



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 07:52 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 validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

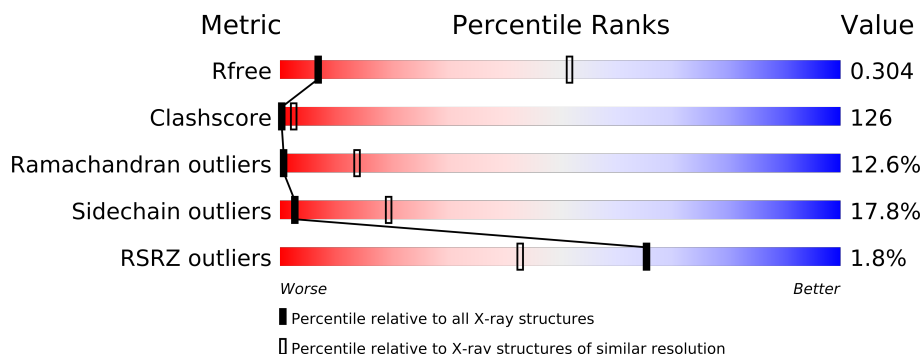
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	1098 (4.00-3.40)
Clashscore	79885	1009 (3.94-3.46)
Ramachandran outliers	78287	1016 (3.98-3.42)
Sidechain outliers	78261	1014 (3.98-3.42)
RSRZ outliers	66119	1099 (4.00-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	
2	B	488	
2	b	488	
3	C	447	
3	c	447	
4	D	340	
4	d	340	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	64	
7	h	64	

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Mol	Chain	Length	Quality of chain
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	
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 that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
23	CLA	A	1003	-	X
23	CLA	A	1006	-	X
23	CLA	B	1012	-	X
23	CLA	B	1021	-	X
23	CLA	C	1025	-	X
23	CLA	C	1028	-	X
23	CLA	C	1032	-	X
23	CLA	D	1004	-	X
23	CLA	a	6007	-	X
23	CLA	b	6013	-	X
23	CLA	b	6023	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
23	CLA	c	6027	-	X
23	CLA	c	6034	-	X
23	CLA	c	6037	-	X
23	CLA	d	6008	-	X
24	PHO	A	1039	-	X
24	PHO	d	6038	-	X
27	BCR	A	1044	-	X
27	BCR	B	1045	-	X
27	BCR	B	1047	-	X
27	BCR	B	1048	-	X
27	BCR	D	1050	-	X
27	BCR	H	1049	-	X
27	BCR	K	1051	-	X
27	BCR	T	6046	-	X
27	BCR	a	6044	-	X
27	BCR	b	6045	-	X
27	BCR	b	6047	-	X
27	BCR	b	6048	-	X
27	BCR	c	6054	-	X
27	BCR	d	6050	-	X
27	BCR	t	1046	-	X
27	BCR	z	6053	-	X
28	DGD	C	1056	-	X
28	DGD	C	1057	-	X
28	DGD	H	1058	-	X
28	DGD	c	6056	-	X
28	DGD	c	6057	-	X
28	DGD	h	6058	-	X
29	MGE	b	6060	-	X
29	MGE	d	6059	-	X
29	MGE	d	6062	-	X
30	LHG	A	1063	-	X
30	LHG	a	6063	-	X

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 47988 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

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			

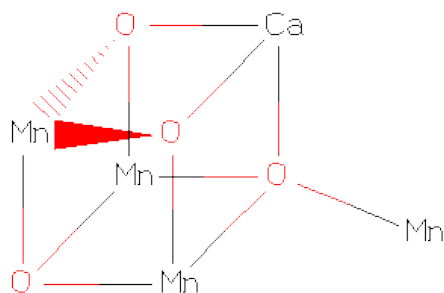
- Molecule 19 is a protein called Photosystem II reaction center protein Y.

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: CaMn_4O_4).

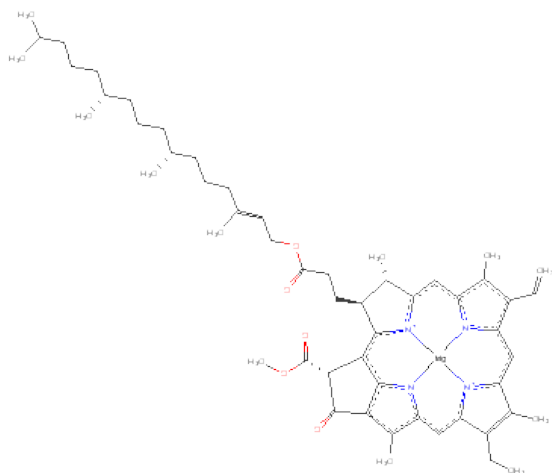


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	0	0
			5	1	4		
21	a	1	Total	Ca	Mn	0	0
			5	1	4		

- 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	a	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	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	D	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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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
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

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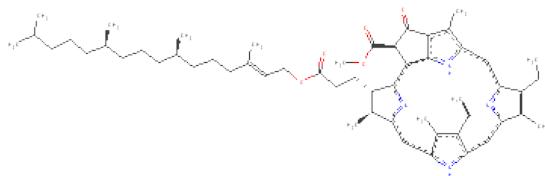
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N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

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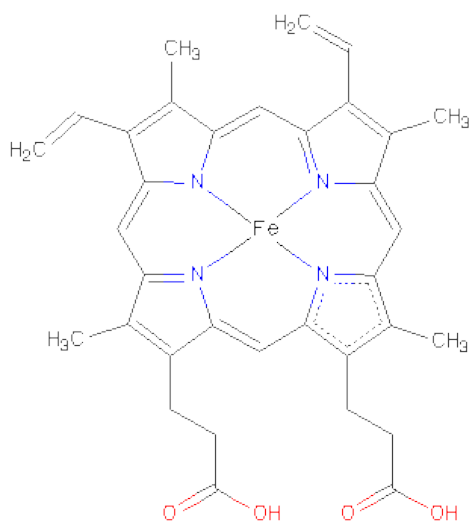
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N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

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



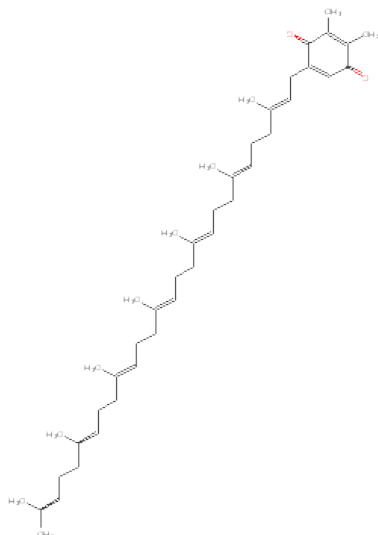
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	d	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 25 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



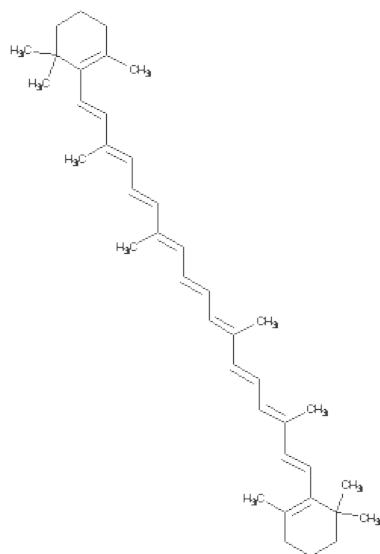
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
25	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
25	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
25	v	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 26 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: C₄₃H₆₄O₂).



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

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



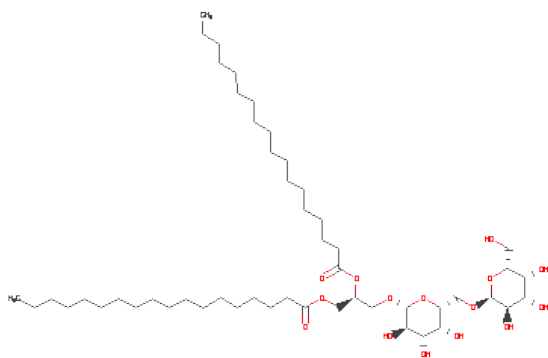
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	t	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	Z	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	a	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	h	1	Total C 40 40	0	0
27	d	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0
27	z	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



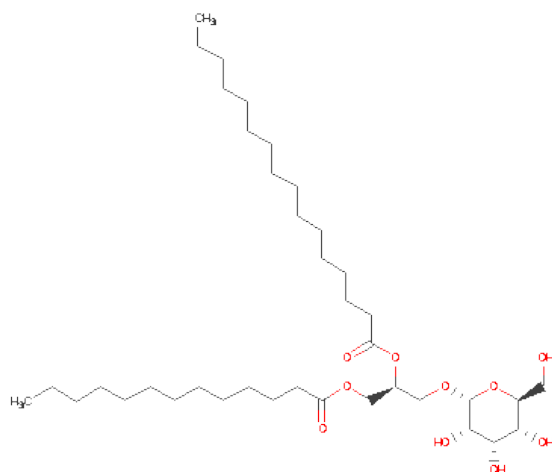
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	C	1	Total C O 66 51 15	0	0
28	C	1	Total C O 66 51 15	0	0
28	C	1	Total C O 66 51 15	0	0

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

- Molecule 29 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYLPALMITATE (three-letter code: MGE) (formula: C₃₈H₇₂O₁₀).



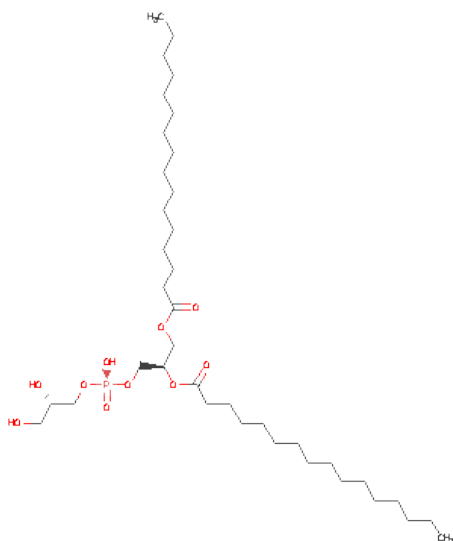
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	J	1	Total	C	O	0	0
			48	38	10		
29	B	1	Total	C	O	0	0
			48	38	10		
29	L	1	Total	C	O	0	0
			48	38	10		
29	D	1	Total	C	O	0	0
			48	38	10		
29	d	1	Total	C	O	0	0
			48	38	10		
29	b	1	Total	C	O	0	0
			48	38	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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

- Molecule 31 is BROMIDE ION (three-letter code: BR) (formula: Br).

