wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 07:52 PM GMT

PDB ID	:	4PBU
Title	:	Serial Time-resolved crystallography of Photosystem II using a femtosecond X-ray laser The S1 state
Authors	:	Kupitz, C.; Basu, S.; Grotjohann, I.; Fromme, R.; Zatsepin, N.; Rendek, K.N.; Hunter, M.; Shoeman, R.L.; White, T.A.; Wang, D.; James, D.; Yang, J.H.; Cobb, D.E.; Reeder, B.; Sierra, R.G.; Liu, H.; Barty, A.; Aquila, A.; Deponte, D.; Kirian, R.A.; Bari, S.; Bergkamp, J.J.; Beyerlein, K.; Bogan, M.J.; Caleman, C.; Chao, T.-C.; Conrad, C.E.; Davis, K.M.; Fleckenstein, H.; Galli, L.; Hau-Riege, S.P.; Kassemeyer, S.; Laksmono, H.; Liang, M.; Lomb, L.; Marchesini, S.; Martin, A.V.; Messerschmidt, M.; Milathianaki, D.; Nass, K.; Ros, A.; Roy-Chowdhury, S.; Schmidt, K.; Seibert, M.; Steinbrener, J.; Stellato, F.; Yan, L.; Yoon, C.; Moore, T.A.; Moore, A.L.; Pushkar, Y.; Williams, G.J.; Boutet, S.; Doak, R.B.; Weierstall, U.; Frank, M.; Chapman, H.N.; Spence, J.C.H.; Fromme, P.
Deposited on	:	2014-04-13
Resolution	:	5.00 Å(reported)

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

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

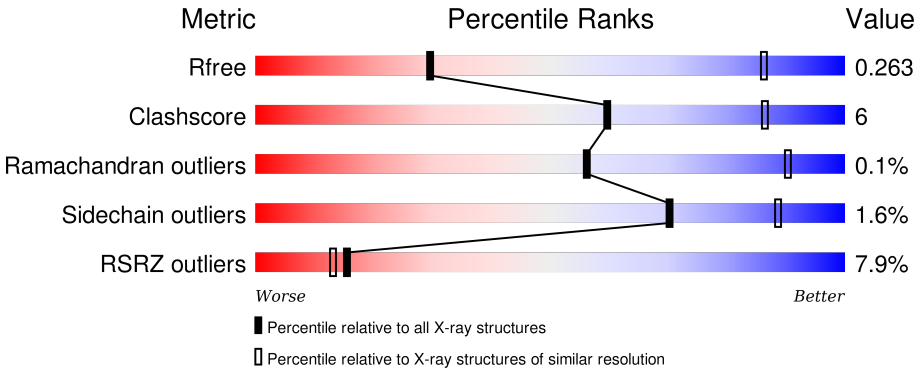
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 5.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1119 (6.22-3.60)
Clashscore	102246	1019 (6.22-3.66)
Ramachandran outliers	100387	1158 (6.22-3.60)
Sidechain outliers	100360	1136 (6.22-3.60)
RSRZ outliers	91569	1122 (6.22-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	334	4% 85% 15%
1	a	334	8% 99%

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CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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Mol	Chain	Length	Quality of chain
2	B	504	7% 88% 12%
2	b	504	12% 99%
3	C	455	11% 84% 15%
3	c	455	6% 98%
4	D	342	8% 85% 15%
4	d	342	8% 99%
5	E	81	14% 77% 23%
5	e	81	11% 98%
6	F	34	3% 74% 26%
6	f	34	9% 91% 6%
7	H	65	17% 80% 15% 5%
7	h	65	22% 98%
8	I	38	8% 84% 16%
8	i	38	8% 100%
9	J	40	15% 78% 18% 5%
9	j	40	8% 100%
10	K	37	68% 30%
10	k	37	8% 95% 5%
11	L	37	11% 73% 24%
11	l	37	97%
12	M	34	21% 79% 21%
12	m	34	9% 100%
13	O	243	3% 81% 19%
13	o	243	7% 97%
14	T	30	10% 87% 13%

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Mol	Chain	Length	Quality of chain
14	t	30	10% 93% 7%
15	U	97	2% 81% 19%
15	u	97	3% 99%
16	V	137	% 85% 15%
16	v	137	7% 98%
17	Y	29	7% 59% 41%
17	y	29	97%
18	X	39	21% 85% 15%
18	x	39	15% 97%
19	Z	62	5% 87% 11%
19	z	62	8% 95% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CL	A	603	-	-	-	X
22	CL	a	404	-	-	-	X
23	BCT	A	605	-	-	-	X
23	BCT	a	414	-	-	-	X
24	CLA	A	606	X	-	-	X
24	CLA	A	607	X	-	-	X
24	CLA	A	609	X	-	-	X
24	CLA	A	614	X	-	-	X
24	CLA	B	602	X	-	-	X
24	CLA	B	603	X	-	-	X
24	CLA	B	604	X	-	-	X
24	CLA	B	605	X	-	-	X
24	CLA	B	606	X	-	-	X
24	CLA	B	607	X	-	-	X
24	CLA	B	608	X	-	-	X
24	CLA	B	609	X	-	-	X
24	CLA	B	610	X	-	-	X
24	CLA	B	611	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	B	612	X	-	-	X
24	CLA	B	613	X	-	-	X
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	X
24	CLA	B	617	X	-	-	X
24	CLA	C	501	X	-	-	X
24	CLA	C	502	X	-	-	X
24	CLA	C	503	X	-	-	X
24	CLA	C	504	X	-	-	X
24	CLA	C	505	X	-	-	X
24	CLA	C	506	X	-	-	X
24	CLA	C	507	X	-	-	X
24	CLA	C	508	X	-	-	X
24	CLA	C	509	X	-	-	X
24	CLA	C	510	X	-	-	X
24	CLA	C	511	X	-	-	X
24	CLA	C	512	X	-	-	X
24	CLA	C	513	X	-	-	X
24	CLA	D	402	X	-	-	X
24	CLA	D	403	X	-	-	X
24	CLA	a	406	X	-	-	X
24	CLA	a	407	X	-	-	X
24	CLA	a	408	X	-	-	X
24	CLA	b	602	X	-	-	X
24	CLA	b	603	X	-	-	X
24	CLA	b	604	X	-	-	X
24	CLA	b	605	X	-	-	X
24	CLA	b	606	X	-	-	X
24	CLA	b	607	X	-	-	X
24	CLA	b	608	X	-	-	X
24	CLA	b	609	X	-	-	X
24	CLA	b	610	-	-	-	X
24	CLA	b	611	X	-	-	X
24	CLA	b	612	X	-	-	X
24	CLA	b	613	X	-	-	X
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	X
24	CLA	b	617	X	-	-	X
24	CLA	c	902	X	-	-	X
24	CLA	c	903	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	c	904	X	-	-	X
24	CLA	c	905	X	-	-	X
24	CLA	c	906	X	-	-	X
24	CLA	c	907	X	-	-	X
24	CLA	c	908	X	-	-	X
24	CLA	c	909	X	-	-	X
24	CLA	c	910	X	-	-	X
24	CLA	c	911	X	-	-	X
24	CLA	c	912	X	-	-	X
24	CLA	c	913	X	-	-	X
24	CLA	c	914	X	-	-	X
24	CLA	d	401	X	-	-	X
24	CLA	d	403	X	-	-	X
24	CLA	d	404	X	-	-	X
25	PHO	A	608	-	-	-	X
25	PHO	D	401	-	-	-	X
25	PHO	a	412	-	-	-	X
25	PHO	d	402	-	-	-	X
26	BCR	A	610	-	-	-	X
26	BCR	B	620	-	-	-	X
26	BCR	C	514	-	-	-	X
26	BCR	C	515	-	-	-	X
26	BCR	D	404	-	-	-	X
26	BCR	H	101	-	-	-	X
26	BCR	K	101	-	-	-	X
26	BCR	T	101	-	-	-	X
26	BCR	T	102	-	-	-	X
26	BCR	Y	101	-	-	-	X
26	BCR	a	409	-	-	-	X
26	BCR	b	618	-	-	-	X
26	BCR	b	619	-	-	-	X
26	BCR	c	915	-	-	-	X
26	BCR	c	918	-	-	-	X
26	BCR	f	101	-	-	-	X
26	BCR	h	101	-	-	-	X
26	BCR	k	101	-	-	-	X
26	BCR	k	102	-	-	-	X
27	PL9	A	611	-	-	-	X
27	PL9	D	405	-	-	-	X
27	PL9	a	410	-	-	-	X
27	PL9	d	405	-	-	-	X
28	SQD	A	612	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	SQD	A	613	-	-	-	X
28	SQD	F	101	-	-	-	X
28	SQD	a	411	-	-	-	X
28	SQD	d	407	-	-	-	X
28	SQD	l	101	-	-	-	X
29	LHG	A	615	-	-	-	X
29	LHG	D	408	-	-	-	X
29	LHG	D	409	-	-	X	X
29	LHG	a	413	-	-	-	X
29	LHG	d	410	-	-	-	X
30	CA	c	901	-	-	-	X
31	DGD	C	516	-	-	-	X
31	DGD	C	517	-	-	-	X
31	DGD	C	518	-	-	-	X
31	DGD	D	406	-	-	-	X
31	DGD	H	102	-	-	-	X
31	DGD	c	916	-	-	-	X
31	DGD	c	917	-	-	-	X
31	DGD	d	406	-	-	-	X
31	DGD	h	102	-	-	-	X
31	DGD	j	101	-	-	-	X
32	HEM	E	101	-	-	-	X
32	HEM	V	202	-	-	-	X
32	HEM	e	101	-	-	-	X
32	HEM	v	202	-	-	-	X

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 48924 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2620	1716	431	458	15			
1	a	334	Total	C	N	O	S	0	0	0
			2620	1716	431	458	15			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	0	0
			3969	2605	661	690	13			
2	b	504	Total	C	N	O	S	0	0	0
			3969	2605	661	690	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	13			
3	c	455	Total	C	N	O	S	0	0	0
			3519	2303	589	614	13			

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	341	Total	C	N	O	S	0	0	0
			2717	1800	444	461	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			662	432	107	123			
5	e	81	Total	C	N	O	0	0	0
			662	432	107	123			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			511	341	82	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	0	0
			312	210	48	53	1			
8	i	38	Total	C	N	O	S	0	0	0
			312	210	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	40	Total	C	N	O	S	0	0	0
			288	192	44	49	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	l	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	4			
13	o	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	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
			256	180	36	38	2			
14	t	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total 774	C 491	N 129	O 154	0	0	0
15	u	97	Total 774	C 491	N 129	O 154	0	0	0

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

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

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

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

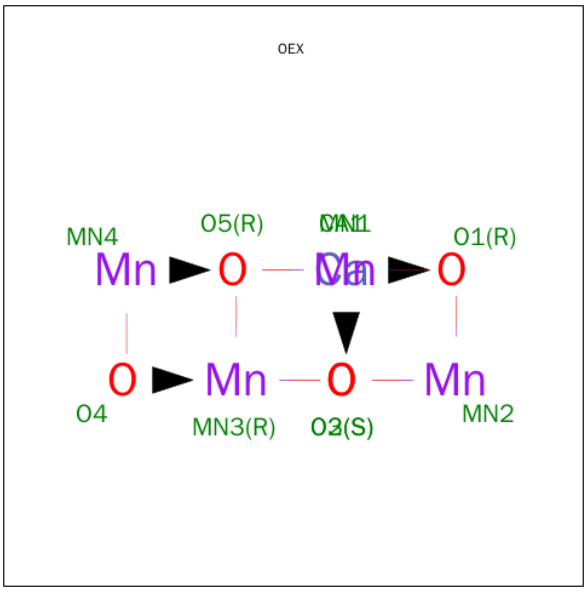
- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	39	Total 287	C 191	N 46	O 50	0	0	0
18	x	39	Total 287	C 191	N 46	O 50	0	0	0

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

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

- Molecule 20 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



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

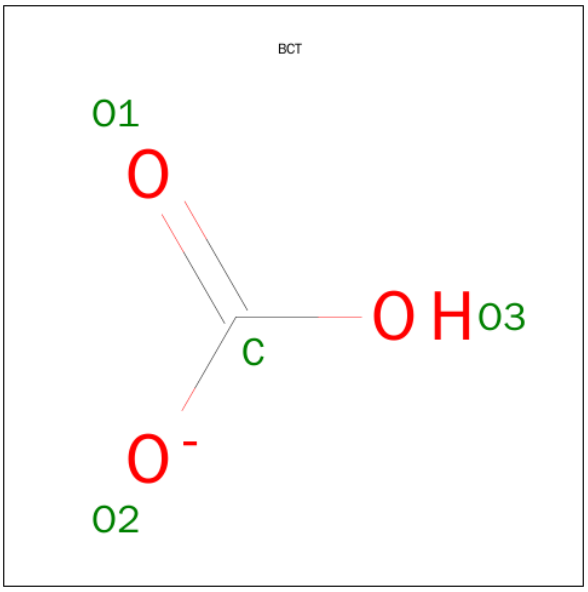
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

