	X	-
23	CLA	C	1034	X	-	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	-	-	-
23	CLA	D	1005	X	-	X	-
23	CLA	D	1008	X	-	X	-
23	CLA	H	1017	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	-	-	-
23	CLA	b	6013	X	-	-	-
23	CLA	b	6014	X	-	-	-
23	CLA	b	6015	X	-	-	-
23	CLA	b	6016	X	-	-	-
23	CLA	b	6017	X	-	-	-
23	CLA	b	6018	X	-	-	-
23	CLA	b	6019	X	-	-	-
23	CLA	b	6020	X	-	-	-
23	CLA	b	6021	X	-	-	-
23	CLA	b	6022	X	-	-	-
23	CLA	b	6023	X	-	-	-
23	CLA	b	6024	X	-	-	X
23	CLA	c	6025	X	-	-	-
23	CLA	c	6026	X	-	-	-
23	CLA	c	6027	X	-	-	X
23	CLA	c	6028	X	-	-	-
23	CLA	c	6029	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	6034	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	6035	X	-	-	-
23	CLA	c	6036	X	-	-	X
23	CLA	c	6037	X	-	-	X
23	CLA	d	6004	X	-	-	-
23	CLA	d	6005	X	-	-	-
23	CLA	d	6008	X	-	-	X
24	PHO	A	1038	X	-	X	-
24	PHO	A	1039	X	-	X	-
24	PHO	a	6039	X	-	-	-
24	PHO	d	6038	X	-	-	X
25	PQ9	D	1042	-	-	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	1054	-	-	X	X
26	BCR	D	1050	-	-	X	-
26	BCR	H	1049	-	-	X	X
26	BCR	K	1051	-	-	X	X
26	BCR	K	1052	-	-	X	X
26	BCR	T	6046	-	-	-	X
26	BCR	Z	1053	-	-	X	X
26	BCR	a	6044	-	-	-	X
26	BCR	b	6047	-	-	-	X
26	BCR	b	6048	-	-	-	X
26	BCR	c	6054	-	-	-	X
26	BCR	d	6050	-	-	-	X
26	BCR	h	6049	-	-	-	X
26	BCR	t	1046	-	-	-	X
26	BCR	z	6053	-	-	-	X
27	LHG	A	1063	-	-	X	X
27	LHG	a	6063	-	-	-	X
28	BR	A	1065	-	-	X	-
29	MGE	B	1060	-	-	X	-
29	MGE	D	1062	-	-	X	-
29	MGE	J	1059	-	-	X	-
29	MGE	L	1061	-	-	X	-
29	MGE	d	6059	-	-	-	X
30	DGD	C	1055	-	-	X	-
30	DGD	C	1056	-	-	X	X
30	DGD	C	1057	-	-	X	X
30	DGD	H	1058	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	DGD	c	6056	-	-	-	X
30	DGD	c	6057	-	-	-	X

## 2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 47988 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	485	Total	C	N	O	S	0	0	0
			3816	2505	635	663	13			
2	b	485	Total	C	N	O	S	0	0	0
			3816	2505	635	663	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
			1841	1152	311	374	4			
13	o	242	Total	C	N	O	S	0	0	0
			1841	1152	311	374	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			

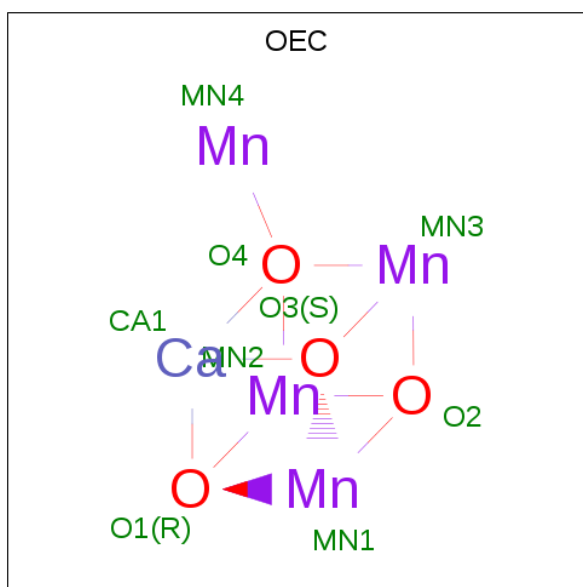
- Molecule 19 is a protein called Photosystem II reaction center protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	N	24	Total	C	N	O		0	0	0
			121	72	24	25				
19	n	24	Total	C	N	O		0	0	0
			121	72	24	25				

- 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:  $\text{CaMn}_4\text{O}_4$ ).



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	a	1	Total	Fe	0	0
			1	1		

- 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>).



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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	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	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	H	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	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	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

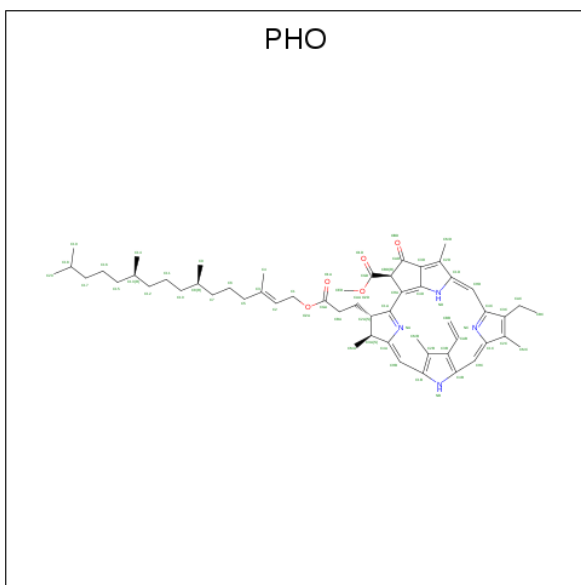
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total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

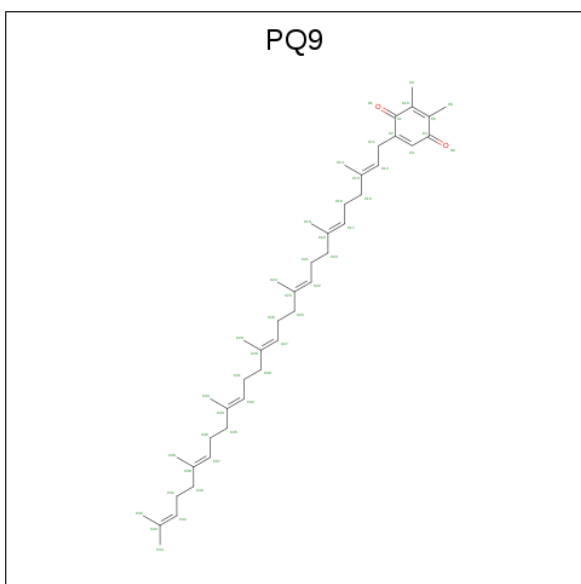
- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).





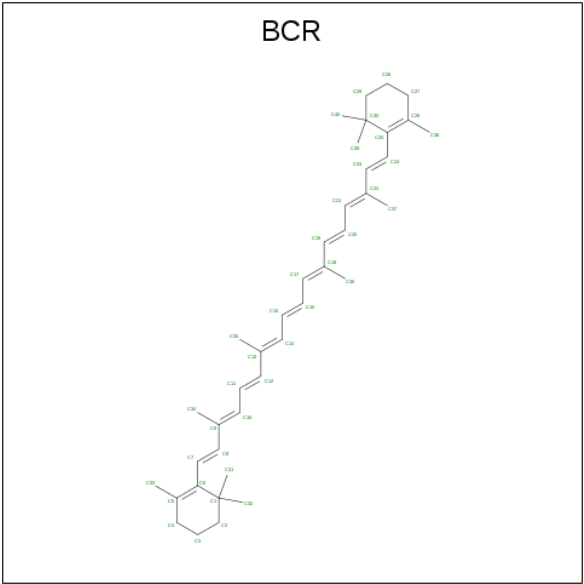
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	d	1	Total	C	N	O	0	0
			64	55	4	5		

- 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:  $C_{43}H_{64}O_2$ ).



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: C<sub>40</sub>H<sub>56</sub>).



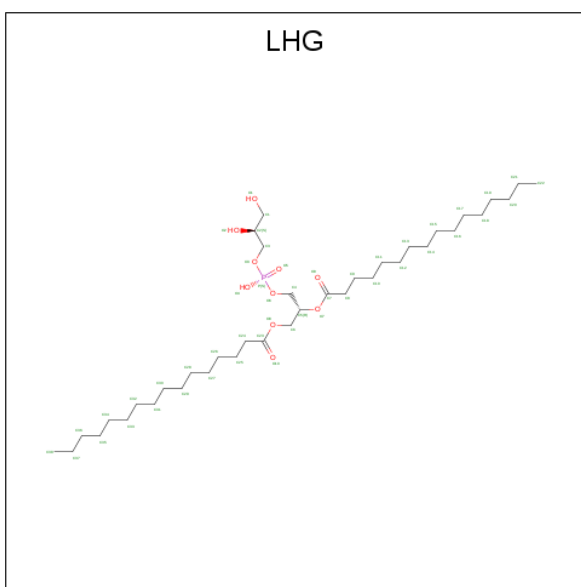
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	A	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	C	1	Total	C	0	0
			40	40		
26	D	1	Total	C	0	0
			40	40		
26	H	1	Total	C	0	0
			40	40		
26	K	1	Total	C	0	0
			40	40		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Z	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	b	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	k	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0
26	z	1	Total C 40 40	0	0

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

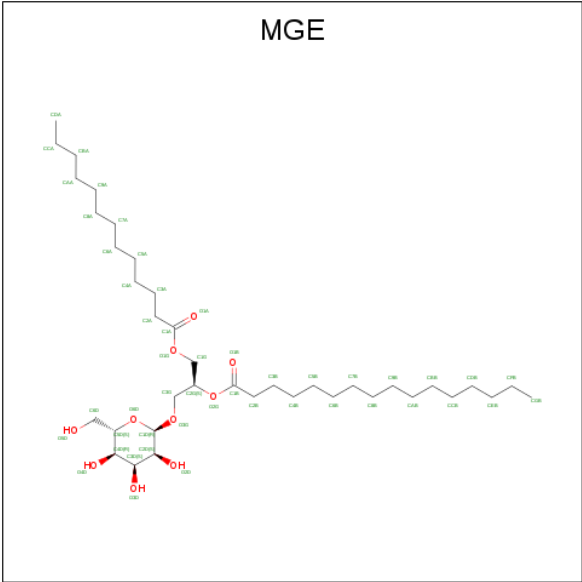


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	P	0	0
			49	38	10	1		
27	a	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 28 is BROMIDE ION (three-letter code: BR) (formula: Br).

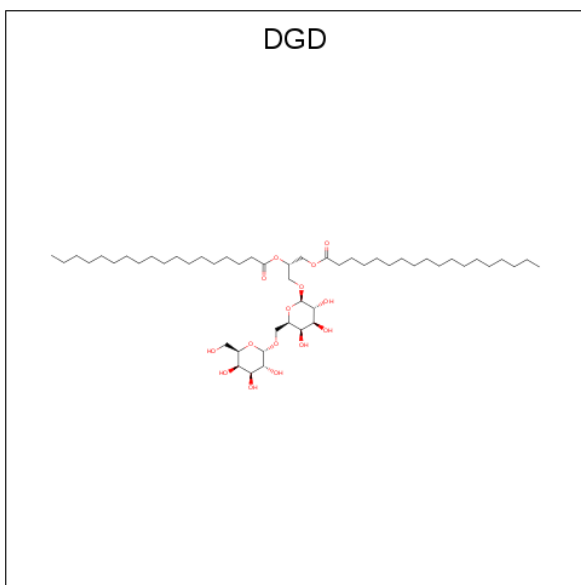
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	2	Total	Br	0	0
			2	2		
28	d	1	Total	Br	0	0
			1	1		
28	a	1	Total	Br	0	0
			1	1		

- Molecule 29 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (three-letter code: MGE) (formula: C<sub>38</sub>H<sub>72</sub>O<sub>10</sub>).