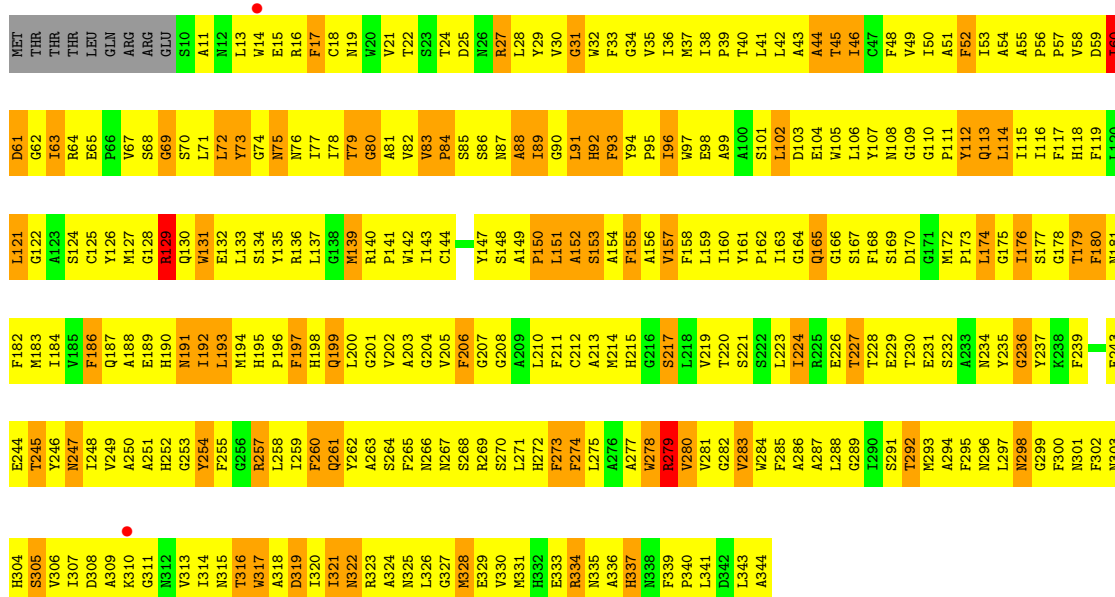
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	A	2	Total	Br	0	0
			2	2		
31	d	1	Total	Br	0	0
			1	1		
31	a	1	Total	Br	0	0
			1	1		

3 Residue-property plots

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

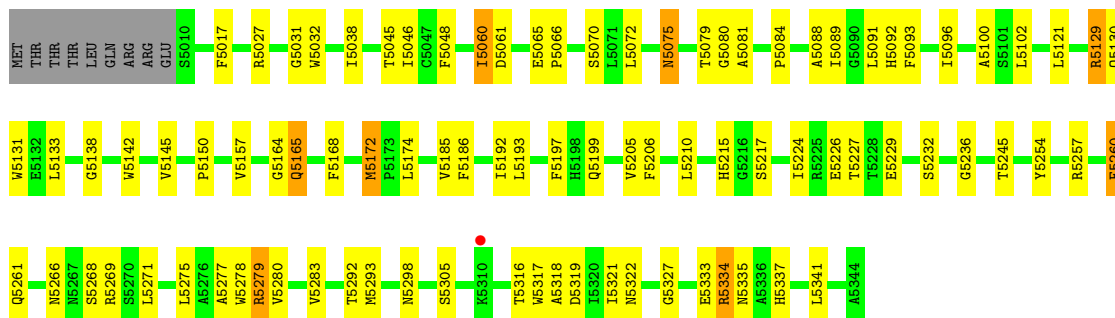
- Molecule 1: Photosystem Q(B) protein

Chain A: 



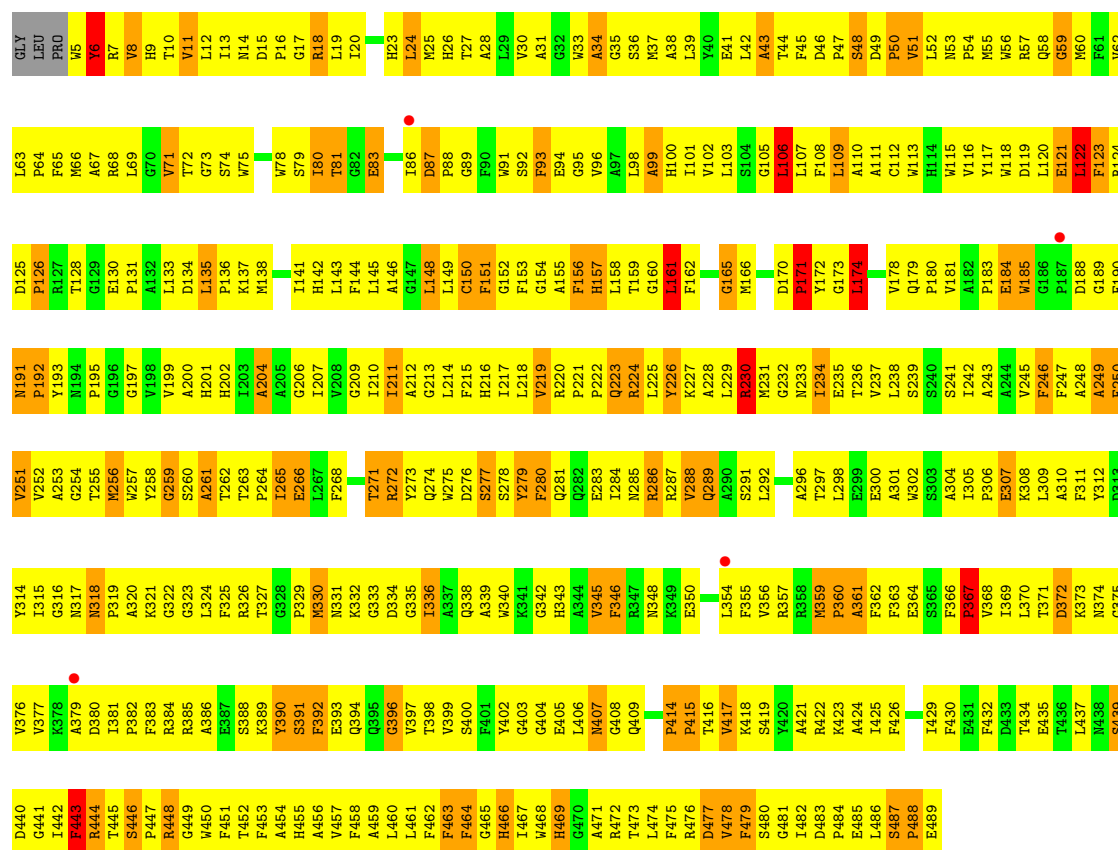
- Molecule 1: Photosystem Q(B) protein

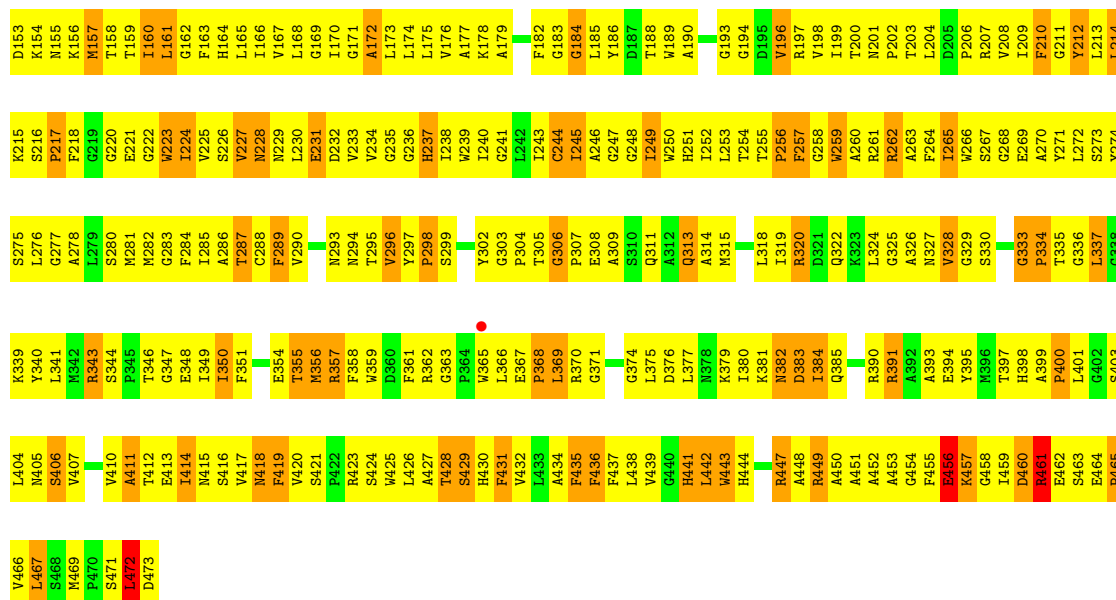
Chain a: 



