



wwPDB X-ray Structure Validation Summary Report (i)

Feb 27, 2014 – 11:37 AM GMT

PDB ID : 2AXT
Title : Crystal Structure of Photosystem II from *Thermosynechococcus elongatus*
Authors : Loll, B.; Kern, J.; Saenger, W.; Zouni, A.; Biesiadka, J.
Deposited on : 2005-09-06
Resolution : 3.00 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>

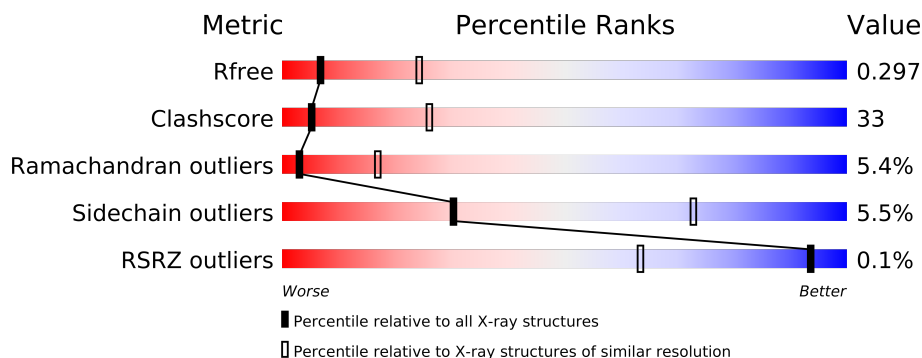
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.00 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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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	510	
2	b	510	
3	C	473	
3	c	473	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	

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Mol	Chain	Length	Quality of chain
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	247	
13	o	247	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	
16	v	137	
17	X	129	
17	x	129	
18	Z	62	
18	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
19	CA	K	56	-	X
21	BCT	D	353	-	X
22	UNK	C	474	-	X
22	UNK	C	478	-	X
22	UNK	C	479	-	X
22	UNK	C	481	-	X
22	UNK	C	483	-	X
22	UNK	C	486	-	X
22	UNK	C	489	-	X
22	UNK	c	5474	-	X
22	UNK	c	5475	-	X
22	UNK	c	5477	-	X
22	UNK	c	5478	-	X
22	UNK	c	5479	-	X
22	UNK	c	5484	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
22	UNK	c	5485	-	X
22	UNK	c	5486	-	X
22	UNK	c	5488	-	X
22	UNK	c	5489	-	X
22	UNK	c	5490	-	X
23	CLA	B	511	-	X
23	CLA	C	495	-	X
23	CLA	a	5560	-	X
23	CLA	a	5563	-	X
23	CLA	b	5511	-	X
23	CLA	b	5516	-	X
23	CLA	c	5503	-	X
26	PQ9	A	564	-	X
26	PQ9	a	5564	-	X
28	BCR	A	566	-	X
28	BCR	C	505	-	X
28	BCR	D	357	-	X
28	BCR	H	107	-	X
28	BCR	X	130	-	X
28	BCR	b	5529	-	X
28	BCR	c	5504	-	X
28	BCR	c	5505	-	X
28	BCR	d	5357	-	X
28	BCR	h	5107	-	X
28	BCR	x	5130	-	X
29	MGE	D	359	-	X
29	MGE	d	5359	-	X
33	LMT	A	569	-	X
33	LMT	T	217	-	X
33	LMT	a	5568	-	X
33	LMT	t	5217	-	X

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 48254 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
			2623	1718	432	458	15			
1	a	335	Total	C	N	O	S	0	0	0
			2623	1718	432	458	15			

- Molecule 2 is a protein called CP47 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	488	Total	C	N	O	S	0	0	0
			3800	2498	632	657	13			
2	b	488	Total	C	N	O	S	0	0	0
			3800	2498	632	657	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
			3421	2244	571	593	13			
3	c	447	Total	C	N	O	S	0	0	0
			3421	2244	571	593	13			

- Molecule 4 is a protein called photosystem II reaction center D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	340	Total	C	N	O	S	0	0	0
			2696	1789	436	459	12			
4	d	340	Total	C	N	O	S	0	0	0
			2696	1789	436	459	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	0	0
			646	424	101	121			
5	e	82	Total	C	N	O	0	0	0
			646	424	101	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			278	189	46	42	1			
6	f	35	Total	C	N	O	S	0	0	0
			278	189	46	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	0	0
			492	330	77	83	2			
7	h	64	Total	C	N	O	S	0	0	0
			492	330	77	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			
8	i	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			240	164	35	40	1			
9	j	34	Total	C	N	O	S	0	0	0
			240	164	35	40	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			289	201	42	46			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total	C	N	O	0	0	0
			289	201	42	46			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	0	0	0
			301	200	48	53			
11	l	37	Total	C	N	O	0	0	0
			301	200	48	53			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	36	Total	C	N	O	S	0	0	0
			276	181	41	53	1			
12	m	36	Total	C	N	O	S	0	0	0
			276	181	41	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
			1772	1113	295	360	4			
13	o	242	Total	C	N	O	S	0	0	0
			1772	1113	295	360	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			254	179	36	37	2			
14	t	30	Total	C	N	O	S	0	0	0
			254	179	36	37	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
			775	492	130	153			
15	u	98	Total	C	N	O	0	0	0
			775	492	130	153			

- 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 Unassigned subunits.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
17	X	104	Total	C	N	Ne	O	S	0	0	0
			687	442	110	3	131	1			
17	x	104	Total	C	N	Ne	O	S	0	0	0
			687	442	110	3	131	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Z	62	Total	C	N	O	S	0	0	0
			442	306	65	69	2			
18	z	62	Total	C	N	O	S	0	0	0
			442	306	65	69	2			

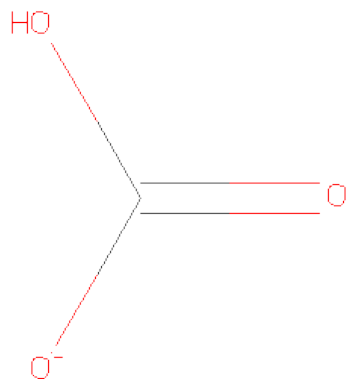
- Molecule 19 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	K	1	Total	Ca	0	0
			1	1		
19	k	1	Total	Ca	0	0
			1	1		

- Molecule 20 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 21 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).

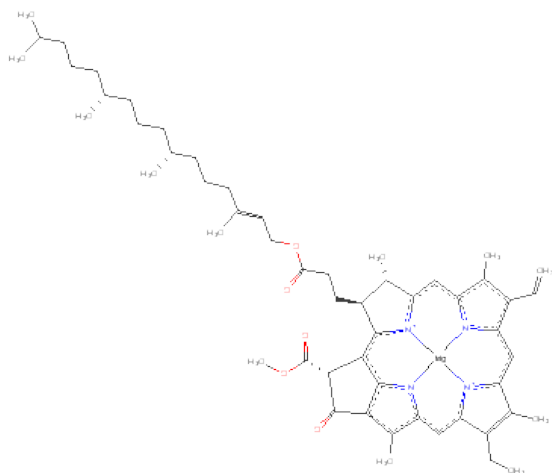


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	D	1	Total	C	O	0	0
			4	1	3		
21	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 22 is UNKNOWN (three-letter code: UNK) (formula: $C_4H_9NO_2$).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	C	17	Total	C	0	0
			152	152		
22	c	17	Total	C	0	0
			152	152		

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
23	D	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
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	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 56	C 46	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 60	C 50	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 46	C 36	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 47	C 37	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 51	C 41	Mg 1	N 4	O 5	0	0
23	C	1	Total 50	C 40	Mg 1	N 4	O 5	0	0

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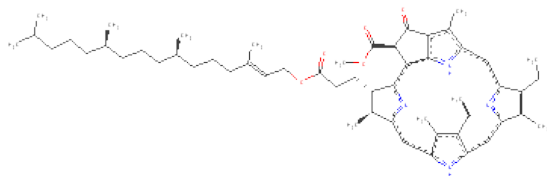
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
23	d	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
23	b	1	Total 41	C 33	Mg 1	N 4	O 3	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 56	C 46	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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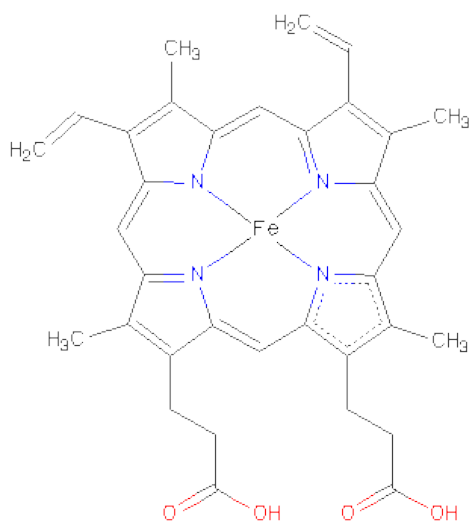
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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



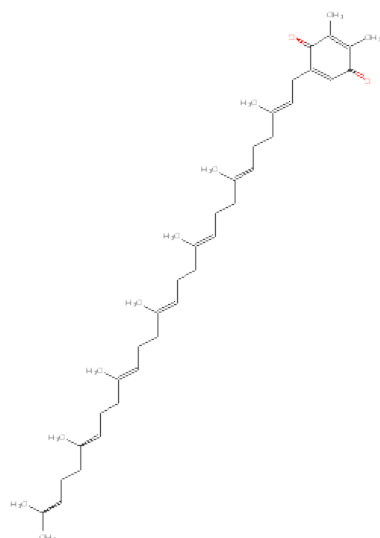
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

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



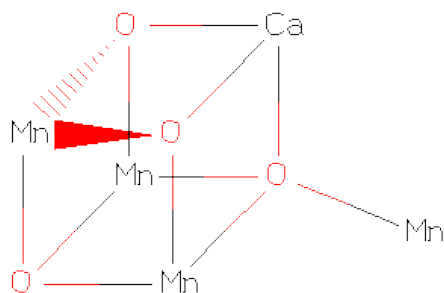
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
25	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
25	f	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
25	v	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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).



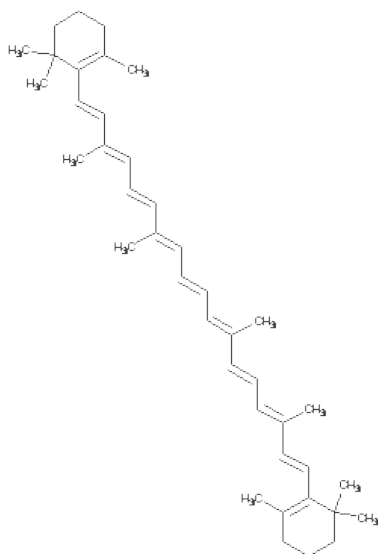
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	D	1	Total	C	O	0	0
			30	28	2		
26	A	1	Total	C	O	0	0
			30	28	2		
26	d	1	Total	C	O	0	0
			30	28	2		
26	a	1	Total	C	O	0	0
			30	28	2		

- Molecule 27 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn₄O₄).