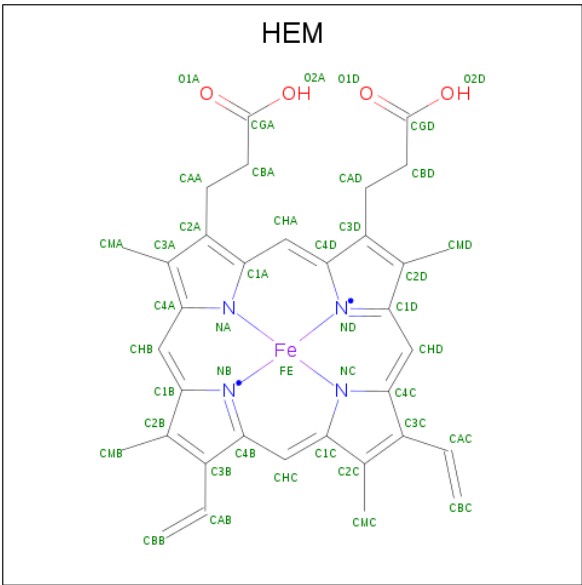
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	B	1	Total	C	O	0	0
			48	38	10		
29	D	1	Total	C	O	0	0
			48	38	10		
29	J	1	Total	C	O	0	0
			48	38	10		
29	L	1	Total	C	O	0	0
			48	38	10		
29	b	1	Total	C	O	0	0
			48	38	10		
29	d	1	Total	C	O	0	0
			48	38	10		
29	d	1	Total	C	O	0	0
			48	38	10		
29	d	1	Total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

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	C	1	Total	C	O	0	0
			66	51	15		
30	C	1	Total	C	O	0	0
			66	51	15		
30	C	1	Total	C	O	0	0
			66	51	15		
30	H	1	Total	C	O	0	0
			66	51	15		
30	c	1	Total	C	O	0	0
			66	51	15		
30	c	1	Total	C	O	0	0
			66	51	15		
30	c	1	Total	C	O	0	0
			66	51	15		
30	h	1	Total	C	O	0	0
			66	51	15		

- Molecule 31 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).

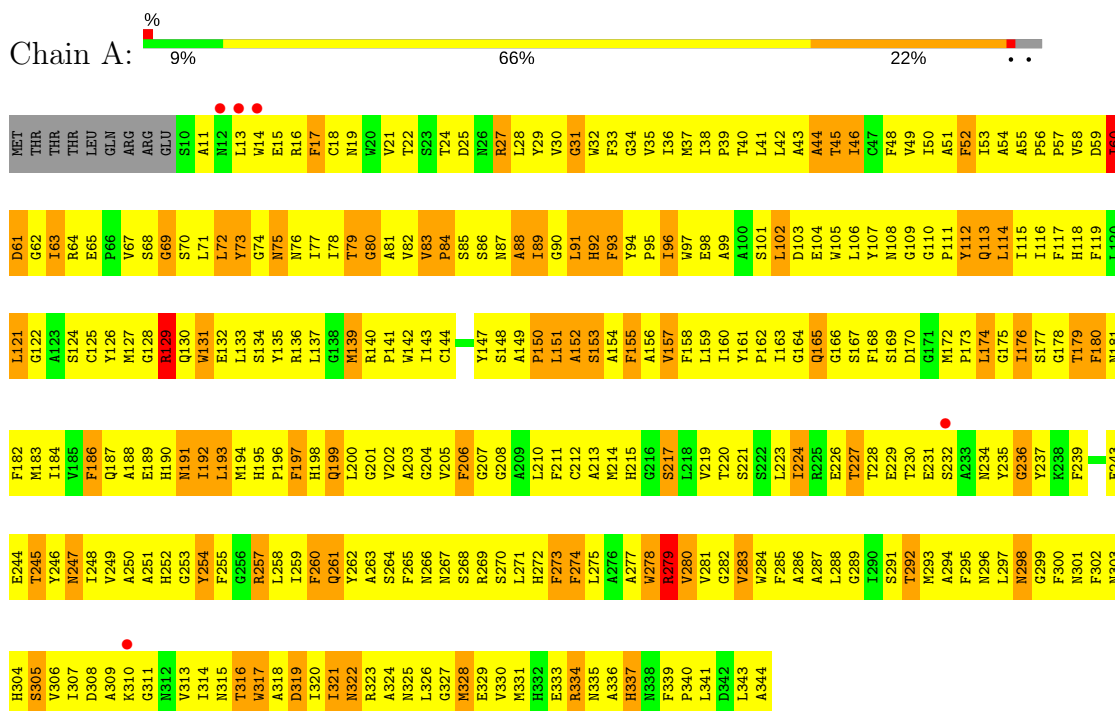


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
31	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
31	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
31	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
31	v	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

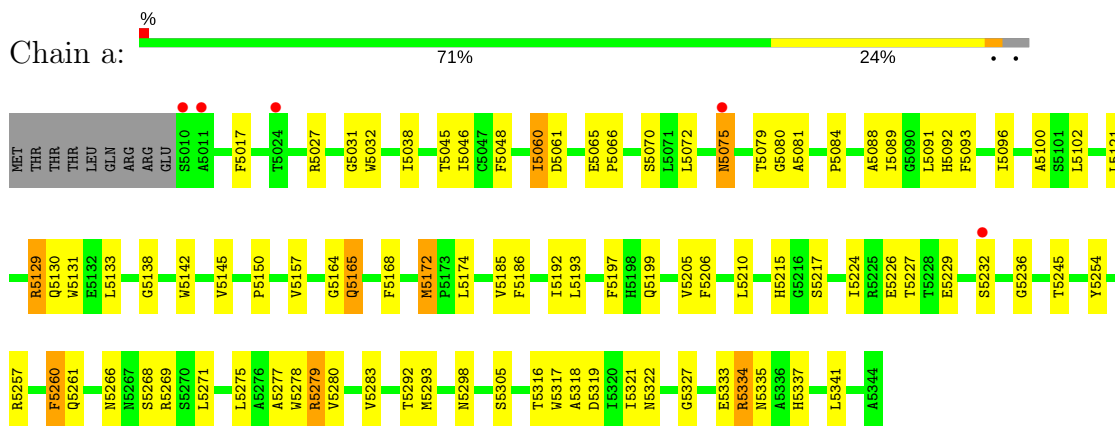
### 3 Residue-property plots

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

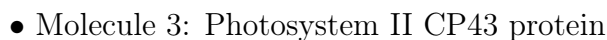


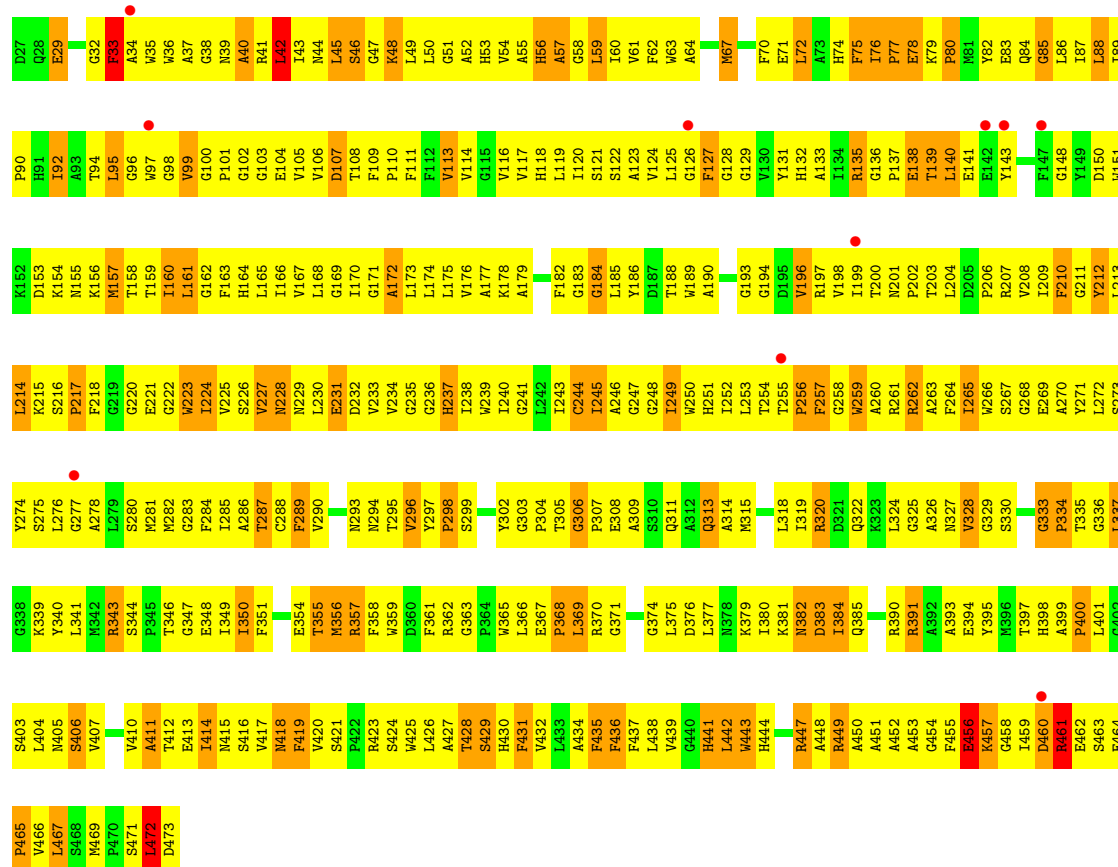
#### • Molecule 1: Photosystem Q(B) protein



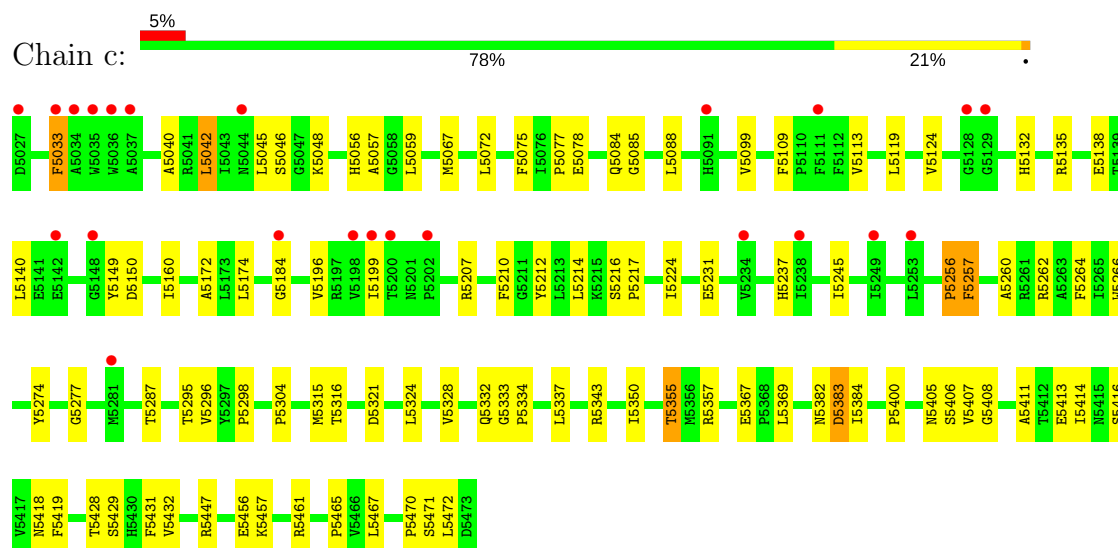
#### • Molecule 2: Photosystem II core light harvesting protein