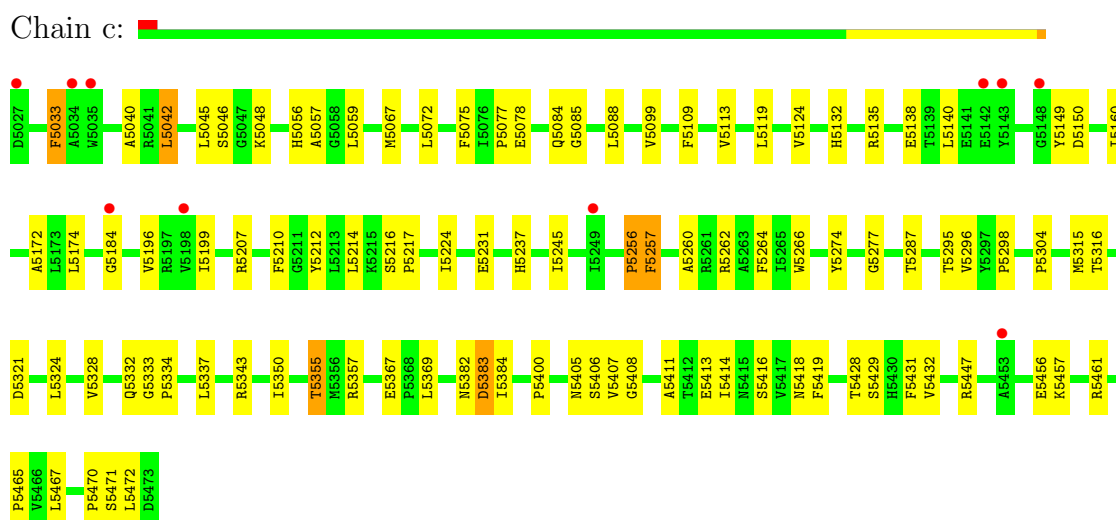
- Molecule 2: Photosystem II core light harvesting protein

Chain B: 

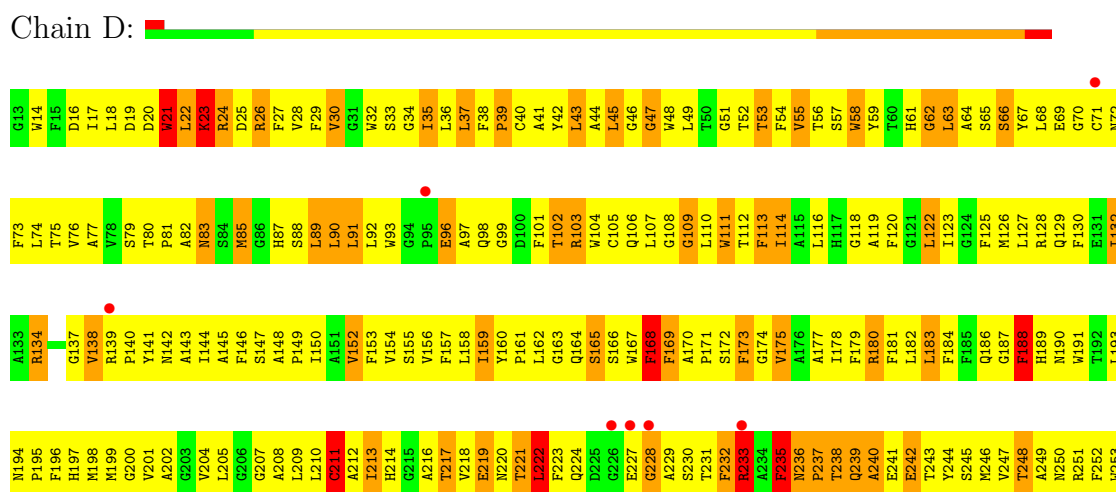


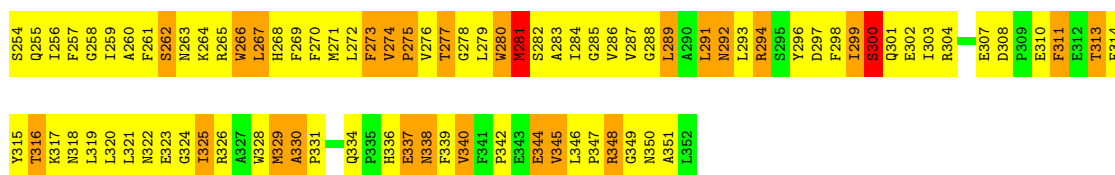


• Molecule 3: Photosystem II CP43 protein



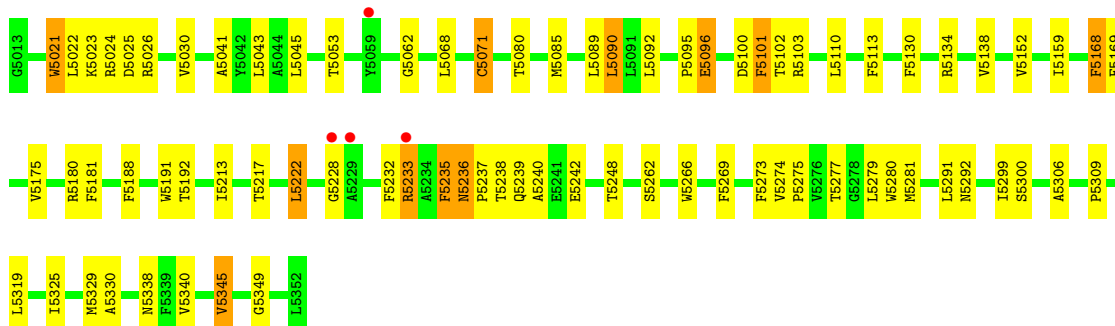
• Molecule 4: Photosystem II D2 protein





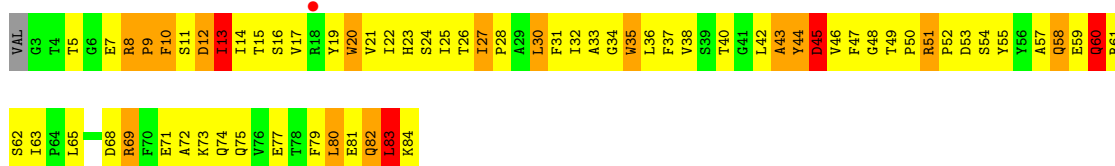
• Molecule 4: Photosystem II D2 protein

Chain d:



• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



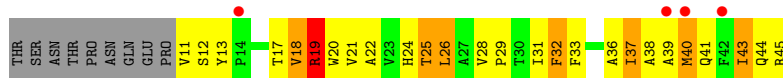
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



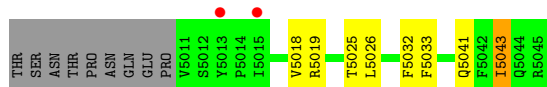
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



• Molecule 6: Cytochrome b559 subunit beta

Chain f:



• Molecule 7: Photosystem II reaction center protein H

- Chain h:

A5002	D5009	E5017	K5063
B5003	E5010	K5020	A5064
B5004	L5011	Y5021	A5065
T5005	B5012	A5022	
W5006	P5013	W5025	
	L5014	G5026	
		V5033	
		L5039	
		T5045	
		Y5049	
		N5050	
		L5055	
		D5056	

- Chain I: 

M1	E2	T3	L4	K5	I6	T7	V8	Y9	I10	V11	V12	T13	F14	F15	L18	F19	V20	F21	G22	G23	L24	S25	G26	P28	A29	R30	N31	P32	K33	R34	K35
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain i:

Category	Count
M5001	10000
I5006	10000
I5010	10000
T5013	10000
F5014	10000
F5023	10000
L5024	10000
D5027	10000
K5033	150000
R5034	150000
K5035	150000

- Chain J:

MET	MET	SER	GLU	GLY	GLY	R7	I8	P9	L10	W11	I12	V13	A14	T15	V16	A17	G18	M19	G20	V21	I22	V23	I24	V25	G26	L27	F28	F29	Y30	G31	A32	Y33	A34	G35	L36	G37	S38	S39	L40
-----	-----	-----	-----	-----	-----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain j:

Diagram illustrating a sequence of amino acids and their corresponding residue numbers:

Amino Acid	Residue Number
MET	
MET	
SER	
GLU	
GLY	
GLY	
	RS007
	RS008
	PS009
	L5010
	WS011
	L5012
	V5013
	I5022
	V5023
	L5024
	GS031
	AS034
	GS035
	L5036
	L5040

- Chain K:

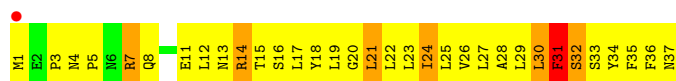
K10	L11	P12	E13	A14	Y15	A16	I17	F18	D19	P20	L21	V22	D23	V24	L25	P26	V27	I28	P29	V30	L31	F32	F33	A34	A35	A36	F37	V38	V39	V43	G44	F45
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain k:



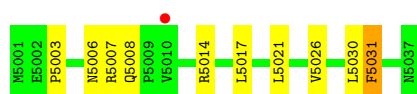
- Molecule 11: Photosystem II reaction center protein L

Chain L:



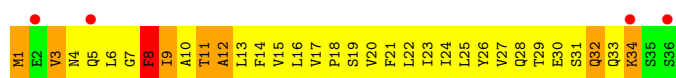
- Molecule 11: Photosystem II reaction center protein L

Chain l:



- Molecule 12: Photosystem II reaction center protein M

Chain M:



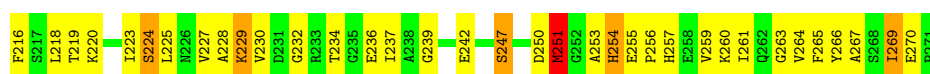
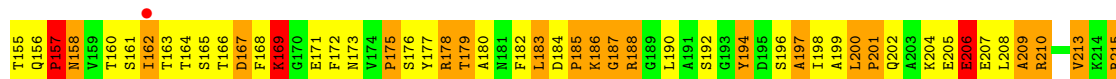
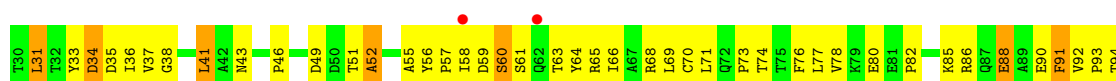
- Molecule 12: Photosystem II reaction center protein M

Chain m:



