



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 06:22 PM GMT

PDB ID : 2WSF
Title : Improved Model of Plant Photosystem I
Authors : Amunts, A.; Toporik, H.; Borovikov, A.; Nelson, N.
Deposited on : 2009-09-05
Resolution : 3.48 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>

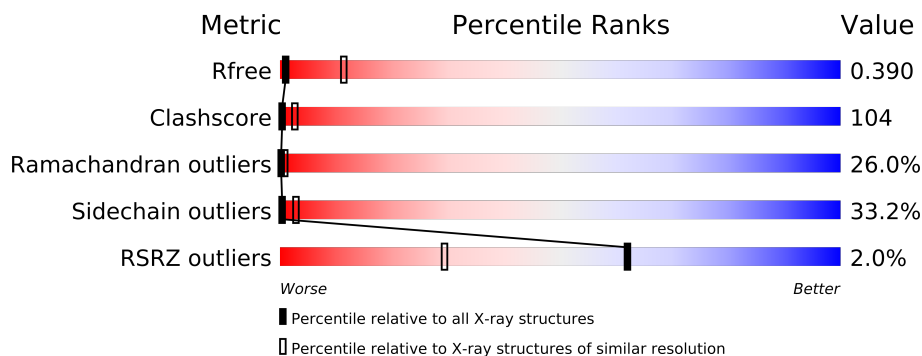
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.48 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	1175 (3.66-3.30)
Clashscore	79885	1001 (3.62-3.34)
Ramachandran outliers	78287	1001 (3.64-3.32)
Sidechain outliers	78261	1002 (3.64-3.32)
RSRZ outliers	66119	1175 (3.66-3.30)

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	1	241	
2	2	269	
3	3	276	
4	4	251	
5	A	758	
6	B	734	
7	C	81	
8	D	212	
9	E	143	
10	F	231	
11	G	167	
12	H	144	
13	I	40	
14	J	44	

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Mol	Chain	Length	Quality of chain
15	K	131	
16	L	216	
17	N	170	
18	R	53	

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	CLA	1	1197	-	X
19	CLA	1	1307	-	X
19	CLA	2	1220	-	X
19	CLA	3	3014	-	X
19	CLA	4	1200	-	X
19	CLA	A	1775	-	X
19	CLA	A	1798	-	X
19	CLA	A	1799	-	X
19	CLA	A	1801	-	X
20	LMU	A	7010	-	X
20	LMU	A	7033	-	X
23	BCR	A	1803	-	X
23	BCR	A	1804	-	X
23	BCR	A	1806	-	X

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 36033 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 AT3G54890.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	165	Total	C	N	O	S	0	0	0
			1264	822	208	230	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	-33	ILE	LYS	CONFLICT	UNP Q9C5R7
1	-1	ARG	LYS	CONFLICT	UNP Q9C5R7

- Molecule 2 is a protein called TYPE II CHLOROPHYLL A/B BINDING PROTEIN FROM PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	176	Total	C	N	O	S	0	0	0
			1374	899	226	245	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	195	ALA	-	INSERTION	UNP Q41038
2	.	-	GLY	DELETION	UNP Q41038

- Molecule 3 is a protein called LHCA3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	153	Total	C	N	O	S	0	0	0
			1186	781	193	207	5			

- Molecule 4 is a protein called CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	166	Total	C	N	O	S	0	0	0
			1319	861	219	236	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	.	-	ALA	DELETION	UNP Q9SQL2

- Molecule 5 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	730	Total	C	N	O	S	0	0	0
			5745	3766	974	987	18			

- Molecule 6 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	733	Total	C	N	O	S	0	0	0
			5848	3843	997	995	13			

- Molecule 7 is a protein called PHOTOSYSTEM I IRON-SULFUR CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	C	81	Total	C	N	O	S	0	0	0
			619	384	108	115	12			

- Molecule 8 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	D	138	Total	C	N	O	S	0	0	0
			1095	704	189	198	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-52	GLY	ALA	CONFLICT	UNP P12353
D	-50	PRO	GLN	CONFLICT	UNP P12353
D	-44	ARG	PRO	CONFLICT	UNP P12353
D	-34	GLU	ASP	CONFLICT	UNP P12353
D	-11	LEU	HIS	CONFLICT	UNP P12353

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	THR	SER	CONFLICT	UNP P12353
D	12	THR	PRO	CONFLICT	UNP P12353
D	14	ALA	GLY	CONFLICT	UNP P12353