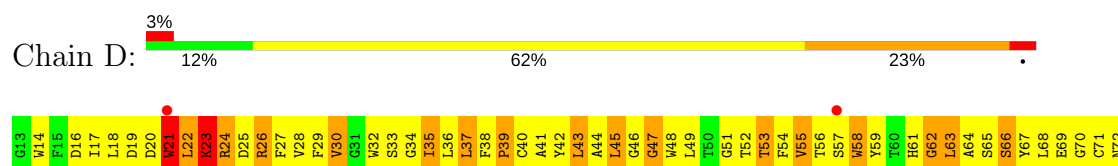


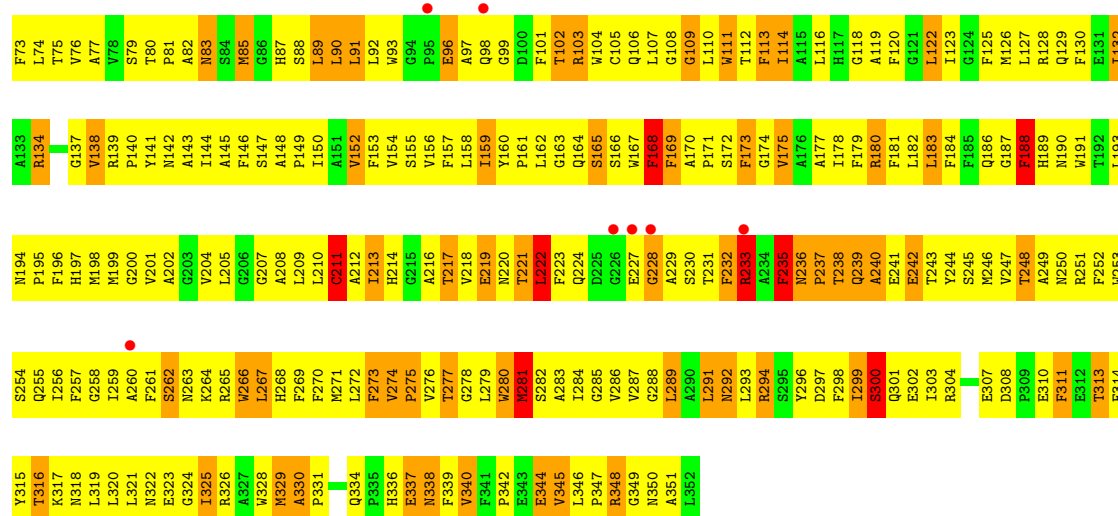


### • Molecule 3: Photosystem II CP43 protein

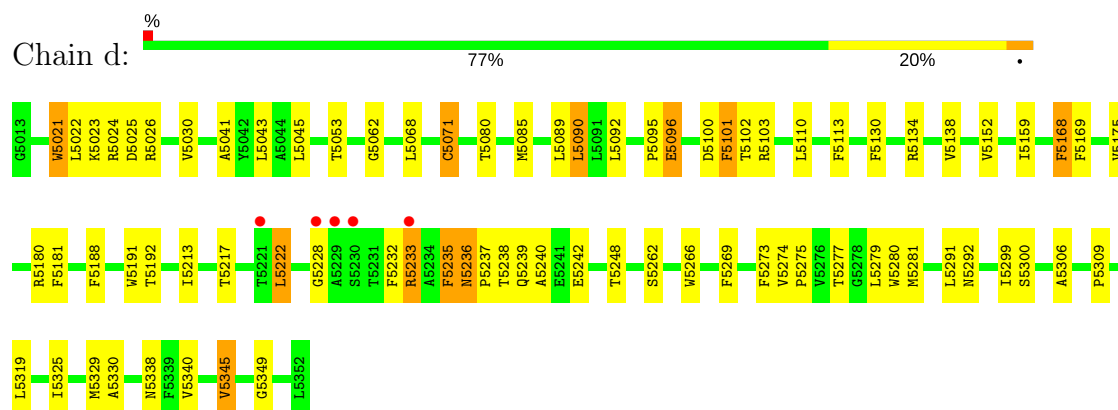


### • Molecule 4: Photosystem II D2 protein

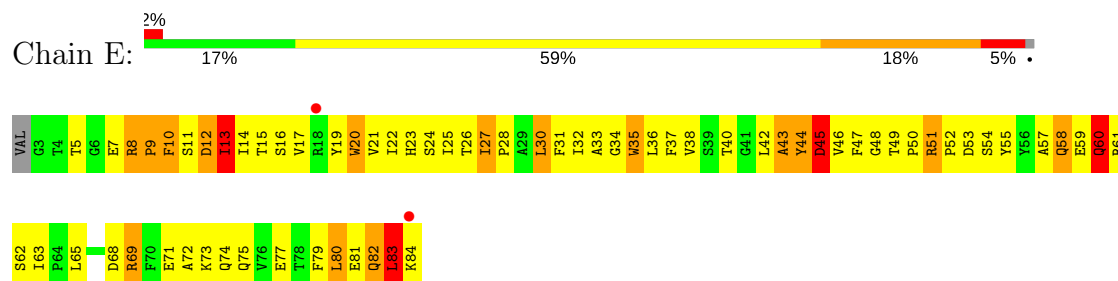




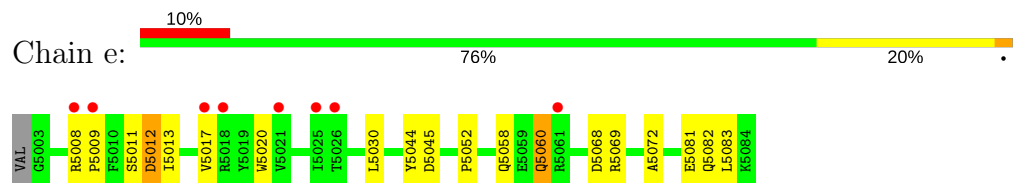
### • Molecule 4: Photosystem II D2 protein



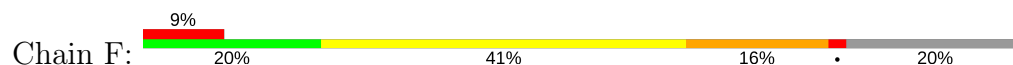
### • Molecule 5: Cytochrome b559 subunit alpha



### • Molecule 5: Cytochrome b559 subunit alpha

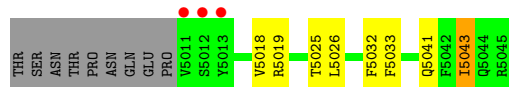


### • Molecule 6: Cytochrome b559 subunit beta

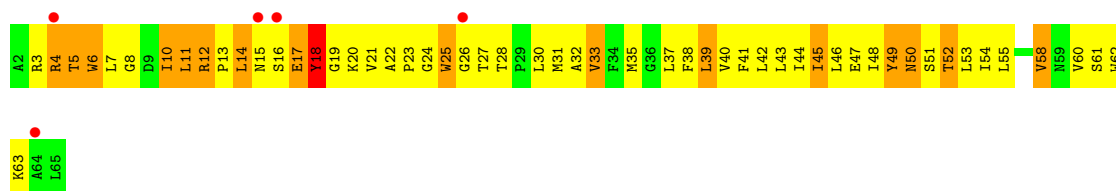
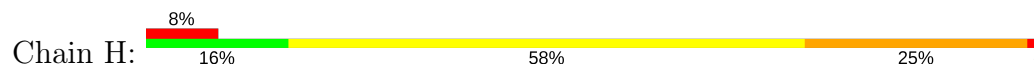




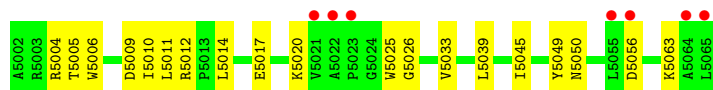
- Molecule 6: Cytochrome b559 subunit beta



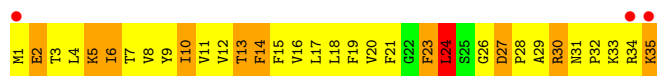
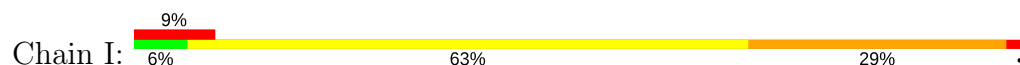
- Molecule 7: Photosystem II reaction center protein H



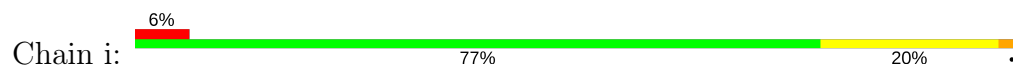
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



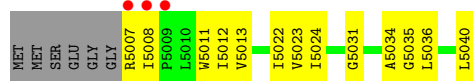
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



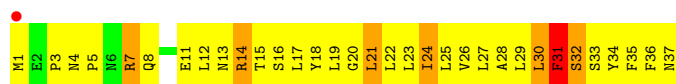
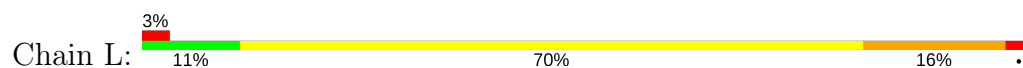
- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K



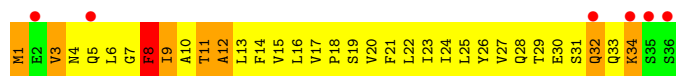
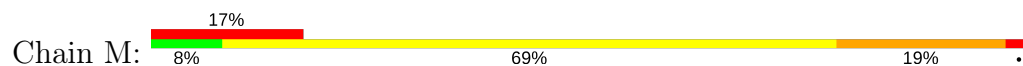
- Molecule 11: Photosystem II reaction center protein L



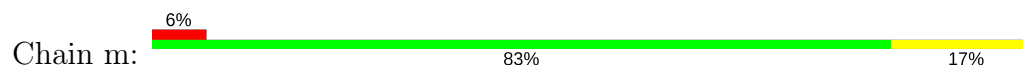
- Molecule 11: Photosystem II reaction center protein L