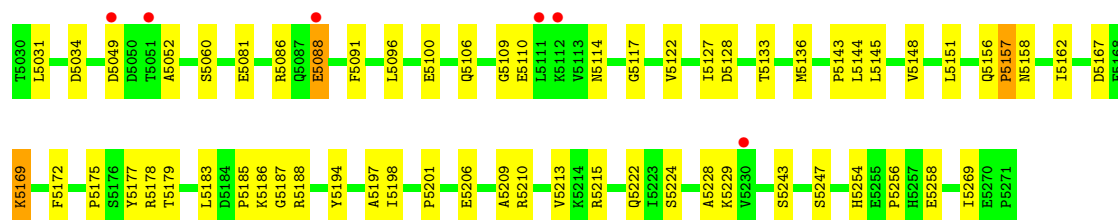
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



• Molecule 14: Photosystem II reaction center protein T

Chain T:



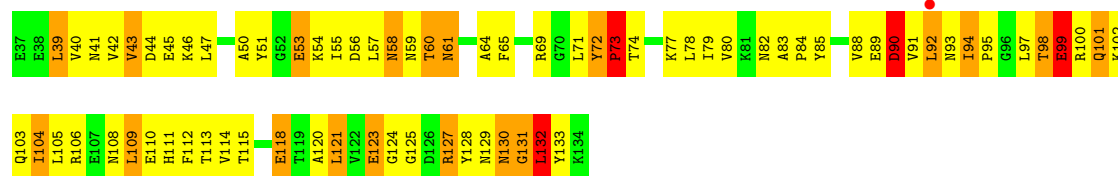
• Molecule 14: Photosystem II reaction center protein T

Chain t:



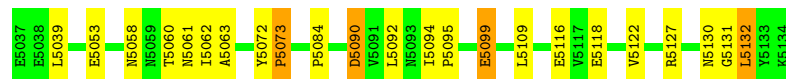
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



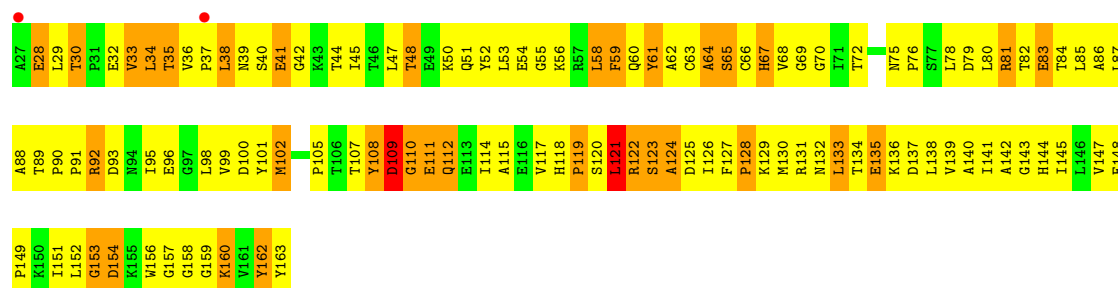
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



• Molecule 16: Cytochrome c-550

Chain V:



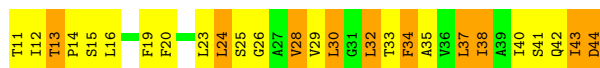
• Molecule 16: Cytochrome c-550

Chain v:



- Molecule 17: Photosystem II reaction center protein X

Chain X:



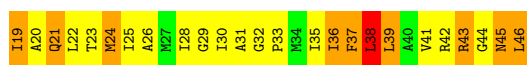
- Molecule 17: Photosystem II reaction center protein X

Chain x:



- Molecule 18: Photosystem II reaction center protein ycf12

Chain Y:



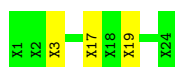
- Molecule 18: Photosystem II reaction center protein ycf12

Chain y:



- Molecule 19: Photosystem II reaction center protein Y

Chain N:



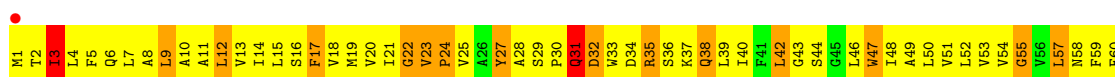
- Molecule 19: Photosystem II reaction center protein Y

Chain n:

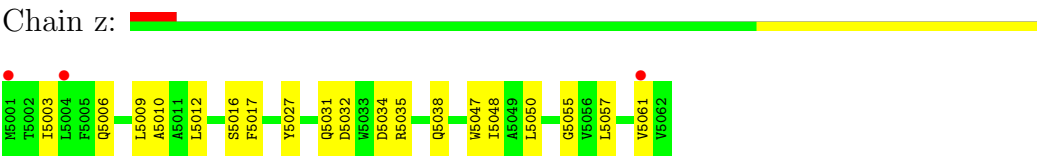
There are no outlier residues recorded for this chain.

- Molecule 20: Photosystem II reaction center protein Z

Chain Z:



- Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 3.66Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.302 , 0.358 0.308 , 0.304	Depositor DCC
R_{free} test set	4216 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	135.2	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 53.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	2 of 83926 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	47988	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, 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 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	282	0	291	74	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	d	195	0	216	0	0
24	A	128	0	148	116	0
24	a	64	0	74	0	0
24	d	64	0	74	0	0
25	E	43	0	30	10	0
25	V	43	0	30	10	0
25	e	43	0	30	0	0
25	v	43	0	30	0	0
26	A	45	0	64	7	0
26	D	45	0	64	32	0
26	a	45	0	64	0	0
26	d	45	0	62	0	0
27	A	40	0	48	25	0
27	B	120	0	141	86	0
27	C	40	0	47	26	0
27	D	40	0	48	62	0
27	H	40	0	47	53	0
27	K	80	0	94	81	0
27	T	40	0	47	18	0
27	Z	40	0	48	41	0
27	a	40	0	48	0	0
27	b	120	0	141	0	0
27	c	40	0	47	0	0
27	d	40	0	48	0	0
27	h	40	0	47	0	0
27	k	80	0	94	0	0
27	t	40	0	47	0	0
27	z	40	0	48	0	0
28	C	198	0	288	149	0
28	H	66	0	96	32	0
28	c	198	0	288	0	0
28	h	66	0	96	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	A	49	0	74	58	0
30	a	49	0	74	0	0
31	A	2	0	0	4	0
31	a	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	d	1	0	0	0	0
All	All	47988	0	48413	6019	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 126.

The worst 5 of 6019 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
27:T:6046:BCR:H371	27:T:6046:BCR:C26	1.34	1.51
23:B:1009:CLA:CMB	27: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

5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	210 (63%)	84 (25%)	39 (12%)	1	15
1	a	333/344 (97%)	214 (64%)	75 (22%)	44 (13%)	0	12
2	B	483/488 (99%)	314 (65%)	109 (23%)	60 (12%)	1	14
2	b	483/488 (99%)	314 (65%)	109 (23%)	60 (12%)	1	14
3	C	445/447 (100%)	306 (69%)	89 (20%)	50 (11%)	1	16
3	c	445/447 (100%)	316 (71%)	82 (18%)	47 (11%)	1	17
4	D	338/340 (99%)	199 (59%)	87 (26%)	52 (15%)	0	8
4	d	338/340 (99%)	214 (63%)	79 (23%)	45 (13%)	0	12
5	E	80/83 (96%)	44 (55%)	22 (28%)	14 (18%)	0	6
5	e	80/83 (96%)	51 (64%)	18 (22%)	11 (14%)	0	11
6	F	33/44 (75%)	26 (79%)	6 (18%)	1 (3%)	7	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	f	33/44 (75%)	26 (79%)	5 (15%)	2 (6%)	2	37
7	H	62/64 (97%)	39 (63%)	15 (24%)	8 (13%)	0	13
7	h	62/64 (97%)	38 (61%)	19 (31%)	5 (8%)	1	27
8	I	33/35 (94%)	19 (58%)	8 (24%)	6 (18%)	0	5
8	i	33/35 (94%)	24 (73%)	6 (18%)	3 (9%)	1	24
9	J	32/40 (80%)	26 (81%)	2 (6%)	4 (12%)	1	14
9	j	32/40 (80%)	26 (81%)	3 (9%)	3 (9%)	1	23
10	K	34/36 (94%)	22 (65%)	8 (24%)	4 (12%)	1	15
10	k	34/36 (94%)	23 (68%)	7 (21%)	4 (12%)	1	15
11	L	35/37 (95%)	20 (57%)	12 (34%)	3 (9%)	1	25
11	l	35/37 (95%)	22 (63%)	9 (26%)	4 (11%)	1	16
12	M	34/36 (94%)	19 (56%)	8 (24%)	7 (21%)	0	3
12	m	34/36 (94%)	24 (71%)	7 (21%)	3 (9%)	1	25
13	O	240/242 (99%)	155 (65%)	47 (20%)	38 (16%)	0	7
13	o	240/242 (99%)	163 (68%)	45 (19%)	32 (13%)	0	12
14	T	28/30 (93%)	18 (64%)	5 (18%)	5 (18%)	0	5
14	t	28/30 (93%)	20 (71%)	7 (25%)	1 (4%)	5	54
15	U	96/98 (98%)	56 (58%)	24 (25%)	16 (17%)	0	7
15	u	96/98 (98%)	55 (57%)	26 (27%)	15 (16%)	0	8
16	V	135/137 (98%)	91 (67%)	25 (18%)	19 (14%)	0	11
16	v	135/137 (98%)	90 (67%)	28 (21%)	17 (13%)	0	14
17	X	32/34 (94%)	29 (91%)	2 (6%)	1 (3%)	7	59
17	x	32/34 (94%)	29 (91%)	2 (6%)	1 (3%)	7	59
18	Y	26/28 (93%)	19 (73%)	5 (19%)	2 (8%)	1	29
18	y	26/28 (93%)	19 (73%)	3 (12%)	4 (15%)	0	8
20	Z	60/62 (97%)	39 (65%)	10 (17%)	11 (18%)	0	5
20	z	60/62 (97%)	46 (77%)	8 (13%)	6 (10%)	1	20
All	All	5118/5250 (98%)	3365 (66%)	1106 (22%)	647 (13%)	0	14