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

- Molecule 28 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



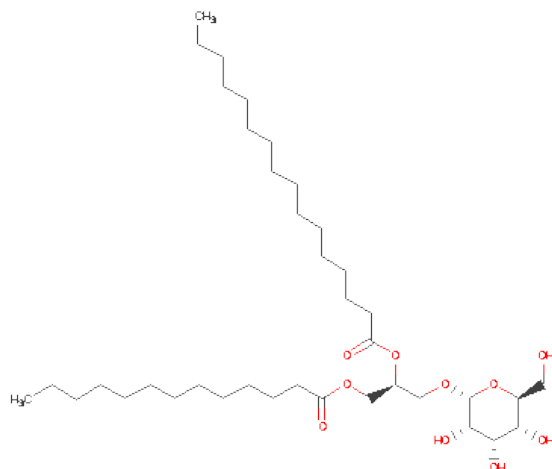
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	1	Total	C	0	0
			40	40		
28	B	1	Total	C	0	0
			40	40		

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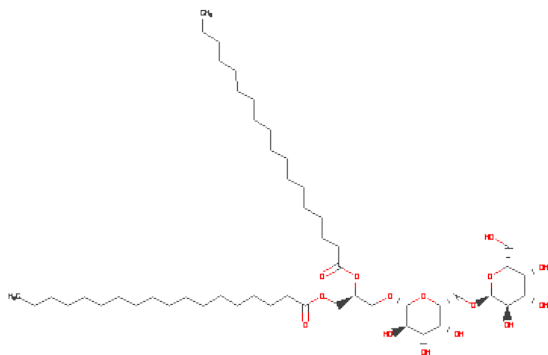
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	t	1	Total C 40 40	0	0
28	B	1	Total C 40 40	0	0
28	B	1	Total C 40 40	0	0
28	H	1	Total C 40 40	0	0
28	D	1	Total C 40 40	0	0
28	X	1	Total C 40 40	0	0
28	C	1	Total C 40 40	0	0
28	C	1	Total C 40 40	0	0
28	C	1	Total C 40 40	0	0
28	a	1	Total C 40 40	0	0
28	b	1	Total C 40 40	0	0
28	T	1	Total C 40 40	0	0
28	b	1	Total C 40 40	0	0
28	b	1	Total C 40 40	0	0
28	h	1	Total C 40 40	0	0
28	d	1	Total C 40 40	0	0
28	x	1	Total C 40 40	0	0
28	c	1	Total C 40 40	0	0
28	c	1	Total C 40 40	0	0
28	c	1	Total C 40 40	0	0

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



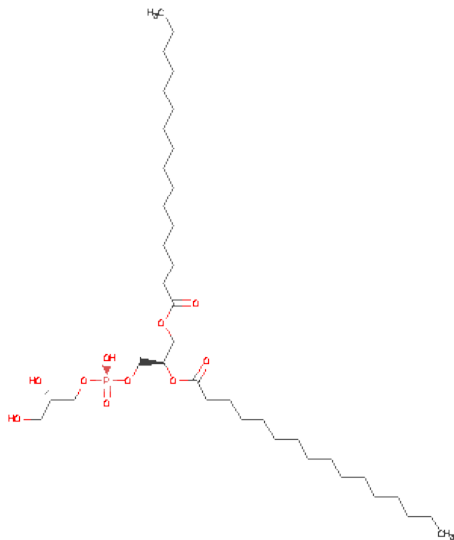
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	I	1	Total	C	O	0	0
			48	38	10		
29	D	1	Total	C	O	0	0
			47	37	10		
29	D	1	Total	C	O	0	0
			41	31	10		
29	L	1	Total	C	O	0	0
			48	38	10		
29	D	1	Total	C	O	0	0
			48	38	10		
29	B	1	Total	C	O	0	0
			48	38	10		
29	i	1	Total	C	O	0	0
			48	38	10		
29	d	1	Total	C	O	0	0
			47	37	10		
29	d	1	Total	C	O	0	0
			41	31	10		
29	l	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		

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



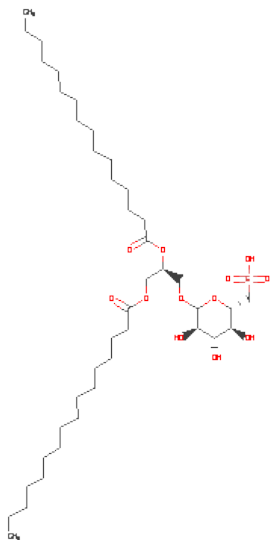
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	C	1	Total	C	O	0	0
			53	38	15		
30	C	1	Total	C	O	0	0
			47	32	15		
30	C	1	Total	C	O	0	0
			57	42	15		
30	H	1	Total	C	O	0	0
			54	39	15		
30	c	1	Total	C	O	0	0
			53	38	15		
30	c	1	Total	C	O	0	0
			47	32	15		
30	c	1	Total	C	O	0	0
			57	42	15		
30	h	1	Total	C	O	0	0
			54	39	15		

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			39	28	10	1		
31	a	1	Total	C	O	P	0	0
			39	28	10	1		

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



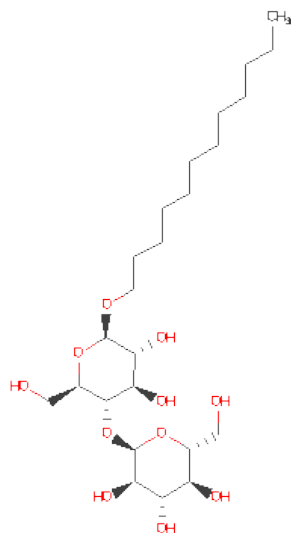
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	O	S	0	0
			54	41	12	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	a	1	Total	C	O	S	0	0
			26	13	12	1		
32	t	1	Total	C	O	S	0	0
			47	34	12	1		
32	d	1	Total	C	O	S	0	0
			54	41	12	1		
32	A	1	Total	C	O	S	0	0
			26	13	12	1		
32	L	1	Total	C	O	S	0	0
			47	34	12	1		

- Molecule 33 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).

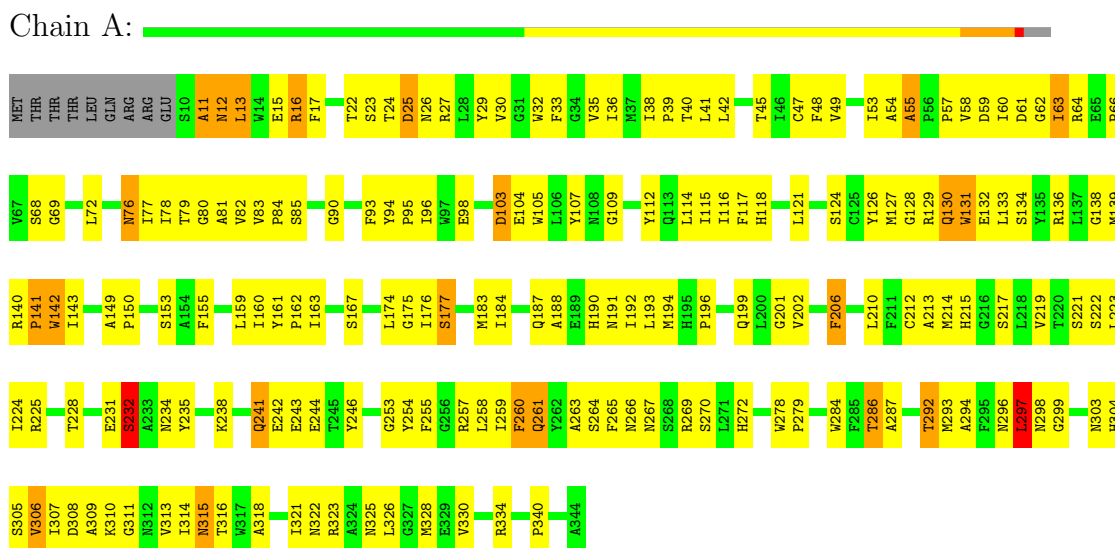


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	A	1	Total	C	O		0	0
			35	24	11			
33	m	1	Total	C	O		0	0
			35	24	11			
33	T	1	Total	C	O		0	0
			35	24	11			
33	a	1	Total	C	O		0	0
			35	24	11			
33	M	1	Total	C	O		0	0
			35	24	11			
33	t	1	Total	C	O		0	0
			35	24	11			

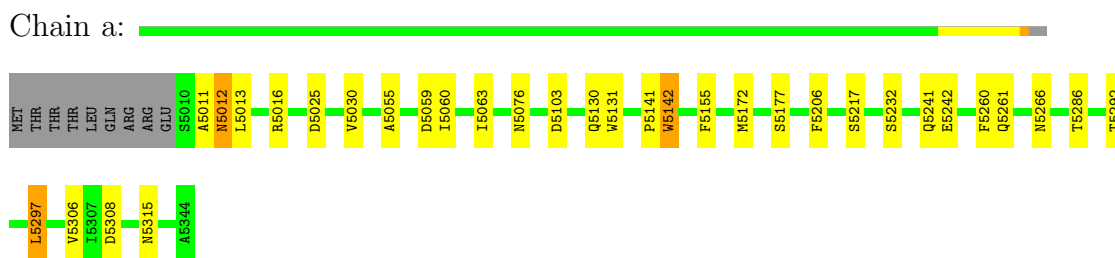
3 Residue-property plots

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.