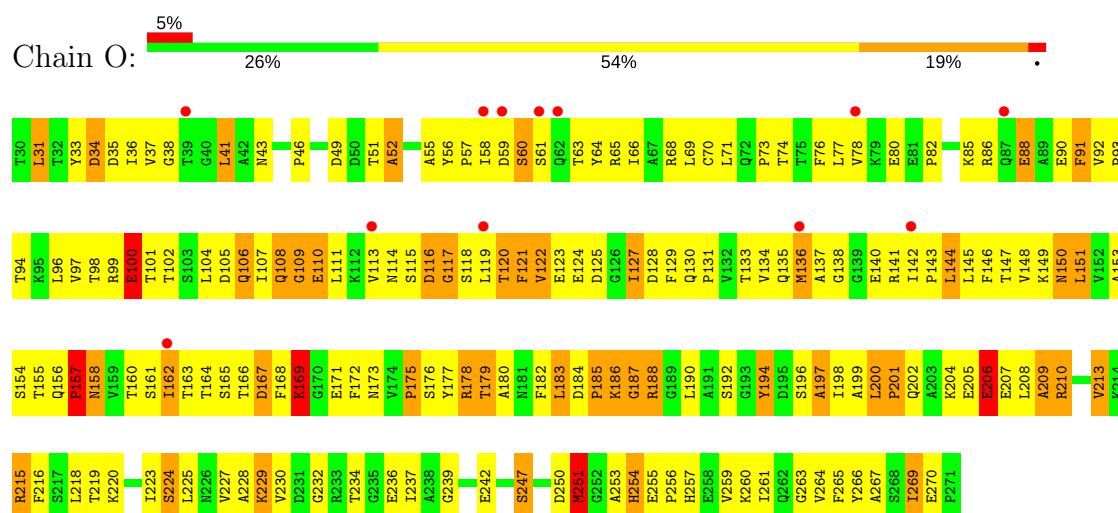
- Molecule 12: Photosystem II reaction center protein M



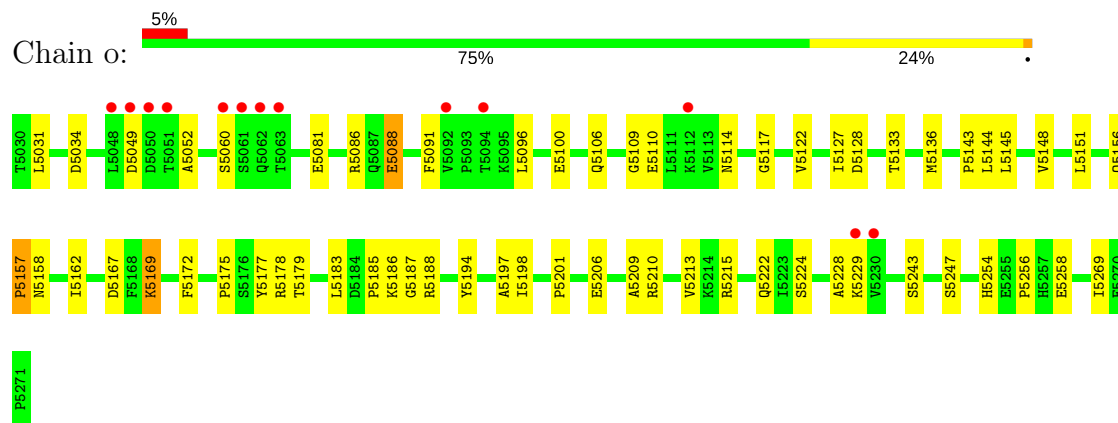
- Molecule 12: Photosystem II reaction center protein M



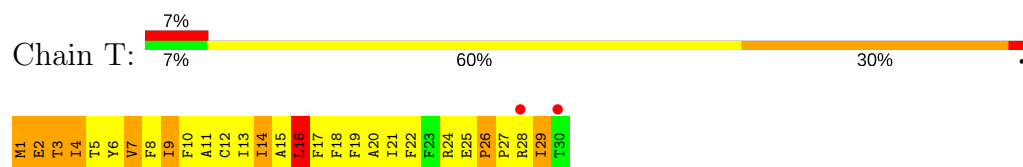
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



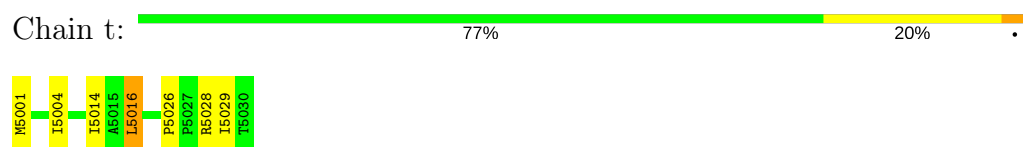
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



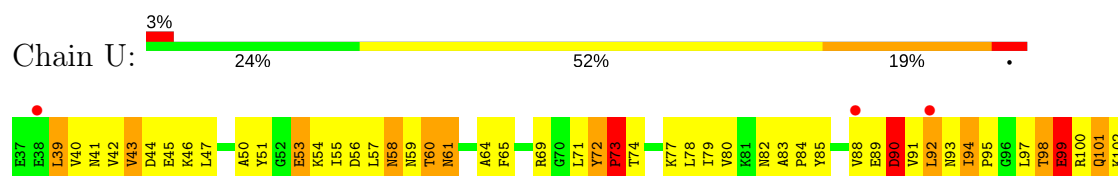
• Molecule 14: Photosystem II reaction center protein T

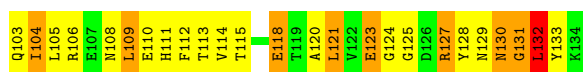


• Molecule 14: Photosystem II reaction center protein T

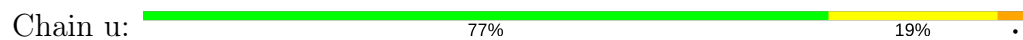


• Molecule 15: Photosystem II 12 kDa extrinsic protein

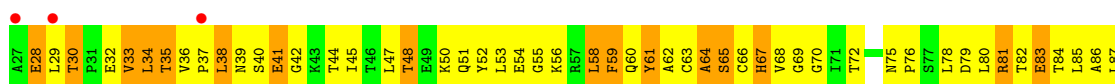
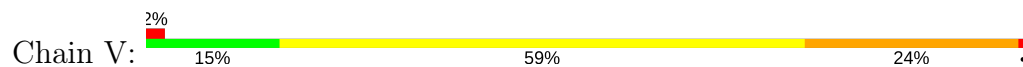




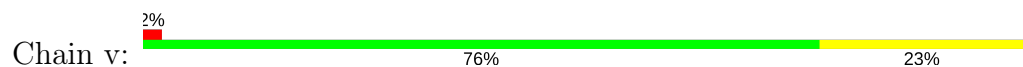
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Cytochrome c-550



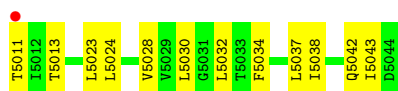
- Molecule 16: Cytochrome c-550



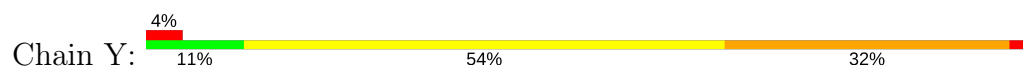
- Molecule 17: Photosystem II reaction center protein X



- Molecule 17: Photosystem II reaction center protein X



- Molecule 18: Photosystem II reaction center protein ycf12

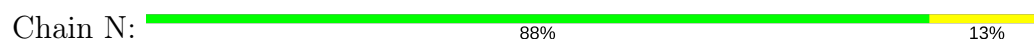




- Molecule 18: Photosystem II reaction center protein ycf12



- Molecule 19: Photosystem II reaction center protein Y

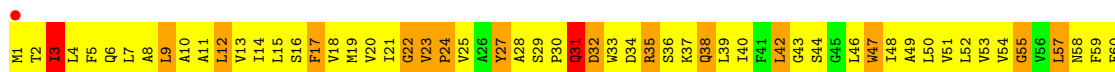
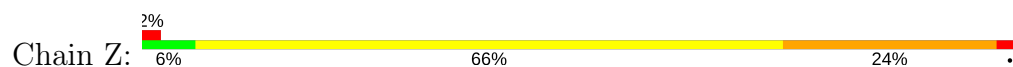


- Molecule 19: Photosystem II reaction center protein Y

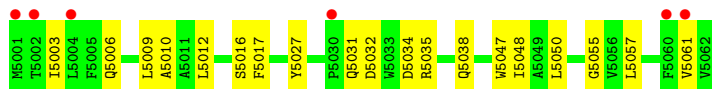


There are no outlier residues recorded for this chain.

- 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, $\alpha$ , $\beta$ , $\gamma$	130.59Å 226.39Å 307.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.70 – 3.70 34.69 – 3.70	Depositor EDS
% Data completeness (in resolution range)	85.8 (34.70-3.70) 85.8 (34.69-3.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.23 (at 3.66Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.302 , 0.358 0.285 , 0.284	Depositor DCC
$R_{free}$ test set	4216 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	135.2	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.21 , 56.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	47988	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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, 0.333 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, BR, PQ9, OEC, HEM, 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	0.51	0/2714	0.77	1/3699 (0.0%)
1	a	0.51	0/2714	0.77	0/3699
2	B	0.51	0/3951	0.79	3/5383 (0.1%)
2	b	0.51	0/3951	0.79	0/5383
3	C	0.48	0/3568	0.74	0/4858
3	c	0.49	0/3568	0.72	1/4858 (0.0%)
4	D	0.52	0/2801	0.77	1/3818 (0.0%)
4	d	0.52	0/2801	0.78	0/3818
5	E	0.46	0/685	0.74	0/933
5	e	0.50	0/685	0.76	0/933
6	F	0.50	0/291	0.77	0/397
6	f	0.58	0/291	0.69	0/397
7	H	0.52	0/520	0.81	0/708
7	h	0.50	0/520	0.82	1/708 (0.1%)
8	I	0.55	0/294	0.68	0/395
8	i	0.55	0/294	0.64	0/395
9	J	0.48	0/255	0.66	0/346
9	j	0.52	0/255	0.72	0/346
10	K	0.54	0/287	0.79	0/394
10	k	0.53	0/287	0.81	0/394
11	L	0.48	0/311	0.76	0/422
11	l	0.49	0/311	0.73	0/422
12	M	0.58	0/287	0.76	0/388
12	m	0.48	0/287	0.76	0/388
13	O	0.48	0/1872	0.79	0/2539
13	o	0.47	0/1872	0.78	0/2539
14	T	0.67	0/266	0.82	0/359
14	t	0.64	0/266	0.74	1/359 (0.3%)
15	U	0.48	0/794	0.77	0/1076
15	u	0.46	0/794	0.81	0/1076
16	V	0.50	0/1085	0.82	1/1473 (0.1%)
16	v	0.50	0/1085	0.82	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	X	0.52	0/249	0.78	0/337
17	x	0.52	0/249	0.71	0/337
18	Y	0.51	0/209	0.88	1/279 (0.4%)
18	y	0.47	0/209	0.83	0/279
20	Z	0.50	0/490	0.75	0/669
20	z	0.51	0/490	0.79	0/669
All	All	0.50	0/41858	0.77	10/56946 (0.0%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	108	TYR	N-CA-C	-5.84	95.24	111.00
2	B	232	GLY	N-CA-C	-5.64	99.00	113.10
2	B	106	LEU	CB-CG-CD1	-5.42	101.78	111.00
18	Y	38	LEU	CA-CB-CG	5.37	127.65	115.30
14	t	5016	LEU	CA-CB-CG	5.32	127.54	115.30