5 of 647 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ILE

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Mol	Chain	Res	Type
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%)	3	20
1	a	270/279 (97%)	216 (80%)	54 (20%)	2	13
2	B	386/388 (100%)	330 (86%)	56 (14%)	5	31
2	b	386/388 (100%)	332 (86%)	54 (14%)	5	33
3	C	349/349 (100%)	285 (82%)	64 (18%)	2	17
3	c	349/349 (100%)	292 (84%)	57 (16%)	3	25
4	D	275/275 (100%)	224 (82%)	51 (18%)	2	17
4	d	275/275 (100%)	231 (84%)	44 (16%)	3	26
5	E	72/73 (99%)	58 (81%)	14 (19%)	2	14
5	e	72/73 (99%)	62 (86%)	10 (14%)	5	34
6	F	29/38 (76%)	21 (72%)	8 (28%)	0	5
6	f	29/38 (76%)	22 (76%)	7 (24%)	1	8
7	H	54/54 (100%)	40 (74%)	14 (26%)	1	7
7	h	54/54 (100%)	41 (76%)	13 (24%)	1	8
8	I	32/32 (100%)	26 (81%)	6 (19%)	2	16
8	i	32/32 (100%)	26 (81%)	6 (19%)	2	16
9	J	24/28 (86%)	15 (62%)	9 (38%)	0	1
9	j	24/28 (86%)	14 (58%)	10 (42%)	0	1
10	K	29/29 (100%)	21 (72%)	8 (28%)	0	5
10	k	29/29 (100%)	21 (72%)	8 (28%)	0	5
11	L	35/35 (100%)	28 (80%)	7 (20%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	l	35/35 (100%)	28 (80%)	7 (20%)	2	13
12	M	33/33 (100%)	30 (91%)	3 (9%)	14	57
12	m	33/33 (100%)	30 (91%)	3 (9%)	14	57
13	O	200/206 (97%)	172 (86%)	28 (14%)	5	33
13	o	200/206 (97%)	168 (84%)	32 (16%)	3	26
14	T	27/27 (100%)	19 (70%)	8 (30%)	0	5
14	t	27/27 (100%)	21 (78%)	6 (22%)	1	10
15	U	85/85 (100%)	72 (85%)	13 (15%)	4	28
15	u	85/85 (100%)	73 (86%)	12 (14%)	5	33
16	V	117/117 (100%)	97 (83%)	20 (17%)	3	22
16	v	117/117 (100%)	100 (86%)	17 (14%)	5	31
17	X	27/27 (100%)	18 (67%)	9 (33%)	0	3
17	x	27/27 (100%)	16 (59%)	11 (41%)	0	1
18	Y	21/21 (100%)	13 (62%)	8 (38%)	0	1
18	y	21/21 (100%)	14 (67%)	7 (33%)	0	3
20	Z	52/52 (100%)	41 (79%)	11 (21%)	1	11
20	z	52/52 (100%)	39 (75%)	13 (25%)	1	7
All	All	4234/4296 (99%)	3479 (82%)	755 (18%)	2	19

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
1	a	5019	ASN

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Mol	Chain	Res	Type
1	a	5130	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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	-	73,73,73	2.04	17 (23%)	95,113,113	2.79	32 (33%)
23	CLA	A	1006	-	73,73,73	2.04	17 (23%)	95,113,113	2.79	32 (33%)
23	CLA	A	1007	-	73,73,73	2.02	18 (24%)	95,113,113	2.83	35 (36%)
24	PHO	A	1038	-	69,69,69	4.17	18 (26%)	91,99,99	2.98	25 (27%)
24	PHO	A	1039	-	69,69,69	4.20	19 (27%)	91,99,99	3.05	25 (27%)
26	PQ9	A	1043	-	45,45,45	4.56	16 (35%)	57,57,57	5.69	26 (45%)
27	BCR	A	1044	-	41,41,41	4.02	16 (39%)	56,56,56	5.93	30 (53%)
30	LHG	A	1063	-	48,48,48	0.89	2 (4%)	54,54,54	0.99	3 (5%)
23	CLA	B	1009	-	73,73,73	2.02	18 (24%)	95,113,113	2.81	33 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	1010	-	73,73,73	2.05	18 (24%)	95,113,113	2.98	33 (34%)
23	CLA	B	1011	2	73,73,73	2.04	17 (23%)	95,113,113	2.78	32 (33%)
23	CLA	B	1012	-	73,73,73	2.04	17 (23%)	95,113,113	2.79	32 (33%)
23	CLA	B	1013	-	73,73,73	2.04	17 (23%)	95,113,113	2.79	32 (33%)
23	CLA	B	1014	-	73,73,73	1.95	17 (23%)	95,113,113	3.01	34 (35%)
23	CLA	B	1015	-	73,73,73	2.05	19 (26%)	95,113,113	3.10	40 (42%)
23	CLA	B	1016	-	73,73,73	2.04	17 (23%)	95,113,113	2.78	31 (32%)
23	CLA	B	1018	-	73,73,73	2.04	17 (23%)	95,113,113	2.79	32 (33%)
23	CLA	B	1019	-	73,73,73	2.08	18 (24%)	95,113,113	3.00	37 (38%)
23	CLA	B	1020	-	73,73,73	2.04	17 (23%)	95,113,113	2.79	31 (32%)
23	CLA	B	1021	-	73,73,73	2.04	17 (23%)	95,113,113	2.78	32 (33%)
23	CLA	B	1022	-	73,73,73	2.00	18 (24%)	95,113,113	2.89	35 (36%)
23	CLA	B	1023	-	73,73,73	2.04	17 (23%)	95,113,113	2.79	32 (33%)
23	CLA	B	1024	-	73,73,73	2.02	17 (23%)	95,113,113	3.00	34 (35%)
27	BCR	B	1045	-	41,41,41	4.22	15 (36%)	56,56,56	6.22	30 (53%)
27	BCR	B	1047	-	41,41,41	4.18	16 (39%)	56,56,56	6.91	25 (44%)
27	BCR	B	1048	-	41,41,41	4.23	17 (41%)	56,56,56	6.10	26 (46%)
29	MGE	B	1060	-	48,48,48	0.91	2 (4%)	56,56,56	1.00	3 (5%)
23	CLA	C	1025	-	73,73,73	2.04	17 (23%)	95,113,113	2.78	31 (32%)
23	CLA	C	1026	-	73,73,73	1.95	17 (23%)	95,113,113	2.89	33 (34%)
23	CLA	C	1027	-	73,73,73	2.04	17 (23%)	95,113,113	2.78	31 (32%)
23	CLA	C	1028	-	73,73,73	2.04	17 (23%)	95,113,113	2.79	31 (32%)
23	CLA	C	1029	-	73,73,73	2.03	18 (24%)	95,113,113	2.90	33 (34%)
23	CLA	C	1030	-	73,73,73	2.04	17 (23%)	95,113,113	2.79	31 (32%)
23	CLA	C	1031	-	73,73,73	2.04	17 (23%)	95,113,113	2.79	32 (33%)
23	CLA	C	1032	-	73,73,73	2.04	17 (23%)	95,113,113	2.79	32 (33%)
23	CLA	C	1033	-	73,73,73	2.05	17 (23%)	95,113,113	2.79	32 (33%)
23	CLA	C	1034	-	73,73,73	2.06	18 (24%)	95,113,113	2.95	33 (34%)
23	CLA	C	1035	-	73,73,73	2.04	17 (23%)	95,113,113	2.79	32 (33%)
23	CLA	C	1036	-	73,73,73	2.04	17 (23%)	95,113,113	2.79	32 (33%)
23	CLA	C	1037	-	73,73,73	2.04	17 (23%)	95,113,113	2.79	32 (33%)
27	BCR	C	1054	-	41,41,41	4.19	17 (41%)	56,56,56	6.62	26 (46%)
28	DGD	C	1055	-	67,67,67	0.81	2 (2%)	81,81,81	0.90	3 (3%)
28	DGD	C	1056	-	67,67,67	0.81	2 (2%)	81,81,81	0.90	3 (3%)
28	DGD	C	1057	-	67,67,67	0.80	2 (2%)	81,81,81	0.90	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	D	1004	-	73,73,73	2.05	17 (23%)	95,113,113	2.79	32 (33%)
23	CLA	D	1005	-	73,73,73	2.04	17 (23%)	95,113,113	2.78	32 (33%)
23	CLA	D	1008	-	73,73,73	2.04	17 (23%)	95,113,113	2.79	32 (33%)
26	PQ9	D	1042	-	45,45,45	4.40	16 (35%)	57,57,57	5.84	26 (45%)
27	BCR	D	1050	-	41,41,41	4.14	16 (39%)	56,56,56	5.97	28 (50%)
29	MGE	D	1062	-	48,48,48	0.91	2 (4%)	56,56,56	1.00	3 (5%)
25	HEM	E	1040	6	49,50,50	2.27	15 (30%)	46,82,82	2.06	8 (17%)
23	CLA	H	1017	-	73,73,73	2.04	17 (23%)	95,113,113	2.80	32 (33%)
27	BCR	H	1049	-	41,41,41	4.23	15 (36%)	56,56,56	5.94	26 (46%)
28	DGD	H	1058	-	67,67,67	0.80	2 (2%)	81,81,81	0.90	3 (3%)
29	MGE	J	1059	-	48,48,48	0.91	2 (4%)	56,56,56	1.00	3 (5%)
27	BCR	K	1051	-	41,41,41	4.19	16 (39%)	56,56,56	6.16	28 (50%)
27	BCR	K	1052	-	41,41,41	4.23	15 (36%)	56,56,56	5.35	26 (46%)
29	MGE	L	1061	-	48,48,48	0.90	2 (4%)	56,56,56	1.00	3 (5%)
27	BCR	T	6046	-	41,41,41	4.24	17 (41%)	56,56,56	7.33	29 (51%)
25	HEM	V	1041	16	49,50,50	2.28	15 (30%)	46,82,82	2.07	8 (17%)
27	BCR	Z	1053	-	41,41,41	4.23	15 (36%)	56,56,56	6.18	32 (57%)
21	OEC	a	6001	1,3	0,0,13	0.00	-	0,0,27	0.00	-
23	CLA	a	6003	-	73,73,73	2.04	17 (23%)	95,113,113	2.79	31 (32%)
23	CLA	a	6006	-	73,73,73	2.04	17 (23%)	95,113,113	2.78	31 (32%)
23	CLA	a	6007	-	73,73,73	2.01	18 (24%)	95,113,113	2.83	35 (36%)
24	PHO	a	6039	-	69,69,69	4.20	19 (27%)	91,99,99	3.05	25 (27%)
26	PQ9	a	6043	-	45,45,45	4.74	21 (46%)	57,57,57	5.66	23 (40%)
27	BCR	a	6044	-	41,41,41	4.02	16 (39%)	56,56,56	5.93	30 (53%)
30	LHG	a	6063	-	48,48,48	0.89	2 (4%)	54,54,54	0.99	3 (5%)
23	CLA	b	6009	-	73,73,73	2.02	17 (23%)	95,113,113	2.81	33 (34%)
23	CLA	b	6010	-	73,73,73	2.06	18 (24%)	95,113,113	2.98	33 (34%)
23	CLA	b	6011	2	73,73,73	2.04	17 (23%)	95,113,113	2.78	32 (33%)
23	CLA	b	6012	-	73,73,73	2.04	17 (23%)	95,113,113	2.79	32 (33%)
23	CLA	b	6013	-	73,73,73	2.04	17 (23%)	95,113,113	2.79	32 (33%)
23	CLA	b	6014	-	73,73,73	1.94	17 (23%)	95,113,113	3.01	34 (35%)
23	CLA	b	6015	-	73,73,73	2.05	19 (26%)	95,113,113	3.10	40 (42%)
23	CLA	b	6016	-	73,73,73	2.05	17 (23%)	95,113,113	2.78	32 (33%)
23	CLA	b	6017	-	73,73,73	2.04	17 (23%)	95,113,113	2.80	32 (33%)
23	CLA	b	6018	-	73,73,73	2.04	17 (23%)	95,113,113	2.79	32 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	6019	-	73,73,73	2.08	18 (24%)	95,113,113	3.00	38 (40%)
23	CLA	b	6020	2	73,73,73	2.04	17 (23%)	95,113,113	2.79	31 (32%)
23	CLA	b	6021	-	73,73,73	2.04	17 (23%)	95,113,113	2.78	31 (32%)
23	CLA	b	6022	-	73,73,73	2.00	18 (24%)	95,113,113	2.88	35 (36%)
23	CLA	b	6023	-	73,73,73	2.05	17 (23%)	95,113,113	2.79	32 (33%)
23	CLA	b	6024	-	73,73,73	2.02	17 (23%)	95,113,113	3.01	35 (36%)
27	BCR	b	6045	-	41,41,41	4.22	15 (36%)	56,56,56	6.22	30 (53%)
27	BCR	b	6047	-	41,41,41	4.18	16 (39%)	56,56,56	6.91	25 (44%)
27	BCR	b	6048	-	41,41,41	4.23	17 (41%)	56,56,56	6.10	26 (46%)
29	MGE	b	6060	-	48,48,48	0.91	2 (4%)	56,56,56	1.00	3 (5%)
23	CLA	c	6025	-	73,73,73	2.04	17 (23%)	95,113,113	2.78	31 (32%)
23	CLA	c	6026	-	73,73,73	1.95	16 (21%)	95,113,113	2.89	33 (34%)
23	CLA	c	6027	-	73,73,73	2.05	17 (23%)	95,113,113	2.79	32 (33%)
23	CLA	c	6028	-	73,73,73	2.04	17 (23%)	95,113,113	2.79	32 (33%)
23	CLA	c	6029	-	73,73,73	2.03	19 (26%)	95,113,113	2.90	33 (34%)
23	CLA	c	6030	-	73,73,73	2.04	17 (23%)	95,113,113	2.79	32 (33%)
23	CLA	c	6031	-	73,73,73	2.05	17 (23%)	95,113,113	2.79	32 (33%)
23	CLA	c	6032	-	73,73,73	2.04	17 (23%)	95,113,113	2.78	31 (32%)
23	CLA	c	6033	-	73,73,73	2.05	17 (23%)	95,113,113	2.79	31 (32%)
23	CLA	c	6034	-	73,73,73	2.03	17 (23%)	95,113,113	2.86	32 (33%)
23	CLA	c	6035	-	73,73,73	2.04	17 (23%)	95,113,113	2.79	31 (32%)
23	CLA	c	6036	-	73,73,73	2.05	17 (23%)	95,113,113	2.80	32 (33%)
23	CLA	c	6037	-	73,73,73	2.05	17 (23%)	95,113,113	2.79	32 (33%)
27	BCR	c	6054	-	41,41,41	4.19	17 (41%)	56,56,56	6.62	26 (46%)
28	DGD	c	6055	-	67,67,67	0.81	2 (2%)	81,81,81	0.89	3 (3%)
28	DGD	c	6056	-	67,67,67	0.81	2 (2%)	81,81,81	0.90	3 (3%)
28	DGD	c	6057	-	67,67,67	0.81	2 (2%)	81,81,81	0.90	3 (3%)
23	CLA	d	6004	-	73,73,73	2.05	17 (23%)	95,113,113	2.79	31 (32%)
23	CLA	d	6005	-	73,73,73	2.04	17 (23%)	95,113,113	2.78	32 (33%)
23	CLA	d	6008	-	73,73,73	2.04	17 (23%)	95,113,113	2.79	32 (33%)
24	PHO	d	6038	-	69,69,69	4.17	18 (26%)	91,99,99	2.98	25 (27%)
26	PQ9	d	6042	-	45,45,45	4.42	16 (35%)	57,57,57	5.85	27 (47%)
27	BCR	d	6050	-	41,41,41	4.14	16 (39%)	56,56,56	5.97	28 (50%)
29	MGE	d	6059	-	48,48,48	0.91	2 (4%)	56,56,56	1.00	3 (5%)
29	MGE	d	6061	-	48,48,48	0.90	2 (4%)	56,56,56	1.00	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	0.91	2 (4%)	56,56,56	0.99	3 (5%)
25	HEM	e	6040	6	49,50,50	2.26	16 (32%)	46,82,82	2.06	8 (17%)
27	BCR	h	6049	-	41,41,41	4.23	15 (36%)	56,56,56	5.94	26 (46%)
28	DGD	h	6058	-	67,67,67	0.80	2 (2%)	81,81,81	0.90	3 (3%)
27	BCR	k	6051	-	41,41,41	4.19	16 (39%)	56,56,56	6.15	28 (50%)
27	BCR	k	6052	-	41,41,41	4.24	15 (36%)	56,56,56	5.02	26 (46%)
27	BCR	t	1046	-	41,41,41	4.24	16 (39%)	56,56,56	6.31	28 (50%)
25	HEM	v	6041	-	49,50,50	2.28	15 (30%)	46,82,82	2.06	8 (17%)
27	BCR	z	6053	-	41,41,41	4.22	15 (36%)	56,56,56	6.18	32 (57%)