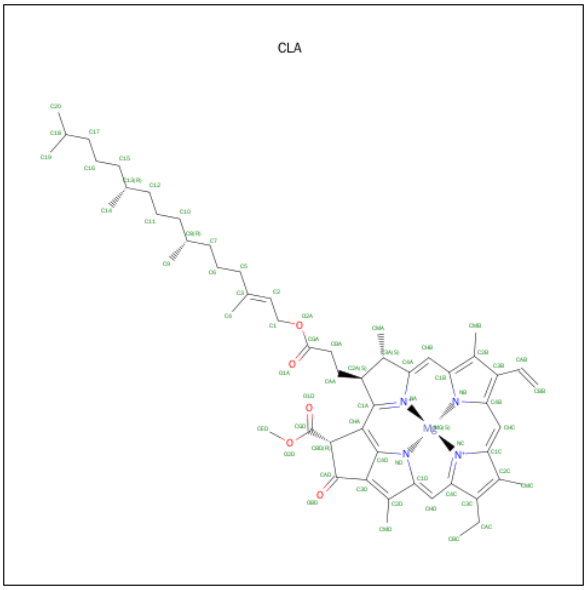
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	a	2	Total	Cl	0	0
			2	2		
22	A	2	Total	Cl	0	0
			2	2		
22	v	1	Total	Cl	0	0
			1	1		
22	V	1	Total	Cl	0	0
			1	1		

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C Mg N O 65 55 1 4 5	0	0
24	A	1	Total C Mg N O 65 55 1 4 5	0	0
24	B	1	Total C Mg N O 65 55 1 4 5	0	0
24	B	1	Total C Mg N O 65 55 1 4 5	0	0
24	B	1	Total C Mg N O 65 55 1 4 5	0	0
24	B	1	Total C Mg N O 65 55 1 4 5	0	0
24	B	1	Total C Mg N O 65 55 1 4 5	0	0
24	B	1	Total C Mg N O 65 55 1 4 5	0	0
24	B	1	Total C Mg N O 65 55 1 4 5	0	0
24	B	1	Total C Mg N O 65 55 1 4 5	0	0
24	B	1	Total C Mg N O 65 55 1 4 5	0	0
24	B	1	Total C Mg N O 65 55 1 4 5	0	0
24	B	1	Total C Mg N O 65 55 1 4 5	0	0
24	B	1	Total C Mg N O 65 55 1 4 5	0	0
24	B	1	Total C Mg N O 65 55 1 4 5	0	0
24	B	1	Total C Mg N O 65 55 1 4 5	0	0
24	B	1	Total C Mg N O 65 55 1 4 5	0	0
24	B	1	Total C Mg N O 65 55 1 4 5	0	0
24	C	1	Total C Mg N O 65 55 1 4 5	0	0
24	C	1	Total C Mg N O 65 55 1 4 5	0	0
24	C	1	Total C Mg N O 65 55 1 4 5	0	0

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

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

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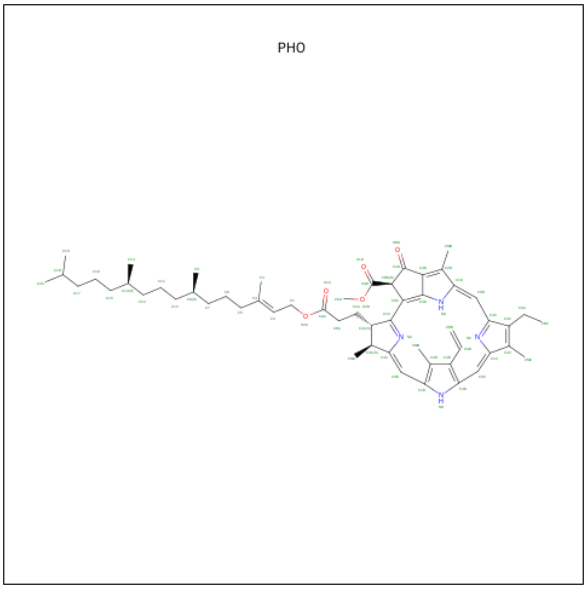
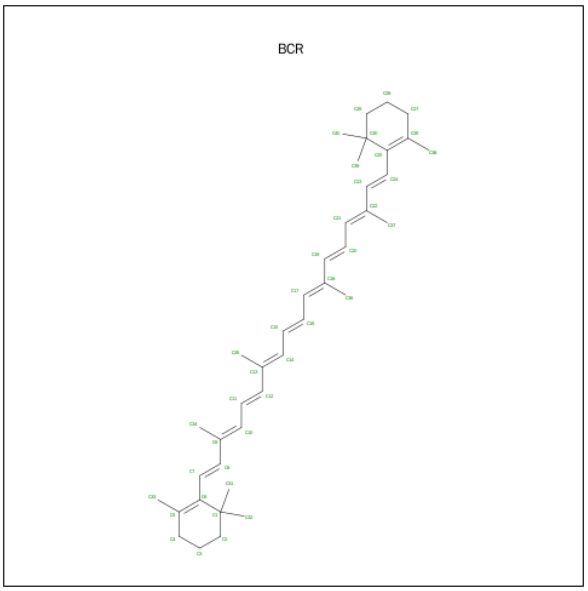
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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	B	1	Total C 40 40	0	0
26	C	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	T	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0

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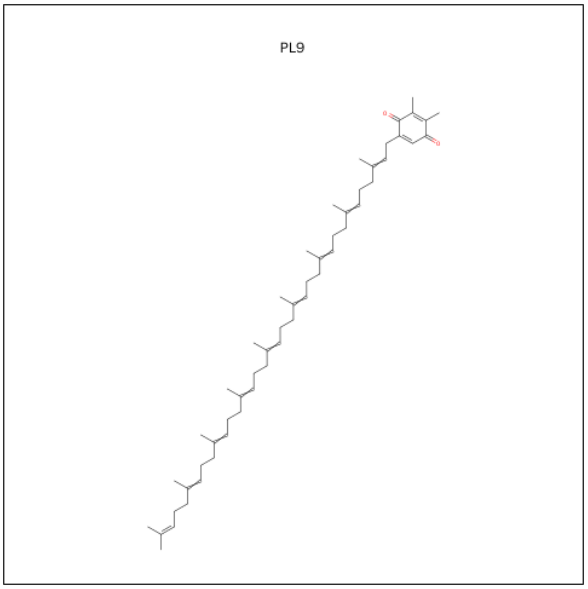
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	f	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0

- Molecule 27 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



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

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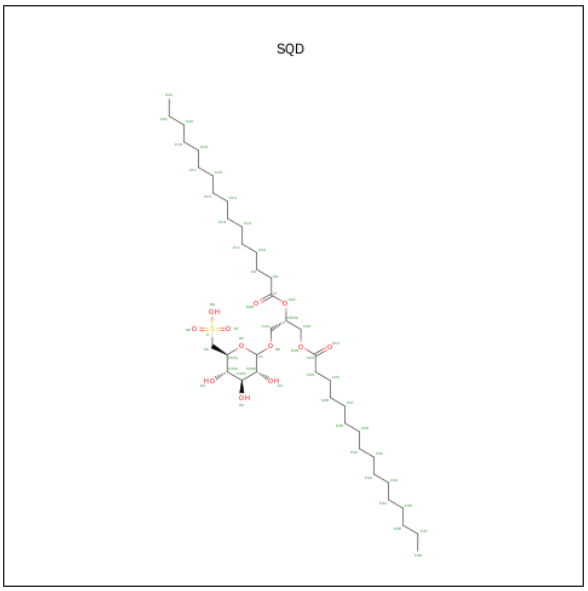
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	a	1	Total C O 55 53 2	0	0
27	d	1	Total C O 55 53 2	0	0

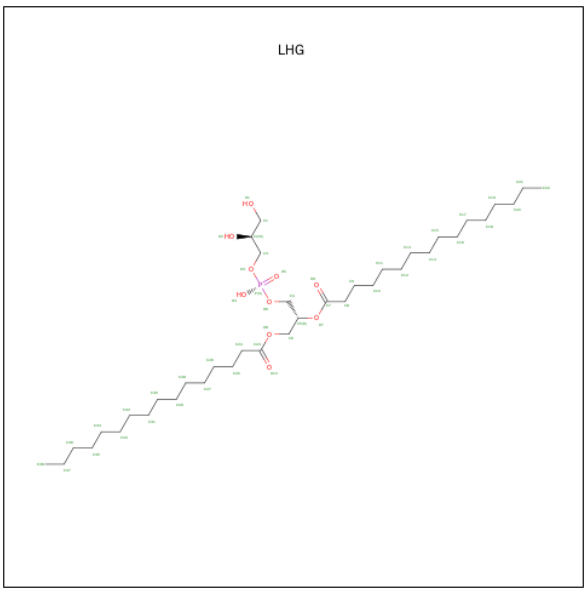
- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O S 54 41 12 1	0	0
28	A	1	Total C O S 54 41 12 1	0	0
28	F	1	Total C O S 43 30 12 1	0	0
28	L	1	Total C O S 54 41 12 1	0	0
28	a	1	Total C O S 54 41 12 1	0	0
28	a	1	Total C O S 54 41 12 1	0	0
28	d	1	Total C O S 43 30 12 1	0	0
28	l	1	Total C O S 54 41 12 1	0	0

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code:

LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	P	0	0
			42	31	10	1		
29	B	1	Total	C	O	P	0	0
			49	38	10	1		
29	D	1	Total	C	O	P	0	0
			49	38	10	1		
29	D	1	Total	C	O	P	0	0
			49	38	10	1		
29	D	1	Total	C	O	P	0	0
			49	38	10	1		
29	a	1	Total	C	O	P	0	0
			42	31	10	1		
29	b	1	Total	C	O	P	0	0
			49	38	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	B	1	Total	Ca	0	0
			1	1		

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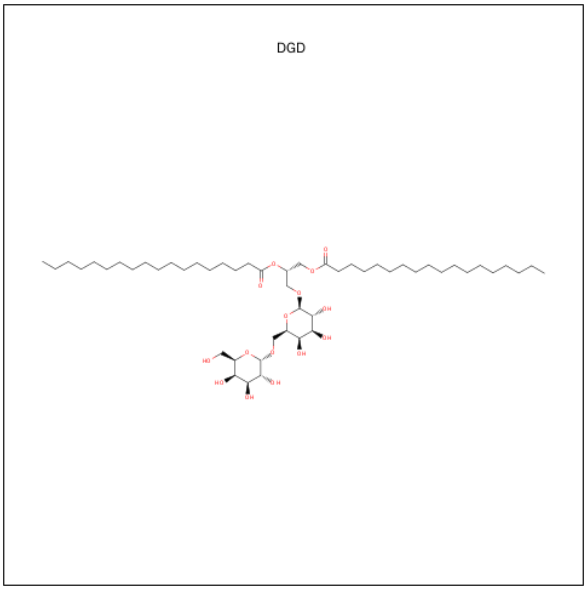
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	c	1	Total Ca 1 1	0	0
30	F	1	Total Ca 1 1	0	0
30	o	1	Total Ca 1 1	0	0
30	O	1	Total Ca 1 1	0	0
30	b	1	Total Ca 1 1	0	0
30	f	1	Total Ca 1 1	0	0

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	C	1	Total C O 62 47 15	0	0
31	C	1	Total C O 62 47 15	0	0
31	C	1	Total C O 62 47 15	0	0
31	D	1	Total C O 62 47 15	0	0
31	H	1	Total C O 62 47 15	0	0

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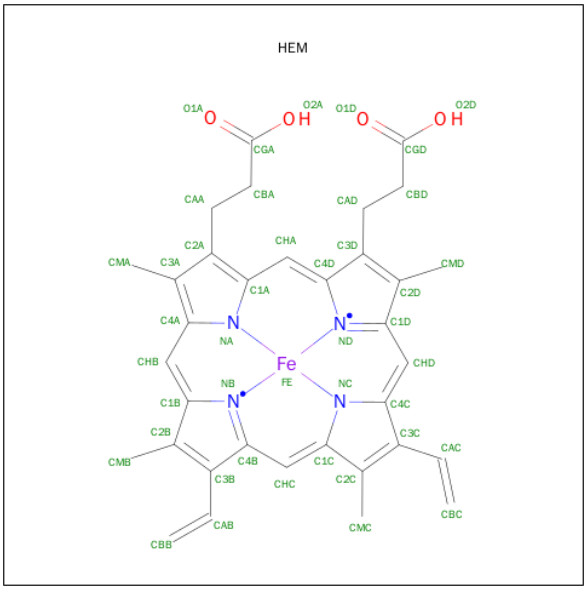
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	c	1	Total C O 62 47 15	0	0
31	c	1	Total C O 62 47 15	0	0
31	d	1	Total C O 62 47 15	0	0
31	h	1	Total C O 62 47 15	0	0
31	j	1	Total C O 62 47 15	0	0

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



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

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

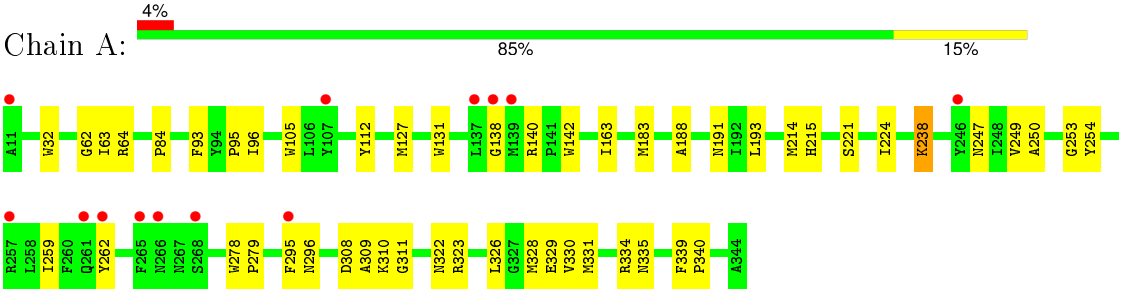
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	j	1	Total Mg 1 1	0	0