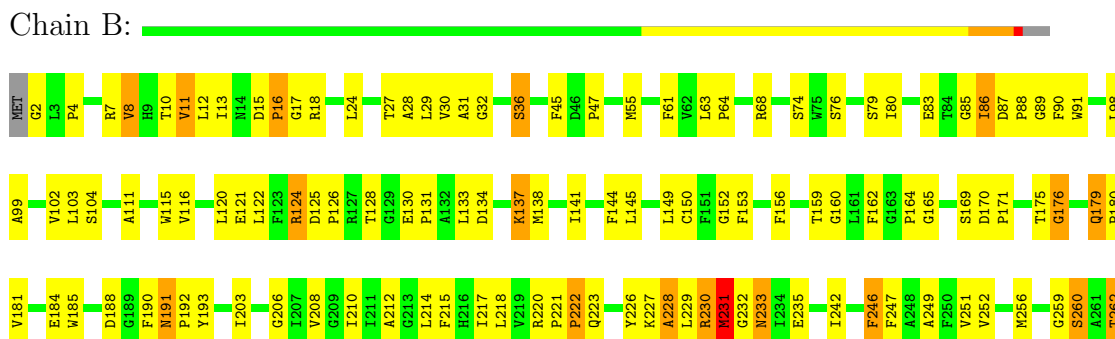
- Molecule 1: Photosystem Q(B) protein

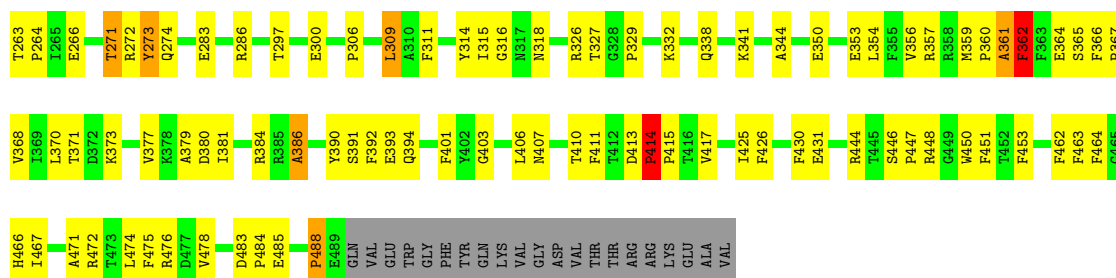


- Molecule 1: Photosystem Q(B) protein



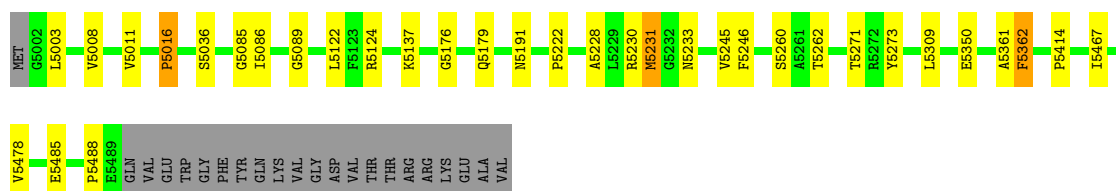
- Molecule 2: CP47 protein





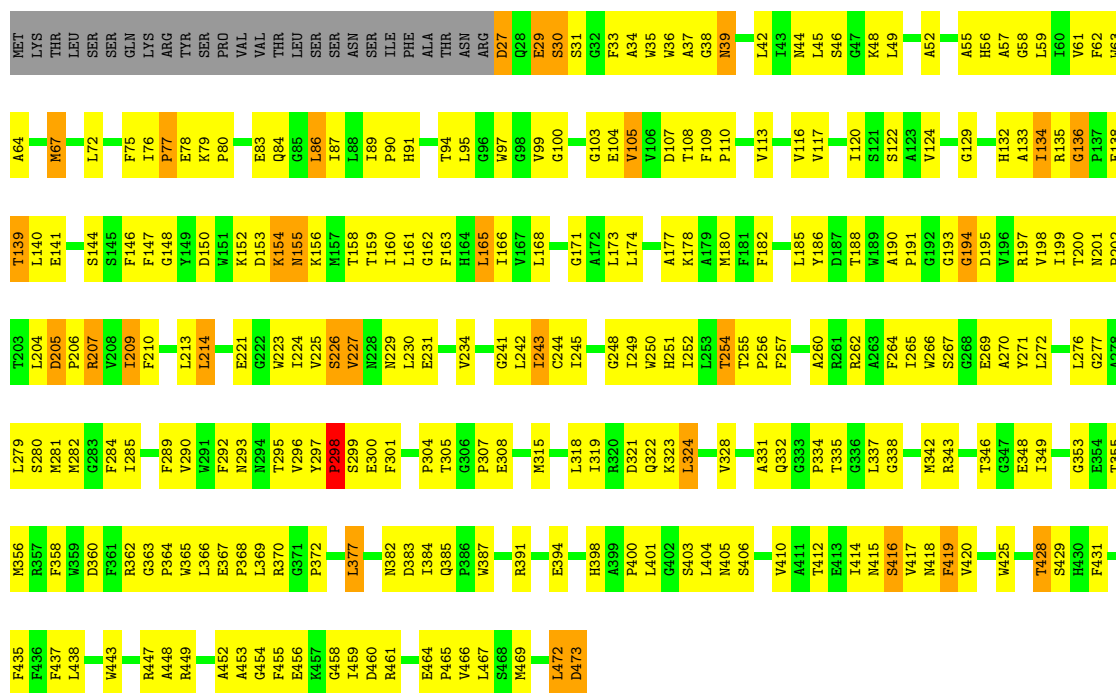
• Molecule 2: CP47 protein

Chain b:



• Molecule 3: photosystem II CP43 protein

Chain C:



• Molecule 3: photosystem II CP43 protein

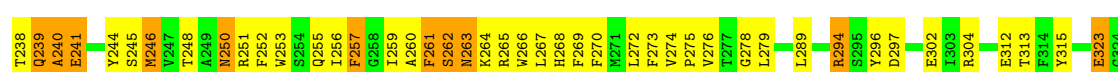
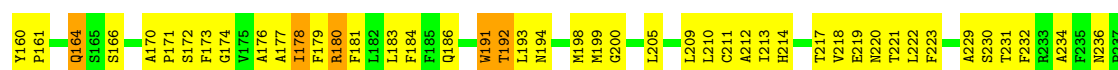
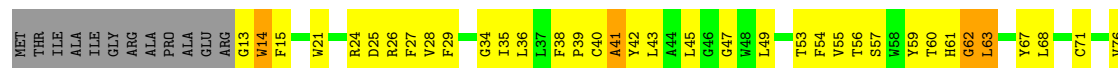
Chain c:





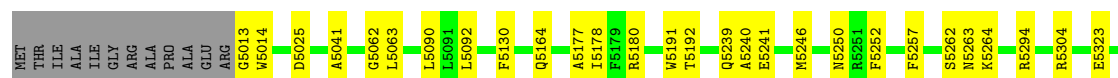
• Molecule 4: photosystem II reaction center D2 protein

Chain D:



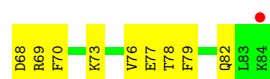
• Molecule 4: photosystem II reaction center D2 protein

Chain d:



• Molecule 5: Cytochrome b559 alpha subunit

Chain E:



• Molecule 5: Cytochrome b559 alpha subunit

Chain e:



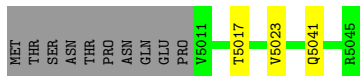
• Molecule 6: Cytochrome b559 beta subunit

Chain F:



- Molecule 6: Cytochrome b559 beta subunit

Chain f:



- Molecule 7: Photosystem II reaction center H protein

Chain H:



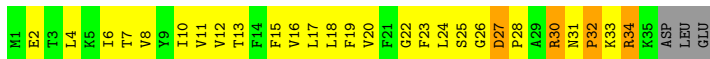
- Molecule 7: Photosystem II reaction center H protein

Chain h:



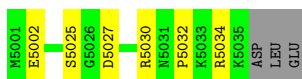
- Molecule 8: Photosystem II reaction center I protein

Chain I:



- Molecule 8: Photosystem II reaction center I protein

Chain i:



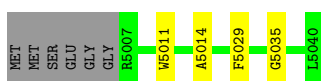
- Molecule 9: Photosystem II reaction center J protein

Chain J:



- Molecule 9: Photosystem II reaction center J protein

Chain j:



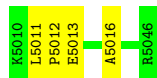
- Molecule 10: Photosystem II reaction center protein K

Chain K:



- Molecule 10: Photosystem II reaction center protein K

Chain k:



- Molecule 11: Photosystem II reaction center L protein

Chain L:



- Molecule 11: Photosystem II reaction center L protein

Chain l:



- Molecule 12: Photosystem II reaction center M protein

Chain M:



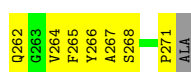
- Molecule 12: Photosystem II reaction center M protein

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 T protein

Chain T:



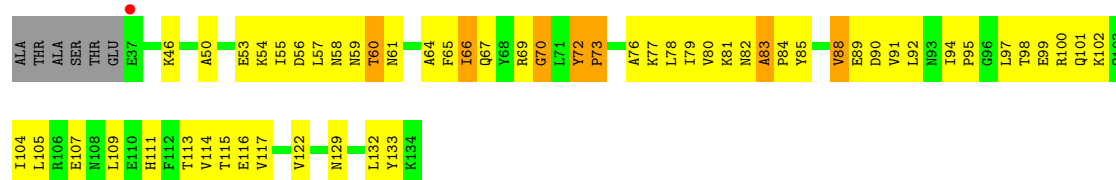
- Molecule 14: Photosystem II reaction center T protein

Chain t:



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



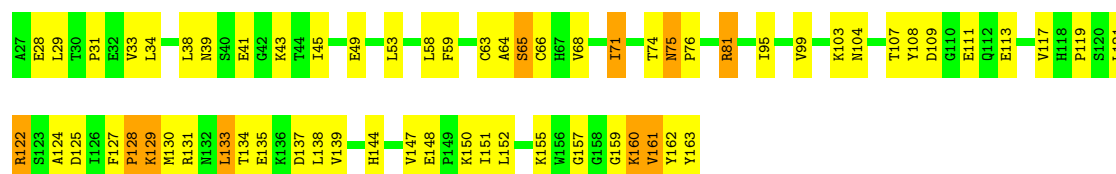
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



- Molecule 16: Cytochrome c-550

Chain V:



- Molecule 16: Cytochrome c-550

Chain v:



- Molecule 17: Unassigned subunits

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	127.69Å 225.40Å 306.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	75.6 (10.00-3.00) 81.7 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.98Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.234 , 0.286 0.250 , 0.297	Depositor DCC
R_{free} test set	1781 reflections (1.25%)	DCC
Wilson B-factor (Å ²)	78.2	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 155340 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	48254	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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, CA, LMT, CLA, BCT, FE2, PQ9, OEC, 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	0.62	0/2708	0.72	1/3694 (0.0%)
1	a	0.62	0/2708	0.74	2/3694 (0.1%)
2	B	0.57	0/3935	0.69	0/5366
2	b	0.56	0/3935	0.70	1/5366 (0.0%)
3	C	0.54	0/3533	0.71	0/4815
3	c	0.57	0/3533	0.72	0/4815
4	D	0.62	1/2791 (0.0%)	0.70	0/3806
4	d	0.60	1/2791 (0.0%)	0.71	0/3806
5	E	0.59	0/665	0.76	0/911
5	e	0.63	0/665	0.77	0/911
6	F	0.66	0/287	0.67	0/392
6	f	0.67	0/287	0.63	0/392
7	H	0.55	0/505	0.73	0/692
7	h	0.55	0/505	0.75	0/692
8	I	0.65	0/293	0.69	0/395
8	i	0.62	0/293	0.69	0/395
9	J	0.57	0/246	0.72	0/335
9	j	0.56	0/246	0.72	0/335
10	K	0.63	0/299	0.72	0/412
10	k	0.74	0/299	0.73	0/412
11	L	0.64	0/308	0.75	0/419
11	l	0.67	0/308	0.74	0/419
12	M	0.71	0/279	0.73	0/379
12	m	0.73	0/279	0.73	0/379
13	O	0.61	0/1803	0.78	2/2461 (0.1%)
13	o	0.60	0/1803	0.77	3/2461 (0.1%)
14	T	0.70	0/263	0.72	0/356
14	t	0.71	0/263	0.72	0/356
15	U	0.62	0/786	0.77	0/1066
15	u	0.60	0/786	0.76	0/1066
16	V	0.58	0/1085	0.71	0/1473
16	v	0.60	0/1085	0.71	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
18	Z	0.66	0/451	0.67	0/620
18	z	0.74	0/451	0.70	0/620
All	All	0.60	2/40474 (0.0%)	0.72	9/55184 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	b	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	5013	GLY	N-CA	5.43	1.54	1.46
4	D	13	GLY	N-CA	5.12	1.53	1.46

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	271	PRO	CA-C-O	7.17	137.40	120.20
1	a	5297	LEU	N-CA-C	-5.78	95.40	111.00
1	A	297	LEU	N-CA-C	-5.56	96.00	111.00
13	o	5271	PRO	CA-C-O	5.23	132.76	120.20
1	a	5142	TRP	N-CA-C	5.22	125.09	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	273	TYR	Sidechain
2	b	5273	TYR	Sidechain

