



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:13 PM GMT

PDB ID : 1S5L
Title : Architecture of the photosynthetic oxygen evolving center
Authors : Ferreira, K.N.; Iverson, T.M.; Maghlaoui, K.; Barber, J.; Iwata, S.
Deposited on : 2004-01-21
Resolution : 3.50 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (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
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

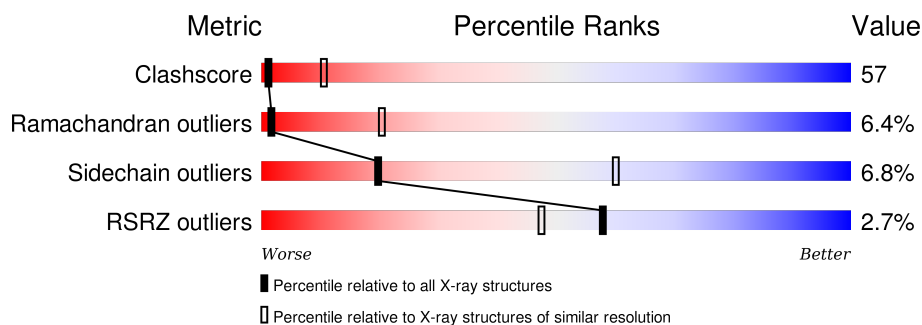
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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))
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div>3%</div> <div>28% 57% 11%</div> <div>• •</div> </div>
1	a	344	<div> <div>%</div> <div>84% 13%</div> <div>•</div> </div>
2	B	510	<div> <div>3%</div> <div>30% 56% 6% 7%</div> <div></div> </div>
2	b	510	<div> <div>2%</div> <div>84% 9% 7%</div> <div></div> </div>
3	C	473	<div> <div>2%</div> <div>22% 57% 9% 11%</div> <div>•</div> </div>
3	c	473	<div> <div>2%</div> <div>79% 9% 11%</div> <div>•</div> </div>
4	D	352	<div> <div>2%</div> <div>30% 59% 7%</div> <div>•</div> </div>

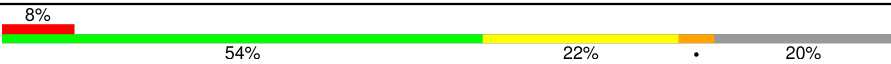

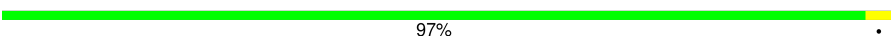
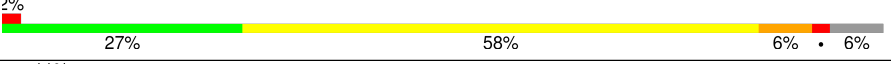
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
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	246	
13	o	246	
14	T	32	
14	t	32	
15	U	134	
15	u	134	
16	V	137	
16	v	137	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
17	X	50	
17	x	50	
18	N	37	
18	n	37	
19	Z	62	
19	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	348	X	-	-	-
23	CLA	A	349	X	-	-	-
23	CLA	A	350	X	-	-	-
23	CLA	A	352	X	-	-	-
23	CLA	B	511	X	-	-	X
23	CLA	B	512	X	-	-	-
23	CLA	B	513	X	-	-	-
23	CLA	B	514	X	-	-	-
23	CLA	B	515	X	-	-	-
23	CLA	B	516	X	-	-	X
23	CLA	B	517	X	-	-	-
23	CLA	B	518	X	-	-	-
23	CLA	B	519	X	-	-	X
23	CLA	B	520	X	-	-	-
23	CLA	B	521	X	-	-	-
23	CLA	B	522	X	-	-	-
23	CLA	B	523	X	-	-	-
23	CLA	B	524	X	-	X	X
23	CLA	B	525	X	-	-	-
23	CLA	B	527	X	-	-	X
23	CLA	C	474	X	-	-	-
23	CLA	C	475	X	-	-	-
23	CLA	C	476	X	-	-	-
23	CLA	C	477	X	-	-	-
23	CLA	C	478	X	-	-	-
23	CLA	C	479	X	-	-	-
23	CLA	C	480	X	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	481	X	-	-	X
23	CLA	C	482	X	-	-	X
23	CLA	C	483	X	-	-	X
23	CLA	C	484	X	-	-	-
23	CLA	C	485	X	-	-	-
23	CLA	C	486	X	-	-	-
23	CLA	C	487	X	-	-	X
23	CLA	D	354	X	-	-	-
23	CLA	D	356	X	-	-	-
23	CLA	a	2348	X	-	-	-
23	CLA	a	2349	X	-	-	X
23	CLA	a	2351	X	-	-	-
23	CLA	b	2511	X	-	-	-
23	CLA	b	2512	X	-	-	-
23	CLA	b	2513	X	-	-	-
23	CLA	b	2514	X	-	-	-
23	CLA	b	2515	X	-	-	-
23	CLA	b	2516	X	-	-	X
23	CLA	b	2517	X	-	-	X
23	CLA	b	2518	X	-	-	-
23	CLA	b	2519	X	-	-	X
23	CLA	b	2520	X	-	-	-
23	CLA	b	2521	X	-	-	-
23	CLA	b	2522	X	-	-	X
23	CLA	b	2523	X	-	-	-
23	CLA	b	2524	X	-	-	X
23	CLA	b	2525	X	-	-	-
23	CLA	b	2526	X	-	-	X
23	CLA	c	2474	X	-	-	-
23	CLA	c	2475	X	-	-	-
23	CLA	c	2476	X	-	-	-
23	CLA	c	2477	X	-	-	X
23	CLA	c	2478	X	-	-	X
23	CLA	c	2479	X	-	-	X
23	CLA	c	2480	X	-	-	-
23	CLA	c	2481	X	-	-	-
23	CLA	c	2482	X	-	-	-
23	CLA	c	2483	X	-	-	-
23	CLA	c	2484	X	-	-	-
23	CLA	c	2485	X	-	-	X
23	CLA	c	2486	X	-	-	X
23	CLA	c	2487	X	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	2354	X	-	-	-
23	CLA	d	2355	X	-	-	X
23	CLA	d	2357	X	-	-	-
25	HEM	e	2084	-	-	-	X
26	PL9	A	353	-	-	-	X
26	PL9	D	357	-	-	-	X
26	PL9	a	2352	-	-	-	X
26	PL9	d	2358	-	-	-	X
27	LMT	d	2359	-	-	-	X
28	BCR	B	528	-	-	-	X
28	BCR	B	529	-	-	-	X
28	BCR	C	488	-	-	-	X
28	BCR	C	489	-	-	-	X
28	BCR	F	48	-	-	-	X
28	BCR	K	50	-	-	-	X
28	BCR	b	2527	-	-	-	X
28	BCR	b	2528	-	-	-	X
28	BCR	c	2488	-	-	-	X
28	BCR	c	2489	-	-	-	X
28	BCR	d	2360	-	-	-	X
28	BCR	k	2050	-	-	-	X

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 45945 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2617	1714	430	458	15			
1	a	333	Total	C	N	O	S	0	0	0
			2616	1714	430	457	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	476	Total	C	N	O	S	0	0	0
			3739	2455	625	646	13			
2	b	476	Total	C	N	O	S	0	0	0
			3739	2455	625	646	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	421	Total	C	N	O	S	0	0	0
			3253	2140	544	557	12			
3	c	421	Total	C	N	O	S	0	0	0
			3253	2140	544	557	12			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	INSERTION	UNP Q8DIF8
C	2	LYS	-	INSERTION	UNP Q8DIF8
C	3	THR	-	INSERTION	UNP Q8DIF8
C	4	LEU	-	INSERTION	UNP Q8DIF8
C	5	SER	-	INSERTION	UNP Q8DIF8
C	6	SER	-	INSERTION	UNP Q8DIF8
C	7	GLN	-	INSERTION	UNP Q8DIF8
C	8	LYS	-	INSERTION	UNP Q8DIF8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	9	ARG	-	INSERTION	UNP Q8DIF8
C	10	TYR	-	INSERTION	UNP Q8DIF8
C	11	SER	-	INSERTION	UNP Q8DIF8
C	12	PRO	-	INSERTION	UNP Q8DIF8
C	13	VAL	-	INSERTION	UNP Q8DIF8
c	2001	MET	-	INSERTION	UNP Q8DIF8
c	2002	LYS	-	INSERTION	UNP Q8DIF8
c	2003	THR	-	INSERTION	UNP Q8DIF8
c	2004	LEU	-	INSERTION	UNP Q8DIF8
c	2005	SER	-	INSERTION	UNP Q8DIF8
c	2006	SER	-	INSERTION	UNP Q8DIF8
c	2007	GLN	-	INSERTION	UNP Q8DIF8
c	2008	LYS	-	INSERTION	UNP Q8DIF8
c	2009	ARG	-	INSERTION	UNP Q8DIF8
c	2010	TYR	-	INSERTION	UNP Q8DIF8
c	2011	SER	-	INSERTION	UNP Q8DIF8
c	2012	PRO	-	INSERTION	UNP Q8DIF8
c	2013	VAL	-	INSERTION	UNP Q8DIF8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	339	Total	C	N	O	S	0	0	0
			2702	1792	439	459	12			
4	d	339	Total	C	N	O	S	0	0	0
			2702	1792	439	459	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	76	Total	C	N	O	0	0	0
			624	411	99	114			
5	e	76	Total	C	N	O	0	0	0
			624	411	99	114			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			
6	f	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			

- Molecule 7 is a protein called photosystem II PsbH protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	53	Total	C	N	O	S	0	0	0
			409	276	60	71	2			
7	h	53	Total	C	N	O	S	0	0	0
			409	276	60	71	2			

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

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 J protein.

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	38	Total	C	N	O	S	0	0	0
			272	182	42	47	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
			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 L protein.

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 M protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	30	Total	C	N	O	S	0	0	0
			234	159	33	41	1			
12	m	30	Total	C	N	O	S	0	0	0
			234	159	33	41	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	246	Total	C	N	O	S	0	0	0
			1888	1179	320	385	4			
13	o	246	Total	C	N	O	S	0	0	0
			1888	1179	320	385	4			

- Molecule 14 is a protein called photosystem II PsbT protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	31	Total	C	N	O	S	0	0	0
			265	186	38	39	2			
14	t	31	Total	C	N	O	S	0	0	0
			265	186	38	39	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	105	Total	C	N	O		0	0	0
			827	521	137	169				
15	u	105	Total	C	N	O		0	0	0
			827	521	137	169				

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

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

- Molecule 17 is a protein called photosystem II PsbX protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	X	40	Total	C	N	O		0	0	0
			296	197	47	52				

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	x	40	Total	C	N	O	0	0	0
			296	197	47	52			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1	MET	-	INSERTION	UNP Q9F1R6
X	2	ILE	-	INSERTION	UNP Q9F1R6
X	3	GLN	-	INSERTION	UNP Q9F1R6
X	4	SER	-	INSERTION	UNP Q9F1R6
X	5	ALA	-	INSERTION	UNP Q9F1R6
X	6	SER	-	INSERTION	UNP Q9F1R6
X	7	SER	-	INSERTION	UNP Q9F1R6
X	8	LEU	-	INSERTION	UNP Q9F1R6
X	9	LEU	-	INSERTION	UNP Q9F1R6
X	10	LEU	-	INSERTION	UNP Q9F1R6
x	2001	MET	-	INSERTION	UNP Q9F1R6
x	2002	ILE	-	INSERTION	UNP Q9F1R6
x	2003	GLN	-	INSERTION	UNP Q9F1R6
x	2004	SER	-	INSERTION	UNP Q9F1R6
x	2005	ALA	-	INSERTION	UNP Q9F1R6
x	2006	SER	-	INSERTION	UNP Q9F1R6
x	2007	SER	-	INSERTION	UNP Q9F1R6
x	2008	LEU	-	INSERTION	UNP Q9F1R6
x	2009	LEU	-	INSERTION	UNP Q9F1R6
x	2010	LEU	-	INSERTION	UNP Q9F1R6

- Molecule 18 is a protein called Photosystem II PsbN protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	N	37	Total	C	N	O	0	0	0
			186	111	37	38			
18	n	37	Total	C	N	O	0	0	0
			186	111	37	38			