- Molecule 9 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	E	65	Total	C	N	O	0	0	0
			520	332	93	95			

- Molecule 10 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	F	154	Total	C	N	O	S	0	0	0
			1221	794	207	217	3			

- Molecule 11 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	G	95	Total	C	N	O	S	0	0	0
			740	481	120	137	2			

- Molecule 12 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	H	69	Total	C	N	O	0	0	0
			529	344	82	103			

- Molecule 13 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	I	30	Total	C	N	O	S	0	0	0
			229	158	34	35	2			

- Molecule 14 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	J	42	Total	C	N	O	S	0	0	0
			338	230	51	56	1			

- Molecule 15 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	K	84	Total	C	N	O	S	0	0	0
			593	374	102	113	4			

- Molecule 16 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	L	162	Total	C	N	O	S	0	0	0
			1215	800	194	216	5			

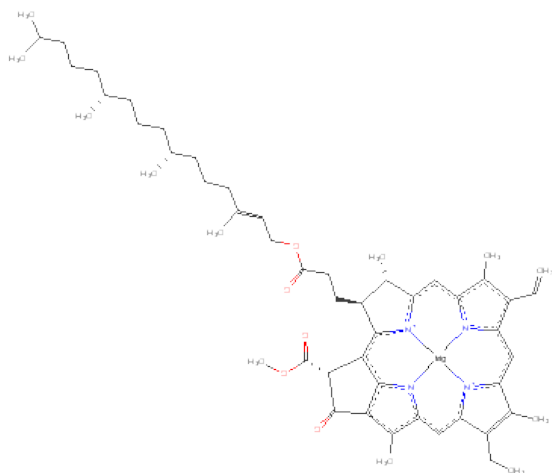
- Molecule 17 is a protein called PHOTOSYSTEM I-N SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	N	85	Total	C	N	O	S	0	0	0
			685	436	113	132	4			

- Molecule 18 is a protein called PHOTOSYSTEM I-N SUBUNIT.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	53	Total	C	N	O	0	0	0
			265	159	53	53			

- Molecule 19 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
19	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	1	1	Total	C	Mg	N		0	0
			25	20	1	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	2	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
19	3	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	A	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
19	B	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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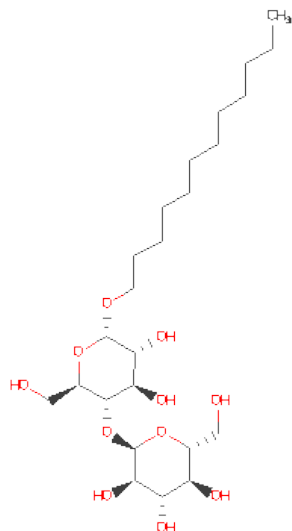
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	F	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	F	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
19	F	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
19	G	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	I	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	R	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
19	R	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N		0	0
			25	20	1	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	1	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
19	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		

- Molecule 20 is DODECYL-ALPHA-D-MALTOSE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	2	1	Total	C	O	0	0
			35	24	11		
20	4	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	B	1	Total	C	O	0	0
			25	14	11		
20	L	1	Total	C	O	0	0
			35	24	11		
20	R	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			34	23	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		

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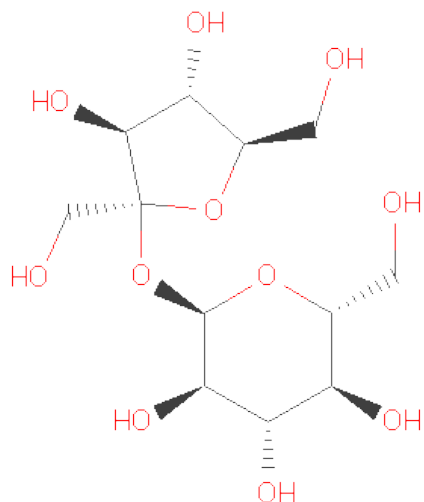
[illegible]

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		
20	A	1	Total	C	O	0	0
			35	24	11		

- Molecule 21 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: C₁₂H₂₂O₁₁).