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	2623	0	2517	223	0
1	a	2623	0	2517	0	0
2	B	3800	0	3637	261	0
2	b	3800	0	3637	0	0
3	C	3421	0	3326	301	0
3	c	3421	0	3326	0	0
4	D	2696	0	2591	237	0
4	d	2696	0	2591	0	0
5	E	646	0	616	52	0
5	e	646	0	616	0	0
6	F	278	0	279	30	0
6	f	278	0	279	0	0
7	H	492	0	495	48	0
7	h	492	0	495	0	0
8	I	286	0	308	31	0
8	i	286	0	305	0	0
9	J	240	0	242	26	0
9	j	240	0	242	0	0
10	K	289	0	294	48	0
10	k	289	0	294	0	0
11	L	301	0	309	24	0
11	l	301	0	306	0	0
12	M	276	0	288	18	0
12	m	276	0	285	0	0
13	O	1772	0	1664	155	0
13	o	1772	0	1664	0	0
14	T	254	0	257	26	0
14	t	254	0	254	0	0
15	U	775	0	771	60	0
15	u	775	0	771	0	0
16	V	1064	0	1072	65	0
16	v	1064	0	1072	0	0
17	X	687	0	268	63	0
17	x	687	0	268	0	0
18	Z	442	0	460	37	0
18	z	442	0	457	0	0
19	K	1	0	0	0	0
19	k	1	0	0	0	0
20	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	a	1	0	0	0	0
21	D	4	0	0	0	0
21	d	4	0	0	0	0
22	C	152	0	17	2	0
22	c	152	0	17	0	0
23	A	250	0	265	15	0
23	B	1007	0	1088	74	0
23	C	774	0	783	51	0
23	D	115	0	111	8	0
23	a	250	0	265	0	0
23	b	1007	0	1088	0	0
23	c	774	0	783	0	0
23	d	115	0	111	0	0
24	A	128	0	148	12	0
24	a	128	0	148	0	0
25	F	43	0	30	3	0
25	V	43	0	30	2	0
25	f	43	0	30	0	0
25	v	43	0	30	0	0
26	A	30	0	37	2	0
26	D	30	0	37	7	0
26	a	30	0	37	0	0
26	d	30	0	37	0	0
27	A	5	0	0	0	0
27	a	5	0	0	0	0
28	A	40	0	56	1	0
28	B	120	0	168	6	0
28	C	120	0	168	20	0
28	D	40	0	56	4	0
28	H	40	0	56	3	0
28	T	40	0	56	5	0
28	X	40	0	56	9	0
28	a	40	0	56	0	0
28	b	120	0	168	0	0
28	c	120	0	168	0	0
28	d	40	0	56	0	0
28	h	40	0	56	0	0
28	t	40	0	56	0	0
28	x	40	0	56	0	0
29	B	48	0	72	1	0
29	D	136	0	194	10	0
29	I	48	0	72	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	L	48	0	72	2	0
29	b	48	0	72	0	0
29	d	136	0	194	0	0
29	i	48	0	72	0	0
29	l	48	0	72	0	0
30	C	157	0	188	18	0
30	H	54	0	66	3	0
30	c	157	0	188	0	0
30	h	54	0	66	0	0
31	A	39	0	51	4	0
31	a	39	0	51	0	0
32	A	80	0	92	0	0
32	L	47	0	60	0	0
32	a	26	0	15	0	0
32	d	54	0	77	0	0
32	t	47	0	60	0	0
33	A	35	0	46	0	0
33	M	35	0	46	0	0
33	T	35	0	46	3	0
33	a	35	0	46	0	0
33	m	35	0	46	0	0
33	t	35	0	46	0	0
All	All	48254	0	47107	1544	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 33.

The worst 5 of 1544 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:X:126:UNK:NE	17:X:126:UNK:CD	1.46	1.53
17:X:126:UNK:CZ	17:X:126:UNK:NE	1.33	1.43
17:X:6:UNK:NE2	17:X:6:UNK:CD	1.33	1.42
17:X:26:UNK:NE2	17:X:26:UNK:CD	1.33	1.41
1:A:76:ASN:HD21	1:A:79:THR:HG23	1.13	1.14

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%)	279 (84%)	39 (12%)	15 (4%)	4	22
1	a	333/344 (97%)	278 (84%)	38 (11%)	17 (5%)	3	18
2	B	486/510 (95%)	407 (84%)	60 (12%)	19 (4%)	5	26
2	b	486/510 (95%)	413 (85%)	56 (12%)	17 (4%)	6	30
3	C	445/473 (94%)	340 (76%)	80 (18%)	25 (6%)	3	16
3	c	445/473 (94%)	342 (77%)	77 (17%)	26 (6%)	3	15
4	D	338/352 (96%)	272 (80%)	50 (15%)	16 (5%)	4	21
4	d	338/352 (96%)	272 (80%)	52 (15%)	14 (4%)	4	24
5	E	80/84 (95%)	60 (75%)	14 (18%)	6 (8%)	2	8
5	e	80/84 (95%)	59 (74%)	15 (19%)	6 (8%)	2	8
6	F	33/45 (73%)	28 (85%)	3 (9%)	2 (6%)	2	14
6	f	33/45 (73%)	28 (85%)	3 (9%)	2 (6%)	2	14
7	H	62/66 (94%)	45 (73%)	11 (18%)	6 (10%)	1	4
7	h	62/66 (94%)	44 (71%)	12 (19%)	6 (10%)	1	4
8	I	33/38 (87%)	22 (67%)	10 (30%)	1 (3%)	7	34
8	i	33/38 (87%)	22 (67%)	10 (30%)	1 (3%)	7	34
9	J	32/40 (80%)	27 (84%)	2 (6%)	3 (9%)	1	5
9	j	32/40 (80%)	25 (78%)	4 (12%)	3 (9%)	1	5
10	K	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	3	16
10	k	35/37 (95%)	28 (80%)	4 (11%)	3 (9%)	1	5
11	L	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	3	16
11	l	35/37 (95%)	28 (80%)	4 (11%)	3 (9%)	1	5
12	M	34/36 (94%)	26 (76%)	6 (18%)	2 (6%)	2	14
12	m	34/36 (94%)	28 (82%)	4 (12%)	2 (6%)	2	14
13	O	240/247 (97%)	185 (77%)	38 (16%)	17 (7%)	2	9
13	o	240/247 (97%)	184 (77%)	39 (16%)	17 (7%)	2	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	T	28/32 (88%)	24 (86%)	4 (14%)	0	100	100
14	t	28/32 (88%)	26 (93%)	2 (7%)	0	100	100
15	U	96/104 (92%)	71 (74%)	18 (19%)	7 (7%)	2	8
15	u	96/104 (92%)	68 (71%)	21 (22%)	7 (7%)	2	8
16	V	135/137 (98%)	110 (82%)	18 (13%)	7 (5%)	3	18
16	v	135/137 (98%)	110 (82%)	18 (13%)	7 (5%)	3	18
18	Z	60/62 (97%)	47 (78%)	9 (15%)	4 (7%)	2	10
18	z	60/62 (97%)	46 (77%)	10 (17%)	4 (7%)	2	10
All	All	5010/5288 (95%)	4001 (80%)	740 (15%)	269 (5%)	3	17

5 of 269 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ALA
1	A	63	ILE
1	A	141	PRO
1	A	142	TRP
1	A	315	ASN

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	269/280 (96%)	251 (93%)	18 (7%)	23	64
1	a	269/280 (96%)	252 (94%)	17 (6%)	25	66
2	B	378/407 (93%)	361 (96%)	17 (4%)	38	81
2	b	378/407 (93%)	360 (95%)	18 (5%)	35	79
3	C	341/374 (91%)	320 (94%)	21 (6%)	26	67
3	c	341/374 (91%)	320 (94%)	21 (6%)	26	67
4	D	273/283 (96%)	259 (95%)	14 (5%)	33	76
4	d	273/283 (96%)	258 (94%)	15 (6%)	30	73
5	E	68/73 (93%)	65 (96%)	3 (4%)	39	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	68/73 (93%)	66 (97%)	2 (3%)	55	90
6	F	27/39 (69%)	26 (96%)	1 (4%)	45	86
6	f	27/39 (69%)	26 (96%)	1 (4%)	45	86
7	H	50/55 (91%)	42 (84%)	8 (16%)	3	17
7	h	50/55 (91%)	43 (86%)	7 (14%)	5	23
8	I	32/35 (91%)	27 (84%)	5 (16%)	4	18
8	i	32/35 (91%)	27 (84%)	5 (16%)	4	18
9	J	22/28 (79%)	21 (96%)	1 (4%)	38	81
9	j	22/28 (79%)	21 (96%)	1 (4%)	38	81
10	K	29/30 (97%)	28 (97%)	1 (3%)	49	88
10	k	29/30 (97%)	28 (97%)	1 (3%)	49	88
11	L	34/35 (97%)	31 (91%)	3 (9%)	14	48
11	l	34/35 (97%)	31 (91%)	3 (9%)	14	48
12	M	32/33 (97%)	32 (100%)	0	100	100
12	m	32/33 (97%)	32 (100%)	0	100	100
13	O	181/208 (87%)	171 (94%)	10 (6%)	30	73
13	o	181/208 (87%)	172 (95%)	9 (5%)	34	77
14	T	26/29 (90%)	25 (96%)	1 (4%)	44	85
14	t	26/29 (90%)	25 (96%)	1 (4%)	44	85
15	U	83/89 (93%)	80 (96%)	3 (4%)	47	86
15	u	83/89 (93%)	80 (96%)	3 (4%)	47	86
16	V	117/117 (100%)	113 (97%)	4 (3%)	49	88
16	v	117/117 (100%)	111 (95%)	6 (5%)	33	76
18	Z	43/52 (83%)	42 (98%)	1 (2%)	63	93
18	z	43/52 (83%)	42 (98%)	1 (2%)	63	93
All	All	4010/4334 (92%)	3788 (94%)	222 (6%)	30	73

5 of 222 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	O	216	PHE
1	a	5286	THR
13	o	5106	GLN

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Mol	Chain	Res	Type
15	U	46	LYS
1	a	5013	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
13	O	130	GLN
1	a	5165	GLN
13	o	5106	GLN
15	U	108	ASN
1	a	5012	ASN