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	773	0
1	a	2630	0	2528	0	0
2	B	3816	0	3680	965	0
2	b	3816	0	3680	0	0
3	C	3455	0	3376	789	0
3	c	3455	0	3376	0	0
4	D	2706	0	2608	774	0
4	d	2706	0	2608	0	0
5	E	666	0	651	140	0
5	e	666	0	651	0	0
6	F	282	0	291	74	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	130	0
7	h	507	0	529	0	0
8	I	287	0	308	77	0
8	i	287	0	305	0	0
9	J	249	0	262	63	0
9	j	249	0	262	0	0
10	K	278	0	289	115	0
10	k	278	0	289	0	0
11	L	304	0	316	100	0
11	l	304	0	313	0	0
12	M	283	0	297	58	0
12	m	283	0	294	0	0
13	O	1841	0	1799	283	0
13	o	1841	0	1799	0	0
14	T	257	0	262	90	0
14	t	257	0	259	0	0
15	U	783	0	779	148	0
15	u	783	0	779	0	0
16	V	1064	0	1072	193	0
16	v	1064	0	1072	0	0
17	X	246	0	269	46	0
17	x	246	0	269	0	0
18	Y	208	0	237	54	0
18	y	208	0	237	0	0
19	N	121	0	26	2	0
19	n	121	0	26	0	0
20	Z	479	0	516	122	0
20	z	479	0	513	0	0
21	A	5	0	0	0	0
21	a	5	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	195	0	216	166	0
23	B	975	0	1079	778	0
23	C	845	0	935	534	0
23	D	195	0	216	119	0
23	H	65	0	72	60	0
23	a	195	0	216	0	0
23	b	1040	0	1151	0	0
23	c	845	0	935	0	0
23	d	195	0	216	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	A	128	0	148	116	0
24	a	64	0	74	0	0
24	d	64	0	74	0	0
25	A	45	0	64	7	0
25	D	45	0	64	32	0
25	a	45	0	64	0	0
25	d	45	0	62	0	0
26	A	40	0	48	25	0
26	B	120	0	141	86	0
26	C	40	0	47	26	0
26	D	40	0	48	62	0
26	H	40	0	47	53	0
26	K	80	0	94	81	0
26	T	40	0	47	18	0
26	Z	40	0	48	41	0
26	a	40	0	48	0	0
26	b	120	0	141	0	0
26	c	40	0	47	0	0
26	d	40	0	48	0	0
26	h	40	0	47	0	0
26	k	80	0	94	0	0
26	t	40	0	47	0	0
26	z	40	0	48	0	0
27	A	49	0	74	58	0
27	a	49	0	74	0	0
28	A	2	0	0	4	0
28	a	1	0	0	0	0
28	d	1	0	0	0	0
29	B	48	0	72	47	0
29	D	48	0	72	23	0
29	J	48	0	72	34	0
29	L	48	0	72	33	0
29	b	48	0	72	0	0
29	d	144	0	216	0	0
30	C	198	0	288	149	0
30	H	66	0	96	32	0
30	c	198	0	288	0	0
30	h	66	0	96	0	0
31	E	43	0	30	10	0
31	V	43	0	30	10	0
31	e	43	0	30	0	0
31	v	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	47988	0	48413	6019	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 126.

The worst 5 of 6019 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)
26:T:6046:BCR:H371	26:T:6046:BCR:C26	1.34	1.51
23:B:1009:CLA:CMB	26:H:1049:BCR:H393	1.41	1.49
23:C:1032:CLA:CED	23:C:1032:CLA:H2A	1.41	1.47
23:A:1003:CLA:H141	24:A:1038:PHO:C9	1.41	1.47
10:K:28:ILE:CG2	10:K:29:PRO:HD3	1.42	1.46

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%)	210 (63%)	84 (25%)	39 (12%)	0	7
1	a	333/344 (97%)	214 (64%)	75 (22%)	44 (13%)	0	5
2	B	483/488 (99%)	314 (65%)	109 (23%)	60 (12%)	0	6
2	b	483/488 (99%)	314 (65%)	109 (23%)	60 (12%)	0	6
3	C	445/447 (100%)	306 (69%)	89 (20%)	50 (11%)	0	7
3	c	445/447 (100%)	316 (71%)	82 (18%)	47 (11%)	0	9
4	D	338/340 (99%)	199 (59%)	87 (26%)	52 (15%)	0	4
4	d	338/340 (99%)	214 (63%)	79 (23%)	45 (13%)	0	5
5	E	80/83 (96%)	44 (55%)	22 (28%)	14 (18%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	e	80/83 (96%)	51 (64%)	18 (22%)	11 (14%)	0	5
6	F	33/44 (75%)	26 (79%)	6 (18%)	1 (3%)	5	38
6	f	33/44 (75%)	26 (79%)	5 (15%)	2 (6%)	1	21
7	H	62/64 (97%)	39 (63%)	15 (24%)	8 (13%)	0	6
7	h	62/64 (97%)	38 (61%)	19 (31%)	5 (8%)	1	14
8	I	33/35 (94%)	19 (58%)	8 (24%)	6 (18%)	0	2
8	i	33/35 (94%)	24 (73%)	6 (18%)	3 (9%)	1	12
9	J	32/40 (80%)	26 (81%)	2 (6%)	4 (12%)	0	6
9	j	32/40 (80%)	26 (81%)	3 (9%)	3 (9%)	1	11
10	K	34/36 (94%)	22 (65%)	8 (24%)	4 (12%)	0	7
10	k	34/36 (94%)	23 (68%)	7 (21%)	4 (12%)	0	7
11	L	35/37 (95%)	20 (57%)	12 (34%)	3 (9%)	1	13
11	l	35/37 (95%)	22 (63%)	9 (26%)	4 (11%)	0	7
12	M	34/36 (94%)	19 (56%)	8 (24%)	7 (21%)	0	2
12	m	34/36 (94%)	24 (71%)	7 (21%)	3 (9%)	1	12
13	O	240/242 (99%)	155 (65%)	47 (20%)	38 (16%)	0	4
13	o	240/242 (99%)	163 (68%)	45 (19%)	32 (13%)	0	5
14	T	28/30 (93%)	18 (64%)	5 (18%)	5 (18%)	0	2
14	t	28/30 (93%)	20 (71%)	7 (25%)	1 (4%)	4	34
15	U	96/98 (98%)	56 (58%)	24 (25%)	16 (17%)	0	3
15	u	96/98 (98%)	55 (57%)	26 (27%)	15 (16%)	0	4
16	V	135/137 (98%)	91 (67%)	25 (18%)	19 (14%)	0	4
16	v	135/137 (98%)	90 (67%)	28 (21%)	17 (13%)	0	6
17	X	32/34 (94%)	29 (91%)	2 (6%)	1 (3%)	4	38
17	x	32/34 (94%)	29 (91%)	2 (6%)	1 (3%)	4	38
18	Y	26/28 (93%)	19 (73%)	5 (19%)	2 (8%)	1	15
18	y	26/28 (93%)	19 (73%)	3 (12%)	4 (15%)	0	4
20	Z	60/62 (97%)	39 (65%)	10 (17%)	11 (18%)	0	2
20	z	60/62 (97%)	46 (77%)	8 (13%)	6 (10%)	0	10
All	All	5118/5250 (98%)	3365 (66%)	1106 (22%)	647 (13%)	0	6

5 of 647 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ILE
1	A	75	ASN
1	A	79	THR
1	A	80	GLY
1	A	84	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/279 (97%)	223 (83%)	47 (17%)	2	14
1	a	270/279 (97%)	216 (80%)	54 (20%)	1	9
2	B	386/388 (100%)	330 (86%)	56 (14%)	3	23
2	b	386/388 (100%)	332 (86%)	54 (14%)	4	25
3	C	349/349 (100%)	285 (82%)	64 (18%)	2	12
3	c	349/349 (100%)	292 (84%)	57 (16%)	2	17
4	D	275/275 (100%)	224 (82%)	51 (18%)	2	11
4	d	275/275 (100%)	231 (84%)	44 (16%)	2	18
5	E	72/73 (99%)	58 (81%)	14 (19%)	1	10
5	e	72/73 (99%)	62 (86%)	10 (14%)	4	25
6	F	29/38 (76%)	21 (72%)	8 (28%)	0	3
6	f	29/38 (76%)	22 (76%)	7 (24%)	1	5
7	H	54/54 (100%)	40 (74%)	14 (26%)	0	4
7	h	54/54 (100%)	41 (76%)	13 (24%)	1	5
8	I	32/32 (100%)	26 (81%)	6 (19%)	1	11
8	i	32/32 (100%)	26 (81%)	6 (19%)	1	11
9	J	24/28 (86%)	15 (62%)	9 (38%)	0	1
9	j	24/28 (86%)	14 (58%)	10 (42%)	0	0
10	K	29/29 (100%)	21 (72%)	8 (28%)	0	3
10	k	29/29 (100%)	21 (72%)	8 (28%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	L	35/35 (100%)	28 (80%)	7 (20%)	1	9
11	l	35/35 (100%)	28 (80%)	7 (20%)	1	9
12	M	33/33 (100%)	30 (91%)	3 (9%)	10	42
12	m	33/33 (100%)	30 (91%)	3 (9%)	10	42
13	O	200/206 (97%)	172 (86%)	28 (14%)	4	25
13	o	200/206 (97%)	168 (84%)	32 (16%)	2	18
14	T	27/27 (100%)	19 (70%)	8 (30%)	0	3
14	t	27/27 (100%)	21 (78%)	6 (22%)	1	7
15	U	85/85 (100%)	72 (85%)	13 (15%)	3	21
15	u	85/85 (100%)	73 (86%)	12 (14%)	4	24
16	V	117/117 (100%)	97 (83%)	20 (17%)	2	15
16	v	117/117 (100%)	100 (86%)	17 (14%)	3	23
17	X	27/27 (100%)	18 (67%)	9 (33%)	0	2
17	x	27/27 (100%)	16 (59%)	11 (41%)	0	0
18	Y	21/21 (100%)	13 (62%)	8 (38%)	0	1
18	y	21/21 (100%)	14 (67%)	7 (33%)	0	2
20	Z	52/52 (100%)	41 (79%)	11 (21%)	1	8
20	z	52/52 (100%)	39 (75%)	13 (25%)	0	5
All	All	4234/4296 (99%)	3479 (82%)	755 (18%)	2	13

5 of 755 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	V	38	LEU
1	a	5266	ASN
15	u	5061	ASN
16	V	119	PRO
20	Z	57	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 121 such sidechains are listed below:

Mol	Chain	Res	Type
16	V	144	HIS
2	b	5055	GLN
15	u	5058	ASN

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Mol	Chain	Res	Type
1	a	5019	ASN
1	a	5130	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 130 ligands modelled in this entry, 6 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	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	A	1006	-	58,73,73	1.88	14 (24%)	66,113,113	2.19	20 (30%)
23	CLA	A	1007	-	58,73,73	1.71	12 (20%)	66,113,113	2.34	21 (31%)
24	PHO	A	1038	-	67,69,69	2.88	24 (35%)	85,99,99	2.88	20 (23%)
24	PHO	A	1039	-	67,69,69	2.89	23 (34%)	85,99,99	2.98	22 (25%)
25	PQ9	A	1043	-	45,45,45	4.00	16 (35%)	57,57,57	5.07	23 (40%)
26	BCR	A	1044	-	41,41,41	4.05	16 (39%)	56,56,56	6.11	30 (53%)
27	LHG	A	1063	-	48,48,48	0.93	2 (4%)	51,54,54	1.05	3 (5%)
23	CLA	B	1009	-	58,73,73	1.85	14 (24%)	66,113,113	2.22	19 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	B	1010	-	58,73,73	1.70	12 (20%)	66,113,113	2.42	22 (33%)
23	CLA	B	1011	2	58,73,73	1.87	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	B	1012	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	B	1013	-	58,73,73	1.87	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	B	1014	-	58,73,73	1.75	14 (24%)	66,113,113	2.33	19 (28%)
23	CLA	B	1015	-	58,73,73	1.78	13 (22%)	66,113,113	2.50	24 (36%)
23	CLA	B	1016	-	58,73,73	1.88	14 (24%)	66,113,113	2.19	20 (30%)
23	CLA	B	1018	-	58,73,73	1.88	14 (24%)	66,113,113	2.21	20 (30%)
23	CLA	B	1019	-	58,73,73	1.80	11 (18%)	66,113,113	2.62	26 (39%)
23	CLA	B	1020	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	B	1021	-	58,73,73	1.87	14 (24%)	66,113,113	2.19	20 (30%)
23	CLA	B	1022	-	58,73,73	1.69	12 (20%)	66,113,113	2.36	23 (34%)
23	CLA	B	1023	-	58,73,73	1.88	14 (24%)	66,113,113	2.21	20 (30%)
23	CLA	B	1024	-	58,73,73	1.72	13 (22%)	66,113,113	2.50	24 (36%)
26	BCR	B	1045	-	41,41,41	4.25	15 (36%)	56,56,56	6.39	28 (50%)
26	BCR	B	1047	-	41,41,41	4.21	16 (39%)	56,56,56	7.04	25 (44%)
26	BCR	B	1048	-	41,41,41	4.26	17 (41%)	56,56,56	6.25	25 (44%)
29	MGE	B	1060	-	48,48,48	0.96	2 (4%)	56,56,56	1.03	3 (5%)
23	CLA	C	1025	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	C	1026	-	58,73,73	1.67	12 (20%)	66,113,113	2.44	21 (31%)
23	CLA	C	1027	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	C	1028	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	C	1029	-	58,73,73	1.74	12 (20%)	66,113,113	2.39	20 (30%)
23	CLA	C	1030	-	58,73,73	1.88	14 (24%)	66,113,113	2.21	20 (30%)
23	CLA	C	1031	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	C	1032	-	58,73,73	1.87	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	C	1033	-	58,73,73	1.88	14 (24%)	66,113,113	2.21	20 (30%)
23	CLA	C	1034	-	58,73,73	1.91	15 (25%)	66,113,113	2.50	21 (31%)
23	CLA	C	1035	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	C	1036	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	C	1037	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
26	BCR	C	1054	-	41,41,41	4.22	17 (41%)	56,56,56	6.76	26 (46%)
30	DGD	C	1055	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
30	DGD	C	1056	-	67,67,67	0.85	2 (2%)	81,81,81	0.92	3 (3%)
30	DGD	C	1057	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	D	1004	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	D	1005	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	D	1008	-	58,73,73	1.87	14 (24%)	66,113,113	2.21	20 (30%)
25	PQ9	D	1042	-	45,45,45	3.85	17 (37%)	57,57,57	5.13	28 (49%)
26	BCR	D	1050	-	41,41,41	4.17	16 (39%)	56,56,56	6.16	28 (50%)
29	MGE	D	1062	-	48,48,48	0.96	2 (4%)	56,56,56	1.03	3 (5%)
31	HEM	E	1040	6	27,50,50	2.17	5 (18%)	17,82,82	1.40	1 (5%)
23	CLA	H	1017	-	58,73,73	1.88	14 (24%)	66,113,113	2.21	20 (30%)
26	BCR	H	1049	-	41,41,41	4.26	16 (39%)	56,56,56	6.11	24 (42%)
30	DGD	H	1058	-	67,67,67	0.84	2 (2%)	81,81,81	0.91	3 (3%)
29	MGE	J	1059	-	48,48,48	0.96	2 (4%)	56,56,56	1.03	3 (5%)
26	BCR	K	1051	-	41,41,41	4.22	16 (39%)	56,56,56	6.33	29 (51%)
26	BCR	K	1052	-	41,41,41	4.26	16 (39%)	56,56,56	5.46	24 (42%)
29	MGE	L	1061	-	48,48,48	0.95	2 (4%)	56,56,56	1.03	3 (5%)
26	BCR	T	6046	-	41,41,41	4.28	17 (41%)	56,56,56	7.47	30 (53%)
31	HEM	V	1041	16	27,50,50	2.18	5 (18%)	17,82,82	1.40	1 (5%)
26	BCR	Z	1053	-	41,41,41	4.26	15 (36%)	56,56,56	6.42	30 (53%)
21	OEC	a	6001	1,3	0,0,13	0.00	-	0,0,27	0.00	-
23	CLA	a	6003	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	a	6006	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	a	6007	-	58,73,73	1.71	11 (18%)	66,113,113	2.34	21 (31%)
24	PHO	a	6039	-	67,69,69	2.89	23 (34%)	85,99,99	2.98	22 (25%)
25	PQ9	a	6043	-	45,45,45	4.13	21 (46%)	57,57,57	5.01	22 (38%)
26	BCR	a	6044	-	41,41,41	4.05	16 (39%)	56,56,56	6.11	30 (53%)
27	LHG	a	6063	-	48,48,48	0.93	2 (4%)	51,54,54	1.05	3 (5%)
23	CLA	b	6009	-	58,73,73	1.85	14 (24%)	66,113,113	2.22	19 (28%)
23	CLA	b	6010	-	58,73,73	1.71	12 (20%)	66,113,113	2.42	22 (33%)
23	CLA	b	6011	2	58,73,73	1.87	14 (24%)	66,113,113	2.21	20 (30%)
23	CLA	b	6012	-	58,73,73	1.88	14 (24%)	66,113,113	2.19	20 (30%)
23	CLA	b	6013	-	58,73,73	1.87	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	b	6014	-	58,73,73	1.75	14 (24%)	66,113,113	2.33	19 (28%)
23	CLA	b	6015	-	58,73,73	1.77	13 (22%)	66,113,113	2.51	24 (36%)
23	CLA	b	6016	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	b	6017	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	b	6018	-	58,73,73	1.88	14 (24%)	66,113,113	2.21	20 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	b	6019	-	58,73,73	1.80	11 (18%)	66,113,113	2.62	25 (37%)
23	CLA	b	6020	2	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	b	6021	-	58,73,73	1.87	14 (24%)	66,113,113	2.19	20 (30%)
23	CLA	b	6022	-	58,73,73	1.69	12 (20%)	66,113,113	2.36	23 (34%)
23	CLA	b	6023	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	b	6024	-	58,73,73	1.72	13 (22%)	66,113,113	2.50	24 (36%)
26	BCR	b	6045	-	41,41,41	4.25	16 (39%)	56,56,56	6.39	28 (50%)
26	BCR	b	6047	-	41,41,41	4.21	16 (39%)	56,56,56	7.04	25 (44%)
26	BCR	b	6048	-	41,41,41	4.26	17 (41%)	56,56,56	6.25	25 (44%)
29	MGE	b	6060	-	48,48,48	0.96	2 (4%)	56,56,56	1.03	3 (5%)
23	CLA	c	6025	-	58,73,73	1.87	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	c	6026	-	58,73,73	1.67	12 (20%)	66,113,113	2.43	21 (31%)
23	CLA	c	6027	-	58,73,73	1.88	14 (24%)	66,113,113	2.21	20 (30%)
23	CLA	c	6028	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	c	6029	-	58,73,73	1.74	12 (20%)	66,113,113	2.40	20 (30%)
23	CLA	c	6030	-	58,73,73	1.88	14 (24%)	66,113,113	2.21	20 (30%)
23	CLA	c	6031	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	c	6032	-	58,73,73	1.87	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	c	6033	-	58,73,73	1.87	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	c	6034	-	58,73,73	1.84	12 (20%)	66,113,113	2.28	17 (25%)
23	CLA	c	6035	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	c	6036	-	58,73,73	1.88	14 (24%)	66,113,113	2.21	20 (30%)
23	CLA	c	6037	-	58,73,73	1.88	14 (24%)	66,113,113	2.19	20 (30%)
26	BCR	c	6054	-	41,41,41	4.22	17 (41%)	56,56,56	6.75	26 (46%)
30	DGD	c	6055	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
30	DGD	c	6056	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
30	DGD	c	6057	-	67,67,67	0.85	2 (2%)	81,81,81	0.92	3 (3%)
23	CLA	d	6004	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	d	6005	-	58,73,73	1.88	14 (24%)	66,113,113	2.20	20 (30%)
23	CLA	d	6008	-	58,73,73	1.87	14 (24%)	66,113,113	2.21	20 (30%)
24	PHO	d	6038	-	67,69,69	2.89	24 (35%)	85,99,99	2.88	20 (23%)
25	PQ9	d	6042	-	45,45,45	3.87	15 (33%)	57,57,57	5.13	27 (47%)
26	BCR	d	6050	-	41,41,41	4.17	16 (39%)	56,56,56	6.16	28 (50%)
29	MGE	d	6059	-	48,48,48	0.96	2 (4%)	56,56,56	1.03	3 (5%)
29	MGE	d	6061	-	48,48,48	0.95	2 (4%)	56,56,56	1.03	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	MGE	d	6062	-	48,48,48	0.96	2 (4%)	56,56,56	1.02	3 (5%)
31	HEM	e	6040	6	27,50,50	2.17	5 (18%)	17,82,82	1.41	1 (5%)
26	BCR	h	6049	-	41,41,41	4.26	16 (39%)	56,56,56	6.11	24 (42%)
30	DGD	h	6058	-	67,67,67	0.84	2 (2%)	81,81,81	0.92	3 (3%)
26	BCR	k	6051	-	41,41,41	4.22	16 (39%)	56,56,56	6.33	29 (51%)
26	BCR	k	6052	-	41,41,41	4.27	16 (39%)	56,56,56	5.11	24 (42%)
26	BCR	t	1046	-	41,41,41	4.27	16 (39%)	56,56,56	6.42	27 (48%)
31	HEM	v	6041	-	27,50,50	2.18	5 (18%)	17,82,82	1.39	1 (5%)
26	BCR	z	6053	-	41,41,41	4.25	15 (36%)	56,56,56	6.42	30 (53%)