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	-	-	0/37/135/135	0/0/9/9
23	CLA	A	1006	-	-	0/37/135/135	0/0/9/9
23	CLA	A	1007	-	1/1/20/25	1/37/135/135	0/0/9/9
24	PHO	A	1038	-	1/1/17/22	1/48/103/103	0/0/6/6
24	PHO	A	1039	-	2/2/17/22	0/48/103/103	0/0/6/6
26	PQ9	A	1043	-	-	0/41/61/61	0/1/1/1
27	BCR	A	1044	-	-	2/29/63/63	0/2/2/2
30	LHG	A	1063	-	-	0/53/53/53	0/0/0/0
23	CLA	B	1009	-	3/3/20/25	1/37/135/135	0/0/9/9
23	CLA	B	1010	-	-	0/37/135/135	0/0/9/9
23	CLA	B	1011	2	-	0/37/135/135	0/0/9/9
23	CLA	B	1012	-	-	1/37/135/135	0/0/9/9
23	CLA	B	1013	-	-	0/37/135/135	0/0/9/9
23	CLA	B	1014	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1015	-	-	0/37/135/135	0/0/9/9
23	CLA	B	1016	-	-	0/37/135/135	0/0/9/9
23	CLA	B	1018	-	-	0/37/135/135	0/0/9/9
23	CLA	B	1019	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1020	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1021	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	B	1022	-	2/2/20/25	1/37/135/135	0/0/9/9
23	CLA	B	1023	-	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	1024	-	1/1/20/25	0/37/135/135	0/0/9/9
27	BCR	B	1045	-	-	0/29/63/63	0/2/2/2
27	BCR	B	1047	-	-	2/29/63/63	0/2/2/2
27	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	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1026	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1027	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1028	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1029	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1030	-	-	0/37/135/135	0/0/9/9
23	CLA	C	1031	-	3/3/20/25	1/37/135/135	0/0/9/9
23	CLA	C	1032	-	-	0/37/135/135	0/0/9/9
23	CLA	C	1033	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1034	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1035	-	-	0/37/135/135	0/0/9/9
23	CLA	C	1036	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	C	1037	-	2/2/20/25	0/37/135/135	0/0/9/9
27	BCR	C	1054	-	-	0/29/63/63	0/2/2/2
28	DGD	C	1055	-	-	0/55/95/95	0/2/2/2
28	DGD	C	1056	-	-	0/55/95/95	0/2/2/2
28	DGD	C	1057	-	-	0/55/95/95	0/2/2/2
23	CLA	D	1004	-	-	0/37/135/135	0/0/9/9
23	CLA	D	1005	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	D	1008	-	-	0/37/135/135	0/0/9/9
26	PQ9	D	1042	-	-	0/41/61/61	0/1/1/1
27	BCR	D	1050	-	-	0/29/63/63	0/2/2/2
29	MGE	D	1062	-	-	0/43/63/63	0/1/1/1
25	HEM	E	1040	6	-	0/14/114/114	0/0/8/8
23	CLA	H	1017	-	1/1/20/25	0/37/135/135	0/0/9/9
27	BCR	H	1049	-	-	0/29/63/63	0/2/2/2
28	DGD	H	1058	-	-	0/55/95/95	1/2/2/2
29	MGE	J	1059	-	-	0/43/63/63	0/1/1/1
27	BCR	K	1051	-	-	0/29/63/63	0/2/2/2
27	BCR	K	1052	-	-	0/29/63/63	0/2/2/2
29	MGE	L	1061	-	-	0/43/63/63	0/1/1/1
27	BCR	T	6046	-	-	0/29/63/63	0/2/2/2
25	HEM	V	1041	16	-	0/14/114/114	0/0/8/8
27	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	6003	-	-	0/37/135/135	0/0/9/9
23	CLA	a	6006	-	-	0/37/135/135	0/0/9/9
23	CLA	a	6007	-	1/1/20/25	1/37/135/135	0/0/9/9
24	PHO	a	6039	-	2/2/17/22	0/48/103/103	0/0/6/6
26	PQ9	a	6043	-	-	0/41/61/61	0/1/1/1
27	BCR	a	6044	-	-	2/29/63/63	0/2/2/2
30	LHG	a	6063	-	-	0/53/53/53	0/0/0/0
23	CLA	b	6009	-	3/3/20/25	1/37/135/135	0/0/9/9
23	CLA	b	6010	-	-	0/37/135/135	0/0/9/9
23	CLA	b	6011	2	-	0/37/135/135	0/0/9/9
23	CLA	b	6012	-	-	1/37/135/135	0/0/9/9
23	CLA	b	6013	-	-	0/37/135/135	0/0/9/9
23	CLA	b	6014	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6015	-	-	0/37/135/135	0/0/9/9
23	CLA	b	6016	-	-	0/37/135/135	0/0/9/9
23	CLA	b	6017	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6018	-	-	0/37/135/135	0/0/9/9
23	CLA	b	6019	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6020	2	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6021	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6022	-	2/2/20/25	1/37/135/135	0/0/9/9
23	CLA	b	6023	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	6024	-	1/1/20/25	0/37/135/135	0/0/9/9
27	BCR	b	6045	-	-	0/29/63/63	0/2/2/2
27	BCR	b	6047	-	-	2/29/63/63	0/2/2/2
27	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	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6026	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6027	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6028	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6029	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6030	-	-	0/37/135/135	0/0/9/9
23	CLA	c	6031	-	3/3/20/25	1/37/135/135	0/0/9/9
23	CLA	c	6032	-	-	0/37/135/135	0/0/9/9
23	CLA	c	6033	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6034	-	4/4/20/25	0/37/135/135	0/0/9/9
23	CLA	c	6035	-	-	0/37/135/135	0/0/9/9
23	CLA	c	6036	-	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	6037	-	2/2/20/25	0/37/135/135	0/0/9/9
27	BCR	c	6054	-	-	0/29/63/63	0/2/2/2
28	DGD	c	6055	-	-	0/55/95/95	0/2/2/2
28	DGD	c	6056	-	-	0/55/95/95	0/2/2/2
28	DGD	c	6057	-	-	0/55/95/95	0/2/2/2
23	CLA	d	6004	-	-	0/37/135/135	0/0/9/9
23	CLA	d	6005	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	d	6008	-	-	0/37/135/135	0/0/9/9
24	PHO	d	6038	-	1/1/17/22	1/48/103/103	0/0/6/6
26	PQ9	d	6042	-	-	0/41/61/61	0/1/1/1
27	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
25	HEM	e	6040	6	-	0/14/114/114	0/0/8/8
27	BCR	h	6049	-	-	0/29/63/63	0/2/2/2
28	DGD	h	6058	-	-	0/55/95/95	1/2/2/2
27	BCR	k	6051	-	-	0/29/63/63	0/2/2/2
27	BCR	k	6052	-	-	0/29/63/63	0/2/2/2
27	BCR	t	1046	-	-	0/29/63/63	0/2/2/2
25	HEM	v	6041	-	-	0/14/114/114	0/0/8/8
27	BCR	z	6053	-	-	1/29/63/63	0/2/2/2