3 Residue-property plots (i)

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

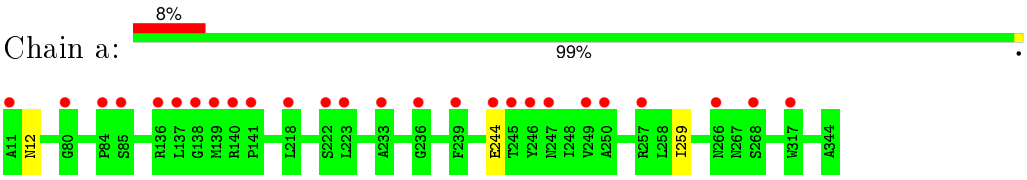
• Molecule 1: Photosystem Q(B) protein 1

Chain A:



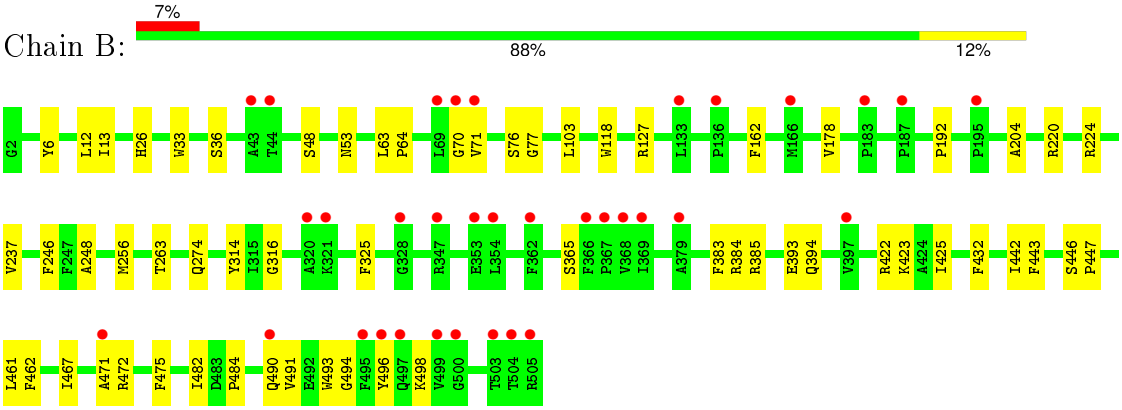
• Molecule 1: Photosystem Q(B) protein 1

Chain a:



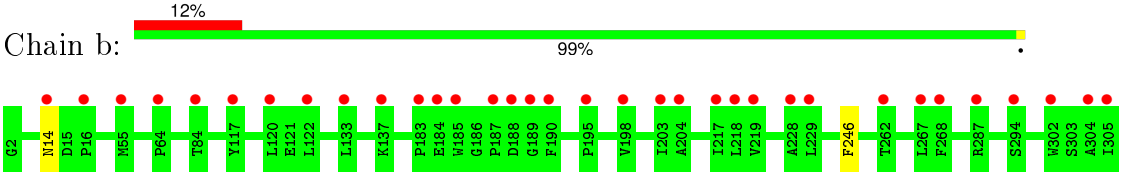
• Molecule 2: Photosystem II core light harvesting protein

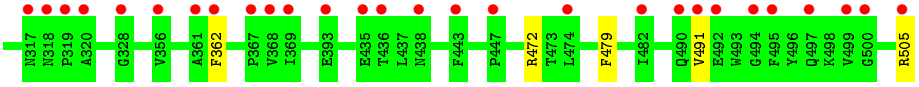
Chain B:



• Molecule 2: Photosystem II core light harvesting protein

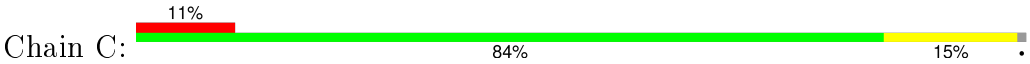
Chain b:

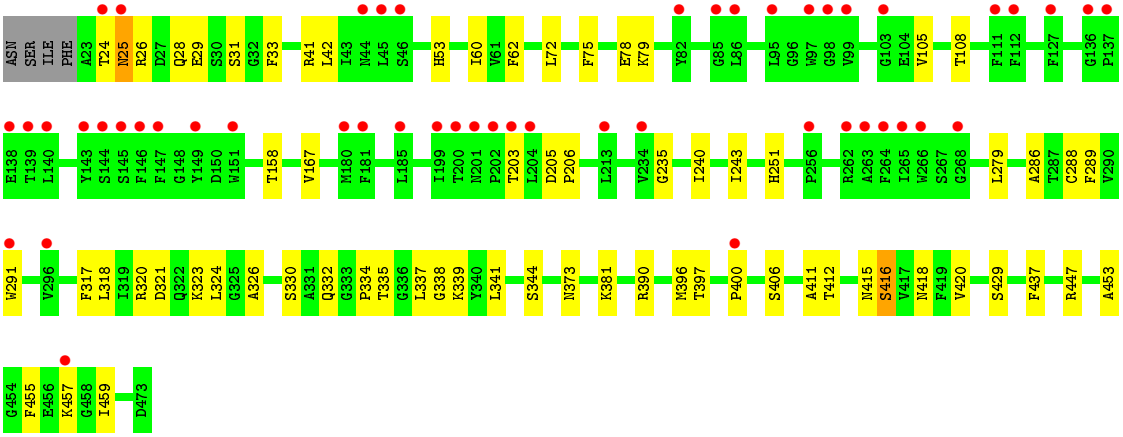




• Molecule 3: Photosystem II CP43 protein

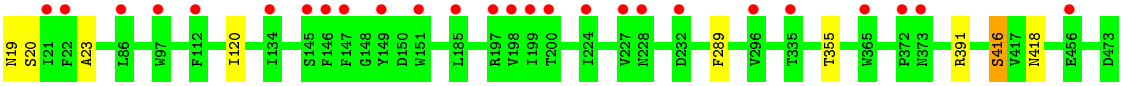
Chain C:





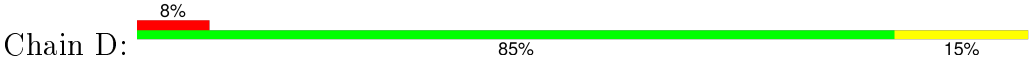
• Molecule 3: Photosystem II CP43 protein

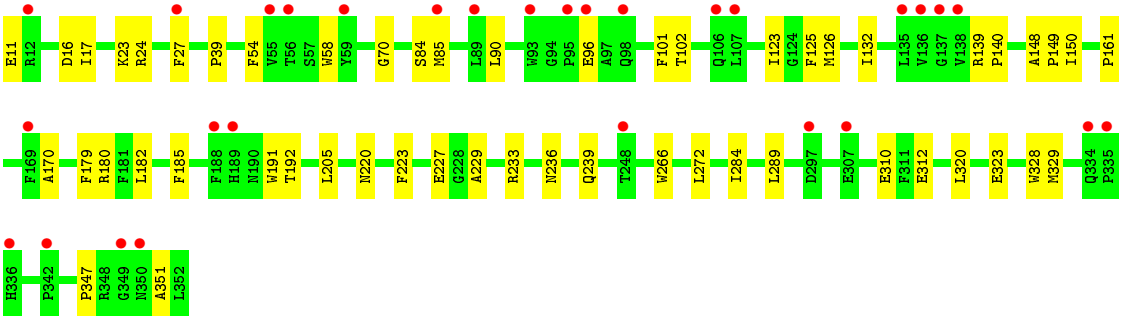
Chain c:



• Molecule 4: Photosystem II D2 protein

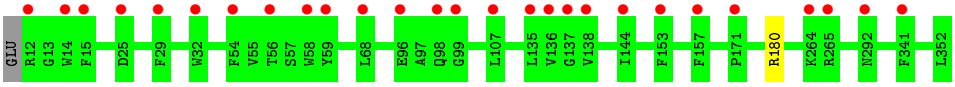
Chain D:





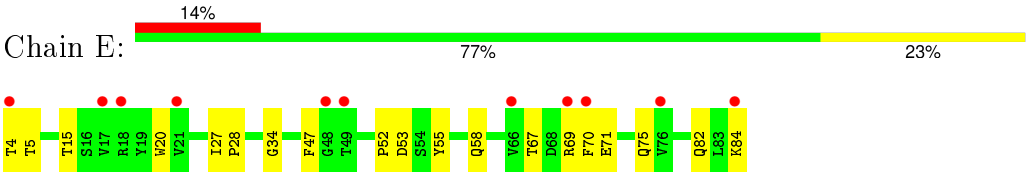
• Molecule 4: Photosystem II D2 protein

Chain d:



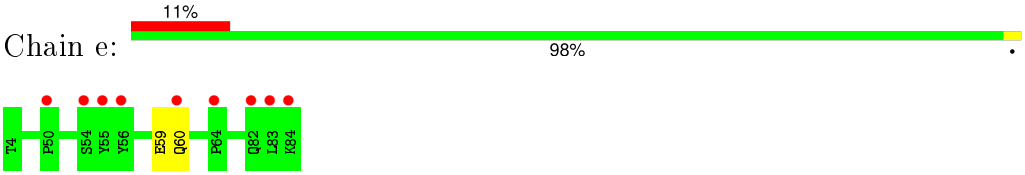
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



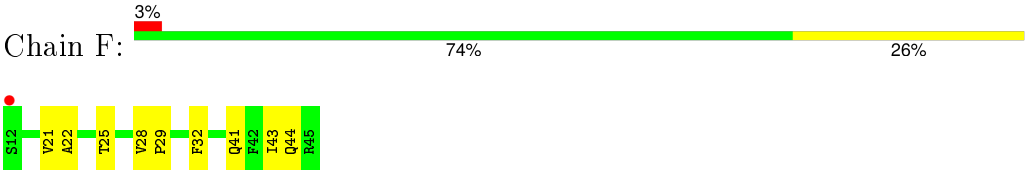
- Molecule 5: Cytochrome b559 subunit alpha

Chain e:



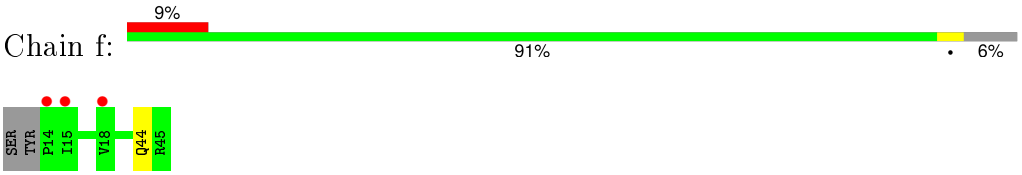
- Molecule 6: Cytochrome b559 subunit beta

Chain F:



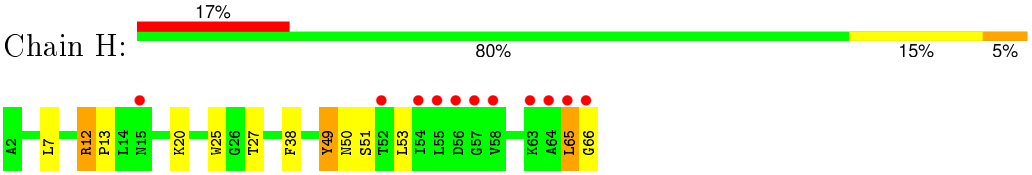
- Molecule 6: Cytochrome b559 subunit beta

Chain f:



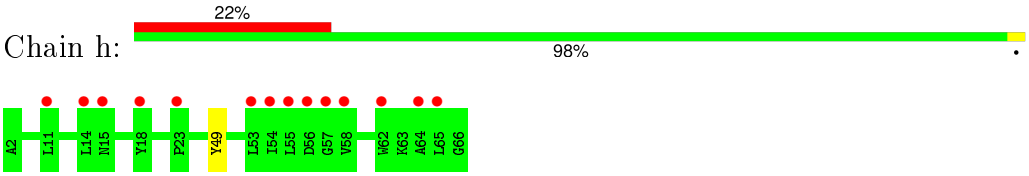
- Molecule 7: Photosystem II reaction center protein H

Chain H:



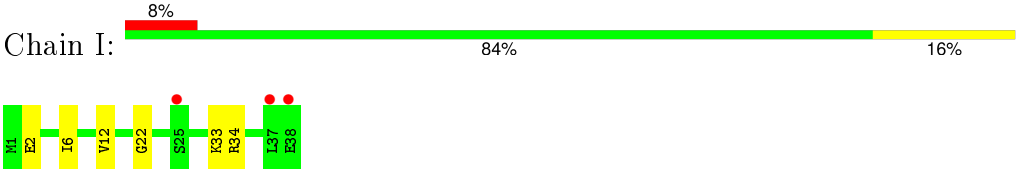
- Molecule 7: Photosystem II reaction center protein H