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	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	A	1006	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	A	1007	-	4/4/20/25	1/37/135/135	0/0/9/9
24	PHO	A	1038	-	2/2/17/22	1/53/103/103	0/5/6/6
24	PHO	A	1039	-	1/1/17/22	0/53/103/103	0/5/6/6
25	PQ9	A	1043	-	-	0/41/61/61	0/1/1/1
26	BCR	A	1044	-	-	2/29/63/63	0/2/2/2
27	LHG	A	1063	-	-	0/53/53/53	0/0/0/0
23	CLA	B	1009	-	6/6/20/25	1/37/135/135	0/0/9/9
23	CLA	B	1010	-	3/3/20/25	1/37/135/135	0/0/9/9
23	CLA	B	1011	2	3/3/20/25	1/37/135/135	0/0/9/9
23	CLA	B	1012	-	3/3/20/25	1/37/135/135	0/0/9/9
23	CLA	B	1013	-	3/3/20/25	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	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1016	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1018	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1019	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1020	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1021	-	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	1022	-	5/5/20/25	1/37/135/135	0/0/9/9
23	CLA	B	1023	-	5/5/20/25	1/37/135/135	0/0/9/9
23	CLA	B	1024	-	4/4/20/25	0/37/135/135	0/0/9/9
26	BCR	B	1045	-	-	0/29/63/63	0/2/2/2
26	BCR	B	1047	-	-	2/29/63/63	0/2/2/2
26	BCR	B	1048	-	-	1/29/63/63	0/2/2/2
29	MGE	B	1060	-	-	1/43/63/63	0/1/1/1
23	CLA	C	1025	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1026	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1027	-	6/6/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1028	-	6/6/20/25	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	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1031	-	6/6/20/25	1/37/135/135	0/0/9/9
23	CLA	C	1032	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1033	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1034	-	7/7/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1035	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1036	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1037	-	5/5/20/25	0/37/135/135	0/0/9/9
26	BCR	C	1054	-	-	0/29/63/63	0/2/2/2
30	DGD	C	1055	-	-	0/55/95/95	0/2/2/2
30	DGD	C	1056	-	-	0/55/95/95	0/2/2/2
30	DGD	C	1057	-	-	0/55/95/95	0/2/2/2
23	CLA	D	1004	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	D	1005	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	D	1008	-	3/3/20/25	0/37/135/135	0/0/9/9
25	PQ9	D	1042	-	-	0/41/61/61	0/1/1/1
26	BCR	D	1050	-	-	0/29/63/63	0/2/2/2
29	MGE	D	1062	-	-	0/43/63/63	0/1/1/1
31	HEM	E	1040	6	-	0/6/54/54	0/0/8/8
23	CLA	H	1017	-	4/4/20/25	0/37/135/135	0/0/9/9
26	BCR	H	1049	-	-	0/29/63/63	0/2/2/2
30	DGD	H	1058	-	-	0/55/95/95	0/2/2/2
29	MGE	J	1059	-	-	0/43/63/63	0/1/1/1
26	BCR	K	1051	-	-	0/29/63/63	0/2/2/2
26	BCR	K	1052	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	MGE	L	1061	-	-	0/43/63/63	0/1/1/1
26	BCR	T	6046	-	-	0/29/63/63	0/2/2/2
31	HEM	V	1041	16	-	0/6/54/54	0/0/8/8
26	BCR	Z	1053	-	-	1/29/63/63	0/2/2/2
21	OEC	a	6001	1,3	-	0/0/0/54	0/0/0/5
23	CLA	a	6003	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	a	6006	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	a	6007	-	4/4/20/25	1/37/135/135	0/0/9/9
24	PHO	a	6039	-	1/1/17/22	0/53/103/103	0/5/6/6
25	PQ9	a	6043	-	-	0/41/61/61	0/1/1/1
26	BCR	a	6044	-	-	2/29/63/63	0/2/2/2
27	LHG	a	6063	-	-	0/53/53/53	0/0/0/0
23	CLA	b	6009	-	6/6/20/25	1/37/135/135	0/0/9/9
23	CLA	b	6010	-	3/3/20/25	1/37/135/135	0/0/9/9
23	CLA	b	6011	2	3/3/20/25	1/37/135/135	0/0/9/9
23	CLA	b	6012	-	3/3/20/25	1/37/135/135	0/0/9/9
23	CLA	b	6013	-	3/3/20/25	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	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6016	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6017	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6018	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6019	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6020	2	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6021	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6022	-	5/5/20/25	1/37/135/135	0/0/9/9
23	CLA	b	6023	-	5/5/20/25	1/37/135/135	0/0/9/9
23	CLA	b	6024	-	4/4/20/25	0/37/135/135	0/0/9/9
26	BCR	b	6045	-	-	0/29/63/63	0/2/2/2
26	BCR	b	6047	-	-	2/29/63/63	0/2/2/2
26	BCR	b	6048	-	-	1/29/63/63	0/2/2/2
29	MGE	b	6060	-	-	1/43/63/63	0/1/1/1
23	CLA	c	6025	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6026	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6027	-	6/6/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6028	-	6/6/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	6029	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6030	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6031	-	6/6/20/25	1/37/135/135	0/0/9/9
23	CLA	c	6032	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6033	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6034	-	7/7/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6035	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6036	-	5/5/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6037	-	5/5/20/25	0/37/135/135	0/0/9/9
26	BCR	c	6054	-	-	0/29/63/63	0/2/2/2
30	DGD	c	6055	-	-	0/55/95/95	0/2/2/2
30	DGD	c	6056	-	-	0/55/95/95	0/2/2/2
30	DGD	c	6057	-	-	0/55/95/95	0/2/2/2
23	CLA	d	6004	-	3/3/20/25	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	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	d	6038	-	2/2/17/22	1/53/103/103	0/5/6/6
25	PQ9	d	6042	-	-	0/41/61/61	0/1/1/1
26	BCR	d	6050	-	-	0/29/63/63	0/2/2/2
29	MGE	d	6059	-	-	0/43/63/63	0/1/1/1
29	MGE	d	6061	-	-	0/43/63/63	0/1/1/1
29	MGE	d	6062	-	-	0/43/63/63	0/1/1/1
31	HEM	e	6040	6	-	0/6/54/54	0/0/8/8
26	BCR	h	6049	-	-	0/29/63/63	0/2/2/2
30	DGD	h	6058	-	-	0/55/95/95	0/2/2/2
26	BCR	k	6051	-	-	0/29/63/63	0/2/2/2
26	BCR	k	6052	-	-	0/29/63/63	0/2/2/2
26	BCR	t	1046	-	-	0/29/63/63	0/2/2/2
31	HEM	v	6041	-	-	0/6/54/54	0/0/8/8
26	BCR	z	6053	-	-	1/29/63/63	0/2/2/2

The worst 5 of 1521 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	6047	BCR	C8-C9	-9.33	1.25	1.45
26	B	1047	BCR	C8-C9	-9.32	1.25	1.45
26	B	1048	BCR	C8-C9	-9.29	1.25	1.45
26	b	6048	BCR	C8-C9	-9.29	1.25	1.45
26	k	6051	BCR	C12-C13	-9.26	1.25	1.45

The worst 5 of 2272 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	6042	PQ9	C29-C28-C30	-23.79	74.25	115.29
25	D	1042	PQ9	C29-C28-C30	-23.27	75.15	115.29
25	a	6043	PQ9	C29-C28-C30	-21.18	78.75	115.29
25	A	1043	PQ9	C29-C28-C30	-20.21	80.43	115.29
26	z	6053	BCR	C40-C30-C25	-15.89	84.54	110.31

5 of 296 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	b	6010	CLA	NC
23	b	6010	CLA	ND
23	b	6010	CLA	NA
23	B	1010	CLA	NC
23	B	1010	CLA	ND

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	b	6047	BCR	C17-C16-C15-C14
26	B	1047	BCR	C17-C16-C15-C14
26	B	1048	BCR	C17-C16-C15-C14
26	b	6048	BCR	C17-C16-C15-C14
26	a	6044	BCR	C21-C20-C19-C18

There are no ring outliers.

61 monomers are involved in 2232 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	1003	CLA	57	0
23	A	1006	CLA	94	0
23	A	1007	CLA	20	0
24	A	1038	PHO	80	0
24	A	1039	PHO	36	0
25	A	1043	PQ9	7	0
26	A	1044	BCR	25	0
27	A	1063	LHG	58	0
23	B	1009	CLA	49	0
23	B	1010	CLA	45	0
23	B	1011	CLA	107	0
23	B	1012	CLA	65	0
23	B	1013	CLA	84	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	1014	CLA	79	0
23	B	1015	CLA	29	0
23	B	1016	CLA	61	0
23	B	1018	CLA	21	0
23	B	1019	CLA	88	0
23	B	1020	CLA	74	0
23	B	1021	CLA	72	0
23	B	1022	CLA	67	0
23	B	1023	CLA	82	0
23	B	1024	CLA	40	0
26	B	1045	BCR	30	0
26	B	1047	BCR	25	0
26	B	1048	BCR	36	0
29	B	1060	MGE	47	0
23	C	1025	CLA	54	0
23	C	1026	CLA	32	0
23	C	1027	CLA	51	0
23	C	1028	CLA	32	0
23	C	1029	CLA	45	0
23	C	1030	CLA	31	0
23	C	1031	CLA	63	0
23	C	1032	CLA	56	0
23	C	1033	CLA	67	0
23	C	1034	CLA	86	0
23	C	1035	CLA	21	0
23	C	1036	CLA	52	0
23	C	1037	CLA	27	0
26	C	1054	BCR	26	0
30	C	1055	DGD	34	0
30	C	1056	DGD	57	0
30	C	1057	DGD	61	0
23	D	1004	CLA	19	0
23	D	1005	CLA	69	0
23	D	1008	CLA	32	0
25	D	1042	PQ9	32	0
26	D	1050	BCR	62	0
29	D	1062	MGE	23	0
31	E	1040	HEM	10	0
23	H	1017	CLA	60	0
26	H	1049	BCR	53	0
30	H	1058	DGD	32	0
29	J	1059	MGE	34	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	K	1051	BCR	43	0
26	K	1052	BCR	47	0
29	L	1061	MGE	33	0
26	T	6046	BCR	18	0
31	V	1041	HEM	10	0
26	Z	1053	BCR	41	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	335/344 (97%)	-0.36	5 (1%) 73 62	97, 127, 162, 173	0
1	a	335/344 (97%)	-0.29	5 (1%) 73 62	101, 131, 166, 178	0
2	B	485/488 (99%)	-0.23	9 (1%) 66 54	94, 130, 157, 181	0
2	b	485/488 (99%)	-0.16	13 (2%) 54 42	102, 129, 161, 183	0
3	C	447/447 (100%)	-0.13	10 (2%) 62 49	100, 143, 170, 185	0
3	c	447/447 (100%)	0.06	23 (5%) 28 20	102, 150, 173, 187	0
4	D	340/340 (100%)	-0.18	9 (2%) 56 43	94, 127, 165, 187	0
4	d	340/340 (100%)	-0.21	5 (1%) 73 62	92, 133, 172, 191	0
5	E	82/83 (98%)	0.03	2 (2%) 59 46	117, 156, 184, 186	0
5	e	82/83 (98%)	0.46	8 (9%) 7 6	126, 160, 181, 186	0
6	F	35/44 (79%)	-0.13	4 (11%) 5 4	139, 147, 160, 163	0
6	f	35/44 (79%)	-0.14	3 (8%) 10 8	143, 152, 160, 163	0
7	H	64/64 (100%)	0.24	5 (7%) 13 9	119, 143, 165, 170	0
7	h	64/64 (100%)	0.27	7 (10%) 5 5	120, 143, 164, 169	0
8	I	35/35 (100%)	-0.07	3 (8%) 10 8	127, 137, 166, 173	0
8	i	35/35 (100%)	-0.09	2 (5%) 24 16	124, 141, 175, 176	0
9	J	34/40 (85%)	-0.43	0 100 100	127, 142, 165, 175	0
9	j	34/40 (85%)	0.05	3 (8%) 10 7	131, 146, 172, 174	0
10	K	36/36 (100%)	-0.33	0 100 100	132, 145, 153, 155	0
10	k	36/36 (100%)	0.02	1 (2%) 53 40	140, 151, 162, 164	0
11	L	37/37 (100%)	-0.29	1 (2%) 54 42	102, 123, 178, 184	0
11	l	37/37 (100%)	-0.31	2 (5%) 26 19	110, 130, 181, 188	0
12	M	36/36 (100%)	0.25	6 (16%) 1 1	101, 119, 171, 174	0
12	m	36/36 (100%)	-0.23	2 (5%) 24 17	100, 121, 171, 179	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	242/242 (100%)	-0.06	12 (4%) 29 21	108, 133, 165, 186	0
13	o	242/242 (100%)	-0.00	13 (5%) 26 19	114, 139, 164, 186	0
14	T	30/30 (100%)	-0.40	2 (6%) 18 12	105, 124, 173, 178	0
14	t	30/30 (100%)	-0.43	0 100 100	101, 115, 173, 181	0
15	U	98/98 (100%)	-0.15	3 (3%) 49 36	108, 123, 143, 158	0
15	u	98/98 (100%)	-0.36	0 100 100	112, 128, 143, 167	0
16	V	137/137 (100%)	-0.32	3 (2%) 62 49	104, 131, 160, 170	0
16	v	137/137 (100%)	-0.12	3 (2%) 62 49	114, 145, 165, 176	0
17	X	34/34 (100%)	-0.20	1 (2%) 51 38	148, 155, 164, 170	0
17	x	34/34 (100%)	-0.19	1 (2%) 51 38	151, 159, 169, 175	0
18	Y	28/28 (100%)	-0.19	1 (3%) 42 31	164, 178, 189, 192	0
18	y	28/28 (100%)	-0.24	1 (3%) 42 31	170, 181, 191, 196	0
19	N	0/24	-	-	-	-
19	n	0/24	-	-	-	-
20	Z	62/62 (100%)	-0.17	1 (1%) 72 60	138, 161, 180, 186	0
20	z	62/62 (100%)	0.06	6 (9%) 8 6	144, 164, 184, 187	0
All	All	5194/5298 (98%)	-0.14	175 (3%) 45 33	92, 136, 172, 196	0