The worst 5 of 1795 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	6039	PHO	CHC-C1C	18.30	1.47	1.35
24	A	1039	PHO	CHC-C1C	18.27	1.47	1.35
24	d	6038	PHO	CHC-C1C	18.00	1.47	1.35
24	A	1038	PHO	CHC-C1C	18.00	1.47	1.35
26	a	6043	PQ9	C27-C28	17.28	1.67	1.32

The worst 5 of 3181 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	1047	BCR	C7-C8-C9	34.32	177.56	126.22
27	b	6047	BCR	C7-C8-C9	34.28	177.50	126.22
27	C	1054	BCR	C7-C8-C9	27.78	167.78	126.22
27	c	6054	BCR	C7-C8-C9	27.76	167.74	126.22
26	d	6042	PQ9	C29-C28-C30	-27.05	74.25	115.39

5 of 86 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	b	6014	CLA	C3A
23	C	1028	CLA	C8
23	C	1028	CLA	C13
23	C	1028	CLA	C3A
23	c	6029	CLA	C8

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1038	PHO	CED-O2D-CGD-CBD
24	d	6038	PHO	CED-O2D-CGD-CBD
23	c	6031	CLA	CED-O2D-CGD-CBD
23	C	1031	CLA	CED-O2D-CGD-CBD
23	A	1007	CLA	CED-O2D-CGD-CBD

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	H	1058	DGD	C1E-C2E-C3E-C4E-C5E-O6E
28	h	6058	DGD	C1E-C2E-C3E-C4E-C5E-O6E

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/344 (97%)	-0.10	2 (0%) 86 69	97, 127, 162, 173	0
1	a	335/344 (97%)	-0.05	1 (0%) 91 83	101, 131, 166, 178	0
2	B	485/488 (99%)	-0.05	4 (0%) 83 63	94, 130, 157, 181	0
2	b	485/488 (99%)	-0.00	4 (0%) 83 63	102, 129, 161, 183	0
3	C	447/447 (100%)	0.09	3 (0%) 84 66	100, 143, 170, 185	0
3	c	447/447 (100%)	0.18	10 (2%) 59 37	102, 150, 173, 187	0
4	D	340/340 (100%)	0.06	7 (2%) 60 38	94, 127, 165, 187	0
4	d	340/340 (100%)	0.03	4 (1%) 75 52	92, 133, 172, 191	0
5	E	82/83 (98%)	0.08	1 (1%) 75 52	117, 156, 184, 186	0
5	e	82/83 (98%)	0.47	4 (4%) 28 18	126, 160, 181, 186	0
6	F	35/44 (79%)	0.16	4 (11%) 6 6	139, 147, 160, 163	0
6	f	35/44 (79%)	0.07	2 (5%) 23 15	143, 152, 160, 163	0
7	H	64/64 (100%)	0.34	4 (6%) 19 13	119, 143, 165, 170	0
7	h	64/64 (100%)	0.12	3 (4%) 30 20	120, 143, 164, 169	0
8	I	35/35 (100%)	0.01	2 (5%) 23 15	127, 137, 166, 173	0
8	i	35/35 (100%)	0.17	3 (8%) 11 9	124, 141, 175, 176	0
9	J	34/40 (85%)	-0.13	1 (2%) 49 31	127, 142, 165, 175	0
9	j	34/40 (85%)	0.24	4 (11%) 5 6	131, 146, 172, 174	0
10	K	36/36 (100%)	-0.06	0 100 100	132, 145, 153, 155	0
10	k	36/36 (100%)	0.29	3 (8%) 11 9	140, 151, 162, 164	0
11	L	37/37 (100%)	-0.15	1 (2%) 52 32	102, 123, 178, 184	0
11	l	37/37 (100%)	-0.01	1 (2%) 52 32	110, 130, 181, 188	0
12	M	36/36 (100%)	0.23	4 (11%) 6 6	101, 119, 171, 174	0
12	m	36/36 (100%)	-0.15	0 100 100	100, 121, 171, 179	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	242/242 (100%)	0.14	5 (2%) 60 38	108, 133, 165, 186	0
13	o	242/242 (100%)	0.19	6 (2%) 54 34	114, 139, 164, 186	0
14	T	30/30 (100%)	0.02	2 (6%) 17 13	105, 124, 173, 178	0
14	t	30/30 (100%)	-0.10	0 100 100	101, 115, 173, 181	0
15	U	98/98 (100%)	0.06	1 (1%) 79 57	108, 123, 143, 158	0
15	u	98/98 (100%)	-0.13	0 100 100	112, 128, 143, 167	0
16	V	137/137 (100%)	-0.15	2 (1%) 70 46	104, 131, 160, 170	0
16	v	137/137 (100%)	0.10	2 (1%) 70 46	114, 145, 165, 176	0
17	X	34/34 (100%)	-0.35	0 100 100	148, 155, 164, 170	0
17	x	34/34 (100%)	-0.12	0 100 100	151, 159, 169, 175	0
18	Y	28/28 (100%)	-0.14	0 100 100	164, 178, 189, 192	0
18	y	28/28 (100%)	-0.04	1 (3%) 41 26	170, 181, 191, 196	0
19	N	0/24	-	-	-	-
19	n	0/24	-	-	-	-
20	Z	62/62 (100%)	0.05	1 (1%) 68 45	138, 161, 180, 186	0
20	z	62/62 (100%)	0.14	3 (4%) 29 19	144, 164, 184, 187	0
All	All	5194/5298 (98%)	0.04	95 (1%) 65 43	92, 136, 172, 196	0

The worst 5 of 95 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	c	5142	GLU	5.5
8	i	5035	LYS	5.2
20	z	5001	MET	4.6
5	e	5018	ARG	4.3
4	d	5228	GLY	4.3