Chain h:



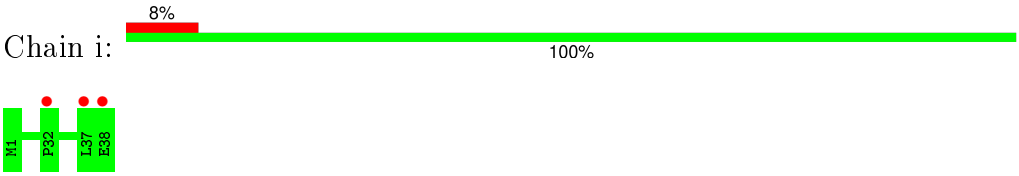
- Molecule 8: Photosystem II reaction center protein I

Chain I:



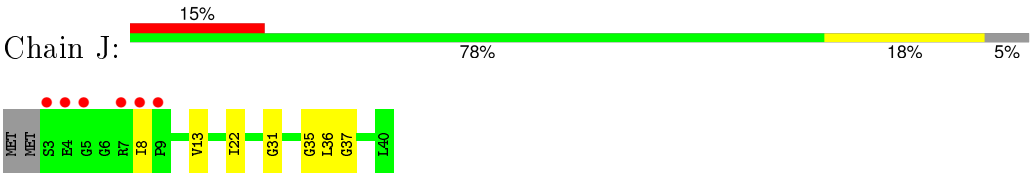
- Molecule 8: Photosystem II reaction center protein I

Chain i:



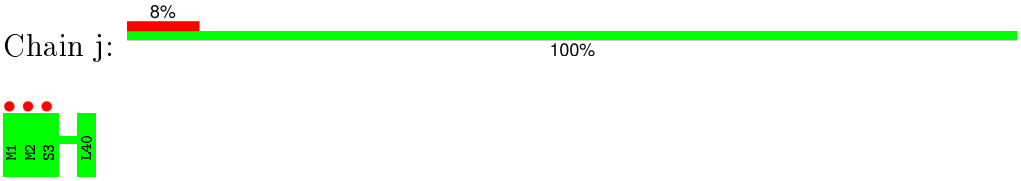
• Molecule 9: Photosystem II reaction center protein J

Chain J:



• Molecule 9: Photosystem II reaction center protein J

Chain j:

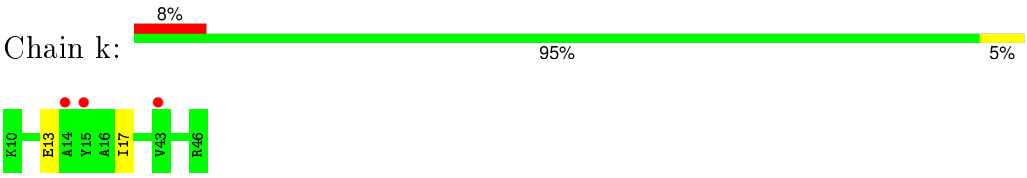


• Molecule 10: Photosystem II reaction center protein K

Chain K:

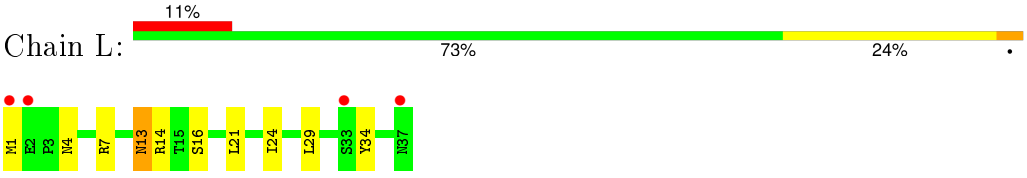
• Molecule 10: Photosystem II reaction center protein K

Chain k:



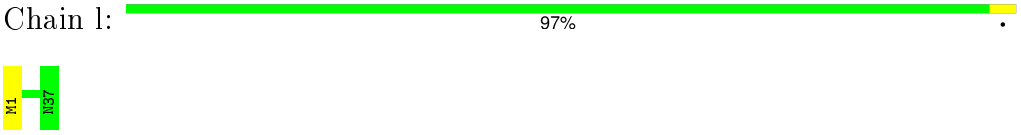
• Molecule 11: Photosystem II reaction center protein L

Chain L:



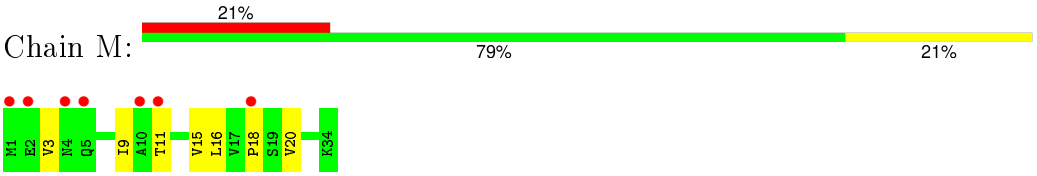
• Molecule 11: Photosystem II reaction center protein L

Chain l:



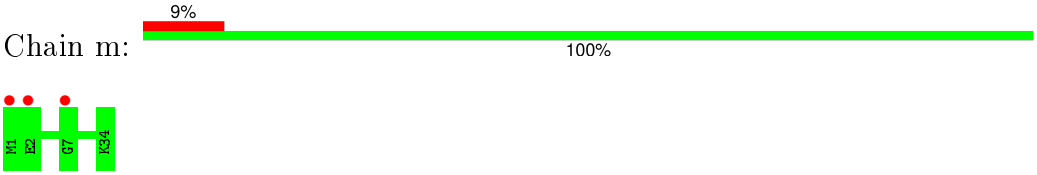
• Molecule 12: Photosystem II reaction center protein M

Chain M:



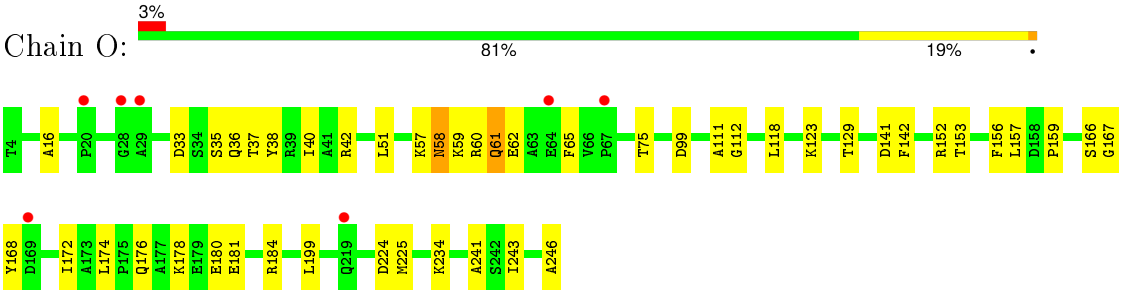
• Molecule 12: Photosystem II reaction center protein M

Chain m:



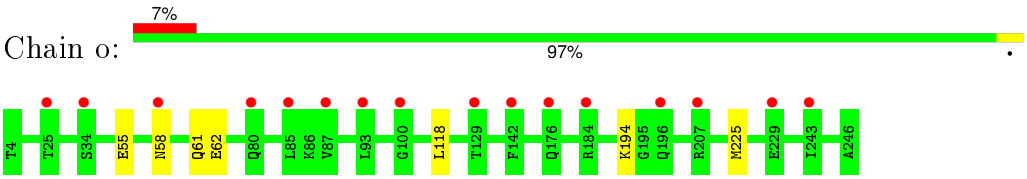
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



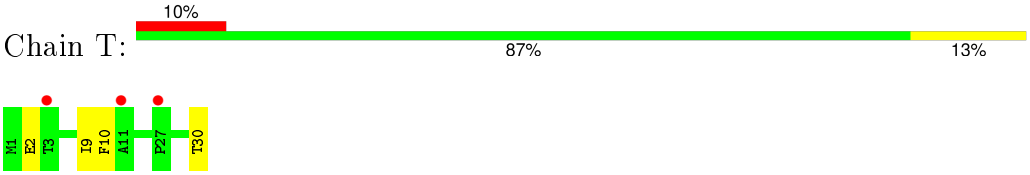
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



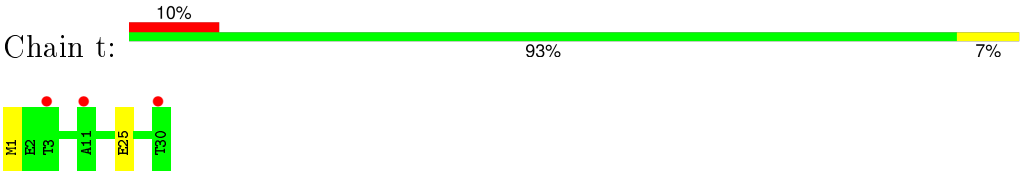
• Molecule 14: Photosystem II reaction center protein T

Chain T:



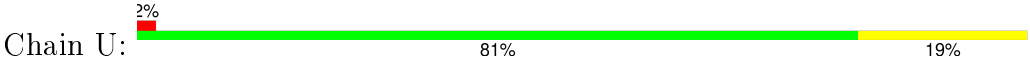
• Molecule 14: Photosystem II reaction center protein T

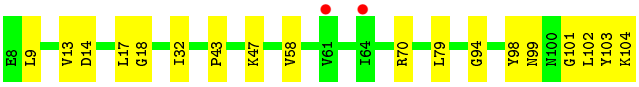
Chain t:



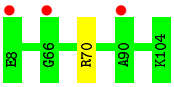
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:

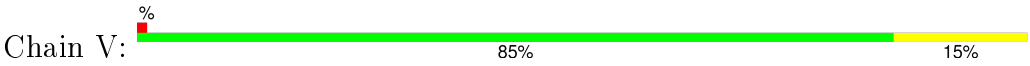


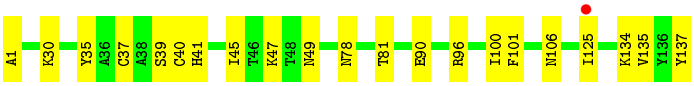


• Molecule 15: Photosystem II 12 kDa extrinsic protein

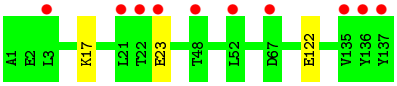


• Molecule 16: Cytochrome c-550

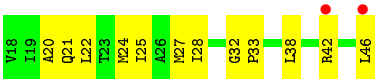




• Molecule 16: Cytochrome c-550

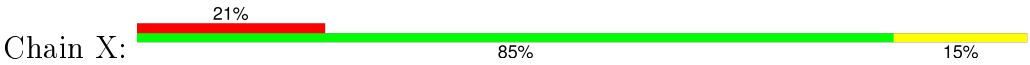


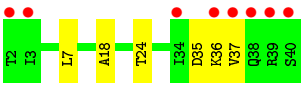
• Molecule 17: Photosystem II reaction center protein Ycf12



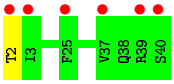
• Molecule 17: Photosystem II reaction center protein Ycf12

• Molecule 18: Photosystem II reaction center X protein



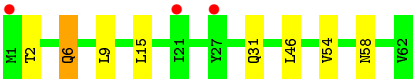


• Molecule 18: Photosystem II reaction center X protein



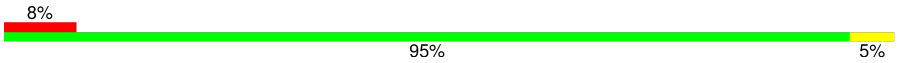
• Molecule 19: Photosystem II reaction center protein Z

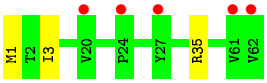
Chain Z:



• Molecule 19: Photosystem II reaction center protein Z

Chain z:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	133.25Å 226.26Å 307.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.64 – 5.00 100.64 – 5.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (100.64-5.00) 100.0 (100.64-5.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 5.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.261 , 0.262 0.259 , 0.263	Depositor DCC
R_{free} test set	2055 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	285.1	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 40956 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	48924	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, MG, OEX, PHO, DGD, CL, CA, CLA, PL9, FE2, BCT, HEM, BCR, SQD

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	0.52	0/2705	0.55	0/3689
1	a	0.51	0/2705	0.54	0/3689
2	B	0.50	0/4109	0.54	0/5600
2	b	0.49	0/4109	0.53	0/5600
3	C	0.47	0/3599	0.51	0/4900
3	c	0.44	0/3633	0.50	0/4946
4	D	0.53	0/2821	0.55	0/3844
4	d	0.49	0/2812	0.53	0/3832
5	E	0.43	0/681	0.51	0/928
5	e	0.42	0/681	0.50	0/928
6	F	0.49	0/284	0.45	0/387
6	f	0.47	0/265	0.44	0/360
7	H	0.47	0/524	0.50	0/713
7	h	0.44	0/524	0.49	0/713
8	I	0.47	0/319	0.51	0/429
8	i	0.46	0/319	0.47	0/429
9	J	0.46	0/278	0.43	0/376
9	j	0.39	0/294	0.45	0/396
10	K	0.43	0/303	0.50	0/416
10	k	0.43	0/303	0.51	0/416
11	L	0.55	0/311	0.51	0/422
11	l	0.54	0/311	0.52	0/422
12	M	0.47	0/270	0.58	0/367
12	m	0.49	0/270	0.52	0/367
13	O	0.45	0/1896	0.58	0/2571
13	o	0.43	0/1896	0.56	0/2571
14	T	0.54	0/265	0.52	0/359
14	t	0.55	0/265	0.52	0/359
15	U	0.46	0/785	0.55	0/1064
15	u	0.45	0/785	0.55	0/1064
16	V	0.47	0/1085	0.53	0/1473
16	v	0.42	0/1085	0.52	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	Y	0.41	0/216	0.45	0/289
17	y	0.35	0/216	0.52	0/289
18	X	0.43	0/290	0.46	0/392
18	x	0.42	0/290	0.48	0/392
19	Z	0.41	0/490	0.45	0/669
19	z	0.40	0/490	0.47	0/669
All	All	0.48	0/42484	0.53	0/57803