The worst 5 of 175 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	c	5142	GLU	6.2
4	d	5228	GLY	5.1
8	i	5035	LYS	5.1
3	c	5034	ALA	5.0
12	M	36	SER	4.8

## 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
25	PQ9	a	6043	45/45	0.35	0.40	135,149,185,185	30
27	LHG	a	6063	49/49	0.43	0.75	186,196,200,200	0
26	BCR	c	6054	40/40	0.46	0.60	174,177,183,183	0
26	BCR	H	1049	40/40	0.52	0.55	155,162,188,188	0
23	CLA	c	6027	65/65	0.55	0.61	178,195,198,200	0
26	BCR	b	6047	40/40	0.56	0.53	114,127,145,147	0
26	BCR	K	1052	40/40	0.59	0.43	153,171,178,179	0
26	BCR	k	6052	40/40	0.59	0.35	158,179,200,200	0
26	BCR	a	6044	40/40	0.60	0.74	154,160,163,166	0
26	BCR	z	6053	40/40	0.60	0.76	159,176,186,187	0
27	LHG	A	1063	49/49	0.60	0.54	181,187,194,195	0
25	PQ9	A	1043	45/45	0.62	0.34	138,151,171,171	30
26	BCR	C	1054	40/40	0.63	0.49	158,165,169,170	0
26	BCR	K	1051	40/40	0.67	0.55	175,179,182,183	0
26	BCR	h	6049	40/40	0.68	0.43	156,175,191,192	0
23	CLA	c	6037	65/65	0.68	0.53	184,188,191,200	0
26	BCR	B	1048	40/40	0.68	0.56	148,155,163,163	0
23	CLA	c	6034	65/65	0.69	0.47	87,162,181,181	0
30	DGD	c	6056	66/66	0.69	0.51	170,175,181,183	0
24	PHO	d	6038	64/64	0.70	0.49	136,147,150,150	0
23	CLA	c	6031	65/65	0.70	0.45	173,182,185,186	0
26	BCR	b	6048	40/40	0.71	0.64	141,147,158,159	0
23	CLA	C	1037	65/65	0.71	0.41	180,185,188,200	0
26	BCR	B	1045	40/40	0.71	0.43	146,156,169,170	0
23	CLA	C	1034	65/65	0.72	0.41	134,147,172,174	0
29	MGE	d	6059	48/48	0.73	0.42	164,168,198,200	0
23	CLA	b	6024	65/65	0.73	0.45	172,183,186,187	0
26	BCR	d	6050	40/40	0.73	0.41	149,160,166,167	0
26	BCR	Z	1053	40/40	0.74	0.45	141,166,178,178	0
26	BCR	b	6045	40/40	0.74	0.39	145,156,167,168	0
30	DGD	c	6057	66/66	0.74	0.56	128,149,183,184	0
23	CLA	C	1032	65/65	0.74	0.44	153,166,174,176	0
30	DGD	C	1056	66/66	0.74	0.44	155,171,183,188	0
23	CLA	B	1024	65/65	0.75	0.40	105,177,179,180	0
30	DGD	C	1057	66/66	0.75	0.47	125,140,187,193	0
26	BCR	T	6046	40/40	0.75	0.45	140,149,154,157	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	a	6003	65/65	0.75	0.38	121,130,145,193	0
26	BCR	t	1046	40/40	0.75	0.41	144,156,163,163	0
26	BCR	A	1044	40/40	0.75	0.58	147,156,158,159	0
30	DGD	H	1058	66/66	0.76	0.43	131,150,165,166	0
26	BCR	B	1047	40/40	0.76	0.40	101,136,157,157	0
23	CLA	B	1009	65/65	0.76	0.39	119,178,184,185	0
23	CLA	c	6036	65/65	0.77	0.45	177,180,184,200	0
23	CLA	b	6009	65/65	0.77	0.48	160,177,200,200	0
23	CLA	b	6017	65/65	0.78	0.36	118,165,168,200	0
29	MGE	d	6061	48/48	0.78	0.38	141,152,165,169	0
23	CLA	B	1023	65/65	0.78	0.39	155,179,185,200	0
30	DGD	h	6058	66/66	0.78	0.39	140,153,163,170	0
23	CLA	d	6008	65/65	0.78	0.41	172,175,185,200	0
26	BCR	D	1050	40/40	0.79	0.32	149,153,161,162	0
23	CLA	b	6023	65/65	0.79	0.39	149,183,189,190	0
23	CLA	C	1025	65/65	0.79	0.39	131,170,180,200	0
23	CLA	C	1030	65/65	0.79	0.38	92,145,175,176	0
23	CLA	C	1027	65/65	0.79	0.43	167,183,190,200	0
23	CLA	C	1031	65/65	0.79	0.39	164,170,179,200	0
23	CLA	a	6007	65/65	0.79	0.74	143,149,179,183	0
25	PQ9	d	6042	45/45	0.80	0.30	137,146,167,168	0
23	CLA	c	6032	65/65	0.80	0.39	144,175,181,182	0
23	CLA	c	6025	65/65	0.80	0.40	145,170,178,200	0
29	MGE	b	6060	48/48	0.81	0.35	158,178,191,192	0
24	PHO	a	6039	64/64	0.81	0.35	151,165,169,170	0
29	MGE	L	1061	48/48	0.81	0.38	141,144,154,155	0
23	CLA	C	1036	65/65	0.81	0.34	162,166,179,200	0
29	MGE	B	1060	48/48	0.81	0.37	151,170,182,184	0
29	MGE	J	1059	48/48	0.82	0.32	152,158,185,186	0
29	MGE	d	6062	48/48	0.82	0.33	130,155,167,168	0
23	CLA	c	6030	65/65	0.82	0.32	100,154,174,175	0
23	CLA	B	1014	65/65	0.82	0.31	123,169,174,176	0
23	CLA	H	1017	65/65	0.82	0.30	116,169,174,200	0
30	DGD	c	6055	66/66	0.82	0.34	147,153,165,166	0
25	PQ9	D	1042	45/45	0.83	0.29	131,145,154,155	0
23	CLA	b	6014	65/65	0.83	0.28	163,171,179,200	0
28	BR	a	6065	1/1	0.83	0.22	164,164,164,164	0
23	CLA	c	6028	65/65	0.83	0.39	147,157,160,162	0
23	CLA	a	6006	65/65	0.83	0.33	140,145,197,200	0
29	MGE	D	1062	48/48	0.84	0.33	129,148,165,165	0
23	CLA	A	1007	65/65	0.85	0.49	137,141,171,183	0
23	CLA	b	6013	65/65	0.85	0.34	139,154,161,172	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	D	1008	65/65	0.85	0.35	159,167,182,200	0
23	CLA	B	1013	65/65	0.85	0.32	131,157,165,168	0
31	HEM	e	6040	43/43	0.85	0.42	171,184,185,185	0
30	DGD	C	1055	66/66	0.85	0.34	131,140,147,152	0
23	CLA	c	6029	65/65	0.86	0.29	151,170,173,200	0
23	CLA	c	6035	65/65	0.86	0.30	170,173,177,200	0
23	CLA	B	1015	65/65	0.86	0.29	133,146,153,175	0
23	CLA	c	6026	65/65	0.86	0.35	140,144,157,170	0
23	CLA	b	6012	65/65	0.86	0.34	146,153,159,198	0
23	CLA	A	1003	65/65	0.86	0.32	122,129,147,149	0
24	PHO	A	1038	64/64	0.86	0.32	122,144,147,148	0
23	CLA	b	6016	65/65	0.87	0.35	76,148,153,155	0
23	CLA	B	1010	65/65	0.87	0.30	115,164,166,169	0
26	BCR	k	6051	40/40	0.87	0.37	187,193,197,197	0
23	CLA	b	6021	65/65	0.87	0.32	125,132,157,160	0
23	CLA	B	1020	65/65	0.87	0.28	113,151,177,179	0
23	CLA	B	1018	65/65	0.87	0.34	111,158,165,168	0
23	CLA	A	1006	65/65	0.87	0.34	119,124,190,192	0
23	CLA	C	1028	65/65	0.87	0.33	141,154,159,168	0
23	CLA	C	1029	65/65	0.87	0.30	146,156,159,200	0
23	CLA	b	6015	65/65	0.87	0.29	137,149,155,164	0
23	CLA	C	1033	65/65	0.88	0.28	117,131,162,164	0
23	CLA	B	1022	65/65	0.88	0.28	135,155,159,161	0
23	CLA	B	1016	65/65	0.88	0.30	87,143,150,150	0
23	CLA	D	1004	65/65	0.88	0.32	101,131,139,142	0
23	CLA	B	1012	65/65	0.88	0.34	148,152,159,176	0
23	CLA	c	6033	65/65	0.89	0.31	84,142,180,180	0
23	CLA	C	1035	65/65	0.89	0.26	155,167,173,200	0
23	CLA	b	6022	65/65	0.90	0.25	133,148,156,157	0
23	CLA	b	6019	65/65	0.90	0.26	124,150,155,193	0
24	PHO	A	1039	64/64	0.90	0.29	149,151,160,161	0
23	CLA	B	1019	65/65	0.90	0.23	121,156,158,200	0
23	CLA	C	1026	65/65	0.90	0.26	128,133,146,149	0
23	CLA	b	6011	65/65	0.90	0.35	156,159,165,170	0
23	CLA	d	6004	65/65	0.90	0.27	111,128,134,134	0
23	CLA	b	6020	65/65	0.90	0.28	75,148,170,173	0
23	CLA	d	6005	65/65	0.91	0.34	90,100,117,118	0
23	CLA	b	6010	65/65	0.91	0.32	93,165,169,170	0
31	HEM	E	1040	43/43	0.91	0.45	141,181,194,198	0
23	CLA	b	6018	65/65	0.91	0.34	142,154,162,165	0
23	CLA	B	1021	65/65	0.91	0.26	104,129,142,146	0
28	BR	A	1065	1/1	0.91	0.22	158,158,158,158	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	D	1005	65/65	0.92	0.29	101,108,116,157	0
31	HEM	V	1041	43/43	0.93	0.32	81,131,132,133	0
23	CLA	B	1011	65/65	0.93	0.34	144,159,161,166	0
31	HEM	v	6041	43/43	0.93	0.28	99,135,139,140	0
28	BR	d	6064	1/1	0.94	0.17	130,130,130,130	0
22	FE2	A	1002	1/1	0.95	0.24	125,125,125,125	0
22	FE2	a	6002	1/1	0.95	0.34	149,149,149,149	0
28	BR	A	1064	1/1	0.96	0.13	113,113,113,113	0
21	OEC	a	6001	5/9	0.98	0.26	87,94,106,107	0
21	OEC	A	1001	5/9	0.99	0.29	79,94,115,119	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.