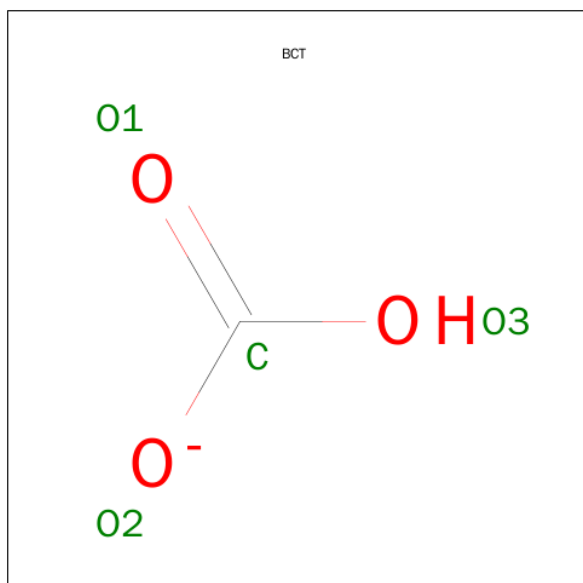
- Molecule 19 is a protein called Photosystem II reaction center Z protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	58	Total	C	N	O	S	0	0	0
			442	300	68	72	2			
19	z	58	Total	C	N	O	S	0	0	0
			442	300	68	72	2			

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

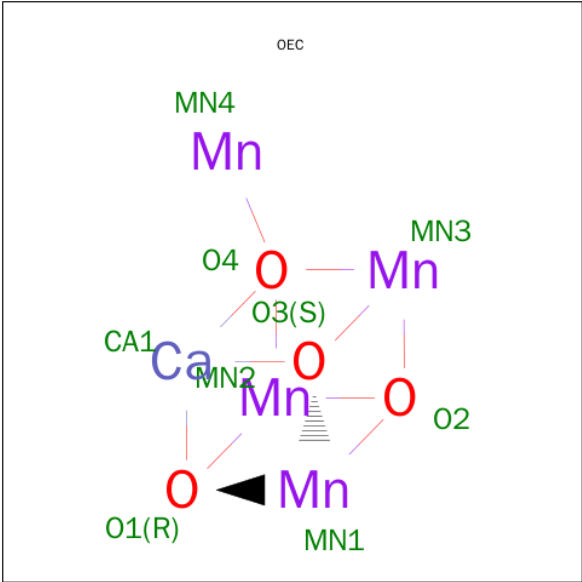
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	1	Total	Fe	0	0
			1	1		
20	a	1	Total	Fe	0	0
			1	1		

- Molecule 21 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



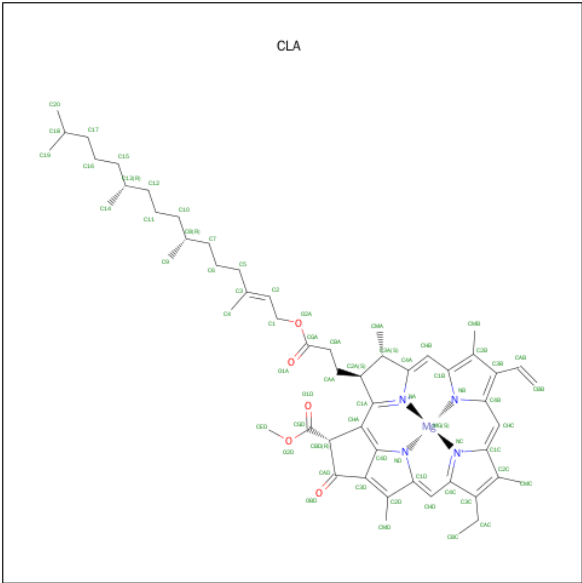
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			4	1	3		
21	D	1	Total	C	O	0	0
			4	1	3		
21	a	1	Total	C	O	0	0
			4	1	3		
21	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 22 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn_4O_4).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	Ca	Mn	O	0	0
			9	1	4	4		
22	a	1	Total	Ca	Mn	O	0	0
			9	1	4	4		

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



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

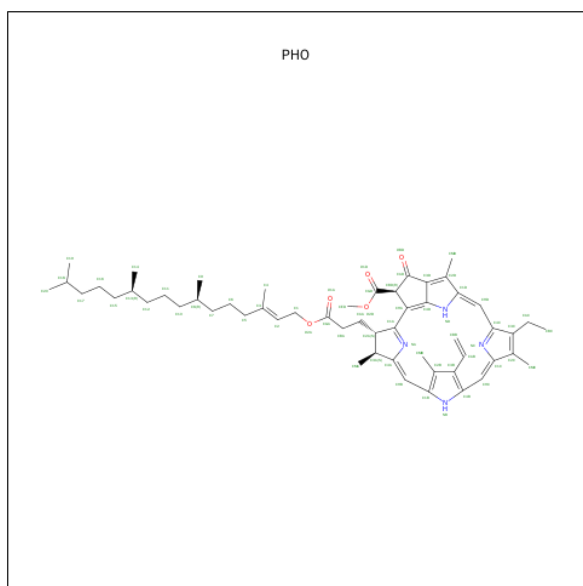
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N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

Continued on next page...

Continued from previous page...

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

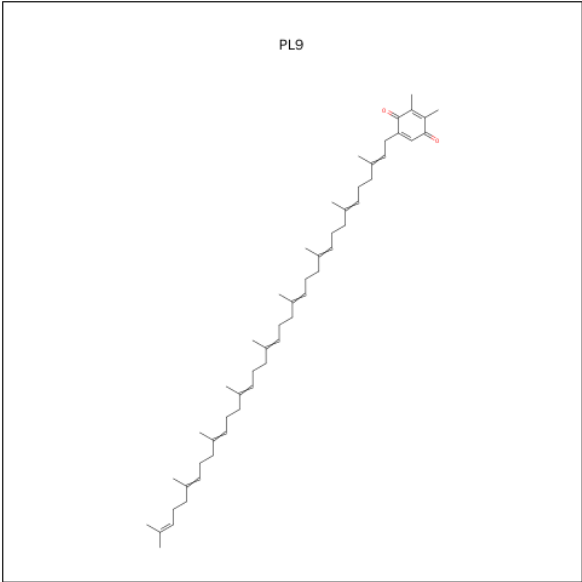
- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

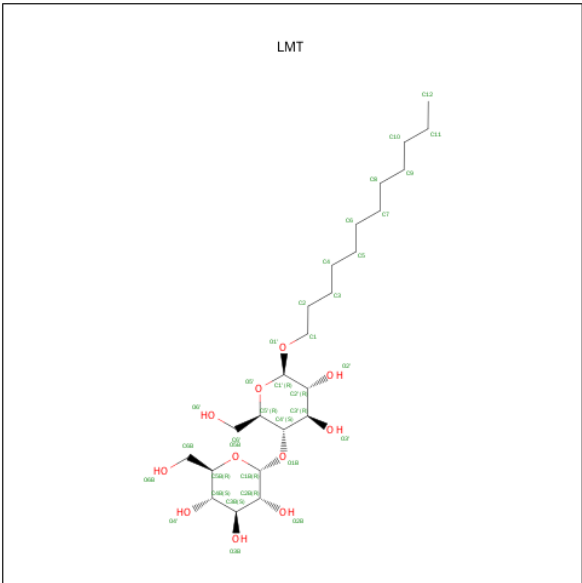
-
- Chemical structure of HEM (Heme) showing a central iron atom coordinated by four nitrogen atoms in a porphyrin-like ring, with various side chains and a central heme group.

- Molecule 26 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: $C_{53}H_{80}O_2$).



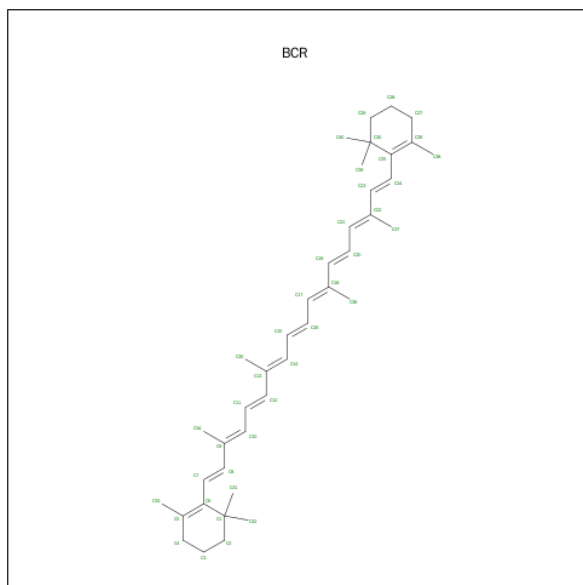
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	D	1	Total	C	O	0	0
			45	43	2		
26	A	1	Total	C	O	0	0
			45	43	2		
26	d	1	Total	C	O	0	0
			45	43	2		
26	a	1	Total	C	O	0	0
			45	43	2		

- Molecule 27 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	B	1	Total	C	O	0	0
			35	24	11		
27	d	1	Total	C	O	0	0
			35	24	11		

- Molecule 28 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	F	1	Total	C	0	0
			40	40		
28	C	1	Total	C	0	0
			40	40		
28	K	1	Total	C	0	0
			40	40		
28	C	1	Total	C	0	0
			40	40		
28	B	1	Total	C	0	0
			40	40		
28	J	1	Total	C	0	0
			40	40		
28	B	1	Total	C	0	0
			40	40		
28	d	1	Total	C	0	0
			40	40		
28	c	1	Total	C	0	0
			40	40		
28	k	1	Total	C	0	0
			40	40		

Continued on next page...

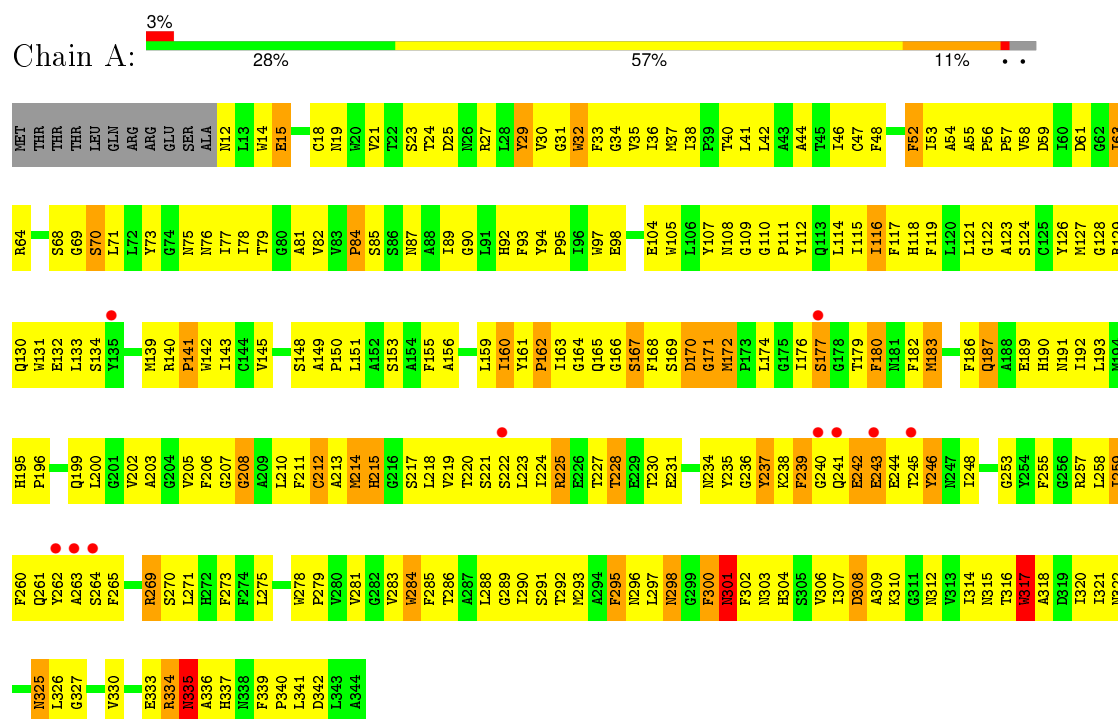
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	c	1	Total C 40 40	0	0
28	b	1	Total C 40 40	0	0
28	j	1	Total C 40 40	0	0
28	b	1	Total C 40 40	0	0