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 180 ligands modelled in this entry, 34 are unknown and 4 are monoatomic - leaving 142 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	$\# Z > 2$
32	SQD	A	5212	-	24,26,54	3.70	13 (54%)	33,37,65	3.01	10 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	A	558	1	73,73,73	1.44	10 (13%)	95,113,113	1.56	19 (20%)
23	CLA	A	559	-	73,73,73	1.32	9 (12%)	95,113,113	1.45	17 (17%)
23	CLA	A	560	-	73,73,73	1.40	10 (13%)	95,113,113	1.53	19 (20%)
24	PHO	A	561	-	69,69,69	1.75	9 (13%)	91,99,99	1.55	18 (19%)
24	PHO	A	562	-	69,69,69	2.09	7 (10%)	91,99,99	1.59	17 (18%)
23	CLA	A	563	-	62,63,73	1.59	13 (20%)	81,101,113	1.58	18 (22%)
26	PQ9	A	564	-	30,30,45	0.96	2 (6%)	37,39,57	1.60	8 (21%)
27	OEC	A	565	1,3	0,0,13	0.00	-	0,0,27	0.00	-
28	BCR	A	566	-	41,41,41	1.55	7 (17%)	56,56,56	2.06	21 (37%)
31	LHG	A	567	-	38,38,48	1.81	5 (13%)	44,44,54	1.42	4 (9%)
32	SQD	A	568	-	54,54,54	2.81	28 (51%)	65,65,65	2.79	18 (27%)
33	LMT	A	569	-	36,36,36	1.47	6 (16%)	47,47,47	1.08	1 (2%)
23	CLA	B	511	-	48,49,73	2.09	13 (27%)	64,84,113	1.56	12 (18%)
23	CLA	B	512	2	73,73,73	1.47	9 (12%)	95,113,113	1.50	18 (18%)
23	CLA	B	513	2	73,73,73	1.55	13 (17%)	95,113,113	1.58	18 (18%)
23	CLA	B	514	2	73,73,73	1.57	11 (15%)	95,113,113	1.50	18 (18%)
23	CLA	B	515	-	73,73,73	1.49	12 (16%)	95,113,113	1.65	21 (22%)
23	CLA	B	516	-	73,73,73	1.54	10 (13%)	95,113,113	1.52	19 (20%)
23	CLA	B	517	-	73,73,73	1.55	12 (16%)	95,113,113	1.66	23 (24%)
23	CLA	B	518	2	73,73,73	1.56	14 (19%)	95,113,113	1.56	20 (21%)
23	CLA	B	519	-	73,73,73	1.64	12 (16%)	95,113,113	1.49	19 (20%)
23	CLA	B	520	-	73,73,73	1.51	13 (17%)	95,113,113	1.48	19 (20%)
23	CLA	B	521	2	73,73,73	1.52	13 (17%)	95,113,113	1.55	19 (20%)
23	CLA	B	522	-	73,73,73	1.57	13 (17%)	95,113,113	1.52	16 (16%)
23	CLA	B	523	-	73,73,73	1.53	12 (16%)	95,113,113	1.49	19 (20%)
23	CLA	B	524	2	64,64,73	2.20	13 (20%)	83,102,113	1.60	19 (22%)
23	CLA	B	525	-	73,73,73	1.59	12 (16%)	95,113,113	1.53	16 (16%)
23	CLA	B	526	-	73,73,73	1.66	16 (21%)	95,113,113	1.51	20 (21%)
28	BCR	B	527	-	41,41,41	1.70	8 (19%)	56,56,56	2.00	16 (28%)
28	BCR	B	528	-	41,41,41	1.82	7 (17%)	56,56,56	1.93	16 (28%)
28	BCR	B	529	-	41,41,41	1.79	8 (19%)	56,56,56	2.14	20 (35%)
29	MGE	B	530	-	48,48,48	1.16	6 (12%)	56,56,56	1.22	6 (10%)
23	CLA	C	491	3	73,73,73	1.45	10 (13%)	95,113,113	1.43	17 (17%)
23	CLA	C	492	3	67,68,73	1.59	13 (19%)	87,107,113	1.58	18 (20%)
23	CLA	C	493	3	73,73,73	1.57	11 (15%)	95,113,113	1.57	20 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	494	-	53,54,73	1.69	11 (20%)	71,90,113	1.82	18 (25%)
23	CLA	C	495	-	73,73,73	1.60	13 (17%)	95,113,113	1.63	20 (21%)
23	CLA	C	496	3	73,73,73	1.61	14 (19%)	95,113,113	1.53	19 (20%)
23	CLA	C	497	-	73,73,73	1.47	12 (16%)	95,113,113	1.53	21 (22%)
23	CLA	C	498	3	73,73,73	1.54	13 (17%)	95,113,113	1.54	18 (18%)
23	CLA	C	499	-	54,55,73	1.69	9 (16%)	72,91,113	1.79	20 (27%)
23	CLA	C	500	-	73,73,73	1.48	11 (15%)	95,113,113	1.45	19 (20%)
23	CLA	C	501	3	73,73,73	1.67	11 (15%)	95,113,113	1.51	19 (20%)
23	CLA	C	502	-	59,59,73	2.07	17 (28%)	77,96,113	1.70	19 (24%)
23	CLA	C	503	3	58,58,73	1.90	14 (24%)	75,95,113	1.58	15 (20%)
28	BCR	C	504	-	41,41,41	1.80	7 (17%)	56,56,56	2.14	23 (41%)
28	BCR	C	505	-	41,41,41	1.90	9 (21%)	56,56,56	2.05	18 (32%)
28	BCR	C	506	-	41,41,41	1.72	9 (21%)	56,56,56	2.14	21 (37%)
30	DGD	C	507	-	54,54,67	1.71	10 (18%)	68,68,81	1.52	7 (10%)
30	DGD	C	508	-	48,48,67	2.02	11 (22%)	62,62,81	1.75	11 (17%)
30	DGD	C	509	-	58,58,67	1.67	8 (13%)	72,72,81	1.43	7 (9%)
21	BCT	D	353	20	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	D	354	4	73,73,73	1.46	15 (20%)	95,113,113	1.62	17 (17%)
23	CLA	D	355	-	58,58,73	1.84	13 (22%)	75,95,113	1.61	17 (22%)
26	PQ9	D	356	-	30,30,45	0.93	1 (3%)	37,39,57	1.79	10 (27%)
28	BCR	D	357	-	41,41,41	1.91	9 (21%)	56,56,56	2.19	20 (35%)
29	MGE	D	358	-	47,47,48	1.26	6 (12%)	55,55,56	0.98	3 (5%)
29	MGE	D	359	-	41,41,48	2.09	6 (14%)	49,49,56	1.09	5 (10%)
29	MGE	D	360	-	48,48,48	0.90	3 (6%)	56,56,56	1.13	4 (7%)
25	HEM	F	51	5,6	49,50,50	3.39	28 (57%)	46,82,82	2.40	13 (28%)
28	BCR	H	107	-	41,41,41	2.03	7 (17%)	56,56,56	2.21	24 (42%)
30	DGD	H	208	-	55,55,67	1.72	11 (20%)	69,69,81	1.58	8 (11%)
29	MGE	I	201	-	48,48,48	1.07	6 (12%)	56,56,56	1.10	4 (7%)
29	MGE	L	210	-	48,48,48	0.94	3 (6%)	56,56,56	1.18	4 (7%)
32	SQD	L	5213	-	47,47,54	3.35	25 (53%)	58,58,65	2.90	14 (24%)
33	LMT	M	5216	-	36,36,36	1.40	7 (19%)	47,47,47	0.91	1 (2%)
33	LMT	T	217	-	36,36,36	1.36	4 (11%)	47,47,47	1.02	4 (8%)
28	BCR	T	5104	-	41,41,41	1.52	9 (21%)	56,56,56	2.23	23 (41%)
25	HEM	V	552	16	49,50,50	3.72	25 (51%)	46,82,82	2.31	14 (30%)
28	BCR	X	130	-	41,41,41	1.88	10 (24%)	56,56,56	2.47	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	SQD	a	212	-	24,26,54	4.07	14 (58%)	33,37,65	3.11	10 (30%)
23	CLA	a	5558	1	73,73,73	1.46	15 (20%)	95,113,113	1.49	19 (20%)
23	CLA	a	5559	-	73,73,73	1.45	11 (15%)	95,113,113	1.47	16 (16%)
23	CLA	a	5560	-	73,73,73	1.51	13 (17%)	95,113,113	1.50	18 (18%)
24	PHO	a	5561	-	69,69,69	1.89	10 (14%)	91,99,99	1.51	14 (15%)
24	PHO	a	5562	-	69,69,69	2.02	8 (11%)	91,99,99	1.56	16 (17%)
23	CLA	a	5563	-	62,63,73	1.71	14 (22%)	81,101,113	1.54	15 (18%)
26	PQ9	a	5564	-	30,30,45	1.01	1 (3%)	37,39,57	1.57	8 (21%)
27	OEC	a	5565	1,3	0,0,13	0.00	-	0,0,27	0.00	-
28	BCR	a	5566	-	41,41,41	1.62	7 (17%)	56,56,56	2.06	22 (39%)
31	LHG	a	5567	-	38,38,48	1.83	5 (13%)	44,44,54	1.38	4 (9%)
33	LMT	a	5568	-	36,36,36	1.40	6 (16%)	47,47,47	1.10	1 (2%)
23	CLA	b	5511	-	48,49,73	2.06	13 (27%)	64,84,113	1.57	14 (21%)
23	CLA	b	5512	2	73,73,73	1.39	10 (13%)	95,113,113	1.49	18 (18%)
23	CLA	b	5513	2	73,73,73	1.49	12 (16%)	95,113,113	1.58	23 (24%)
23	CLA	b	5514	2	73,73,73	1.52	12 (16%)	95,113,113	1.53	20 (21%)
23	CLA	b	5515	-	73,73,73	1.43	12 (16%)	95,113,113	1.60	22 (23%)
23	CLA	b	5516	-	73,73,73	1.56	12 (16%)	95,113,113	1.54	21 (22%)
23	CLA	b	5517	-	73,73,73	1.58	10 (13%)	95,113,113	1.59	20 (21%)
23	CLA	b	5518	2	73,73,73	1.61	11 (15%)	95,113,113	1.56	20 (21%)
23	CLA	b	5519	-	73,73,73	1.54	15 (20%)	95,113,113	1.51	21 (22%)
23	CLA	b	5520	-	73,73,73	1.52	14 (19%)	95,113,113	1.48	18 (18%)
23	CLA	b	5521	2	73,73,73	1.45	7 (9%)	95,113,113	1.56	20 (21%)
23	CLA	b	5522	-	73,73,73	1.57	14 (19%)	95,113,113	1.50	14 (14%)
23	CLA	b	5523	-	73,73,73	1.48	10 (13%)	95,113,113	1.55	21 (22%)
23	CLA	b	5524	2	64,64,73	2.34	13 (20%)	83,102,113	1.56	17 (20%)
23	CLA	b	5525	-	73,73,73	1.48	13 (17%)	95,113,113	1.50	18 (18%)
23	CLA	b	5526	-	73,73,73	1.71	18 (24%)	95,113,113	1.56	20 (21%)
28	BCR	b	5527	-	41,41,41	1.50	8 (19%)	56,56,56	1.92	14 (25%)
28	BCR	b	5528	-	41,41,41	1.66	8 (19%)	56,56,56	1.96	17 (30%)
28	BCR	b	5529	-	41,41,41	1.65	9 (21%)	56,56,56	2.06	19 (33%)
29	MGE	b	5530	-	48,48,48	1.15	8 (16%)	56,56,56	1.15	6 (10%)
23	CLA	c	5491	3	73,73,73	1.65	12 (16%)	95,113,113	1.49	17 (17%)
23	CLA	c	5492	3	67,68,73	1.56	11 (16%)	87,107,113	1.60	19 (21%)
23	CLA	c	5493	3	73,73,73	1.65	13 (17%)	95,113,113	1.56	19 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	5494	-	53,54,73	1.63	11 (20%)	71,90,113	1.76	18 (25%)
23	CLA	c	5495	-	73,73,73	1.73	13 (17%)	95,113,113	1.62	23 (24%)
23	CLA	c	5496	-	73,73,73	1.58	16 (21%)	95,113,113	1.50	18 (18%)
23	CLA	c	5497	-	73,73,73	1.49	13 (17%)	95,113,113	1.49	20 (21%)
23	CLA	c	5498	3	73,73,73	1.72	15 (20%)	95,113,113	1.57	18 (18%)
23	CLA	c	5499	-	54,55,73	1.78	11 (20%)	72,91,113	1.76	19 (26%)
23	CLA	c	5500	-	73,73,73	1.48	13 (17%)	95,113,113	1.49	19 (20%)