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2620	0	2517	64	0
1	a	2620	0	2517	0	0
2	B	3969	0	3828	85	0
2	b	3969	0	3828	0	0
3	C	3486	0	3407	73	0
3	c	3519	0	3437	0	23
4	D	2726	0	2627	69	0
4	d	2717	0	2621	0	0
5	E	662	0	648	18	0
5	e	662	0	648	0	0
6	F	275	0	282	6	0
6	f	257	0	269	0	0
7	H	511	0	532	14	0
7	h	511	0	532	0	0
8	I	312	0	329	6	0
8	i	312	0	329	0	0
9	J	272	0	279	7	0
9	j	288	0	300	0	0
10	K	293	0	305	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	k	293	0	305	0	0
11	L	304	0	316	11	0
11	l	304	0	316	0	0
12	M	267	0	289	9	0
12	m	267	0	289	0	0
13	O	1865	0	1838	48	23
13	o	1865	0	1838	0	0
14	T	256	0	262	5	0
14	t	256	0	262	0	0
15	U	774	0	773	32	0
15	u	774	0	773	0	0
16	V	1064	0	1073	34	0
16	v	1064	0	1075	0	0
17	Y	215	0	246	11	0
17	y	215	0	246	0	0
18	X	287	0	317	7	0
18	x	287	0	317	0	0
19	Z	479	0	516	4	0
19	z	479	0	516	0	0
20	A	10	0	0	0	0
20	a	10	0	0	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	V	1	0	0	0	0
22	a	2	0	0	0	0
22	v	1	0	0	0	0
23	A	4	0	0	0	0
23	a	4	0	0	0	0
24	A	260	0	288	11	0
24	B	1040	0	1152	48	0
24	C	845	0	936	43	0
24	D	130	0	144	6	0
24	a	195	0	216	0	0
24	b	1040	0	1152	0	0
24	c	845	0	936	0	0
24	d	195	0	216	0	0
25	A	64	0	74	4	0
25	D	64	0	74	4	0
25	a	64	0	74	0	0
25	d	64	0	74	0	0
26	A	40	0	48	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	B	160	0	188	9	0
26	C	80	0	93	0	0
26	D	40	0	48	2	0
26	H	40	0	46	2	0
26	K	40	0	46	5	0
26	T	80	0	94	2	0
26	Y	40	0	47	1	0
26	a	40	0	48	0	0
26	b	80	0	92	0	0
26	c	80	0	95	0	0
26	f	40	0	46	0	0
26	h	40	0	46	0	0
26	k	80	0	90	0	0
27	A	55	0	80	9	0
27	D	55	0	80	2	0
27	a	55	0	80	0	0
27	d	55	0	80	0	0
28	A	108	0	156	6	0
28	F	43	0	53	0	0
28	L	54	0	78	10	0
28	a	108	0	156	0	0
28	d	43	0	53	0	0
28	l	54	0	78	0	0
29	A	42	0	57	3	0
29	B	49	0	74	3	0
29	D	147	0	222	28	0
29	a	42	0	57	0	0
29	b	49	0	74	0	0
29	d	147	0	222	0	0
30	B	1	0	0	0	0
30	F	1	0	0	0	0
30	O	1	0	0	0	0
30	b	1	0	0	0	0
30	c	1	0	0	0	0
30	f	1	0	0	0	0
30	o	1	0	0	0	0
31	C	186	0	246	6	0
31	D	62	0	82	4	0
31	H	62	0	82	3	0
31	c	124	0	164	0	0
31	d	62	0	82	0	0
31	h	62	0	82	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	j	62	0	82	0	0
32	E	43	0	30	0	0
32	V	43	0	30	9	0
32	e	43	0	30	0	0
32	v	43	0	30	0	0
33	j	1	0	0	0	0
All	All	48924	0	49705	447	23

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 6.

The worst 5 of 447 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)
16:V:37:CYS:SG	32:V:202:HEM:HAB	1.52	1.49
16:V:40:CYS:SG	32:V:202:HEM:HAC	1.56	1.46
16:V:37:CYS:SG	32:V:202:HEM:CAB	2.03	1.46
16:V:40:CYS:SG	32:V:202:HEM:CAC	2.03	1.44
1:A:214:MET:HG2	27:A:611:PL9:H102	1.20	1.18

The worst 5 of 23 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:37:THR:O	3:c:19:ASN:CG[2_455]	0.56	1.64
13:O:37:THR:O	3:c:19:ASN:ND2[2_455]	0.91	1.29
13:O:36:GLN:NE2	3:c:19:ASN:CA[2_455]	0.99	1.21
13:O:37:THR:N	3:c:19:ASN:OD1[2_455]	1.04	1.16
13:O:36:GLN:NE2	3:c:19:ASN:C[2_455]	1.05	1.15

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	332/334 (99%)	328 (99%)	3 (1%)	1 (0%)	46 83
1	a	332/334 (99%)	325 (98%)	6 (2%)	1 (0%)	46 83
2	B	502/504 (100%)	496 (99%)	6 (1%)	0	100 100
2	b	502/504 (100%)	492 (98%)	10 (2%)	0	100 100
3	C	449/455 (99%)	440 (98%)	8 (2%)	1 (0%)	52 86
3	c	453/455 (100%)	440 (97%)	12 (3%)	1 (0%)	52 86
4	D	340/342 (99%)	332 (98%)	8 (2%)	0	100 100
4	d	339/342 (99%)	333 (98%)	6 (2%)	0	100 100
5	E	79/81 (98%)	78 (99%)	1 (1%)	0	100 100
5	e	79/81 (98%)	78 (99%)	1 (1%)	0	100 100
6	F	32/34 (94%)	32 (100%)	0	0	100 100
6	f	30/34 (88%)	30 (100%)	0	0	100 100
7	H	63/65 (97%)	58 (92%)	5 (8%)	0	100 100
7	h	63/65 (97%)	56 (89%)	7 (11%)	0	100 100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100 100
8	i	36/38 (95%)	35 (97%)	1 (3%)	0	100 100
9	J	36/40 (90%)	36 (100%)	0	0	100 100
9	j	38/40 (95%)	38 (100%)	0	0	100 100
10	K	35/37 (95%)	35 (100%)	0	0	100 100
10	k	35/37 (95%)	35 (100%)	0	0	100 100
11	L	35/37 (95%)	35 (100%)	0	0	100 100
11	l	35/37 (95%)	35 (100%)	0	0	100 100
12	M	32/34 (94%)	32 (100%)	0	0	100 100
12	m	32/34 (94%)	32 (100%)	0	0	100 100
13	O	241/243 (99%)	233 (97%)	7 (3%)	1 (0%)	39 80
13	o	241/243 (99%)	231 (96%)	9 (4%)	1 (0%)	39 80
14	T	28/30 (93%)	27 (96%)	1 (4%)	0	100 100
14	t	28/30 (93%)	28 (100%)	0	0	100 100
15	U	95/97 (98%)	93 (98%)	2 (2%)	0	100 100
15	u	95/97 (98%)	93 (98%)	2 (2%)	0	100 100
16	V	135/137 (98%)	132 (98%)	3 (2%)	0	100 100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Y	27/29 (93%)	27 (100%)	0	0	100	100
17	y	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
18	X	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
18	x	37/39 (95%)	35 (95%)	2 (5%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	5191/5276 (98%)	5072 (98%)	113 (2%)	6 (0%)	56	90

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	58	ASN
13	o	58	ASN
3	C	416	SER
3	c	416	SER
1	A	259	ILE

5.3.2 Protein sidechains (i)

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	269/269 (100%)	268 (100%)	1 (0%)	93	96
1	a	269/269 (100%)	267 (99%)	2 (1%)	88	94
2	B	402/402 (100%)	399 (99%)	3 (1%)	88	94
2	b	402/402 (100%)	395 (98%)	7 (2%)	68	88
3	C	352/356 (99%)	348 (99%)	4 (1%)	80	91
3	c	356/356 (100%)	350 (98%)	6 (2%)	68	88
4	D	277/277 (100%)	274 (99%)	3 (1%)	80	91
4	d	276/277 (100%)	275 (100%)	1 (0%)	93	96
5	E	72/72 (100%)	71 (99%)	1 (1%)	74	89
5	e	72/72 (100%)	70 (97%)	2 (3%)	51	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	F	28/28 (100%)	27 (96%)	1 (4%)	42 75
6	f	26/28 (93%)	25 (96%)	1 (4%)	40 74
7	H	54/54 (100%)	51 (94%)	3 (6%)	26 65
7	h	54/54 (100%)	53 (98%)	1 (2%)	65 86
8	I	35/35 (100%)	35 (100%)	0	100 100
8	i	35/35 (100%)	35 (100%)	0	100 100
9	J	26/28 (93%)	26 (100%)	0	100 100
9	j	28/28 (100%)	28 (100%)	0	100 100
10	K	30/30 (100%)	28 (93%)	2 (7%)	20 59
10	k	30/30 (100%)	28 (93%)	2 (7%)	20 59
11	L	35/35 (100%)	33 (94%)	2 (6%)	25 64
11	l	35/35 (100%)	34 (97%)	1 (3%)	50 79
12	M	31/31 (100%)	30 (97%)	1 (3%)	46 77
12	m	31/31 (100%)	31 (100%)	0	100 100
13	O	206/206 (100%)	202 (98%)	4 (2%)	65 86
13	o	206/206 (100%)	200 (97%)	6 (3%)	50 79
14	T	27/27 (100%)	27 (100%)	0	100 100
14	t	27/27 (100%)	25 (93%)	2 (7%)	17 55
15	U	84/84 (100%)	83 (99%)	1 (1%)	78 90
15	u	84/84 (100%)	83 (99%)	1 (1%)	78 90
16	V	117/117 (100%)	116 (99%)	1 (1%)	84 93
16	v	117/117 (100%)	114 (97%)	3 (3%)	54 81
17	Y	22/22 (100%)	21 (96%)	1 (4%)	34 70
17	y	22/22 (100%)	21 (96%)	1 (4%)	34 70
18	X	32/32 (100%)	32 (100%)	0	100 100
18	x	32/32 (100%)	31 (97%)	1 (3%)	47 78
19	Z	52/52 (100%)	50 (96%)	2 (4%)	40 74
19	z	52/52 (100%)	49 (94%)	3 (6%)	25 63
All	All	4305/4314 (100%)	4235 (98%)	70 (2%)	70 88

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	244	GLU
3	c	120	ILE
16	v	122	GLU
2	b	14	ASN
2	b	472	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
13	O	147	ASN
1	a	315	ASN
13	o	124	ASN
19	Z	58	ASN
2	b	53	ASN