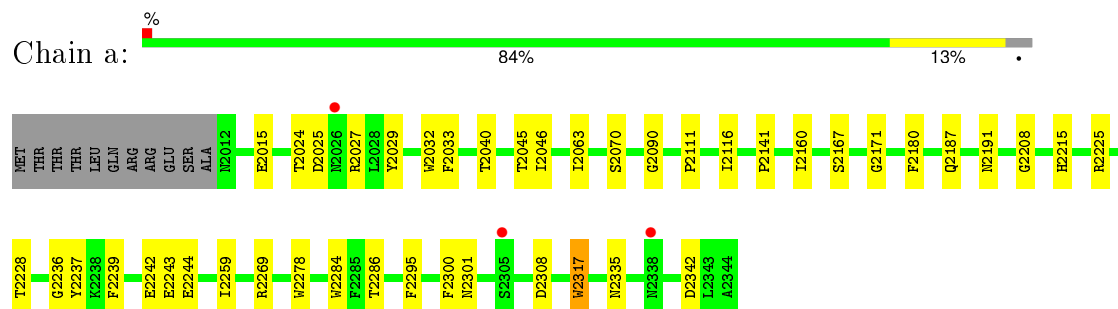
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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

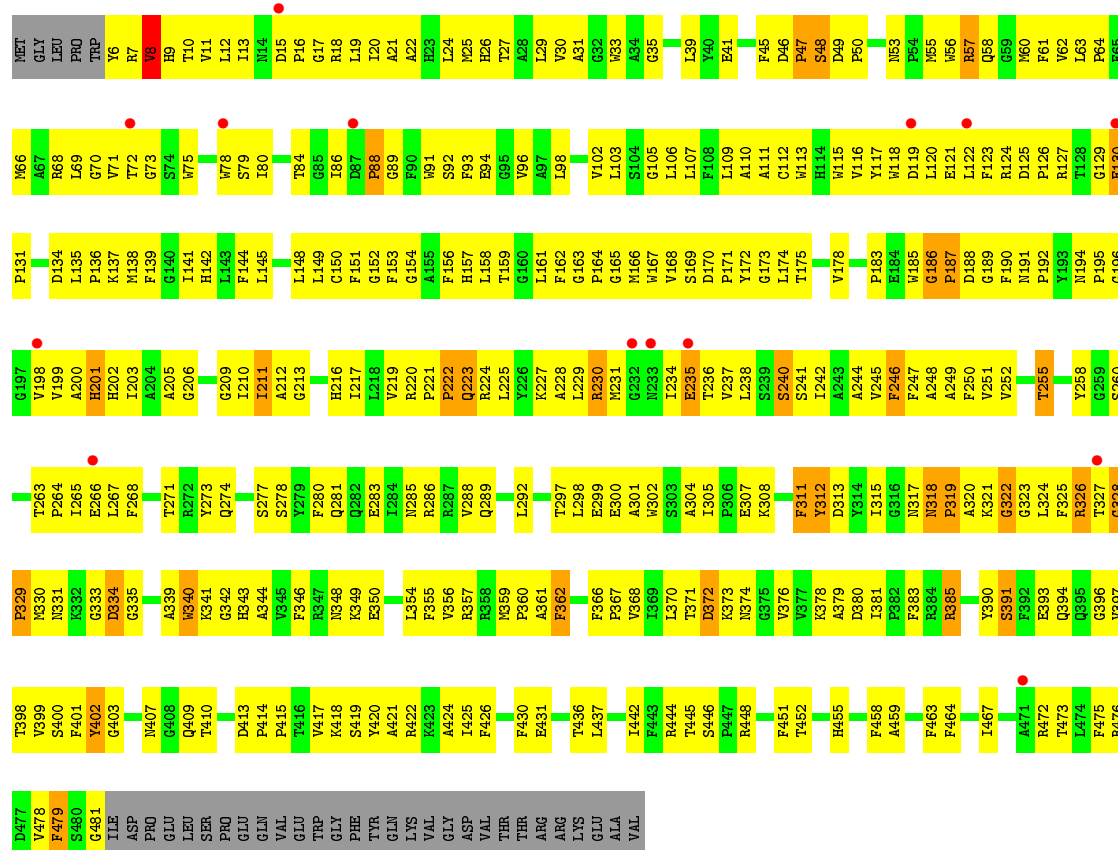


• Molecule 1: Photosystem Q(B) protein

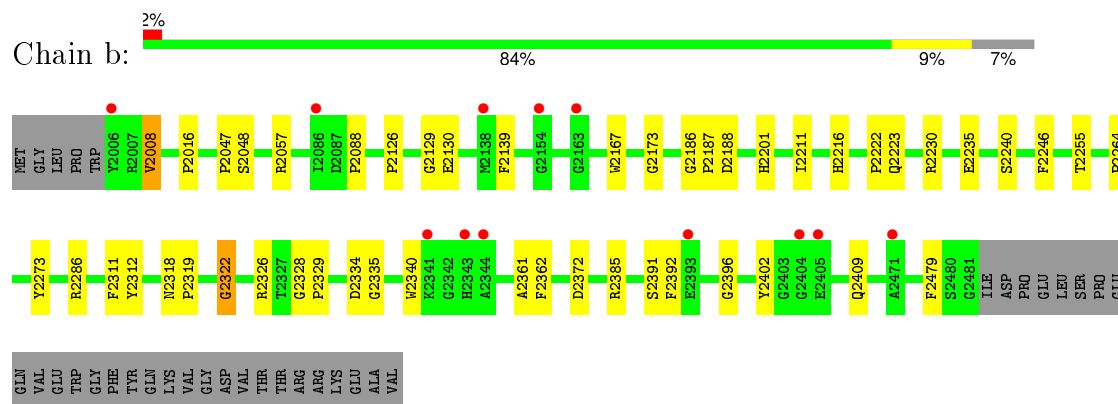


• Molecule 2: photosystem II core light harvesting protein

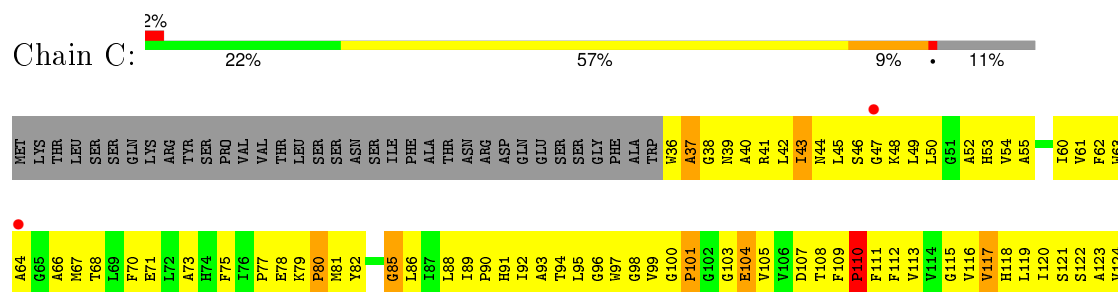


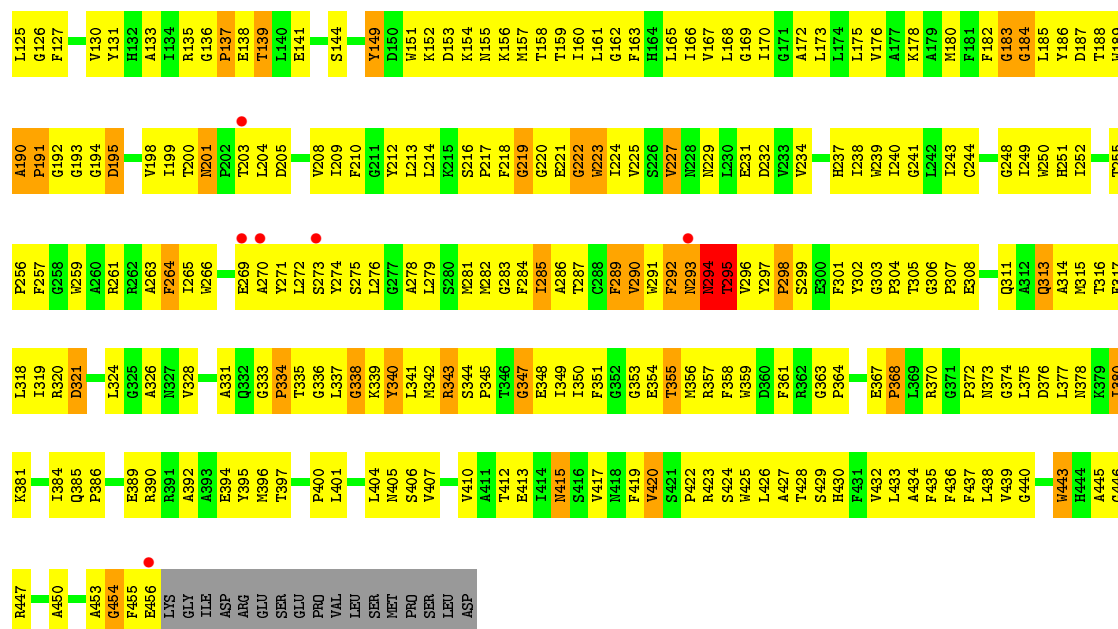


• Molecule 2: photosystem II core light harvesting protein

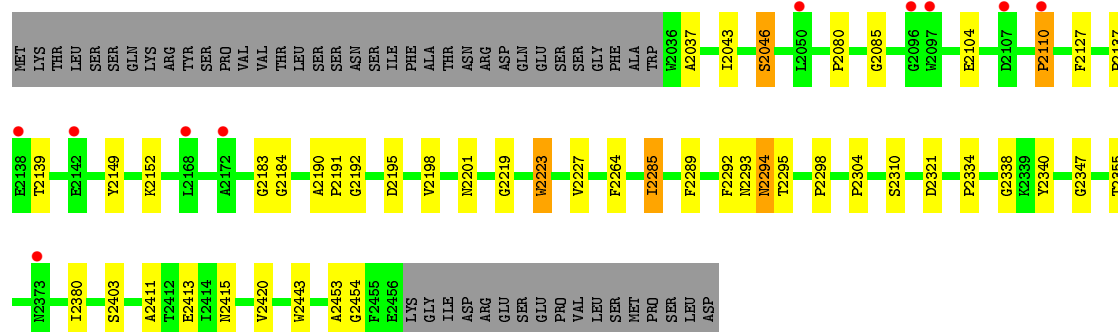
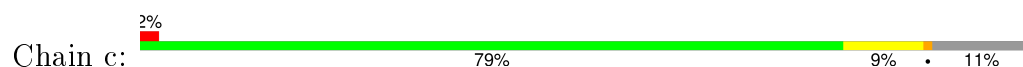