23	CLA	c	5501	3	73,73,73	1.76	14 (19%)	95,113,113	1.50	19 (20%)
23	CLA	c	5502	-	59,59,73	2.12	18 (30%)	77,96,113	1.69	18 (23%)
23	CLA	c	5503	3	58,58,73	1.95	15 (25%)	75,95,113	1.60	16 (21%)
28	BCR	c	5504	-	41,41,41	2.04	7 (17%)	56,56,56	2.11	23 (41%)
28	BCR	c	5505	-	41,41,41	1.92	9 (21%)	56,56,56	2.06	18 (32%)
28	BCR	c	5506	-	41,41,41	1.92	9 (21%)	56,56,56	2.07	20 (35%)
30	DGD	c	5507	-	54,54,67	1.52	11 (20%)	68,68,81	1.51	6 (8%)
30	DGD	c	5508	-	48,48,67	1.72	10 (20%)	62,62,81	1.80	12 (19%)
30	DGD	c	5509	-	58,58,67	1.55	6 (10%)	72,72,81	1.41	5 (6%)
21	BCT	d	5353	20	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	d	5354	4	73,73,73	1.47	11 (15%)	95,113,113	1.61	20 (21%)
23	CLA	d	5355	-	58,58,73	1.83	15 (25%)	75,95,113	1.59	14 (18%)
26	PQ9	d	5356	-	30,30,45	0.85	1 (3%)	37,39,57	1.77	9 (24%)
28	BCR	d	5357	-	41,41,41	1.94	9 (21%)	56,56,56	2.25	21 (37%)
32	SQD	d	5358	-	54,54,54	2.96	26 (48%)	65,65,65	2.73	20 (30%)
29	MGE	d	5359	-	47,47,48	1.33	6 (12%)	55,55,56	0.98	3 (5%)
29	MGE	d	5360	-	41,41,48	2.00	6 (14%)	49,49,56	1.11	6 (12%)
29	MGE	d	5361	-	48,48,48	1.01	4 (8%)	56,56,56	1.07	3 (5%)
25	HEM	f	5051	5,6	49,50,50	3.40	27 (55%)	46,82,82	2.52	15 (32%)
28	BCR	h	5107	-	41,41,41	1.93	7 (17%)	56,56,56	2.21	25 (44%)
30	DGD	h	5208	-	55,55,67	1.93	9 (16%)	69,69,81	1.60	8 (11%)
29	MGE	i	5201	-	48,48,48	1.21	8 (16%)	56,56,56	1.11	5 (8%)
29	MGE	l	5210	-	48,48,48	0.87	3 (6%)	56,56,56	1.15	4 (7%)
33	LMT	m	216	-	36,36,36	1.42	7 (19%)	47,47,47	0.97	1 (2%)
28	BCR	t	104	-	41,41,41	1.63	9 (21%)	56,56,56	2.20	23 (41%)
32	SQD	t	213	-	47,47,54	3.33	24 (51%)	58,58,65	2.98	15 (25%)
33	LMT	t	5217	-	36,36,36	1.42	5 (13%)	47,47,47	1.00	3 (6%)
25	HEM	v	5552	16	49,50,50	4.00	26 (53%)	46,82,82	2.31	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	BCR	x	5130	-	41,41,41	1.93	9 (21%)	56,56,56	2.45	24 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	SQD	A	5212	-	-	0/19/39/69	0/1/1/1
23	CLA	A	558	1	-	0/37/135/135	0/0/9/9
23	CLA	A	559	-	-	0/37/135/135	0/0/9/9
23	CLA	A	560	-	-	0/37/135/135	0/0/9/9
24	PHO	A	561	-	3/3/17/22	0/48/103/103	0/0/6/6
24	PHO	A	562	-	3/3/17/22	0/48/103/103	0/0/6/6
23	CLA	A	563	-	-	0/25/123/135	0/0/9/9
26	PQ9	A	564	-	-	0/23/43/61	0/1/1/1
27	OEC	A	565	1,3	-	0/0/0/54	0/0/0/5
28	BCR	A	566	-	-	0/29/63/63	0/2/2/2
31	LHG	A	567	-	-	0/43/43/53	0/0/0/0
32	SQD	A	568	-	-	0/49/69/69	0/1/1/1
33	LMT	A	569	-	-	0/21/61/61	0/2/2/2
23	CLA	B	511	-	-	0/8/106/135	0/0/9/9
23	CLA	B	512	2	-	0/37/135/135	0/0/9/9
23	CLA	B	513	2	-	0/37/135/135	0/0/9/9
23	CLA	B	514	2	-	0/37/135/135	0/0/9/9
23	CLA	B	515	-	-	0/37/135/135	0/0/9/9
23	CLA	B	516	-	-	0/37/135/135	0/0/9/9
23	CLA	B	517	-	-	0/37/135/135	0/0/9/9
23	CLA	B	518	2	-	0/37/135/135	0/0/9/9
23	CLA	B	519	-	-	0/37/135/135	0/0/9/9
23	CLA	B	520	-	-	0/37/135/135	0/0/9/9
23	CLA	B	521	2	-	0/37/135/135	0/0/9/9
23	CLA	B	522	-	-	0/37/135/135	0/0/9/9
23	CLA	B	523	-	-	0/37/135/135	0/0/9/9
23	CLA	B	524	2	-	0/27/125/135	0/0/9/9
23	CLA	B	525	-	-	0/37/135/135	0/0/9/9
23	CLA	B	526	-	-	0/37/135/135	0/0/9/9
28	BCR	B	527	-	-	0/29/63/63	0/2/2/2
28	BCR	B	528	-	-	0/29/63/63	0/2/2/2
28	BCR	B	529	-	-	0/29/63/63	0/2/2/2
29	MGE	B	530	-	-	0/43/63/63	0/1/1/1
23	CLA	C	491	3	-	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	492	3	-	0/31/129/135	0/0/9/9
23	CLA	C	493	3	-	0/37/135/135	0/0/9/9
23	CLA	C	494	-	-	0/15/113/135	0/0/9/9
23	CLA	C	495	-	-	0/37/135/135	0/0/9/9
23	CLA	C	496	3	-	0/37/135/135	0/0/9/9
23	CLA	C	497	-	-	0/37/135/135	0/0/9/9
23	CLA	C	498	3	-	0/37/135/135	0/0/9/9
23	CLA	C	499	-	-	0/16/114/135	0/0/9/9
23	CLA	C	500	-	-	0/37/135/135	0/0/9/9
23	CLA	C	501	3	-	0/37/135/135	0/0/9/9
23	CLA	C	502	-	-	0/21/119/135	0/0/9/9
23	CLA	C	503	3	-	1/19/117/135	0/0/9/9
28	BCR	C	504	-	-	0/29/63/63	0/2/2/2
28	BCR	C	505	-	-	0/29/63/63	0/2/2/2
28	BCR	C	506	-	-	0/29/63/63	0/2/2/2
30	DGD	C	507	-	3/3/13/13	0/42/82/95	0/2/2/2
30	DGD	C	508	-	3/3/13/13	0/36/76/95	0/2/2/2
30	DGD	C	509	-	3/3/13/13	0/46/86/95	0/2/2/2
21	BCT	D	353	20	-	0/0/0/0	0/0/0/0
23	CLA	D	354	4	-	1/37/135/135	0/0/9/9
23	CLA	D	355	-	-	0/19/117/135	0/0/9/9
26	PQ9	D	356	-	-	0/23/43/61	0/1/1/1
28	BCR	D	357	-	-	0/29/63/63	0/2/2/2
29	MGE	D	358	-	-	0/42/62/63	0/1/1/1
29	MGE	D	359	-	-	0/36/56/63	0/1/1/1
29	MGE	D	360	-	-	0/43/63/63	0/1/1/1
25	HEM	F	51	5,6	-	0/14/114/114	0/0/8/8
28	BCR	H	107	-	-	0/29/63/63	0/2/2/2
30	DGD	H	208	-	3/3/13/13	0/43/83/95	0/2/2/2
29	MGE	I	201	-	-	0/43/63/63	0/1/1/1
29	MGE	L	210	-	-	0/43/63/63	0/1/1/1
32	SQD	L	5213	-	-	0/42/62/69	0/1/1/1
33	LMT	M	5216	-	-	0/21/61/61	0/2/2/2
33	LMT	T	217	-	-	0/21/61/61	0/2/2/2
28	BCR	T	5104	-	-	0/29/63/63	0/2/2/2
25	HEM	V	552	16	-	0/14/114/114	0/0/8/8
28	BCR	X	130	-	-	0/29/63/63	0/2/2/2
32	SQD	a	212	-	-	0/19/39/69	0/1/1/1
23	CLA	a	5558	1	-	0/37/135/135	0/0/9/9
23	CLA	a	5559	-	-	0/37/135/135	0/0/9/9
23	CLA	a	5560	-	-	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PHO	a	5561	-	3/3/17/22	0/48/103/103	0/0/6/6
24	PHO	a	5562	-	3/3/17/22	0/48/103/103	0/0/6/6
23	CLA	a	5563	-	-	0/25/123/135	0/0/9/9
26	PQ9	a	5564	-	-	0/23/43/61	0/1/1/1
27	OEC	a	5565	1,3	-	0/0/0/54	0/0/0/5
28	BCR	a	5566	-	-	0/29/63/63	0/2/2/2
31	LHG	a	5567	-	-	0/43/43/53	0/0/0/0
33	LMT	a	5568	-	-	0/21/61/61	0/2/2/2
23	CLA	b	5511	-	-	0/8/106/135	0/0/9/9
23	CLA	b	5512	2	-	0/37/135/135	0/0/9/9
23	CLA	b	5513	2	-	0/37/135/135	0/0/9/9
23	CLA	b	5514	2	-	0/37/135/135	0/0/9/9
23	CLA	b	5515	-	-	0/37/135/135	0/0/9/9
23	CLA	b	5516	-	-	0/37/135/135	0/0/9/9
23	CLA	b	5517	-	-	0/37/135/135	0/0/9/9
23	CLA	b	5518	2	-	0/37/135/135	0/0/9/9
23	CLA	b	5519	-	-	0/37/135/135	0/0/9/9
23	CLA	b	5520	-	-	0/37/135/135	0/0/9/9
23	CLA	b	5521	2	-	0/37/135/135	0/0/9/9
23	CLA	b	5522	-	-	0/37/135/135	0/0/9/9
23	CLA	b	5523	-	-	0/37/135/135	0/0/9/9
23	CLA	b	5524	2	-	0/27/125/135	0/0/9/9
23	CLA	b	5525	-	-	0/37/135/135	0/0/9/9
23	CLA	b	5526	-	-	0/37/135/135	0/0/9/9
28	BCR	b	5527	-	-	0/29/63/63	0/2/2/2
28	BCR	b	5528	-	-	0/29/63/63	0/2/2/2
28	BCR	b	5529	-	-	0/29/63/63	0/2/2/2
29	MGE	b	5530	-	-	0/43/63/63	0/1/1/1
23	CLA	c	5491	3	-	0/37/135/135	0/0/9/9
23	CLA	c	5492	3	-	0/31/129/135	0/0/9/9
23	CLA	c	5493	3	-	0/37/135/135	0/0/9/9
23	CLA	c	5494	-	-	0/15/113/135	0/0/9/9
23	CLA	c	5495	-	-	0/37/135/135	0/0/9/9
23	CLA	c	5496	-	-	0/37/135/135	0/0/9/9
23	CLA	c	5497	-	-	0/37/135/135	0/0/9/9
23	CLA	c	5498	3	-	0/37/135/135	0/0/9/9
23	CLA	c	5499	-	-	0/16/114/135	0/0/9/9
23	CLA	c	5500	-	-	0/37/135/135	0/0/9/9
23	CLA	c	5501	3	-	0/37/135/135	0/0/9/9
23	CLA	c	5502	-	-	0/21/119/135	0/0/9/9
23	CLA	c	5503	3	-	1/19/117/135	0/0/9/9
28	BCR	c	5504	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	BCR	c	5505	-	-	0/29/63/63	0/2/2/2
28	BCR	c	5506	-	-	0/29/63/63	0/2/2/2
30	DGD	c	5507	-	3/3/13/13	0/42/82/95	0/2/2/2
30	DGD	c	5508	-	3/3/13/13	0/36/76/95	0/2/2/2
30	DGD	c	5509	-	3/3/13/13	0/46/86/95	0/2/2/2
21	BCT	d	5353	20	-	0/0/0/0	0/0/0/0
23	CLA	d	5354	4	-	1/37/135/135	0/0/9/9
23	CLA	d	5355	-	-	0/19/117/135	0/0/9/9
26	PQ9	d	5356	-	-	0/23/43/61	0/1/1/1
28	BCR	d	5357	-	-	0/29/63/63	0/2/2/2
32	SQD	d	5358	-	-	0/49/69/69	0/1/1/1
29	MGE	d	5359	-	-	0/42/62/63	0/1/1/1
29	MGE	d	5360	-	-	0/36/56/63	0/1/1/1
29	MGE	d	5361	-	-	0/43/63/63	0/1/1/1
25	HEM	f	5051	5,6	-	0/14/114/114	0/0/8/8
28	BCR	h	5107	-	-	0/29/63/63	0/2/2/2
30	DGD	h	5208	-	3/3/13/13	0/43/83/95	0/2/2/2
29	MGE	i	5201	-	-	0/43/63/63	0/1/1/1
29	MGE	l	5210	-	-	0/43/63/63	0/1/1/1
33	LMT	m	216	-	-	0/21/61/61	0/2/2/2
28	BCR	t	104	-	-	0/29/63/63	0/2/2/2
32	SQD	t	213	-	-	0/42/62/69	0/1/1/1
33	LMT	t	5217	-	-	0/21/61/61	0/2/2/2
25	HEM	v	5552	16	-	0/14/114/114	0/0/8/8
28	BCR	x	5130	-	-	0/29/63/63	0/2/2/2