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 152 ligands modelled in this entry, 16 are monoatomic - leaving 136 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	OEX	A	601	1,3	0,15,15	0.00	-	0,32,32	0.00	-
23	BCT	A	605	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	A	606	-	55,73,73	1.80	10 (18%)	61,113,113	1.76	14 (22%)
24	CLA	A	607	-	55,73,73	1.72	10 (18%)	61,113,113	2.07	16 (26%)
25	PHO	A	608	-	67,69,69	1.88	14 (20%)	84,99,99	1.97	20 (23%)
24	CLA	A	609	-	55,73,73	1.84	10 (18%)	61,113,113	1.89	16 (26%)
26	BCR	A	610	-	41,41,41	3.66	14 (34%)	56,56,56	7.57	38 (67%)
27	PL9	A	611	-	55,55,55	0.71	2 (3%)	68,69,69	1.64	13 (19%)
28	SQD	A	612	-	53,54,54	1.33	3 (5%)	61,65,65	1.67	10 (16%)
28	SQD	A	613	-	53,54,54	1.36	3 (5%)	61,65,65	1.33	5 (8%)
24	CLA	A	614	-	55,73,73	1.74	10 (18%)	61,113,113	2.06	16 (26%)
29	LHG	A	615	-	41,41,48	1.01	2 (4%)	42,47,54	1.10	3 (7%)
24	CLA	B	602	-	55,73,73	1.90	11 (20%)	61,113,113	1.90	14 (22%)
24	CLA	B	603	-	55,73,73	1.89	11 (20%)	61,113,113	1.69	11 (18%)
24	CLA	B	604	-	55,73,73	1.82	10 (18%)	61,113,113	2.02	15 (24%)
24	CLA	B	605	-	55,73,73	1.71	10 (18%)	61,113,113	1.96	15 (24%)
24	CLA	B	606	-	55,73,73	1.76	10 (18%)	61,113,113	1.79	14 (22%)
24	CLA	B	607	-	55,73,73	1.85	11 (20%)	61,113,113	1.90	12 (19%)
24	CLA	B	608	-	55,73,73	1.78	10 (18%)	61,113,113	1.81	13 (21%)
24	CLA	B	609	-	55,73,73	1.77	10 (18%)	61,113,113	2.04	17 (27%)
24	CLA	B	610	-	55,73,73	1.78	10 (18%)	61,113,113	1.84	13 (21%)
24	CLA	B	611	-	55,73,73	1.81	10 (18%)	61,113,113	1.77	14 (22%)
24	CLA	B	612	-	55,73,73	1.66	10 (18%)	61,113,113	1.84	13 (21%)
24	CLA	B	613	-	55,73,73	1.81	11 (20%)	61,113,113	1.87	15 (24%)
24	CLA	B	614	-	55,73,73	1.79	11 (20%)	61,113,113	1.74	15 (24%)
24	CLA	B	615	-	55,73,73	1.77	11 (20%)	61,113,113	1.91	15 (24%)
24	CLA	B	616	-	55,73,73	1.82	11 (20%)	61,113,113	1.69	11 (18%)
24	CLA	B	617	-	55,73,73	1.85	10 (18%)	61,113,113	1.82	17 (27%)
26	BCR	B	618	-	41,41,41	3.60	14 (34%)	56,56,56	7.30	38 (67%)
26	BCR	B	619	-	41,41,41	3.60	14 (34%)	56,56,56	7.55	41 (73%)
26	BCR	B	620	-	41,41,41	3.67	14 (34%)	56,56,56	8.19	41 (73%)
29	LHG	B	621	-	48,48,48	0.86	2 (4%)	49,54,54	1.00	2 (4%)
26	BCR	B	622	-	41,41,41	3.73	15 (36%)	56,56,56	7.41	34 (60%)
24	CLA	C	501	-	55,73,73	1.85	11 (20%)	61,113,113	1.98	14 (22%)
24	CLA	C	502	-	55,73,73	1.79	10 (18%)	61,113,113	1.79	14 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	C	503	-	55,73,73	1.87	11 (20%)	61,113,113	1.71	12 (19%)
24	CLA	C	504	-	55,73,73	1.83	10 (18%)	61,113,113	1.93	13 (21%)
24	CLA	C	505	-	55,73,73	1.85	12 (21%)	61,113,113	1.78	13 (21%)
24	CLA	C	506	-	55,73,73	1.87	11 (20%)	61,113,113	1.89	15 (24%)
24	CLA	C	507	-	55,73,73	1.93	11 (20%)	61,113,113	1.88	14 (22%)
24	CLA	C	508	-	55,73,73	1.92	12 (21%)	61,113,113	1.80	11 (18%)
24	CLA	C	509	-	55,73,73	1.85	12 (21%)	61,113,113	1.91	16 (26%)
24	CLA	C	510	-	55,73,73	1.82	11 (20%)	61,113,113	1.85	15 (24%)
24	CLA	C	511	3	55,73,73	1.86	11 (20%)	61,113,113	1.78	11 (18%)
24	CLA	C	512	-	55,73,73	1.90	12 (21%)	61,113,113	1.83	15 (24%)
24	CLA	C	513	-	55,73,73	1.95	11 (20%)	61,113,113	1.69	13 (21%)
26	BCR	C	514	-	41,41,41	3.80	15 (36%)	56,56,56	8.21	35 (62%)
26	BCR	C	515	-	41,41,41	3.76	14 (34%)	56,56,56	8.00	39 (69%)
31	DGD	C	516	-	63,63,67	0.84	2 (3%)	77,77,81	0.99	3 (3%)
31	DGD	C	517	-	63,63,67	0.85	2 (3%)	77,77,81	0.86	3 (3%)
31	DGD	C	518	-	63,63,67	0.76	3 (4%)	77,77,81	0.91	3 (3%)
25	PHO	D	401	-	67,69,69	1.98	15 (22%)	84,99,99	1.97	21 (25%)
24	CLA	D	402	-	55,73,73	1.79	10 (18%)	61,113,113	1.87	18 (29%)
24	CLA	D	403	-	55,73,73	1.86	12 (21%)	61,113,113	1.73	12 (19%)
26	BCR	D	404	-	41,41,41	3.75	14 (34%)	56,56,56	7.56	41 (73%)
27	PL9	D	405	-	55,55,55	0.82	1 (1%)	68,69,69	1.42	9 (13%)
31	DGD	D	406	-	63,63,67	0.96	4 (6%)	77,77,81	1.07	6 (7%)
29	LHG	D	407	-	48,48,48	0.84	2 (4%)	49,54,54	1.01	3 (6%)
29	LHG	D	408	-	48,48,48	0.87	2 (4%)	49,54,54	0.86	2 (4%)
29	LHG	D	409	-	48,48,48	0.91	2 (4%)	49,54,54	0.90	2 (4%)
32	HEM	E	101	5,6	30,50,50	2.21	8 (26%)	24,82,82	2.44	9 (37%)
28	SQD	F	101	-	42,43,54	1.54	3 (7%)	50,54,65	1.66	7 (14%)
26	BCR	H	101	-	41,41,41	3.74	14 (34%)	56,56,56	8.04	40 (71%)
31	DGD	H	102	-	63,63,67	0.88	3 (4%)	77,77,81	0.94	6 (7%)
26	BCR	K	101	-	41,41,41	3.70	14 (34%)	56,56,56	7.54	41 (73%)
28	SQD	L	101	-	53,54,54	1.35	4 (7%)	61,65,65	1.61	8 (13%)
26	BCR	T	101	-	41,41,41	3.74	14 (34%)	56,56,56	6.87	38 (67%)
26	BCR	T	102	-	41,41,41	3.62	15 (36%)	56,56,56	7.04	38 (67%)
32	HEM	V	202	16	30,50,50	2.26	9 (30%)	24,82,82	2.41	9 (37%)
26	BCR	Y	101	-	41,41,41	3.78	14 (34%)	56,56,56	7.85	36 (64%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	OEX	a	401	1,3	0,15,15	0.00	-	0,32,32	0.00	-
28	SQD	a	402	-	53,54,54	1.38	3 (5%)	61,65,65	1.33	5 (8%)
24	CLA	a	406	-	55,73,73	1.75	10 (18%)	61,113,113	1.86	14 (22%)
24	CLA	a	407	-	55,73,73	1.72	10 (18%)	61,113,113	1.97	16 (26%)
24	CLA	a	408	-	55,73,73	1.84	10 (18%)	61,113,113	1.91	16 (26%)
26	BCR	a	409	-	41,41,41	3.59	14 (34%)	56,56,56	7.59	36 (64%)
27	PL9	a	410	-	55,55,55	0.71	2 (3%)	68,69,69	1.61	16 (23%)
28	SQD	a	411	-	53,54,54	1.33	3 (5%)	61,65,65	1.73	9 (14%)
25	PHO	a	412	-	67,69,69	2.01	15 (22%)	84,99,99	1.97	19 (22%)
29	LHG	a	413	-	41,41,48	1.02	2 (4%)	42,47,54	0.93	2 (4%)
23	BCT	a	414	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	b	602	-	55,73,73	1.95	11 (20%)	61,113,113	1.84	14 (22%)
24	CLA	b	603	-	55,73,73	1.86	11 (20%)	61,113,113	1.71	12 (19%)
24	CLA	b	604	-	55,73,73	1.79	10 (18%)	61,113,113	1.99	18 (29%)
24	CLA	b	605	-	55,73,73	1.77	11 (20%)	61,113,113	1.96	17 (27%)
24	CLA	b	606	-	55,73,73	1.72	11 (20%)	61,113,113	1.98	15 (24%)
24	CLA	b	607	-	55,73,73	1.89	11 (20%)	61,113,113	1.85	13 (21%)
24	CLA	b	608	-	55,73,73	1.82	10 (18%)	61,113,113	1.83	15 (24%)
24	CLA	b	609	-	55,73,73	1.84	11 (20%)	61,113,113	1.87	14 (22%)
24	CLA	b	610	-	55,73,73	1.88	12 (21%)	61,113,113	1.81	12 (19%)
24	CLA	b	611	-	55,73,73	1.84	12 (21%)	61,113,113	1.71	10 (16%)
24	CLA	b	612	-	55,73,73	1.78	10 (18%)	61,113,113	1.81	13 (21%)
24	CLA	b	613	-	55,73,73	1.78	10 (18%)	61,113,113	1.90	14 (22%)
24	CLA	b	614	-	55,73,73	1.83	11 (20%)	61,113,113	1.81	13 (21%)
24	CLA	b	615	-	55,73,73	1.78	11 (20%)	61,113,113	2.03	19 (31%)
24	CLA	b	616	-	55,73,73	1.83	10 (18%)	61,113,113	1.83	15 (24%)
24	CLA	b	617	-	55,73,73	1.88	11 (20%)	61,113,113	1.88	16 (26%)
26	BCR	b	618	-	41,41,41	3.65	14 (34%)	56,56,56	7.79	41 (73%)
26	BCR	b	619	-	41,41,41	3.75	15 (36%)	56,56,56	8.34	40 (71%)
29	LHG	b	620	-	48,48,48	0.87	2 (4%)	49,54,54	1.00	2 (4%)
24	CLA	c	902	-	55,73,73	1.87	12 (21%)	61,113,113	1.92	12 (19%)
24	CLA	c	903	-	55,73,73	1.84	11 (20%)	61,113,113	1.86	13 (21%)
24	CLA	c	904	-	55,73,73	1.88	12 (21%)	61,113,113	1.66	14 (22%)
24	CLA	c	905	-	55,73,73	1.88	12 (21%)	61,113,113	1.85	14 (22%)
24	CLA	c	906	-	55,73,73	1.86	11 (20%)	61,113,113	1.80	16 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	c	907	-	55,73,73	1.87	11 (20%)	61,113,113	1.71	11 (18%)
24	CLA	c	908	-	55,73,73	1.87	11 (20%)	61,113,113	1.93	12 (19%)
24	CLA	c	909	-	55,73,73	1.84	13 (23%)	61,113,113	1.69	10 (16%)
24	CLA	c	910	-	55,73,73	1.89	11 (20%)	61,113,113	1.91	14 (22%)
24	CLA	c	911	-	55,73,73	1.84	10 (18%)	61,113,113	1.78	14 (22%)
24	CLA	c	912	3	55,73,73	1.89	11 (20%)	61,113,113	1.78	12 (19%)
24	CLA	c	913	-	55,73,73	1.90	12 (21%)	61,113,113	1.85	13 (21%)
24	CLA	c	914	-	55,73,73	1.96	12 (21%)	61,113,113	1.70	13 (21%)
26	BCR	c	915	-	41,41,41	3.73	15 (36%)	56,56,56	8.32	40 (71%)
31	DGD	c	916	-	63,63,67	0.83	2 (3%)	77,77,81	0.91	3 (3%)
31	DGD	c	917	-	63,63,67	0.85	2 (3%)	77,77,81	0.81	2 (2%)
26	BCR	c	918	-	41,41,41	3.56	15 (36%)	56,56,56	7.37	36 (64%)
24	CLA	d	401	-	55,73,73	1.75	10 (18%)	61,113,113	1.86	14 (22%)
25	PHO	d	402	-	67,69,69	1.92	14 (20%)	84,99,99	1.90	19 (22%)
24	CLA	d	403	-	55,73,73	1.76	11 (20%)	61,113,113	1.92	16 (26%)
24	CLA	d	404	-	55,73,73	1.88	12 (21%)	61,113,113	1.82	13 (21%)
27	PL9	d	405	-	55,55,55	0.85	3 (5%)	68,69,69	1.39	11 (16%)
31	DGD	d	406	-	63,63,67	0.93	3 (4%)	77,77,81	0.98	3 (3%)
28	SQD	d	407	-	42,43,54	1.57	3 (7%)	50,54,65	1.59	7 (14%)
29	LHG	d	408	-	48,48,48	0.87	2 (4%)	49,54,54	0.98	4 (8%)
29	LHG	d	409	-	48,48,48	0.82	2 (4%)	49,54,54	0.92	3 (6%)
29	LHG	d	410	-	48,48,48	0.89	2 (4%)	49,54,54	0.96	3 (6%)
32	HEM	e	101	5,6	30,50,50	2.14	9 (30%)	24,82,82	2.48	9 (37%)
26	BCR	f	101	-	41,41,41	3.77	15 (36%)	56,56,56	7.74	47 (83%)
26	BCR	h	101	-	41,41,41	3.73	14 (34%)	56,56,56	8.15	41 (73%)
31	DGD	h	102	-	63,63,67	0.87	3 (4%)	77,77,81	0.86	3 (3%)
31	DGD	j	101	-	63,63,67	0.85	3 (4%)	77,77,81	0.88	3 (3%)
26	BCR	k	101	-	41,41,41	3.82	14 (34%)	56,56,56	8.29	42 (75%)
26	BCR	k	102	-	41,41,41	3.74	14 (34%)	56,56,56	8.23	42 (75%)
28	SQD	l	101	-	53,54,54	1.30	4 (7%)	61,65,65	1.51	6 (9%)
32	HEM	v	202	16	30,50,50	2.27	11 (36%)	24,82,82	2.43	10 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	OEX	A	601	1,3	-	0/0/68/68	0/0/6/6
23	BCT	A	605	21	-	0/0/0/0	0/0/0/0
24	CLA	A	606	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	A	607	-	2/2/20/25	0/37/135/135	0/0/9/9
25	PHO	A	608	-	-	0/53/103/103	0/1/6/6
24	CLA	A	609	-	1/1/20/25	0/37/135/135	0/0/9/9
26	BCR	A	610	-	-	0/29/63/63	0/2/2/2
27	PL9	A	611	-	-	0/53/73/73	0/1/1/1
28	SQD	A	612	-	-	0/49/69/69	0/1/1/1
28	SQD	A	613	-	-	0/49/69/69	0/1/1/1
24	CLA	A	614	-	1/1/20/25	0/37/135/135	0/0/9/9
29	LHG	A	615	-	-	0/46/46/53	0/0/0/0
24	CLA	B	602	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	607	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	609	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	B	610	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	612	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	617	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	B	618	-	-	0/29/63/63	0/2/2/2
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
29	LHG	B	621	-	-	0/53/53/53	0/0/0/0
26	BCR	B	622	-	-	0/29/63/63	0/2/2/2
24	CLA	C	501	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	C	502	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	505	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	508	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	511	3	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	C	512	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	513	-	2/2/20/25	0/37/135/135	0/0/9/9
26	BCR	C	514	-	-	0/29/63/63	0/2/2/2
26	BCR	C	515	-	-	0/29/63/63	0/2/2/2
31	DGD	C	516	-	-	0/51/91/95	0/2/2/2
31	DGD	C	517	-	-	0/51/91/95	0/2/2/2
31	DGD	C	518	-	-	0/51/91/95	0/2/2/2
25	PHO	D	401	-	-	0/53/103/103	0/1/6/6
24	CLA	D	402	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	D	403	-	2/2/20/25	0/37/135/135	0/0/9/9
26	BCR	D	404	-	-	0/29/63/63	0/2/2/2
27	PL9	D	405	-	-	0/53/73/73	0/1/1/1
31	DGD	D	406	-	-	0/51/91/95	0/2/2/2
29	LHG	D	407	-	-	0/53/53/53	0/0/0/0
29	LHG	D	408	-	-	0/53/53/53	0/0/0/0
29	LHG	D	409	-	-	0/53/53/53	0/0/0/0
32	HEM	E	101	5,6	-	0/10/54/54	0/0/8/8
28	SQD	F	101	-	-	0/38/58/69	0/1/1/1
26	BCR	H	101	-	-	0/29/63/63	0/2/2/2
31	DGD	H	102	-	-	0/51/91/95	0/2/2/2
26	BCR	K	101	-	-	0/29/63/63	0/2/2/2
28	SQD	L	101	-	-	0/49/69/69	0/1/1/1
26	BCR	T	101	-	-	0/29/63/63	0/2/2/2
26	BCR	T	102	-	-	0/29/63/63	0/2/2/2
32	HEM	V	202	16	-	0/10/54/54	0/0/8/8
26	BCR	Y	101	-	-	0/29/63/63	0/2/2/2
20	OEX	a	401	1,3	-	0/0/68/68	0/0/6/6
28	SQD	a	402	-	-	0/49/69/69	0/1/1/1
24	CLA	a	406	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	a	407	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	a	408	-	1/1/20/25	0/37/135/135	0/0/9/9
26	BCR	a	409	-	-	0/29/63/63	0/2/2/2
27	PL9	a	410	-	-	0/53/73/73	0/1/1/1
28	SQD	a	411	-	-	0/49/69/69	0/1/1/1
25	PHO	a	412	-	-	0/53/103/103	0/1/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LHG	a	413	-	-	0/46/46/53	0/0/0/0
23	BCT	a	414	21	-	0/0/0/0	0/0/0/0
24	CLA	b	602	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	603	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	604	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	607	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	609	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	b	610	-	-	0/37/135/135	0/0/9/9
24	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	612	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	b	618	-	-	0/29/63/63	0/2/2/2
26	BCR	b	619	-	-	0/29/63/63	0/2/2/2
29	LHG	b	620	-	-	0/53/53/53	0/0/0/0
24	CLA	c	902	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	903	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	c	904	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	c	905	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	c	906	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	c	907	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	c	908	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	909	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	c	910	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	911	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	912	3	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	c	913	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	914	-	2/2/20/25	0/37/135/135	0/0/9/9
26	BCR	c	915	-	-	0/29/63/63	0/2/2/2
31	DGD	c	916	-	-	0/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DGD	c	917	-	-	0/51/91/95	0/2/2/2
26	BCR	c	918	-	-	0/29/63/63	0/2/2/2
24	CLA	d	401	-	1/1/20/25	0/37/135/135	0/0/9/9
25	PHO	d	402	-	-	0/53/103/103	0/1/6/6
24	CLA	d	403	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	d	404	-	1/1/20/25	0/37/135/135	0/0/9/9
27	PL9	d	405	-	-	0/53/73/73	0/1/1/1
31	DGD	d	406	-	-	0/51/91/95	0/2/2/2
28	SQD	d	407	-	-	0/38/58/69	0/1/1/1
29	LHG	d	408	-	-	0/53/53/53	0/0/0/0
29	LHG	d	409	-	-	0/53/53/53	0/0/0/0
29	LHG	d	410	-	-	0/53/53/53	0/0/0/0
32	HEM	e	101	5,6	-	0/10/54/54	0/0/8/8
26	BCR	f	101	-	-	0/29/63/63	0/2/2/2
26	BCR	h	101	-	-	1/29/63/63	0/2/2/2
31	DGD	h	102	-	-	0/51/91/95	0/2/2/2
31	DGD	j	101	-	-	0/51/91/95	0/2/2/2
26	BCR	k	101	-	-	0/29/63/63	0/2/2/2
26	BCR	k	102	-	-	0/29/63/63	0/2/2/2
28	SQD	l	101	-	-	0/49/69/69	0/1/1/1
32	HEM	v	202	16	-	0/10/54/54	0/0/8/8