• Molecule 3: photosystem II CP43 protein

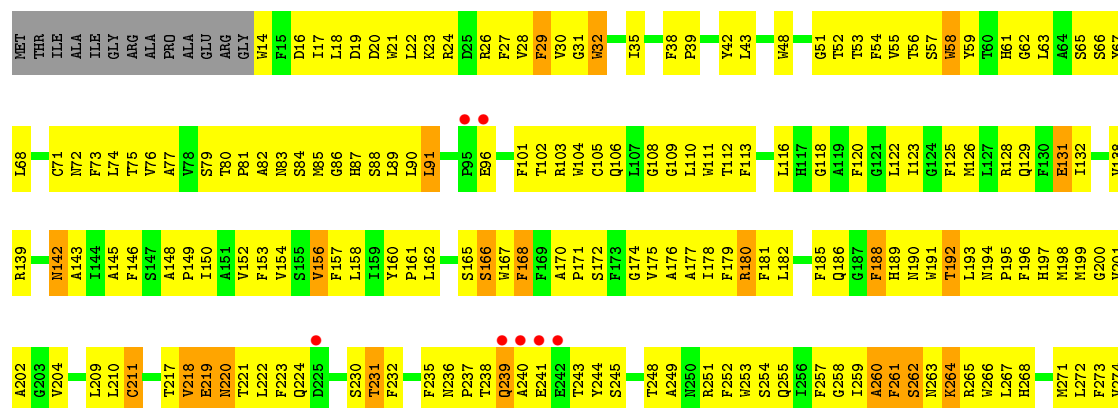


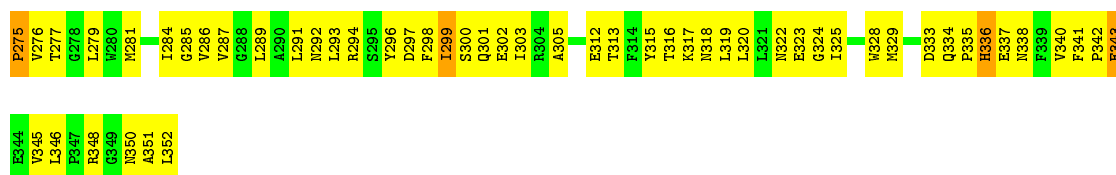


• Molecule 3: photosystem II CP43 protein

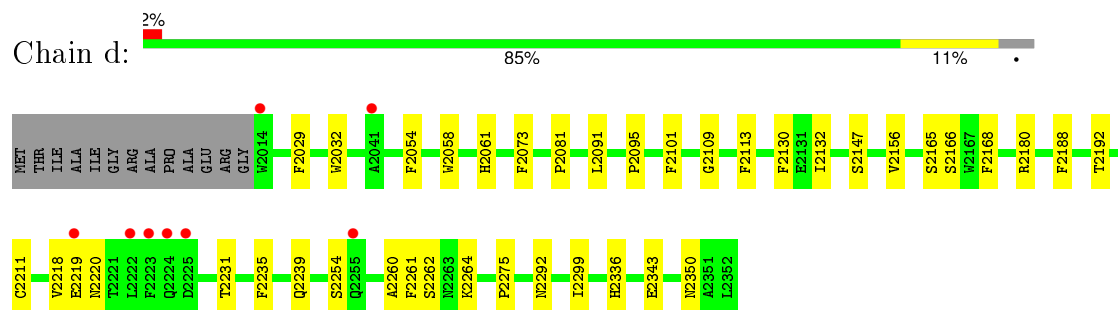


• Molecule 4: photosystem II reaction center D2 protein

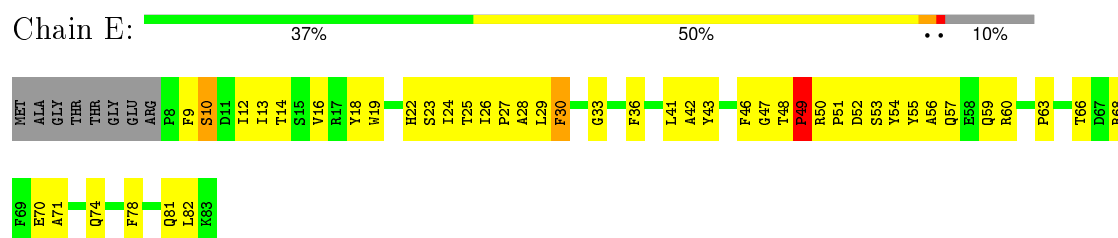




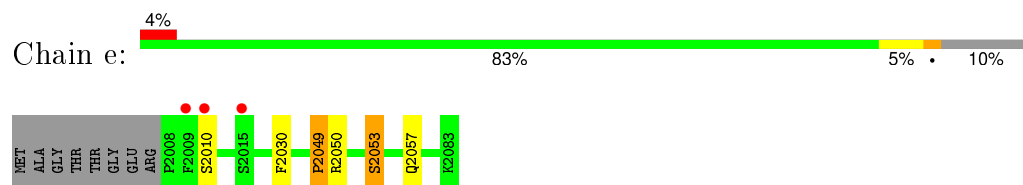
- Molecule 4: photosystem II reaction center D2 protein



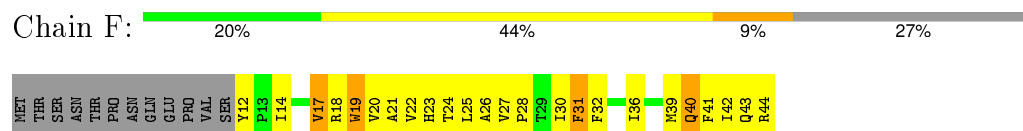
- Molecule 5: Cytochrome b559 alpha subunit



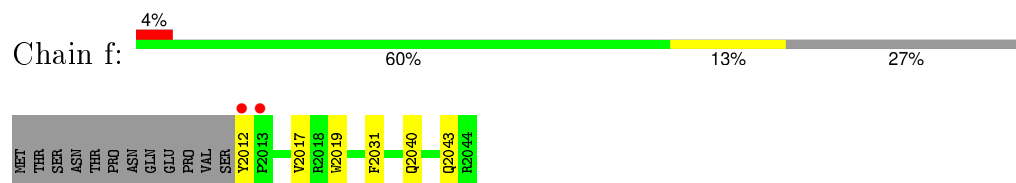
- Molecule 5: Cytochrome b559 alpha subunit



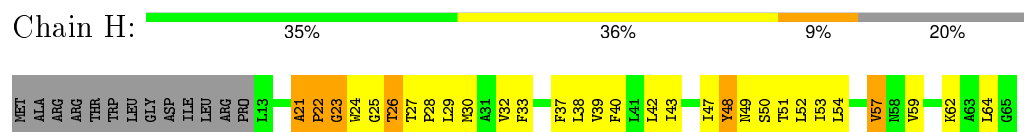
- Molecule 6: Cytochrome b559 beta subunit



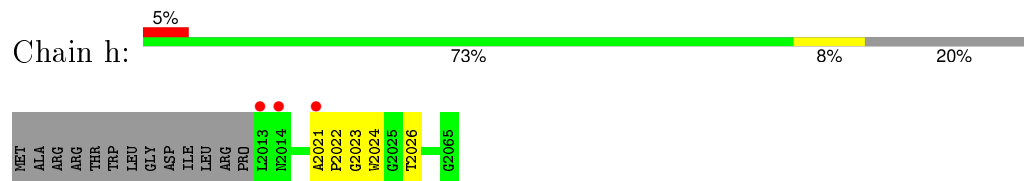
- Molecule 6: Cytochrome b559 beta subunit



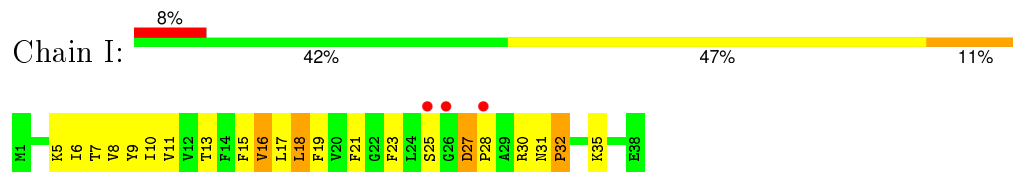
- Molecule 7: photosystem II PsbH protein



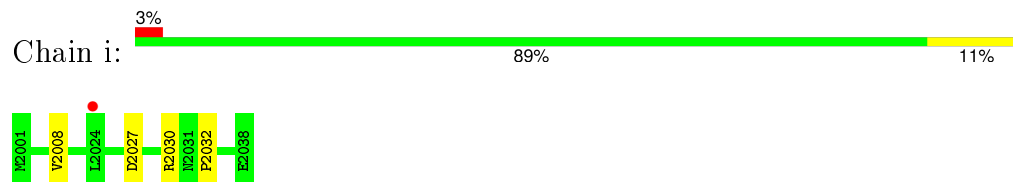
- Molecule 7: photosystem II PsbH protein



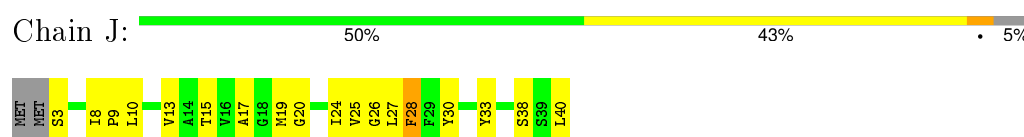
- Molecule 8: Photosystem II reaction center I protein



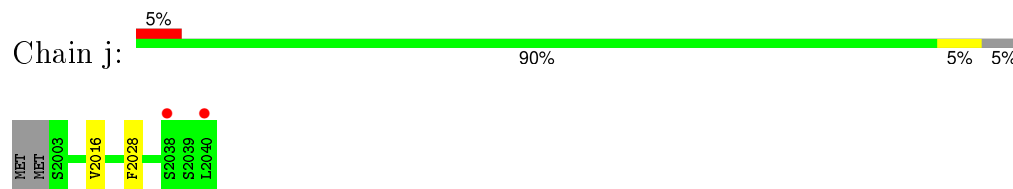
- Molecule 8: Photosystem II reaction center I protein



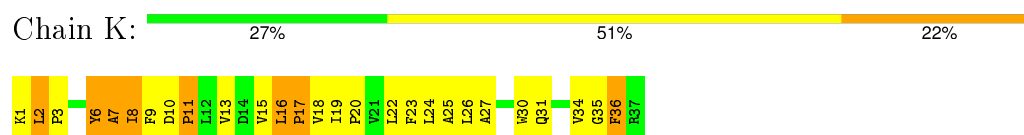
- Molecule 9: Photosystem II reaction center J protein




- Molecule 9: Photosystem II reaction center J protein



- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K

Chain k:  84% 16%




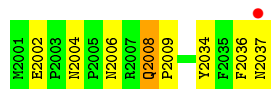
- Molecule 11: Photosystem II reaction center L protein

Chain L:  5% 30% 51% 14% 5%



- Molecule 11: Photosystem II reaction center L protein

Chain l:  3% 78% 19% .



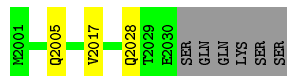
- Molecule 12: Photosystem II reaction center M protein

Chain M:  28% 50% 6% 17%



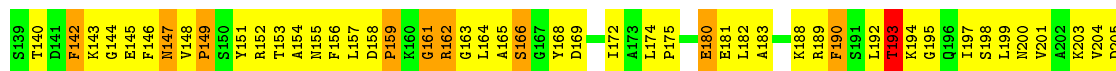
- Molecule 12: Photosystem II reaction center M protein

Chain m:  75% 8% 17%

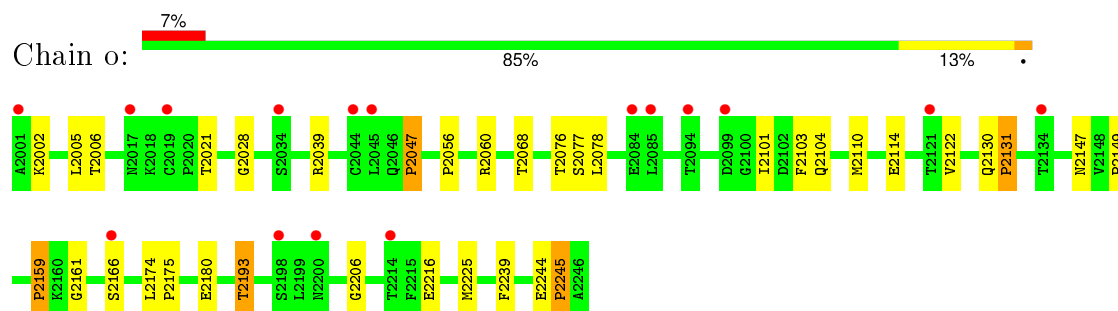


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

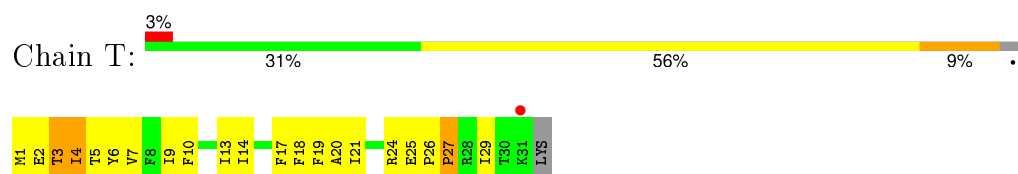
Chain O:  2% 30% 55% 13% .