The worst 5 of 1519 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	V	552	HEM	C2D-C1D	-17.32	1.40	1.44
25	v	5552	HEM	C2D-C1D	-16.89	1.40	1.44
25	F	51	HEM	C2D-C1D	-14.18	1.41	1.44
32	d	5358	SQD	C6-C5	-13.55	1.38	1.52
25	v	5552	HEM	C2B-C1B	13.48	1.47	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	t	213	SQD	O6-C1-C2	9.46	120.22	108.18
32	L	5213	SQD	C5-C6-S	9.40	128.29	114.45
32	A	568	SQD	C5-C6-S	9.08	127.83	114.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	t	213	SQD	C5-C6-S	9.07	127.82	114.45
32	L	5213	SQD	O6-C1-C2	9.01	119.65	108.18

5 of 36 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	562	PHO	C2A
24	A	562	PHO	C13
24	A	562	PHO	C8
30	c	5507	DGD	C2D
30	c	5507	DGD	C5D

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	D	354	CLA	C1-C2-C3-C4
23	d	5354	CLA	C1-C2-C3-C4
23	C	503	CLA	C1-C2-C3-C4
23	c	5503	CLA	C1-C2-C3-C4

There are no ring outliers.

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%)	-0.39	0 100 100	40, 58, 78, 87	0
1	a	335/344 (97%)	-0.36	0 100 100	48, 65, 82, 98	0
2	B	488/510 (95%)	-0.36	0 100 100	40, 61, 78, 91	0
2	b	488/510 (95%)	-0.36	0 100 100	40, 62, 79, 91	0
3	C	447/473 (94%)	-0.34	0 100 100	46, 68, 80, 88	0
3	c	447/473 (94%)	-0.24	1 (0%) 93 54	53, 75, 86, 98	0
4	D	340/352 (96%)	-0.37	0 100 100	35, 58, 76, 89	0
4	d	340/352 (96%)	-0.38	0 100 100	42, 65, 83, 95	0
5	E	82/84 (97%)	-0.15	1 (1%) 75 20	55, 70, 86, 94	0
5	e	82/84 (97%)	-0.06	1 (1%) 75 20	65, 77, 90, 94	0
6	F	35/45 (77%)	-0.20	0 100 100	55, 67, 82, 85	0
6	f	35/45 (77%)	-0.11	0 100 100	67, 75, 87, 89	0
7	H	64/66 (96%)	-0.28	0 100 100	57, 72, 81, 87	0
7	h	64/66 (96%)	-0.17	0 100 100	62, 71, 81, 93	0
8	I	35/38 (92%)	-0.29	0 100 100	57, 65, 80, 88	0
8	i	35/38 (92%)	-0.23	0 100 100	62, 72, 86, 88	0
9	J	34/40 (85%)	-0.40	0 100 100	55, 68, 72, 74	0
9	j	34/40 (85%)	-0.30	0 100 100	68, 74, 79, 86	0
10	K	37/37 (100%)	-0.36	0 100 100	60, 68, 80, 87	0
10	k	37/37 (100%)	-0.29	0 100 100	76, 80, 93, 97	0
11	L	37/37 (100%)	-0.11	0 100 100	43, 61, 95, 100	0
11	l	37/37 (100%)	-0.21	1 (2%) 52 10	45, 57, 86, 91	0
12	M	36/36 (100%)	-0.35	0 100 100	52, 58, 89, 94	0
12	m	36/36 (100%)	-0.29	0 100 100	54, 60, 86, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	242/247 (97%)	-0.29	0 100 100	44, 65, 88, 101	0
13	o	242/247 (97%)	-0.24	1 (0%) 90 41	43, 71, 88, 97	0
14	T	30/32 (93%)	-0.26	0 100 100	47, 61, 91, 97	0
14	t	30/32 (93%)	-0.45	0 100 100	48, 60, 89, 93	0
15	U	98/104 (94%)	-0.25	1 (1%) 79 22	44, 60, 76, 83	0
15	u	98/104 (94%)	-0.34	0 100 100	52, 64, 74, 89	0
16	V	137/137 (100%)	-0.36	0 100 100	47, 60, 75, 84	0
16	v	137/137 (100%)	-0.20	0 100 100	54, 74, 87, 99	0
17	X	0/129	-	-	-	-
17	x	0/129	-	-	-	-
18	Z	62/62 (100%)	-0.19	0 100 100	67, 76, 93, 96	0
18	z	62/62 (100%)	-0.16	0 100 100	73, 87, 94, 97	0
All	All	5078/5546 (91%)	-0.31	6 (0%) 93 63	35, 66, 85, 101	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	l	5001	MET	3.9
5	E	84	LYS	3.2
13	o	5049	ASP	2.7
3	c	5029	GLU	2.5
15	U	37	GLU	2.3