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
27	BCR	b	6045	40/40	0.56	8.24	145,156,167,168	0
27	BCR	a	6044	40/40	0.77	6.44	154,160,163,166	0
27	BCR	T	6046	40/40	0.51	6.12	140,149,154,157	0
27	BCR	A	1044	40/40	0.61	6.02	147,156,158,159	0
27	BCR	b	6048	40/40	0.71	5.93	141,147,158,159	0
28	DGD	C	1056	66/66	0.51	5.82	155,171,183,188	0
27	BCR	H	1049	40/40	0.59	5.15	155,162,188,188	0
27	BCR	b	6047	40/40	0.46	5.07	114,127,145,147	0
27	BCR	B	1045	40/40	0.46	4.54	146,156,169,170	0
23	CLA	a	6007	65/65	0.58	4.47	143,149,179,183	0
27	BCR	B	1047	40/40	0.36	4.46	101,136,157,157	0
23	CLA	d	6008	65/65	0.44	4.05	172,175,185,200	0
27	BCR	z	6053	40/40	0.85	4.05	159,176,186,187	0
30	LHG	A	1063	49/49	0.56	3.90	181,187,194,195	0
23	CLA	b	6023	65/65	0.51	3.81	149,183,189,190	0
29	MGE	b	6060	48/48	0.40	3.78	158,178,191,192	0
27	BCR	K	1051	40/40	0.47	3.73	175,179,182,183	0
28	DGD	c	6057	66/66	0.63	3.70	128,149,183,184	0
27	BCR	d	6050	40/40	0.49	3.65	149,160,166,167	0
27	BCR	B	1048	40/40	0.58	3.64	148,155,163,163	0
23	CLA	C	1025	65/65	0.44	3.35	131,170,180,200	0
28	DGD	c	6056	66/66	0.54	3.34	170,175,181,183	0
28	DGD	C	1057	66/66	0.46	3.18	125,140,187,193	0
27	BCR	c	6054	40/40	0.58	3.07	174,177,183,183	0
23	CLA	C	1028	65/65	0.39	3.02	141,154,159,168	0
29	MGE	d	6059	48/48	0.52	3.01	164,168,198,200	0
30	LHG	a	6063	49/49	0.82	2.90	186,196,200,200	0
23	CLA	B	1021	65/65	0.27	2.84	104,129,142,146	0
23	CLA	b	6013	65/65	0.33	2.82	139,154,161,172	0
24	PHO	d	6038	64/64	0.48	2.79	136,147,150,150	0
27	BCR	D	1050	40/40	0.32	2.63	149,153,161,162	0
23	CLA	A	1006	65/65	0.32	2.62	119,124,190,192	0
27	BCR	t	1046	40/40	0.33	2.61	144,156,163,163	0
28	DGD	H	1058	66/66	0.41	2.47	131,150,165,166	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	D	1004	65/65	0.31	2.36	101,131,139,142	0
23	CLA	B	1012	65/65	0.33	2.28	148,152,159,176	0
29	MGE	d	6062	48/48	0.32	2.23	130,155,167,168	0
28	DGD	h	6058	66/66	0.35	2.23	140,153,163,170	0
24	PHO	A	1039	64/64	0.30	2.19	149,151,160,161	0
23	CLA	c	6027	65/65	0.63	2.18	178,195,198,200	0
23	CLA	C	1032	65/65	0.47	2.03	153,166,174,176	0
23	CLA	A	1003	65/65	0.32	2.00	122,129,147,149	0
27	BCR	h	6049	40/40	0.44	1.98	156,175,191,192	0
29	MGE	d	6061	48/48	0.45	1.98	141,152,165,169	0
23	CLA	c	6032	65/65	0.43	1.97	144,175,181,182	0
23	CLA	b	6012	65/65	0.37	1.95	146,153,159,198	0
23	CLA	b	6017	65/65	0.31	1.86	118,165,168,200	0
23	CLA	b	6011	65/65	0.35	1.85	156,159,165,170	0
23	CLA	b	6016	65/65	0.36	1.85	76,148,153,155	0
23	CLA	c	6031	65/65	0.40	1.76	173,182,185,186	0
23	CLA	a	6006	65/65	0.31	1.71	140,145,197,200	0
27	BCR	C	1054	40/40	0.44	1.71	158,165,169,170	0
23	CLA	A	1007	65/65	0.44	1.71	137,141,171,183	0
29	MGE	L	1061	48/48	0.39	1.71	141,144,154,155	0
25	HEM	V	1041	43/43	0.28	1.71	81,131,132,133	0
23	CLA	D	1008	65/65	0.29	1.66	159,167,182,200	0
29	MGE	D	1062	48/48	0.34	1.64	129,148,165,165	0
23	CLA	c	6037	65/65	0.54	1.63	184,188,191,200	0
23	CLA	b	6021	65/65	0.32	1.62	125,132,157,160	0
23	CLA	d	6004	65/65	0.28	1.62	111,128,134,134	0
23	CLA	d	6005	65/65	0.29	1.58	90,100,117,118	0
23	CLA	c	6028	65/65	0.39	1.57	147,157,160,162	0
23	CLA	b	6015	65/65	0.27	1.54	137,149,155,164	0
26	PQ9	A	1043	45/45	0.31	1.52	138,151,171,171	30
28	DGD	c	6055	66/66	0.35	1.48	147,153,165,166	0
23	CLA	B	1013	65/65	0.29	1.46	131,157,165,168	0
23	CLA	C	1034	65/65	0.40	1.44	134,147,172,174	0
27	BCR	K	1052	40/40	0.40	1.34	153,171,178,179	0
26	PQ9	d	6042	45/45	0.28	1.32	137,146,167,168	0
23	CLA	c	6034	65/65	0.52	1.27	87,162,181,181	0
24	PHO	a	6039	64/64	0.31	1.27	151,165,169,170	0
26	PQ9	a	6043	45/45	0.34	1.24	135,149,185,185	30
28	DGD	C	1055	66/66	0.37	1.18	131,140,147,152	0
27	BCR	Z	1053	40/40	0.42	1.18	141,166,178,178	0
23	CLA	c	6025	65/65	0.40	1.17	145,170,178,200	0
23	CLA	b	6024	65/65	0.42	1.13	172,183,186,187	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
23	CLA	c	6036	65/65	0.47	1.08	177,180,184,200	0
23	CLA	C	1037	65/65	0.49	1.08	180,185,188,200	0
23	CLA	a	6003	65/65	0.31	1.07	121,130,145,193	0
23	CLA	B	1024	65/65	0.40	1.07	105,177,179,180	0
23	CLA	C	1027	65/65	0.47	1.02	167,183,190,200	0
23	CLA	B	1023	65/65	0.41	0.99	155,179,185,200	0
23	CLA	B	1018	65/65	0.33	0.98	111,158,165,168	0
23	CLA	B	1019	65/65	0.25	0.97	121,156,158,200	0
23	CLA	B	1015	65/65	0.30	0.88	133,146,153,175	0
23	CLA	B	1016	65/65	0.30	0.86	87,143,150,150	0
23	CLA	D	1005	65/65	0.29	0.84	101,108,116,157	0
23	CLA	b	6018	65/65	0.33	0.82	142,154,162,165	0
23	CLA	C	1031	65/65	0.40	0.80	164,170,179,200	0
23	CLA	C	1036	65/65	0.37	0.80	162,166,179,200	0
25	HEM	E	1040	43/43	0.40	0.74	141,181,194,198	0
29	MGE	B	1060	48/48	0.36	0.72	151,170,182,184	0
27	BCR	k	6051	40/40	0.31	0.71	187,193,197,197	0
23	CLA	b	6010	65/65	0.29	0.70	93,165,169,170	0
26	PQ9	D	1042	45/45	0.28	0.68	131,145,154,155	0
23	CLA	B	1022	65/65	0.29	0.67	135,155,159,161	0
23	CLA	B	1010	65/65	0.28	0.67	115,164,166,169	0
23	CLA	B	1011	65/65	0.28	0.66	144,159,161,166	0
23	CLA	c	6030	65/65	0.29	0.59	100,154,174,175	0
25	HEM	e	6040	43/43	0.38	0.55	171,184,185,185	0
24	PHO	A	1038	64/64	0.30	0.54	122,144,147,148	0
23	CLA	H	1017	65/65	0.27	0.53	116,169,174,200	0
29	MGE	J	1059	48/48	0.34	0.52	152,158,185,186	0
23	CLA	c	6026	65/65	0.35	0.45	140,144,157,170	0
23	CLA	b	6020	65/65	0.32	0.44	75,148,170,173	0
27	BCR	k	6052	40/40	0.36	0.41	158,179,200,200	0
23	CLA	B	1014	65/65	0.27	0.40	123,169,174,176	0
23	CLA	b	6009	65/65	0.43	0.33	160,177,200,200	0
23	CLA	C	1026	65/65	0.27	0.32	128,133,146,149	0
25	HEM	v	6041	43/43	0.27	0.31	99,135,139,140	0
23	CLA	c	6029	65/65	0.28	0.30	151,170,173,200	0
23	CLA	b	6019	65/65	0.28	0.29	124,150,155,193	0
23	CLA	B	1009	65/65	0.38	0.27	119,178,184,185	0
23	CLA	C	1030	65/65	0.31	0.22	92,145,175,176	0
23	CLA	B	1020	65/65	0.26	0.21	113,151,177,179	0
23	CLA	c	6033	65/65	0.27	0.10	84,142,180,180	0
23	CLA	b	6014	65/65	0.24	0.10	163,171,179,200	0
21	OEC	a	6001	5/9	0.26	0.08	87,94,106,107	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	OEC	A	1001	5/9	0.24	0.05	79,94,115,119	0
23	CLA	c	6035	65/65	0.31	0.01	170,173,177,200	0
23	CLA	C	1029	65/65	0.29	0.00	146,156,159,200	0
23	CLA	C	1035	65/65	0.27	0.00	155,167,173,200	0
23	CLA	C	1033	65/65	0.27	-0.03	117,131,162,164	0
31	BR	a	6065	1/1	0.18	-0.22	164,164,164,164	0
22	FE2	a	6002	1/1	0.26	-0.32	149,149,149,149	0
23	CLA	b	6022	65/65	0.25	-0.36	133,148,156,157	0
31	BR	A	1065	1/1	0.26	-0.43	158,158,158,158	0
22	FE2	A	1002	1/1	0.20	-0.54	125,125,125,125	0
31	BR	A	1064	1/1	0.16	-1.04	113,113,113,113	0
31	BR	d	6064	1/1	0.14	-2.14	130,130,130,130	0

6.5 Other polymers ⓘ

There are no such residues in this entry.