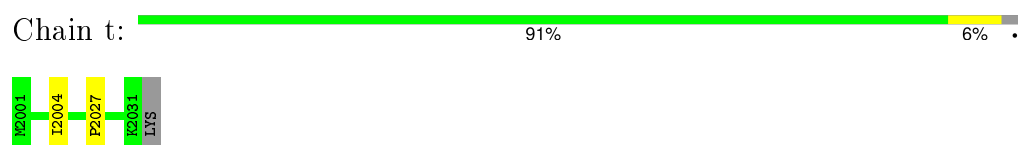
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



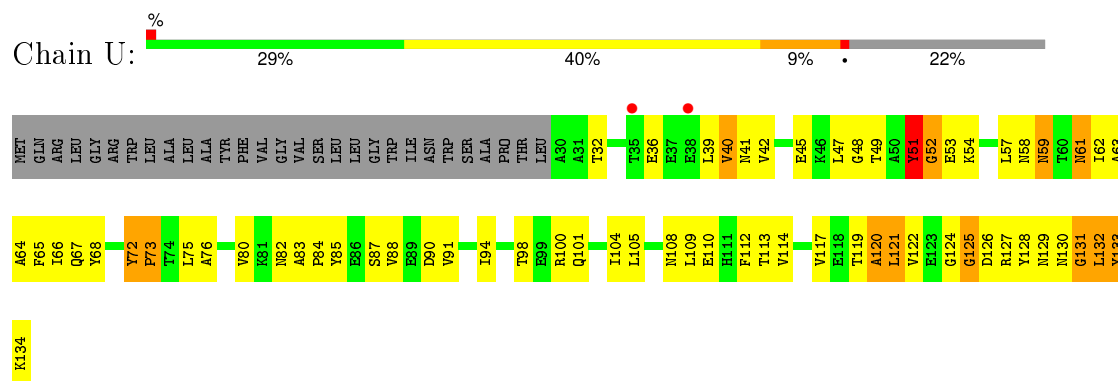
- Molecule 14: photosystem II PsbT protein



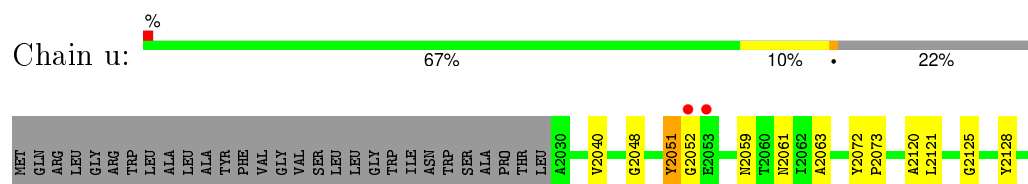
- Molecule 14: photosystem II PsbT protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein

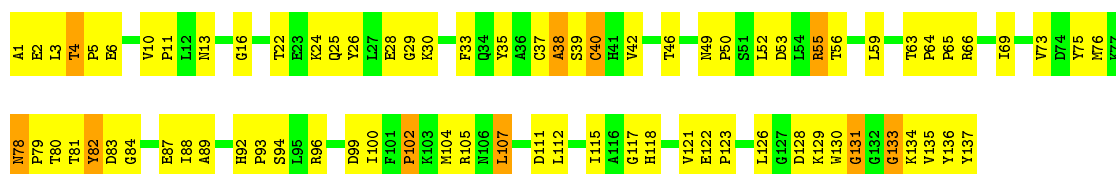


- Molecule 15: Photosystem II 12 kDa extrinsic protein

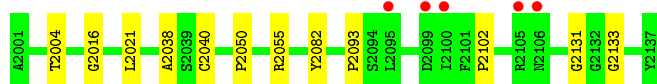
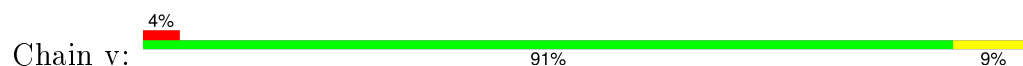


- Molecule 16: Cytochrome c-550





- Molecule 16: Cytochrome c-550



- Molecule 17: photosystem II PsbX protein



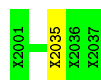
- Molecule 17: photosystem II PsbX protein



- Molecule 18: Photosystem II PsbN protein



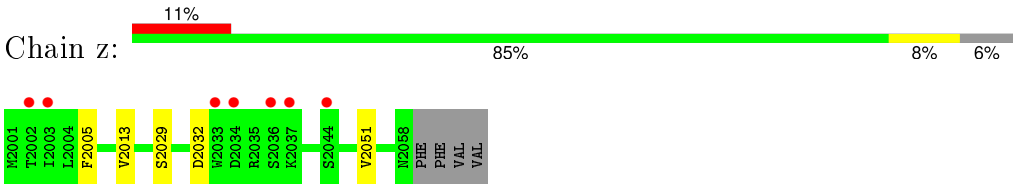
- Molecule 18: Photosystem II PsbN protein



- Molecule 19: Photosystem II reaction center Z protein



- Molecule 19: Photosystem II reaction center Z protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.99Å 228.85Å 309.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 74.07 – 3.47	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.50) 84.1 (74.07-3.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.296 , 0.342 0.307 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	118.3	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 97.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 105247 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	45945	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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: PHO, LMT, CLA, PL9, BCT, FE, OEC, HEM, BCR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.65	0/2702	0.85	2/3685 (0.1%)
1	a	0.62	0/2701	0.83	2/3685 (0.1%)
2	B	0.57	0/3870	0.80	3/5271 (0.1%)
2	b	0.56	0/3870	0.80	4/5271 (0.1%)
3	C	0.60	0/3361	0.81	3/4579 (0.1%)
3	c	0.57	0/3361	0.80	3/4579 (0.1%)
4	D	0.62	0/2797	0.82	1/3813 (0.0%)
4	d	0.62	0/2797	0.83	2/3813 (0.1%)
5	E	0.59	0/643	0.89	1/876 (0.1%)
5	e	0.61	0/643	0.87	1/876 (0.1%)
6	F	0.74	0/278	0.84	0/379
6	f	0.68	0/278	0.84	0/379
7	H	0.58	0/419	0.81	0/570
7	h	0.60	0/419	0.81	0/570
8	I	0.63	0/319	0.73	0/429
8	i	0.61	0/319	0.73	0/429
9	J	0.60	0/278	0.80	0/376
9	j	0.62	0/278	0.84	0/376
10	K	0.66	0/303	0.92	0/416
10	k	0.63	0/303	0.86	0/416
11	L	0.74	1/311 (0.3%)	0.87	0/422
11	l	0.73	1/311 (0.3%)	0.91	0/422
12	M	0.63	0/237	0.77	0/324
12	m	0.70	0/237	0.80	0/324
13	O	0.67	0/1919	0.97	4/2601 (0.2%)
13	o	0.68	0/1919	0.96	3/2601 (0.1%)
14	T	0.71	0/274	0.78	0/370
14	t	0.74	0/274	0.80	0/370
15	U	0.68	0/838	0.91	1/1137 (0.1%)
15	u	0.62	0/838	0.87	0/1137
16	V	0.62	0/1085	0.78	0/1473
16	v	0.56	0/1085	0.77	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	X	0.57	0/299	0.72	0/403
17	x	0.61	0/299	0.75	0/403
19	Z	0.54	0/451	0.74	0/617
19	z	0.54	0/451	0.72	0/617
All	All	0.61	2/40767 (0.0%)	0.83	30/55482 (0.1%)

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
1	A	0	1
2	B	0	1
2	b	0	1
11	l	0	1
13	O	0	1
15	U	0	2
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	l	2037	ASN	C-OXT	5.21	1.33	1.23
11	L	37	ASN	C-OXT	5.18	1.33	1.23

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	2171	GLY	N-CA-C	-7.28	94.91	113.10
1	A	171	GLY	N-CA-C	-7.27	94.93	113.10
13	O	131	PRO	N-CA-C	6.48	128.95	112.10
1	a	2236	GLY	N-CA-C	6.41	129.12	113.10
4	D	231	THR	N-CA-C	-6.30	93.98	111.00

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	246	TYR	Sidechain
2	B	273	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
13	O	240	TYR	Sidechain
15	U	133	TYR	Sidechain
15	U	51	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2617	0	2514	451	0
1	a	2616	0	2514	0	0
2	B	3739	0	3613	450	0
2	b	3739	0	3613	0	0
3	C	3253	0	3192	532	0
3	c	3253	0	3192	0	0
4	D	2702	0	2605	412	0
4	d	2702	0	2605	0	0
5	E	624	0	613	95	0
5	e	624	0	613	0	0
6	F	269	0	277	43	0
6	f	269	0	277	0	0
7	H	409	0	424	52	0
7	h	409	0	424	0	0
8	I	312	0	329	25	0
8	i	312	0	326	0	0
9	J	272	0	279	43	0
9	j	272	0	279	0	0
10	K	293	0	308	57	0
10	k	293	0	305	0	0
11	L	304	0	316	49	0
11	l	304	0	313	0	0
12	M	234	0	255	32	0
12	m	234	0	252	0	0
13	O	1888	0	1867	274	6
13	o	1888	0	1864	0	0
14	T	265	0	275	41	0
14	t	265	0	272	0	0
15	U	827	0	819	121	0
15	u	827	0	819	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	V	1064	0	1075	124	0
16	v	1064	0	1070	0	0
17	X	296	0	328	14	0
17	x	296	0	328	0	0
18	N	186	0	40	10	0
18	n	186	0	40	0	6
19	Z	442	0	480	61	0
19	z	442	0	477	0	0
20	A	1	0	0	0	0
20	a	1	0	0	0	0
21	A	4	0	0	0	0
21	D	4	0	0	0	0
21	a	4	0	0	0	0
21	d	4	0	0	0	0
22	A	9	0	0	1	0
22	a	9	0	0	0	0
23	A	260	0	288	29	0
23	B	1040	0	1152	116	0
23	C	910	0	1008	104	0
23	D	130	0	144	18	0
23	a	195	0	216	0	0
23	b	1040	0	1152	0	0
23	c	910	0	1008	0	0
23	d	195	0	216	0	0
24	A	64	0	74	6	0
24	D	64	0	74	8	0
24	a	64	0	74	0	0
24	d	64	0	74	0	0
25	E	43	0	30	16	0
25	V	43	0	30	10	0
25	e	43	0	30	0	0
25	v	43	0	30	0	0
26	A	45	0	61	8	0
26	D	45	0	61	5	0
26	a	45	0	61	0	0
26	d	45	0	61	0	0
27	B	35	0	46	0	0
27	d	35	0	46	0	0
28	B	80	0	112	16	0
28	C	80	0	112	23	0
28	F	40	0	56	3	0
28	J	40	0	56	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	K	40	0	56	13	0
28	b	80	0	112	0	0
28	c	80	0	112	0	0
28	d	40	0	56	0	0
28	j	40	0	56	0	0
28	k	40	0	56	0	0
All	All	45945	0	45912	2600	6

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 57.

The worst 5 of 2600 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)
25:V:138:HEM:CMB	25:V:138:HEM:C2B	1.74	1.63
25:V:138:HEM:C2C	25:V:138:HEM:CMC	1.75	1.62
16:V:37:CYS:SG	25:V:138:HEM:HAB	1.57	1.44
5:E:12:ILE:CG2	5:E:18:TYR:HB2	1.44	1.43
5:E:12:ILE:HD12	25:E:84:HEM:O2D	1.31	1.25

The worst 5 of 6 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:246:ALA:C	18:n:2035:UNK:O[2_555]	1.76	0.44
13:O:246:ALA:N	18:n:2035:UNK:O[2_555]	1.97	0.23
13:O:246:ALA:O	18:n:2035:UNK:O[2_555]	2.07	0.13
13:O:246:ALA:O	18:n:2035:UNK:CB[2_555]	2.15	0.05
13:O:246:ALA:N	18:n:2035:UNK:C[2_555]	2.17	0.03