The worst 5 of 1250 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	918	BCR	C8-C9	-8.63	1.26	1.45
26	b	619	BCR	C8-C9	-8.58	1.26	1.45
26	B	622	BCR	C8-C9	-8.53	1.27	1.45
26	C	514	BCR	C8-C9	-8.51	1.27	1.45
26	C	514	BCR	C12-C13	-8.48	1.27	1.45

The worst 5 of 2127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	620	BCR	C36-C18-C17	-10.02	108.10	122.90
26	A	610	BCR	C37-C22-C21	-9.26	109.22	122.90
26	D	404	BCR	C30-C25-C26	-8.76	109.80	122.66
26	Y	101	BCR	C33-C5-C4	-8.54	97.23	113.43
26	B	619	BCR	C36-C18-C19	-8.30	104.28	118.10

5 of 163 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	a	408	CLA	NC
24	b	602	CLA	NC
24	b	602	CLA	ND
24	b	602	CLA	NA
24	C	509	CLA	NC

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	h	101	BCR	C21-C20-C19-C18

There are no ring outliers.

60 monomers are involved in 188 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	606	CLA	4	0
24	A	607	CLA	2	0
25	A	608	PHO	4	0
24	A	609	CLA	3	0
27	A	611	PL9	9	0
28	A	612	SQD	5	0
28	A	613	SQD	1	0
24	A	614	CLA	4	0
29	A	615	LHG	3	0
24	B	603	CLA	5	0
24	B	604	CLA	2	0
24	B	605	CLA	2	0
24	B	606	CLA	6	0
24	B	607	CLA	6	0
24	B	609	CLA	3	0
24	B	610	CLA	2	0
24	B	611	CLA	7	0
24	B	612	CLA	5	0
24	B	613	CLA	5	0
24	B	614	CLA	4	0
24	B	615	CLA	1	0
24	B	616	CLA	3	0
24	B	617	CLA	4	0
26	B	618	BCR	2	0
26	B	619	BCR	5	0
26	B	620	BCR	1	0
29	B	621	LHG	3	0
26	B	622	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	501	CLA	2	0
24	C	502	CLA	3	0
24	C	503	CLA	3	0
24	C	504	CLA	5	0
24	C	505	CLA	3	0
24	C	506	CLA	5	0
24	C	507	CLA	2	0
24	C	508	CLA	8	0
24	C	509	CLA	2	0
24	C	510	CLA	7	0
24	C	511	CLA	3	0
24	C	512	CLA	3	0
24	C	513	CLA	1	0
31	C	516	DGD	2	0
31	C	517	DGD	1	0
31	C	518	DGD	3	0
25	D	401	PHO	4	0
24	D	402	CLA	1	0
24	D	403	CLA	5	0
26	D	404	BCR	2	0
27	D	405	PL9	2	0
31	D	406	DGD	4	0
29	D	407	LHG	4	0
29	D	408	LHG	1	0
29	D	409	LHG	23	0
26	H	101	BCR	2	0
31	H	102	DGD	3	0
26	K	101	BCR	5	0
28	L	101	SQD	10	0
26	T	101	BCR	2	0
32	V	202	HEM	9	0
26	Y	101	BCR	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	334/334 (100%)	0.43	13 (3%) 43 36	16, 22, 43, 53	0
1	a	334/334 (100%)	0.50	26 (7%) 16 13	19, 24, 45, 62	0
2	B	504/504 (100%)	0.39	34 (6%) 21 16	18, 27, 49, 70	0
2	b	504/504 (100%)	0.66	62 (12%) 5 7	20, 29, 52, 93	0
3	C	451/455 (99%)	0.51	50 (11%) 7 8	21, 31, 44, 56	0
3	c	455/455 (100%)	0.34	26 (5%) 27 22	24, 34, 45, 59	0
4	D	342/342 (100%)	0.70	29 (8%) 13 12	17, 23, 39, 61	0
4	d	341/342 (99%)	0.59	27 (7%) 15 13	19, 26, 42, 59	0
5	E	81/81 (100%)	0.75	11 (13%) 4 5	27, 40, 57, 63	0
5	e	81/81 (100%)	0.42	9 (11%) 7 8	34, 45, 67, 76	0
6	F	34/34 (100%)	-0.01	1 (2%) 55 45	28, 33, 58, 61	0
6	f	32/34 (94%)	0.05	3 (9%) 11 10	30, 36, 60, 62	0
7	H	65/65 (100%)	0.79	11 (16%) 2 4	23, 34, 40, 58	0
7	h	65/65 (100%)	1.20	14 (21%) 1 3	28, 37, 48, 58	0
8	I	38/38 (100%)	0.37	3 (7%) 15 13	26, 33, 65, 68	0
8	i	38/38 (100%)	0.16	3 (7%) 15 13	29, 34, 62, 65	0
9	J	38/40 (95%)	0.64	6 (15%) 3 4	26, 37, 68, 72	0
9	j	40/40 (100%)	-0.08	3 (7%) 17 15	31, 42, 76, 80	0
10	K	37/37 (100%)	0.08	0 100 100	33, 38, 45, 47	0
10	k	37/37 (100%)	0.36	3 (8%) 15 13	38, 43, 55, 58	0
11	L	37/37 (100%)	0.62	4 (10%) 8 8	17, 22, 50, 59	0
11	l	37/37 (100%)	0.47	0 100 100	19, 22, 55, 62	0
12	M	34/34 (100%)	1.07	7 (20%) 1 3	21, 23, 36, 52	0
12	m	34/34 (100%)	0.79	3 (8%) 12 11	21, 25, 37, 53	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/243 (100%)	0.36	7 (2%) 55 45	18, 32, 55, 71	0
13	o	243/243 (100%)	0.48	16 (6%) 22 17	21, 35, 61, 72	0
14	T	30/30 (100%)	0.70	3 (10%) 9 9	19, 23, 44, 52	0
14	t	30/30 (100%)	0.78	3 (10%) 9 9	20, 24, 44, 51	0
15	U	97/97 (100%)	0.13	2 (2%) 67 58	23, 30, 48, 50	0
15	u	97/97 (100%)	0.29	3 (3%) 52 43	25, 31, 37, 47	0
16	V	137/137 (100%)	0.14	1 (0%) 89 84	23, 28, 39, 48	0
16	v	137/137 (100%)	0.25	10 (7%) 18 15	27, 37, 51, 57	0
17	Y	29/29 (100%)	0.48	2 (6%) 20 16	42, 48, 75, 77	0
17	y	29/29 (100%)	0.08	0 100 100	50, 56, 75, 76	0
18	X	39/39 (100%)	0.84	8 (20%) 1 3	33, 40, 66, 68	0
18	x	39/39 (100%)	1.17	6 (15%) 3 4	37, 43, 75, 77	0
19	Z	62/62 (100%)	0.43	3 (4%) 34 28	39, 48, 68, 72	0
19	z	62/62 (100%)	0.53	5 (8%) 15 13	53, 61, 82, 87	0
All	All	5267/5276 (99%)	0.48	417 (7%) 15 13	16, 30, 56, 93	0

The worst 5 of 417 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	x	40	SER	8.1
7	H	65	LEU	7.0
4	d	136	VAL	6.5
9	J	3	SER	6.3
4	D	59	TYR	6.3