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
22	UNK	c	5486	8/-	0.39	29.92	63,64,65,66	0
22	UNK	C	486	8/-	0.27	28.09	55,56,59,60	0
22	UNK	c	5484	5/-	0.76	12.72	69,69,70,72	0
22	UNK	c	5489	7/-	0.38	9.65	73,73,74,74	0
22	UNK	C	478	11/-	0.35	9.32	58,65,66,66	0
33	LMT	A	569	35/35	0.46	9.04	80,89,92,93	0
22	UNK	c	5485	5/-	0.44	8.96	68,69,69,70	0
28	BCR	H	107	40/40	0.34	7.10	77,83,88,89	0
33	LMT	a	5568	35/35	0.47	6.95	79,92,94,96	0
19	CA	K	56	1/1	0.14	6.16	119,119,119,119	0
33	LMT	t	5217	35/35	0.42	5.68	76,95,104,105	0
22	UNK	c	5479	11/-	0.33	5.47	76,77,77,77	0
22	UNK	c	5478	11/-	0.47	5.41	76,79,81,81	0
22	UNK	C	489	7/-	0.34	5.30	75,76,77,78	0
33	LMT	T	217	35/35	0.35	5.19	83,93,96,97	0
28	BCR	x	5130	40/40	0.48	5.07	77,81,85,86	0
22	UNK	c	5490	4/-	0.38	4.94	91,92,92,92	0
28	BCR	h	5107	40/40	0.35	4.89	74,79,82,83	0
26	PQ9	A	564	30/45	0.36	4.69	54,57,63,64	30
22	UNK	c	5474	15/-	0.26	4.43	39,50,56,56	0
23	CLA	B	511	41/65	0.34	4.20	88,90,92,98	0
22	UNK	C	483	13/-	0.29	4.12	61,68,78,78	0
23	CLA	b	5511	41/65	0.40	4.11	88,92,95,96	0
28	BCR	C	505	40/40	0.41	3.91	75,81,91,92	0
28	BCR	X	130	40/40	0.35	3.45	68,71,80,81	0
28	BCR	b	5529	40/40	0.41	3.37	69,72,74,74	0
22	UNK	c	5488	5/-	0.27	3.11	59,59,59,60	0
28	BCR	d	5357	40/40	0.37	3.09	61,72,86,88	0
28	BCR	D	357	40/40	0.28	3.05	61,66,78,80	0
28	BCR	c	5505	40/40	0.39	3.01	84,87,91,92	0
22	UNK	C	481	13/-	0.36	2.94	61,64,68,69	0
23	CLA	a	5560	65/65	0.22	2.76	62,68,100,101	0
26	PQ9	a	5564	30/45	0.28	2.69	51,55,62,62	30
29	MGE	d	5359	47/48	0.31	2.66	72,81,96,98	0
22	UNK	c	5475	12/-	0.42	2.66	74,78,84,84	0
22	UNK	C	474	15/-	0.22	2.65	26,37,40,40	0
22	UNK	c	5477	7/-	0.29	2.60	67,68,70,70	0
23	CLA	a	5563	55/65	0.34	2.57	59,65,102,103	0
28	BCR	c	5504	40/40	0.30	2.39	73,80,88,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
29	MGE	D	359	41/48	0.26	2.28	60,67,76,79	0
22	UNK	C	479	11/-	0.30	2.26	58,64,67,67	0
23	CLA	b	5516	65/65	0.28	2.20	62,66,84,86	0
23	CLA	c	5503	50/65	0.28	2.14	88,91,92,93	0
21	BCT	D	353	4/4	0.24	2.13	72,73,73,74	0
23	CLA	C	495	65/65	0.24	2.03	58,68,74,76	0
28	BCR	A	566	40/40	0.28	2.02	50,57,64,66	0
23	CLA	B	519	65/65	0.25	1.99	73,82,85,87	0
22	UNK	C	485	5/-	0.29	1.92	57,59,61,61	0
23	CLA	c	5501	65/65	0.26	1.91	82,91,94,95	0
23	CLA	b	5515	65/65	0.22	1.88	46,51,74,76	0
22	UNK	C	475	12/-	0.38	1.88	68,69,72,73	0
29	MGE	D	358	47/48	0.25	1.86	65,72,79,81	0
28	BCR	B	528	40/40	0.22	1.86	54,68,74,75	0
23	CLA	B	526	65/65	0.29	1.83	71,82,97,98	0
23	CLA	A	563	55/65	0.25	1.76	43,49,75,78	0
26	PQ9	D	356	30/45	0.24	1.76	49,67,80,83	0
32	SQD	A	568	54/54	0.33	1.75	76,82,90,90	0
30	DGD	C	507	53/66	0.26	1.73	55,66,86,88	0
33	LMT	m	216	35/35	0.29	1.69	62,87,89,91	0
23	CLA	c	5497	65/65	0.26	1.67	66,82,84,87	0
28	BCR	C	504	40/40	0.21	1.65	57,64,70,70	0
23	CLA	c	5498	65/65	0.27	1.62	81,90,93,93	0
33	LMT	M	5216	35/35	0.28	1.61	58,83,90,90	0
29	MGE	b	5530	48/48	0.18	1.54	59,64,71,73	0
22	UNK	C	482	13/-	0.23	1.53	64,66,67,67	0
22	UNK	c	5487	7/-	0.28	1.49	57,57,58,58	0
22	UNK	c	5476	9/-	0.30	1.49	58,60,62,62	0
24	PHO	a	5562	64/64	0.22	1.46	70,75,81,82	0
28	BCR	T	5104	40/40	0.23	1.42	67,71,78,79	0
23	CLA	B	512	65/65	0.25	1.41	68,75,78,79	0
23	CLA	B	515	65/65	0.21	1.41	55,66,71,72	0
28	BCR	t	104	40/40	0.21	1.40	65,72,84,85	0
23	CLA	D	355	50/65	0.22	1.38	63,65,68,70	0
28	BCR	b	5527	40/40	0.21	1.35	58,63,72,72	0
28	BCR	B	527	40/40	0.19	1.34	58,65,68,69	0
28	BCR	B	529	40/40	0.27	1.34	62,69,80,80	0
25	HEM	F	51	43/43	0.26	1.31	78,84,92,95	0
29	MGE	l	5210	48/48	0.22	1.29	59,69,78,81	0
28	BCR	c	5506	40/40	0.32	1.29	75,81,86,86	0
23	CLA	B	516	65/65	0.27	1.28	61,76,92,97	0
23	CLA	b	5512	65/65	0.24	1.28	68,72,75,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
29	MGE	d	5361	48/48	0.20	1.28	61,68,78,83	0
23	CLA	C	497	65/65	0.27	1.27	74,78,80,82	0
23	CLA	b	5513	65/65	0.21	1.25	54,61,84,90	0
31	LHG	A	567	39/49	0.22	1.25	57,73,79,81	0
23	CLA	C	501	65/65	0.24	1.21	70,78,83,85	0
23	CLA	c	5495	65/65	0.23	1.20	74,81,86,88	0
22	UNK	C	487	7/-	0.28	1.18	49,52,52,53	0
22	UNK	C	476	9/-	0.31	1.16	61,62,63,64	0
30	DGD	c	5509	57/66	0.28	1.16	67,72,77,78	0
22	UNK	C	477	7/-	0.17	1.14	47,49,51,51	0
23	CLA	d	5354	65/65	0.18	1.12	39,47,64,65	0
23	CLA	b	5519	65/65	0.22	1.11	70,75,80,81	0
28	BCR	a	5566	40/40	0.25	1.10	59,75,78,79	0
30	DGD	C	508	47/66	0.20	1.09	61,71,80,83	0
29	MGE	i	5201	48/48	0.28	1.08	67,83,88,90	0
23	CLA	b	5520	65/65	0.23	1.08	63,72,74,76	0
25	HEM	f	5051	43/43	0.28	1.06	80,84,97,101	0
30	DGD	H	208	54/66	0.21	1.04	61,69,75,76	0
23	CLA	B	522	65/65	0.23	1.04	54,65,75,77	0
32	SQD	t	213	47/54	0.31	1.03	61,95,116,117	0
30	DGD	c	5507	53/66	0.23	1.01	66,74,90,91	0
31	LHG	a	5567	39/49	0.28	1.00	65,68,74,80	0
32	SQD	L	5213	47/54	0.31	1.00	52,85,106,108	0
29	MGE	D	360	48/48	0.20	0.99	52,60,63,68	0
29	MGE	d	5360	41/48	0.22	0.94	68,72,78,80	0
23	CLA	B	520	65/65	0.24	0.93	62,67,76,79	0
23	CLA	c	5496	65/65	0.25	0.93	79,83,95,97	0
22	UNK	c	5483	13/-	0.29	0.93	71,75,80,82	0
32	SQD	a	212	26/54	0.29	0.91	82,94,101,103	0
23	CLA	A	560	65/65	0.20	0.90	49,57,86,88	0
25	HEM	V	552	43/43	0.19	0.88	37,54,58,59	0
22	UNK	C	484	5/-	0.30	0.83	47,51,52,53	0
29	MGE	L	210	48/48	0.22	0.83	59,68,73,75	0
22	UNK	c	5482	13/-	0.22	0.82	60,61,71,72	0
23	CLA	C	493	65/65	0.21	0.81	67,71,77,79	0
24	PHO	A	561	64/64	0.18	0.78	32,52,55,59	0
26	PQ9	d	5356	30/45	0.18	0.77	51,57,66,66	0
24	PHO	a	5561	64/64	0.18	0.75	51,55,66,68	0
23	CLA	C	503	50/65	0.27	0.75	83,86,88,94	0
23	CLA	C	498	65/65	0.21	0.70	64,74,98,101	0
22	UNK	c	5481	13/-	0.22	0.65	60,62,66,66	0
23	CLA	c	5500	65/65	0.21	0.65	64,69,82,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	DGD	h	5208	54/66	0.20	0.65	57,68,73,75	0
28	BCR	b	5528	40/40	0.18	0.62	61,64,72,73	0
23	CLA	C	496	65/65	0.24	0.62	71,78,88,89	0
23	CLA	d	5355	50/65	0.23	0.59	74,77,80,81	0
25	HEM	v	5552	43/43	0.19	0.58	65,67,70,70	0
32	SQD	A	5212	26/54	0.25	0.56	75,100,107,107	0
23	CLA	c	5502	51/65	0.26	0.53	93,96,97,98	0
23	CLA	B	525	65/65	0.21	0.51	67,84,91,92	0
32	SQD	d	5358	54/54	0.29	0.49	74,85,106,107	0
23	CLA	C	502	51/65	0.22	0.49	74,80,83,84	0
23	CLA	b	5526	65/65	0.30	0.46	66,71,92,95	0
23	CLA	b	5514	65/65	0.18	0.41	41,51,74,75	0
30	DGD	C	509	57/66	0.20	0.40	52,60,69,70	0
23	CLA	B	514	65/65	0.19	0.39	59,64,82,83	0
29	MGE	B	530	48/48	0.18	0.37	55,64,70,72	0
28	BCR	C	506	40/40	0.24	0.37	68,72,79,80	0
23	CLA	b	5522	65/65	0.19	0.37	60,66,75,76	0
23	CLA	c	5499	47/65	0.22	0.33	60,69,76,78	0
23	CLA	B	513	65/65	0.18	0.30	56,61,67,67	0
24	PHO	A	562	64/64	0.16	0.27	47,53,63,66	0
29	MGE	I	201	48/48	0.20	0.19	73,81,89,90	0
23	CLA	b	5517	65/65	0.16	0.15	54,58,66,71	0
23	CLA	b	5525	65/65	0.20	0.09	71,77,80,82	0
23	CLA	C	491	65/65	0.18	0.04	63,70,77,79	0
23	CLA	c	5493	65/65	0.22	0.02	67,81,86,86	0
23	CLA	B	521	65/65	0.18	0.02	58,63,66,68	0
23	CLA	C	499	47/65	0.17	0.01	57,60,66,69	0
27	OEC	a	5565	5/9	0.15	-0.03	63,64,71,87	0
30	DGD	c	5508	47/66	0.17	-0.06	66,76,82,84	0
23	CLA	a	5559	65/65	0.15	-0.11	42,49,60,60	0
23	CLA	A	559	65/65	0.15	-0.11	39,43,49,52	0
23	CLA	C	492	60/65	0.17	-0.14	53,58,76,77	0
23	CLA	B	524	56/65	0.18	-0.19	67,72,77,80	0
23	CLA	D	354	65/65	0.15	-0.22	35,43,63,66	0
23	CLA	B	518	65/65	0.18	-0.23	53,64,79,79	0
27	OEC	A	565	5/9	0.14	-0.24	62,63,65,66	0
23	CLA	b	5523	65/65	0.15	-0.25	45,52,74,75	0
23	CLA	b	5524	56/65	0.18	-0.26	63,68,89,91	0
23	CLA	B	523	65/65	0.16	-0.28	47,56,73,74	0
23	CLA	b	5518	65/65	0.17	-0.30	60,64,69,75	0
23	CLA	c	5491	65/65	0.17	-0.35	70,78,81,86	0
23	CLA	a	5558	65/65	0.15	-0.36	41,50,55,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	c	5494	46/65	0.17	-0.39	72,77,86,88	0
23	CLA	C	494	46/65	0.14	-0.40	59,66,68,72	0
23	CLA	c	5492	60/65	0.16	-0.40	57,61,83,84	0
23	CLA	C	500	65/65	0.15	-0.42	59,63,73,74	0
22	UNK	C	488	5/-	0.14	-0.46	41,45,47,47	0
23	CLA	B	517	65/65	0.14	-0.56	37,44,56,57	0
23	CLA	b	5521	65/65	0.16	-0.57	48,57,63,64	0
23	CLA	A	558	65/65	0.13	-0.69	41,46,50,51	0
22	UNK	C	490	4/-	0.11	-1.54	67,67,68,68	0
19	CA	k	5056	1/1	0.14	-1.62	119,119,119,119	0
21	BCT	d	5353	4/4	0.12	-2.37	75,75,76,77	0
20	FE2	a	5557	1/1	0.09	-3.13	75,75,75,75	0
20	FE2	A	557	1/1	0.05	-3.80	60,60,60,60	0
22	UNK	c	5480	7/-	0.26	-	65,66,66,67	0
22	UNK	C	480	7/-	0.22	-	35,36,38,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.