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	331/344 (96%)	251 (76%)	58 (18%)	22 (7%)	1	19
1	a	331/344 (96%)	253 (76%)	56 (17%)	22 (7%)	1	19
2	B	474/510 (93%)	367 (77%)	84 (18%)	23 (5%)	3	27
2	b	474/510 (93%)	367 (77%)	83 (18%)	24 (5%)	2	26
3	C	419/473 (89%)	326 (78%)	60 (14%)	33 (8%)	1	14
3	c	419/473 (89%)	326 (78%)	62 (15%)	31 (7%)	1	16
4	D	337/352 (96%)	274 (81%)	49 (14%)	14 (4%)	3	32
4	d	337/352 (96%)	270 (80%)	51 (15%)	16 (5%)	3	29
5	E	74/84 (88%)	62 (84%)	10 (14%)	2 (3%)	6	44
5	e	74/84 (88%)	57 (77%)	14 (19%)	3 (4%)	3	33
6	F	31/45 (69%)	23 (74%)	5 (16%)	3 (10%)	1	10
6	f	31/45 (69%)	22 (71%)	6 (19%)	3 (10%)	1	10
7	H	51/66 (77%)	35 (69%)	13 (26%)	3 (6%)	2	22
7	h	51/66 (77%)	35 (69%)	13 (26%)	3 (6%)	2	22
8	I	36/38 (95%)	25 (69%)	10 (28%)	1 (3%)	6	43
8	i	36/38 (95%)	27 (75%)	7 (19%)	2 (6%)	2	24
9	J	36/40 (90%)	32 (89%)	3 (8%)	1 (3%)	6	43
9	j	36/40 (90%)	30 (83%)	4 (11%)	2 (6%)	2	24
10	K	35/37 (95%)	27 (77%)	2 (6%)	6 (17%)	0	3
10	k	35/37 (95%)	26 (74%)	3 (9%)	6 (17%)	0	3
11	L	35/37 (95%)	28 (80%)	3 (9%)	4 (11%)	0	7
11	l	35/37 (95%)	27 (77%)	5 (14%)	3 (9%)	1	12
12	M	28/36 (78%)	22 (79%)	5 (18%)	1 (4%)	4	37
12	m	28/36 (78%)	22 (79%)	4 (14%)	2 (7%)	1	17
13	O	244/246 (99%)	180 (74%)	44 (18%)	20 (8%)	1	13
13	o	244/246 (99%)	179 (73%)	45 (18%)	20 (8%)	1	13
14	T	29/32 (91%)	23 (79%)	3 (10%)	3 (10%)	1	9
14	t	29/32 (91%)	22 (76%)	5 (17%)	2 (7%)	1	18
15	U	103/134 (77%)	78 (76%)	14 (14%)	11 (11%)	0	8
15	u	103/134 (77%)	81 (79%)	11 (11%)	11 (11%)	0	8
16	V	135/137 (98%)	111 (82%)	16 (12%)	8 (6%)	2	22
16	v	135/137 (98%)	106 (78%)	22 (16%)	7 (5%)	2	25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	X	38/50 (76%)	36 (95%)	1 (3%)	1 (3%)	7	45
17	x	38/50 (76%)	35 (92%)	2 (5%)	1 (3%)	7	45
19	Z	56/62 (90%)	39 (70%)	15 (27%)	2 (4%)	4	37
19	z	56/62 (90%)	40 (71%)	13 (23%)	3 (5%)	2	25
All	All	4984/5446 (92%)	3864 (78%)	801 (16%)	319 (6%)	2	20

5 of 319 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	GLY
1	A	228	THR
1	A	242	GLU
1	A	308	ASP
2	B	88	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	244 (90%)	26 (10%)	10	43
1	a	270/280 (96%)	249 (92%)	21 (8%)	16	53
2	B	377/407 (93%)	355 (94%)	22 (6%)	25	65
2	b	377/407 (93%)	355 (94%)	22 (6%)	25	65
3	C	326/374 (87%)	306 (94%)	20 (6%)	23	64
3	c	326/374 (87%)	307 (94%)	19 (6%)	25	65
4	D	275/283 (97%)	257 (94%)	18 (6%)	21	62
4	d	275/283 (97%)	253 (92%)	22 (8%)	15	52
5	E	68/73 (93%)	65 (96%)	3 (4%)	35	73
5	e	68/73 (93%)	64 (94%)	4 (6%)	24	65
6	F	27/39 (69%)	25 (93%)	2 (7%)	17	56
6	f	27/39 (69%)	24 (89%)	3 (11%)	8	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	44/55 (80%)	41 (93%)	3 (7%)	20	60
7	h	44/55 (80%)	42 (96%)	2 (4%)	34	73
8	I	35/35 (100%)	31 (89%)	4 (11%)	7	33
8	i	35/35 (100%)	33 (94%)	2 (6%)	25	66
9	J	26/28 (93%)	25 (96%)	1 (4%)	40	76
9	j	26/28 (93%)	26 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	20	61
10	k	30/30 (100%)	30 (100%)	0	100	100
11	L	35/35 (100%)	31 (89%)	4 (11%)	7	33
11	l	35/35 (100%)	31 (89%)	4 (11%)	7	33
12	M	27/33 (82%)	26 (96%)	1 (4%)	41	76
12	m	27/33 (82%)	26 (96%)	1 (4%)	41	76
13	O	208/208 (100%)	187 (90%)	21 (10%)	9	40
13	o	208/208 (100%)	190 (91%)	18 (9%)	13	48
14	T	28/29 (97%)	28 (100%)	0	100	100
14	t	28/29 (97%)	28 (100%)	0	100	100
15	U	89/112 (80%)	85 (96%)	4 (4%)	34	73
15	u	89/112 (80%)	84 (94%)	5 (6%)	26	66
16	V	117/117 (100%)	112 (96%)	5 (4%)	35	74
16	v	117/117 (100%)	112 (96%)	5 (4%)	35	74
17	X	33/42 (79%)	30 (91%)	3 (9%)	12	46
17	x	33/42 (79%)	29 (88%)	4 (12%)	6	30
19	Z	48/52 (92%)	42 (88%)	6 (12%)	6	29
19	z	48/52 (92%)	46 (96%)	2 (4%)	36	74
All	All	4126/4464 (92%)	3847 (93%)	279 (7%)	20	60