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
26	BCR	K	101	40/40	0.86	1.84	9.84	29,33,37,37	0
26	BCR	Y	101	40/40	0.65	1.57	9.31	34,38,39,39	0
27	PL9	A	611	55/55	0.56	2.04	8.80	52,69,78,78	0
26	BCR	k	102	40/40	0.54	2.03	7.08	33,44,47,48	0
27	PL9	a	410	55/55	0.17	1.70	6.74	63,80,85,85	0
26	BCR	c	915	40/40	0.73	1.85	6.49	30,37,41,42	0
31	DGD	D	406	62/66	0.53	1.38	6.11	77,89,103,103	0
24	CLA	B	603	65/65	0.89	1.13	5.55	23,26,32,32	0
26	BCR	c	918	40/40	0.74	1.76	5.55	50,52,58,58	0
26	BCR	f	101	40/40	0.45	0.98	5.34	30,34,48,49	0
26	BCR	k	101	40/40	0.32	1.08	4.76	37,41,45,45	0
26	BCR	b	619	40/40	0.55	1.06	4.74	30,34,41,42	0
24	CLA	c	902	65/65	0.78	1.54	4.41	30,33,41,45	0
22	CL	a	404	1/1	0.81	0.64	4.37	28,28,28,28	0
26	BCR	C	515	40/40	0.81	1.90	4.26	30,37,40,41	0
24	CLA	c	908	65/65	0.85	1.08	4.24	28,32,50,51	0
26	BCR	D	404	40/40	0.53	0.96	4.09	25,30,48,49	0
24	CLA	c	906	65/65	0.90	0.81	3.71	28,31,44,44	0
28	SQD	F	101	43/54	0.83	0.82	3.52	67,74,78,79	0
25	PHO	D	401	64/64	0.81	0.98	3.48	19,22,28,32	0
24	CLA	b	604	65/65	0.95	1.13	3.36	23,26,35,38	0
24	CLA	a	408	65/65	0.73	0.77	3.33	20,24,75,75	0
31	DGD	H	102	62/66	0.91	1.00	3.32	26,32,38,40	0
29	LHG	a	413	42/49	0.47	0.68	3.26	95,107,110,111	0
26	BCR	C	514	40/40	0.72	1.34	3.25	37,43,47,47	0
24	CLA	b	609	65/65	0.92	1.08	3.10	22,27,38,39	0
24	CLA	c	907	65/65	0.87	0.86	3.09	30,35,64,64	0
29	LHG	D	409	49/49	0.84	0.81	3.02	26,33,62,64	0
24	CLA	A	609	65/65	0.88	0.65	3.01	21,24,71,72	0
24	CLA	d	403	65/65	0.88	0.73	2.95	18,21,38,39	0
24	CLA	c	913	65/65	0.77	1.26	2.91	38,42,62,63	0
24	CLA	b	606	65/65	0.81	0.82	2.89	21,24,32,33	0
24	CLA	b	605	65/65	0.81	0.80	2.85	20,25,53,55	0
24	CLA	B	611	65/65	0.90	0.86	2.82	21,25,32,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
31	DGD	d	406	62/66	0.59	0.94	2.81	80,91,105,105	0
24	CLA	c	914	65/65	0.76	1.07	2.77	46,51,73,74	0
24	CLA	D	403	65/65	0.72	1.01	2.76	24,27,65,67	0
24	CLA	D	402	65/65	0.85	0.81	2.73	13,18,34,35	0
26	BCR	A	610	40/40	0.62	0.62	2.72	22,27,32,32	0
24	CLA	C	509	65/65	0.89	1.01	2.65	29,32,46,47	0
31	DGD	h	102	62/66	0.87	0.88	2.64	29,36,43,44	0
25	PHO	a	412	64/64	0.84	0.80	2.63	20,25,30,33	0
24	CLA	C	512	65/65	0.74	1.36	2.61	37,41,62,63	0
24	CLA	B	613	65/65	0.88	0.57	2.60	20,24,30,31	0
24	CLA	c	910	65/65	0.86	0.86	2.59	27,30,46,46	0
24	CLA	C	507	65/65	0.81	1.31	2.57	29,33,52,53	0
24	CLA	d	404	65/65	0.81	0.84	2.56	26,31,67,68	0
24	CLA	b	603	65/65	0.87	1.05	2.56	26,29,36,37	0
26	BCR	H	101	40/40	0.66	1.44	2.55	26,33,42,42	0
24	CLA	C	501	65/65	0.88	1.01	2.54	29,32,44,46	0
29	LHG	A	615	42/49	0.63	1.14	2.51	69,83,86,86	0
24	CLA	A	607	65/65	0.79	0.85	2.51	19,21,63,65	0
24	CLA	b	616	65/65	0.80	1.17	2.47	27,30,45,46	0
24	CLA	B	610	65/65	0.90	0.84	2.46	23,28,31,32	0
24	CLA	C	508	65/65	0.82	0.71	2.40	25,29,54,58	0
24	CLA	B	604	65/65	0.89	0.87	2.39	18,22,31,35	0
24	CLA	C	511	65/65	0.93	0.93	2.38	29,34,37,38	0
24	CLA	c	911	65/65	0.92	0.66	2.38	26,30,39,40	0
24	CLA	c	903	65/65	0.77	0.82	2.27	25,28,42,45	0
24	CLA	c	904	65/65	0.84	0.86	2.25	26,37,39,40	0
24	CLA	C	510	65/65	0.90	0.69	2.25	24,28,35,37	0
28	SQD	A	612	54/54	0.65	0.83	2.17	49,57,66,67	0
24	CLA	c	909	65/65	0.90	0.59	2.14	27,29,57,60	0
26	BCR	B	620	40/40	0.59	0.55	2.09	27,33,39,39	0
24	CLA	c	912	65/65	0.87	0.78	2.05	32,37,43,44	0
24	CLA	a	407	65/65	0.63	0.75	2.00	19,23,63,65	0
24	CLA	B	609	65/65	0.85	0.92	1.92	20,24,31,31	0
24	CLA	b	610	65/65	0.93	0.88	1.91	28,31,33,36	0
23	BCT	a	414	4/4	0.97	0.94	1.78	34,34,35,37	0
24	CLA	b	602	65/65	0.68	1.23	1.75	38,46,68,68	0
24	CLA	B	606	65/65	0.83	0.72	1.72	19,23,34,35	0
29	LHG	d	410	49/49	0.87	0.71	1.72	28,34,66,67	0
24	CLA	b	617	65/65	0.61	0.93	1.65	27,33,74,75	0
24	CLA	b	607	65/65	0.60	0.59	1.59	26,30,41,42	0
26	BCR	b	618	40/40	0.73	0.43	1.58	24,28,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
24	CLA	B	602	65/65	0.62	0.91	1.49	32,41,66,66	0
24	CLA	C	504	65/65	0.80	0.66	1.45	25,28,54,54	0
24	CLA	A	606	65/65	0.86	0.65	1.45	15,19,25,34	0
28	SQD	d	407	43/54	0.69	1.01	1.42	84,90,93,94	0
32	HEM	E	101	43/43	0.93	0.70	1.41	39,42,45,47	0
24	CLA	b	613	65/65	0.84	0.64	1.41	21,26,33,35	0
26	BCR	h	101	40/40	0.78	1.18	1.39	29,37,45,45	0
32	HEM	V	202	43/43	0.90	0.56	1.38	23,24,27,29	0
28	SQD	a	411	54/54	0.72	0.51	1.35	50,60,75,76	0
24	CLA	b	611	65/65	0.91	0.75	1.29	25,28,34,37	0
24	CLA	B	605	65/65	0.91	0.50	1.26	19,22,50,51	0
24	CLA	a	406	65/65	0.77	0.52	1.23	18,20,28,33	0
31	DGD	C	518	62/66	0.85	0.52	1.20	22,31,52,56	0
32	HEM	e	101	43/43	0.92	0.42	1.19	43,46,52,55	0
32	HEM	v	202	43/43	0.93	0.61	1.18	28,31,34,36	0
24	CLA	C	513	65/65	0.70	1.16	1.16	39,45,64,64	0
27	PL9	D	405	55/55	0.70	0.55	1.16	19,23,29,32	0
28	SQD	A	613	54/54	0.76	0.50	1.14	50,63,68,68	0
25	PHO	d	402	64/64	0.85	0.50	1.10	18,22,24,25	0
24	CLA	C	505	65/65	0.93	0.76	1.02	28,30,44,45	0
26	BCR	a	409	40/40	0.53	0.48	1.02	21,26,29,29	0
24	CLA	C	502	65/65	0.90	0.67	1.01	24,26,39,42	0
25	PHO	A	608	64/64	0.79	0.54	0.98	16,21,25,26	0
24	CLA	B	616	65/65	0.78	0.62	0.96	25,27,45,46	0
29	LHG	D	408	49/49	0.80	0.52	0.90	24,28,37,40	0
24	CLA	C	506	65/65	0.88	0.81	0.90	31,38,74,75	0
31	DGD	j	101	62/66	0.90	0.43	0.89	25,34,52,55	0
24	CLA	c	905	65/65	0.89	0.56	0.88	28,30,55,56	0
24	CLA	C	503	65/65	0.88	0.66	0.85	27,31,35,36	0
24	CLA	B	617	65/65	0.74	0.46	0.82	22,29,77,78	0
31	DGD	C	516	62/66	0.90	0.44	0.75	23,33,61,62	0
24	CLA	B	612	65/65	0.85	0.46	0.70	19,21,32,34	0
24	CLA	A	614	65/65	0.84	0.49	0.69	14,18,29,35	0
24	CLA	b	612	65/65	0.76	0.47	0.66	20,23,37,41	0
24	CLA	B	607	65/65	0.72	0.55	0.60	24,28,40,41	0
31	DGD	C	517	62/66	0.78	0.46	0.37	23,35,62,63	0
31	DGD	c	916	62/66	0.86	0.48	0.36	24,35,60,61	0
26	BCR	T	101	40/40	0.67	0.44	0.21	25,37,44,45	0
28	SQD	a	402	54/54	0.78	0.40	0.19	51,67,75,76	0
31	DGD	c	917	62/66	0.82	0.42	0.17	28,36,64,65	0
30	CA	c	901	1/1	0.57	0.44	0.15	46,46,46,46	0
26	BCR	T	102	40/40	0.75	0.41	0.10	25,29,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
24	CLA	b	608	65/65	0.74	0.46	0.05	19,23,30,32	0
24	CLA	b	614	65/65	0.82	0.38	0.04	21,24,44,45	0
24	CLA	d	401	65/65	0.84	0.46	0.03	17,20,27,31	0
22	CL	A	603	1/1	0.79	0.42	-0.02	24,24,24,24	0
29	LHG	d	409	49/49	0.84	0.34	-0.03	23,27,38,40	0
27	PL9	d	405	55/55	0.75	0.41	-0.07	19,25,29,31	0
28	SQD	l	101	54/54	0.72	0.41	-0.07	57,69,84,85	0
23	BCT	A	605	4/4	0.96	0.46	-0.08	39,39,40,42	0
20	OEX	a	401	10/10	0.95	0.35	-0.23	25,27,28,28	0
28	SQD	L	101	54/54	0.78	0.38	-0.25	58,66,80,80	0
29	LHG	D	407	49/49	0.74	0.40	-0.36	29,34,41,41	0
29	LHG	b	620	49/49	0.85	0.33	-0.46	24,31,46,50	0
29	LHG	d	408	49/49	0.80	0.40	-0.46	29,37,41,42	0
33	MG	j	102	1/1	0.59	0.20	-0.47	34,34,34,34	0
24	CLA	B	608	65/65	0.75	0.41	-0.49	17,20,32,34	0
26	BCR	B	618	40/40	0.67	0.36	-0.50	23,27,28,29	0
24	CLA	B	615	65/65	0.78	0.40	-0.61	20,24,60,61	0
30	CA	O	301	1/1	0.88	0.19	-0.69	49,49,49,49	0
20	OEX	A	601	10/10	0.93	0.35	-0.70	22,23,26,26	0
26	BCR	B	622	40/40	0.62	0.40	-0.72	23,34,41,41	0
22	CL	A	604	1/1	0.91	0.32	-0.74	21,21,21,21	0
24	CLA	B	614	65/65	0.92	0.33	-0.76	19,22,45,47	0
29	LHG	B	621	49/49	0.90	0.31	-0.78	23,31,43,44	0
24	CLA	b	615	65/65	0.78	0.35	-0.93	22,26,65,66	0
22	CL	a	405	1/1	0.94	0.20	-1.55	26,26,26,26	0
26	BCR	B	619	40/40	0.78	0.31	-2.35	21,28,40,40	0
30	CA	o	301	1/1	0.95	0.09	-2.35	51,51,51,51	0
21	FE2	A	602	1/1	0.99	0.11	-2.56	26,26,26,26	0
30	CA	F	102	1/1	0.56	0.46	-	56,56,56,56	0
30	CA	f	102	1/1	0.20	0.38	-	58,58,58,58	0
22	CL	v	201	1/1	0.48	0.38	-	60,60,60,60	0
30	CA	B	601	1/1	0.53	0.72	-	76,76,76,76	0
30	CA	b	601	1/1	0.36	1.06	-	77,77,77,77	0
22	CL	V	201	1/1	0.69	0.15	-	50,50,50,50	0
21	FE2	a	403	1/1	0.94	0.20	-	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.