5 of 279 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	O	245	PRO
1	a	2187	GLN
13	o	2166	SER
15	U	61	ASN
19	Z	34	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
13	O	219	GLN
1	a	2296	ASN
13	o	2147	ASN
15	U	59	ASN
19	Z	6	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 108 ligands modelled in this entry, 2 are monoatomic - leaving 106 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
21	BCT	A	346	22	0,3,3	0.00	-	0,3,3	0.00	-
22	OEC	A	347	1,3,21	0,13,13	0.00	-	0,27,27	0.00	-
23	CLA	A	348	1	55,73,73	1.08	6 (10%)	61,113,113	1.52	13 (21%)
23	CLA	A	349	-	55,73,73	1.03	5 (9%)	61,113,113	1.71	14 (22%)
23	CLA	A	350	-	55,73,73	0.97	1 (1%)	61,113,113	1.56	13 (21%)
24	PHO	A	351	-	67,69,69	1.11	5 (7%)	84,99,99	1.34	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	A	352	1	55,73,73	1.03	4 (7%)	61,113,113	1.49	11 (18%)
26	PL9	A	353	-	45,45,55	2.59	19 (42%)	56,57,69	2.52	19 (33%)
23	CLA	B	511	2	55,73,73	1.22	9 (16%)	61,113,113	1.79	16 (26%)
23	CLA	B	512	2	55,73,73	1.04	3 (5%)	61,113,113	1.52	10 (16%)
23	CLA	B	513	2	55,73,73	1.12	4 (7%)	61,113,113	1.89	15 (24%)
23	CLA	B	514	-	55,73,73	1.29	8 (14%)	61,113,113	1.73	14 (22%)
23	CLA	B	515	2	55,73,73	1.13	5 (9%)	61,113,113	1.68	15 (24%)
23	CLA	B	516	2	55,73,73	1.40	8 (14%)	61,113,113	1.62	12 (19%)
23	CLA	B	517	2	55,73,73	1.07	5 (9%)	61,113,113	1.66	15 (24%)
23	CLA	B	518	2	55,73,73	1.07	3 (5%)	61,113,113	1.75	10 (16%)
23	CLA	B	519	2	55,73,73	1.38	9 (16%)	61,113,113	1.97	11 (18%)
23	CLA	B	520	2	55,73,73	1.28	7 (12%)	61,113,113	2.27	10 (16%)
23	CLA	B	521	2	55,73,73	1.06	4 (7%)	61,113,113	1.39	8 (13%)
23	CLA	B	522	2	55,73,73	0.95	3 (5%)	61,113,113	1.56	14 (22%)
23	CLA	B	523	2	55,73,73	1.14	6 (10%)	61,113,113	1.74	15 (24%)
23	CLA	B	524	-	55,73,73	1.03	3 (5%)	61,113,113	1.66	13 (21%)
23	CLA	B	525	2	55,73,73	1.15	6 (10%)	61,113,113	1.63	11 (18%)
27	LMT	B	526	-	36,36,36	1.31	4 (11%)	47,47,47	1.80	9 (19%)
23	CLA	B	527	-	55,73,73	1.19	8 (14%)	61,113,113	1.64	12 (19%)
28	BCR	B	528	-	41,41,41	1.98	6 (14%)	56,56,56	2.25	18 (32%)
28	BCR	B	529	-	41,41,41	2.05	9 (21%)	56,56,56	2.30	23 (41%)
23	CLA	C	474	3	55,73,73	1.07	4 (7%)	61,113,113	1.67	14 (22%)
23	CLA	C	475	-	55,73,73	1.44	9 (16%)	61,113,113	1.68	13 (21%)
23	CLA	C	476	3	55,73,73	1.00	3 (5%)	61,113,113	1.50	9 (14%)
23	CLA	C	477	3	55,73,73	1.14	5 (9%)	61,113,113	2.15	14 (22%)
23	CLA	C	478	3	55,73,73	1.14	5 (9%)	61,113,113	1.57	9 (14%)
23	CLA	C	479	3	55,73,73	1.04	3 (5%)	61,113,113	1.82	15 (24%)
23	CLA	C	480	3	55,73,73	0.94	2 (3%)	61,113,113	1.56	13 (21%)
23	CLA	C	481	3	55,73,73	0.95	3 (5%)	61,113,113	1.91	11 (18%)
23	CLA	C	482	3	55,73,73	1.11	4 (7%)	61,113,113	1.57	10 (16%)
23	CLA	C	483	3	55,73,73	1.15	6 (10%)	61,113,113	1.83	12 (19%)
23	CLA	C	484	3	55,73,73	1.11	4 (7%)	61,113,113	1.49	10 (16%)
23	CLA	C	485	-	55,73,73	1.06	3 (5%)	61,113,113	1.71	14 (22%)
23	CLA	C	486	3	55,73,73	1.07	4 (7%)	61,113,113	1.59	12 (19%)
23	CLA	C	487	-	55,73,73	1.27	5 (9%)	61,113,113	1.61	13 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	BCR	C	488	-	41,41,41	1.80	10 (24%)	56,56,56	2.01	18 (32%)
28	BCR	C	489	-	41,41,41	1.73	7 (17%)	56,56,56	1.99	17 (30%)
21	BCT	D	353	20	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	D	354	4	55,73,73	1.02	4 (7%)	61,113,113	1.47	10 (16%)
24	PHO	D	355	-	67,69,69	0.98	4 (5%)	84,99,99	1.54	15 (17%)
23	CLA	D	356	4	55,73,73	1.12	4 (7%)	61,113,113	1.45	9 (14%)
26	PL9	D	357	-	45,45,55	2.52	18 (40%)	56,57,69	1.95	13 (23%)
25	HEM	E	84	5,6	30,50,50	3.02	15 (50%)	24,82,82	3.86	15 (62%)
28	BCR	F	48	-	41,41,41	1.97	8 (19%)	56,56,56	2.53	23 (41%)
28	BCR	J	53	-	41,41,41	1.89	6 (14%)	56,56,56	2.15	20 (35%)
28	BCR	K	50	-	41,41,41	2.06	17 (41%)	56,56,56	1.94	15 (26%)
25	HEM	V	138	16	30,50,50	5.60	16 (53%)	24,82,82	3.74	16 (66%)
21	BCT	a	2346	22	0,3,3	0.00	-	0,3,3	0.00	-
22	OEC	a	2347	1,3,21	0,13,13	0.00	-	0,27,27	0.00	-
23	CLA	a	2348	1	55,73,73	1.05	5 (9%)	61,113,113	1.50	13 (21%)
23	CLA	a	2349	-	55,73,73	0.95	1 (1%)	61,113,113	1.52	13 (21%)
24	PHO	a	2350	-	67,69,69	1.13	5 (7%)	84,99,99	1.31	10 (11%)
23	CLA	a	2351	1	55,73,73	1.12	4 (7%)	61,113,113	1.49	10 (16%)
26	PL9	a	2352	-	45,45,55	2.61	19 (42%)	56,57,69	2.53	18 (32%)
23	CLA	b	2511	2	55,73,73	1.21	6 (10%)	61,113,113	1.80	15 (24%)
23	CLA	b	2512	2	55,73,73	1.04	3 (5%)	61,113,113	1.58	11 (18%)
23	CLA	b	2513	2	55,73,73	1.13	4 (7%)	61,113,113	1.86	14 (22%)
23	CLA	b	2514	-	55,73,73	1.30	7 (12%)	61,113,113	1.75	14 (22%)
23	CLA	b	2515	2	55,73,73	1.13	5 (9%)	61,113,113	1.66	16 (26%)
23	CLA	b	2516	2	55,73,73	1.45	9 (16%)	61,113,113	1.63	13 (21%)
23	CLA	b	2517	2	55,73,73	1.03	5 (9%)	61,113,113	1.67	12 (19%)
23	CLA	b	2518	2	55,73,73	1.15	8 (14%)	61,113,113	1.71	10 (16%)
23	CLA	b	2519	2	55,73,73	1.33	6 (10%)	61,113,113	1.95	12 (19%)
23	CLA	b	2520	2	55,73,73	1.30	7 (12%)	61,113,113	2.29	10 (16%)
23	CLA	b	2521	2	55,73,73	1.15	5 (9%)	61,113,113	1.39	9 (14%)
23	CLA	b	2522	2	55,73,73	1.06	4 (7%)	61,113,113	1.53	13 (21%)
23	CLA	b	2523	2	55,73,73	1.19	7 (12%)	61,113,113	1.72	14 (22%)
23	CLA	b	2524	-	55,73,73	1.01	3 (5%)	61,113,113	1.65	12 (19%)
23	CLA	b	2525	2	55,73,73	1.14	5 (9%)	61,113,113	1.66	11 (18%)
23	CLA	b	2526	-	55,73,73	1.10	4 (7%)	61,113,113	1.68	12 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	BCR	b	2527	-	41,41,41	1.88	7 (17%)	56,56,56	2.27	20 (35%)
28	BCR	b	2528	-	41,41,41	2.03	8 (19%)	56,56,56	2.22	21 (37%)
23	CLA	c	2474	3	55,73,73	1.08	4 (7%)	61,113,113	1.67	12 (19%)
23	CLA	c	2475	-	55,73,73	1.47	10 (18%)	61,113,113	1.64	12 (19%)
23	CLA	c	2476	3	55,73,73	1.04	5 (9%)	61,113,113	1.49	9 (14%)
23	CLA	c	2477	3	55,73,73	1.17	4 (7%)	61,113,113	2.14	16 (26%)
23	CLA	c	2478	3	55,73,73	1.12	6 (10%)	61,113,113	1.59	12 (19%)
23	CLA	c	2479	3	55,73,73	1.12	5 (9%)	61,113,113	1.84	16 (26%)
23	CLA	c	2480	3	55,73,73	0.96	4 (7%)	61,113,113	1.57	10 (16%)
23	CLA	c	2481	3	55,73,73	0.97	5 (9%)	61,113,113	1.90	12 (19%)
23	CLA	c	2482	3	55,73,73	1.14	4 (7%)	61,113,113	1.49	11 (18%)
23	CLA	c	2483	3	55,73,73	1.18	5 (9%)	61,113,113	1.82	12 (19%)
23	CLA	c	2484	3	55,73,73	1.13	4 (7%)	61,113,113	1.47	11 (18%)
23	CLA	c	2485	-	55,73,73	1.09	4 (7%)	61,113,113	1.72	15 (24%)
23	CLA	c	2486	3	55,73,73	1.07	4 (7%)	61,113,113	1.62	12 (19%)
23	CLA	c	2487	-	55,73,73	1.22	7 (12%)	61,113,113	1.64	13 (21%)
28	BCR	c	2488	-	41,41,41	1.95	11 (26%)	56,56,56	1.99	18 (32%)
28	BCR	c	2489	-	41,41,41	1.91	8 (19%)	56,56,56	2.01	17 (30%)
21	BCT	d	2353	20	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	d	2354	4	55,73,73	0.98	3 (5%)	61,113,113	1.51	9 (14%)
23	CLA	d	2355	-	55,73,73	1.05	3 (5%)	61,113,113	1.65	13 (21%)
24	PHO	d	2356	-	67,69,69	1.02	3 (4%)	84,99,99	1.51	15 (17%)
23	CLA	d	2357	4	55,73,73	1.12	5 (9%)	61,113,113	1.44	10 (16%)
26	PL9	d	2358	-	45,45,55	2.60	18 (40%)	56,57,69	1.94	14 (25%)
27	LMT	d	2359	-	36,36,36	1.31	4 (11%)	47,47,47	1.78	8 (17%)
28	BCR	d	2360	-	41,41,41	1.98	8 (19%)	56,56,56	2.48	22 (39%)
25	HEM	e	2084	5,6	30,50,50	3.06	16 (53%)	24,82,82	3.68	10 (41%)
28	BCR	j	2053	-	41,41,41	2.13	8 (19%)	56,56,56	2.15	19 (33%)
28	BCR	k	2050	-	41,41,41	2.11	18 (43%)	56,56,56	1.91	14 (25%)
25	HEM	v	2138	16	30,50,50	3.80	18 (60%)	24,82,82	4.29	16 (66%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCT	A	346	22	-	0/0/0/0	0/0/0/0
22	OEC	A	347	1,3,21	-	0/0/54/54	0/3/5/5
23	CLA	A	348	1	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	A	349	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	A	350	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	A	351	-	-	0/53/103/103	0/1/6/6
23	CLA	A	352	1	3/3/20/25	0/37/135/135	0/0/9/9
26	PL9	A	353	-	-	0/41/61/73	0/1/1/1
23	CLA	B	511	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	512	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	513	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	514	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	515	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	516	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	517	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	518	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	519	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	520	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	521	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	522	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	523	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	524	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	525	2	3/3/20/25	0/37/135/135	0/0/9/9
27	LMT	B	526	-	-	0/21/61/61	0/2/2/2
23	CLA	B	527	-	3/3/20/25	0/37/135/135	0/0/9/9
28	BCR	B	528	-	-	0/29/63/63	0/2/2/2
28	BCR	B	529	-	-	0/29/63/63	0/2/2/2
23	CLA	C	474	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	475	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	476	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	477	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	478	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	479	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	480	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	481	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	482	3	3/3/20/25	0/37/135/135	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	483	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	484	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	485	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	486	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	487	-	3/3/20/25	0/37/135/135	0/0/9/9
28	BCR	C	488	-	-	0/29/63/63	0/2/2/2
28	BCR	C	489	-	-	0/29/63/63	0/2/2/2
21	BCT	D	353	20	-	0/0/0/0	0/0/0/0
23	CLA	D	354	4	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	D	355	-	-	0/53/103/103	0/1/6/6
23	CLA	D	356	4	3/3/20/25	0/37/135/135	0/0/9/9
26	PL9	D	357	-	-	0/41/61/73	0/1/1/1
25	HEM	E	84	5,6	-	0/10/54/54	0/0/8/8
28	BCR	F	48	-	-	0/29/63/63	0/2/2/2
28	BCR	J	53	-	-	0/29/63/63	0/2/2/2
28	BCR	K	50	-	-	0/29/63/63	0/2/2/2
25	HEM	V	138	16	-	0/10/54/54	0/0/8/8
21	BCT	a	2346	22	-	0/0/0/0	0/0/0/0
22	OEC	a	2347	1,3,21	-	0/0/54/54	0/3/5/5
23	CLA	a	2348	1	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	a	2349	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	a	2350	-	-	0/53/103/103	0/1/6/6
23	CLA	a	2351	1	3/3/20/25	0/37/135/135	0/0/9/9
26	PL9	a	2352	-	-	0/41/61/73	0/1/1/1
23	CLA	b	2511	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2512	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2513	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2514	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2515	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2516	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2517	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2518	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2519	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2520	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2521	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2522	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2523	2	3/3/20/25	0/37/135/135	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	2524	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2525	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	2526	-	3/3/20/25	0/37/135/135	0/0/9/9
28	BCR	b	2527	-	-	0/29/63/63	0/2/2/2
28	BCR	b	2528	-	-	0/29/63/63	0/2/2/2
23	CLA	c	2474	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2475	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2476	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2477	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2478	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2479	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2480	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2481	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2482	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2483	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2484	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2485	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2486	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	2487	-	3/3/20/25	0/37/135/135	0/0/9/9
28	BCR	c	2488	-	-	0/29/63/63	0/2/2/2
28	BCR	c	2489	-	-	0/29/63/63	0/2/2/2
21	BCT	d	2353	20	-	0/0/0/0	0/0/0/0
23	CLA	d	2354	4	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	d	2355	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	d	2356	-	-	0/53/103/103	0/1/6/6
23	CLA	d	2357	4	3/3/20/25	0/37/135/135	0/0/9/9
26	PL9	d	2358	-	-	0/41/61/73	0/1/1/1
27	LMT	d	2359	-	-	0/21/61/61	0/2/2/2
28	BCR	d	2360	-	-	0/29/63/63	0/2/2/2
25	HEM	e	2084	5,6	-	0/10/54/54	0/0/8/8
28	BCR	j	2053	-	-	0/29/63/63	0/2/2/2
28	BCR	k	2050	-	-	0/29/63/63	0/2/2/2
25	HEM	v	2138	16	-	0/10/54/54	0/0/8/8

The worst 5 of 650 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	v	2138	HEM	C3D-C4D	-7.90	1.41	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	v	2138	HEM	C3B-C4B	-7.44	1.45	1.51
25	e	2084	HEM	C2D-C3D	-6.18	1.36	1.54
26	d	2358	PL9	C53-C6	-5.28	1.39	1.50
26	D	357	PL9	C53-C6	-5.16	1.40	1.50

The worst 5 of 1333 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	E	84	HEM	C3B-CAB-CBB	-11.71	106.50	124.46
25	e	2084	HEM	C3B-CAB-CBB	-11.63	106.62	124.46
25	v	2138	HEM	C3B-CAB-CBB	-11.62	106.63	124.46
25	V	138	HEM	C3B-CAB-CBB	-10.38	108.53	124.46
25	v	2138	HEM	CAA-C2A-C1A	-7.18	119.21	127.01

5 of 216 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	B	520	CLA	NC
23	B	520	CLA	ND
23	B	520	CLA	NA
23	c	2478	CLA	NC
23	c	2478	CLA	ND

There are no torsion outliers.

There are no ring outliers.

50 monomers are involved in 359 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	347	OEC	1	0
23	A	348	CLA	14	0
23	A	349	CLA	5	0
23	A	350	CLA	10	0
24	A	351	PHO	6	0
23	A	352	CLA	1	0
26	A	353	PL9	8	0
23	B	511	CLA	5	0
23	B	512	CLA	7	0
23	B	513	CLA	7	0
23	B	514	CLA	4	0
23	B	515	CLA	8	0
23	B	516	CLA	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	517	CLA	3	0
23	B	518	CLA	16	0
23	B	519	CLA	7	0
23	B	520	CLA	10	0
23	B	521	CLA	9	0
23	B	522	CLA	12	0
23	B	523	CLA	7	0
23	B	524	CLA	22	0
23	B	525	CLA	7	0
23	B	527	CLA	5	0
28	B	528	BCR	3	0
28	B	529	BCR	13	0
23	C	474	CLA	11	0
23	C	475	CLA	5	0
23	C	476	CLA	4	0
23	C	477	CLA	8	0
23	C	478	CLA	6	0
23	C	479	CLA	13	0
23	C	480	CLA	6	0
23	C	481	CLA	4	0
23	C	482	CLA	6	0
23	C	483	CLA	11	0
23	C	484	CLA	1	0
23	C	485	CLA	10	0
23	C	486	CLA	18	0
23	C	487	CLA	17	0
28	C	488	BCR	12	0
28	C	489	BCR	11	0
23	D	354	CLA	10	0
24	D	355	PHO	8	0
23	D	356	CLA	8	0
26	D	357	PL9	5	0
25	E	84	HEM	16	0
28	F	48	BCR	3	0
28	J	53	BCR	2	0
28	K	50	BCR	13	0
25	V	138	HEM	10	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	333/344 (96%)	0.14	10 (3%) 54 43	33, 60, 91, 104	0
1	a	333/344 (96%)	-0.14	3 (0%) 85 78	39, 63, 92, 105	0
2	B	476/510 (93%)	-0.04	14 (2%) 55 45	39, 65, 89, 105	0
2	b	476/510 (93%)	-0.02	12 (2%) 61 50	39, 65, 89, 106	0
3	C	421/473 (89%)	-0.12	8 (1%) 70 60	34, 69, 89, 103	0
3	c	421/473 (89%)	-0.07	10 (2%) 62 52	36, 71, 90, 107	0
4	D	339/352 (96%)	-0.09	7 (2%) 67 58	22, 60, 92, 106	0
4	d	339/352 (96%)	-0.16	8 (2%) 62 52	31, 62, 92, 106	0
5	E	76/84 (90%)	-0.18	0 100 100	55, 76, 94, 107	0
5	e	76/84 (90%)	-0.13	3 (3%) 43 35	60, 79, 96, 107	0
6	F	33/45 (73%)	-0.42	0 100 100	49, 68, 92, 107	0
6	f	33/45 (73%)	-0.20	2 (6%) 25 19	49, 70, 92, 101	0
7	H	53/66 (80%)	-0.33	0 100 100	46, 73, 104, 106	0
7	h	53/66 (80%)	-0.29	3 (5%) 27 21	56, 74, 106, 109	0
8	I	38/38 (100%)	0.19	3 (7%) 15 13	60, 76, 100, 102	0
8	i	38/38 (100%)	-0.53	1 (2%) 59 49	59, 76, 100, 104	0
9	J	38/40 (95%)	-0.30	0 100 100	60, 79, 99, 103	0
9	j	38/40 (95%)	0.11	2 (5%) 30 23	61, 82, 98, 107	0
10	K	37/37 (100%)	-0.60	0 100 100	61, 71, 95, 95	0
10	k	37/37 (100%)	-0.25	0 100 100	65, 73, 96, 97	0
11	L	37/37 (100%)	-0.06	2 (5%) 29 23	39, 58, 101, 104	0
11	l	37/37 (100%)	0.14	1 (2%) 58 47	34, 61, 99, 101	0
12	M	30/36 (83%)	0.00	0 100 100	45, 56, 79, 88	0
12	m	30/36 (83%)	0.06	0 100 100	44, 56, 79, 88	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	246/246 (100%)	0.01	5 (2%) 68 59	41, 75, 100, 110	0
13	o	246/246 (100%)	0.21	16 (6%) 22 17	46, 75, 99, 107	0
14	T	31/32 (96%)	0.20	1 (3%) 51 42	27, 54, 86, 89	0
14	t	31/32 (96%)	-0.42	0 100 100	32, 53, 90, 93	0
15	U	105/134 (78%)	0.04	2 (1%) 70 60	41, 67, 91, 104	0
15	u	105/134 (78%)	-0.14	2 (1%) 70 60	46, 68, 92, 103	0
16	V	137/137 (100%)	-0.30	0 100 100	42, 66, 80, 88	0
16	v	137/137 (100%)	0.00	5 (3%) 46 37	46, 70, 85, 90	0
17	X	40/50 (80%)	-0.09	4 (10%) 9 9	67, 74, 102, 109	0
17	x	40/50 (80%)	0.21	3 (7%) 17 14	67, 77, 104, 108	0
18	N	0/37	-	-	-	-
18	n	0/37	-	-	-	-
19	Z	58/62 (93%)	-0.32	1 (1%) 73 64	62, 80, 93, 102	0
19	z	58/62 (93%)	0.31	7 (12%) 6 6	70, 81, 94, 106	0
All	All	5056/5520 (91%)	-0.06	135 (2%) 58 47	22, 68, 95, 110	0

The worst 5 of 135 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	a	2026	ASN	6.9
8	I	25	SER	6.6
1	A	264	SER	5.6
16	v	2100	ILE	5.4
4	D	242	GLU	5.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
23	CLA	C	487	65/65	0.57	0.78	8.16	87,101,114,118	0
28	BCR	K	50	40/40	0.67	0.61	7.85	79,85,96,101	0
28	BCR	C	489	40/40	0.73	0.49	6.64	85,90,100,100	0
28	BCR	b	2527	40/40	0.74	0.44	5.49	64,78,84,86	0
28	BCR	k	2050	40/40	0.64	0.72	4.99	80,85,97,101	0
28	BCR	c	2488	40/40	0.76	0.71	4.88	76,84,93,96	0
28	BCR	B	528	40/40	0.73	0.41	4.47	63,79,85,87	0
26	PL9	D	357	45/55	0.75	0.42	4.32	71,80,86,88	0
28	BCR	F	48	40/40	0.76	0.37	3.80	66,80,91,92	0
23	CLA	c	2487	65/65	0.52	0.63	3.60	88,101,114,118	0
28	BCR	d	2360	40/40	0.75	0.39	3.35	67,79,91,93	0
28	BCR	C	488	40/40	0.83	0.42	3.28	75,83,92,95	0
23	CLA	b	2526	65/65	0.82	0.45	2.87	82,89,106,110	0
28	BCR	B	529	40/40	0.39	0.69	2.53	76,93,105,106	0
23	CLA	b	2517	65/65	0.89	0.47	2.48	64,71,80,89	0
23	CLA	C	481	65/65	0.87	0.36	2.47	54,60,84,88	0
27	LMT	d	2359	35/35	0.77	0.38	2.42	73,82,91,92	0
23	CLA	d	2355	65/65	0.90	0.40	2.35	19,32,75,86	0
23	CLA	B	516	65/65	0.84	0.37	2.34	44,55,92,93	0
23	CLA	c	2486	65/65	0.76	0.50	2.33	79,84,92,94	0
23	CLA	a	2349	65/65	0.87	0.33	2.06	36,54,93,95	0
23	CLA	b	2516	65/65	0.91	0.28	2.05	42,54,93,94	0
28	BCR	b	2528	40/40	0.62	0.57	2.03	77,92,105,106	0
26	PL9	d	2358	45/55	0.73	0.40	1.95	70,80,87,89	0
23	CLA	b	2521	65/65	0.85	0.39	1.85	67,71,80,82	0
28	BCR	c	2489	40/40	0.70	0.51	1.85	85,90,100,100	0
23	CLA	C	480	65/65	0.84	0.48	1.83	64,79,82,87	0
26	PL9	a	2352	45/55	0.68	0.45	1.81	77,85,90,91	0
23	CLA	B	527	65/65	0.79	0.43	1.80	84,89,106,109	0
23	CLA	C	475	65/65	0.86	0.38	1.79	66,80,97,103	0
23	CLA	c	2477	65/65	0.82	0.44	1.78	73,79,98,101	0
23	CLA	C	485	65/65	0.81	0.39	1.78	64,75,91,95	0
23	CLA	b	2519	65/65	0.90	0.43	1.76	60,66,90,91	0
23	CLA	B	518	65/65	0.91	0.39	1.75	51,61,86,89	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	c	2485	65/65	0.86	0.46	1.69	61,75,90,94	0
23	CLA	a	2348	65/65	0.93	0.32	1.62	44,50,65,69	0
23	CLA	A	352	65/65	0.79	0.36	1.59	48,65,101,102	0
25	HEM	V	138	43/43	0.95	0.27	1.58	44,49,56,57	0
23	CLA	B	511	65/65	0.88	0.41	1.48	58,81,92,97	0
27	LMT	B	526	35/35	0.83	0.39	1.43	72,82,90,91	0
23	CLA	B	524	65/65	0.88	0.54	1.36	56,68,75,88	0
25	HEM	e	2084	43/43	0.89	0.47	1.32	75,79,100,108	0
23	CLA	B	519	65/65	0.82	0.46	1.30	58,67,90,91	0
23	CLA	d	2354	65/65	0.94	0.29	1.29	40,47,75,80	0
23	CLA	c	2483	65/65	0.85	0.31	1.26	68,74,100,106	0
24	PHO	D	355	64/64	0.87	0.32	1.23	62,69,103,111	0
23	CLA	c	2475	65/65	0.85	0.33	1.23	66,80,97,102	0
23	CLA	C	482	65/65	0.79	0.42	1.22	71,80,97,98	0
23	CLA	C	476	65/65	0.85	0.33	1.18	49,62,75,78	0
23	CLA	a	2351	65/65	0.84	0.27	1.16	50,66,101,102	0
23	CLA	c	2478	65/65	0.91	0.50	1.11	55,66,87,92	0
23	CLA	C	483	65/65	0.70	0.42	1.11	67,73,101,106	0
23	CLA	b	2513	65/65	0.88	0.29	1.10	45,57,102,106	0
24	PHO	a	2350	64/64	0.82	0.35	1.07	56,66,81,82	0
26	PL9	A	353	45/55	0.62	0.57	1.04	77,86,91,92	0
23	CLA	b	2511	65/65	0.82	0.39	1.02	58,81,92,97	0
23	CLA	C	486	65/65	0.88	0.31	0.99	78,84,91,95	0
23	CLA	D	354	65/65	0.92	0.33	0.97	42,46,76,81	0
23	CLA	D	356	65/65	0.87	0.28	0.89	69,77,90,95	0
23	CLA	d	2357	65/65	0.80	0.37	0.88	68,77,91,95	0
23	CLA	b	2518	65/65	0.89	0.37	0.87	53,60,86,88	0
23	CLA	b	2514	65/65	0.87	0.38	0.85	59,67,79,82	0
24	PHO	d	2356	64/64	0.86	0.32	0.80	62,70,103,111	0
23	CLA	B	514	65/65	0.80	0.38	0.78	60,67,79,82	0
23	CLA	c	2479	65/65	0.89	0.44	0.76	57,76,80,84	0
23	CLA	C	479	65/65	0.91	0.33	0.75	57,76,80,83	0
23	CLA	B	517	65/65	0.89	0.40	0.75	65,71,79,89	0
23	CLA	b	2525	65/65	0.83	0.30	0.71	73,80,89,91	0
23	CLA	c	2480	65/65	0.87	0.39	0.70	65,80,82,87	0
23	CLA	b	2522	65/65	0.88	0.44	0.67	69,75,87,88	0
23	CLA	c	2476	65/65	0.85	0.28	0.64	50,64,75,78	0
23	CLA	B	513	65/65	0.93	0.37	0.63	46,57,102,106	0
23	CLA	c	2481	65/65	0.87	0.33	0.59	55,60,85,89	0
23	CLA	C	484	65/65	0.78	0.39	0.58	76,87,101,102	0
23	CLA	B	512	65/65	0.93	0.26	0.55	37,50,63,67	0
23	CLA	C	478	65/65	0.91	0.40	0.53	55,65,87,91	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	b	2524	65/65	0.88	0.44	0.52	56,68,76,89	0
25	HEM	E	84	43/43	0.95	0.31	0.47	64,79,100,108	0
23	CLA	c	2474	65/65	0.87	0.30	0.46	70,76,88,89	0
23	CLA	B	521	65/65	0.85	0.33	0.44	67,72,80,81	0
23	CLA	A	349	65/65	0.93	0.35	0.43	19,31,76,86	0
23	CLA	A	348	65/65	0.93	0.34	0.38	44,50,65,70	0
23	CLA	b	2512	65/65	0.91	0.26	0.24	34,50,63,66	0
23	CLA	C	477	65/65	0.84	0.31	0.08	71,79,97,100	0
25	HEM	v	2138	43/43	0.94	0.25	0.06	40,50,55,57	0
23	CLA	A	350	65/65	0.87	0.37	0.05	36,52,92,95	0
23	CLA	b	2520	65/65	0.85	0.31	0.05	61,68,78,79	0
23	CLA	B	523	65/65	0.88	0.29	-0.05	60,64,94,109	0
23	CLA	B	515	65/65	0.87	0.28	-0.05	45,66,84,87	0
23	CLA	B	522	65/65	0.90	0.27	-0.06	71,75,87,88	0
23	CLA	B	520	65/65	0.85	0.28	-0.06	63,68,79,79	0
24	PHO	A	351	64/64	0.91	0.26	-0.10	55,65,80,82	0
23	CLA	b	2523	65/65	0.88	0.27	-0.12	59,64,94,108	0
23	CLA	C	474	65/65	0.86	0.24	-0.14	69,76,87,89	0
23	CLA	B	525	65/65	0.87	0.27	-0.20	72,80,89,92	0
23	CLA	c	2482	65/65	0.86	0.40	-0.24	72,81,97,98	0
23	CLA	c	2484	65/65	0.81	0.32	-0.27	77,87,101,102	0
21	BCT	D	353	4/4	0.96	0.20	-0.34	66,66,69,69	0
23	CLA	b	2515	65/65	0.90	0.24	-0.54	43,66,84,87	0
21	BCT	a	2346	4/4	0.93	0.22	-0.92	71,72,73,76	0
21	BCT	A	346	4/4	0.97	0.18	-1.65	70,70,71,74	0
21	BCT	d	2353	4/4	0.97	0.13	-1.66	66,68,69,69	0
22	OEC	A	347	9/9	0.93	0.21	-1.92	66,69,73,74	0
20	FE	A	345	1/1	0.97	0.11	-2.05	58,58,58,58	0
22	OEC	a	2347	9/9	0.94	0.17	-2.15	68,70,74,75	0
20	FE	a	2345	1/1	0.91	0.10	-2.18	67,67,67,67	0
28	BCR	J	53	40/40	0.70	0.51	-	70,88,100,100	0
28	BCR	j	2053	40/40	0.73	0.51	-	71,87,100,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.