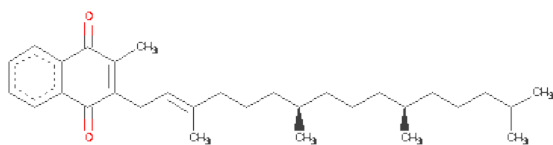
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	2	1	Total	C	O	0	0
			22	12	10		
21	3	1	Total	C	O	0	0
			23	12	11		
21	H	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			22	12	10		

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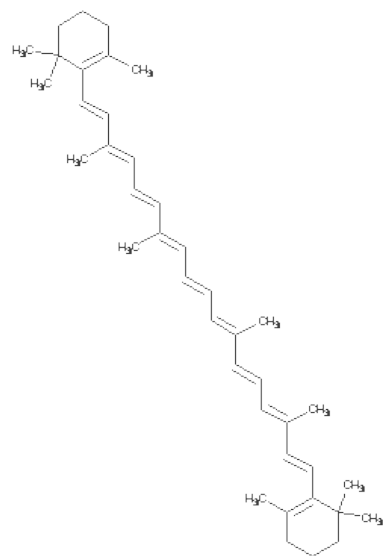
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		
21	B	1	Total	C	O	0	0
			23	12	11		

- Molecule 22 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	C	O	0	0
			33	31	2		
22	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 23 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



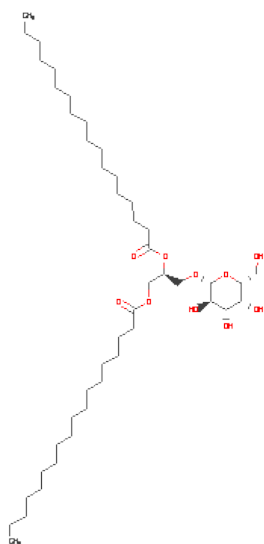
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C 40 40	0	0
23	A	1	Total C 40 40	0	0
23	A	1	Total C 40 40	0	0
23	A	1	Total C 40 40	0	0
23	A	1	Total C 39 39	0	0
23	A	1	Total C 40 40	0	0
23	A	1	Total C 40 40	0	0
23	B	1	Total C 40 40	0	0
23	B	1	Total C 40 40	0	0
23	B	1	Total C 40 40	0	0
23	B	1	Total C 40 40	0	0
23	B	1	Total C 40 40	0	0
23	B	1	Total C 40 40	0	0
23	B	1	Total C 40 40	0	0

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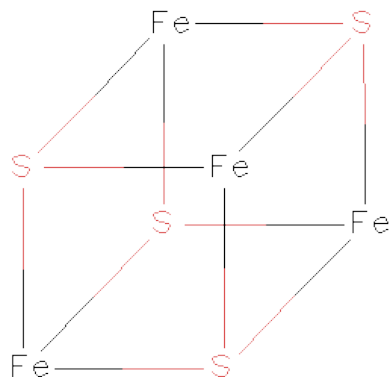
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	I	1	Total C 40 40	0	0
23	L	1	Total C 40 40	0	0

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	B	1	Total C O 49 39 10	0	0

- Molecule 25 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	Fe	S	0	0
			8	4	4		
25	C	1	Total	Fe	S	0	0
			8	4	4		
25	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 26 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

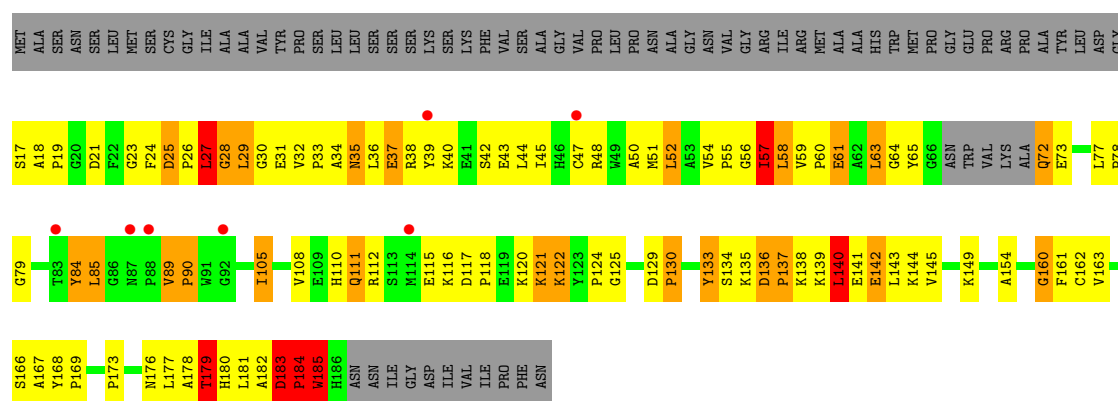
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	B	1	Total	C	O	0	0
			23	12	11		

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.

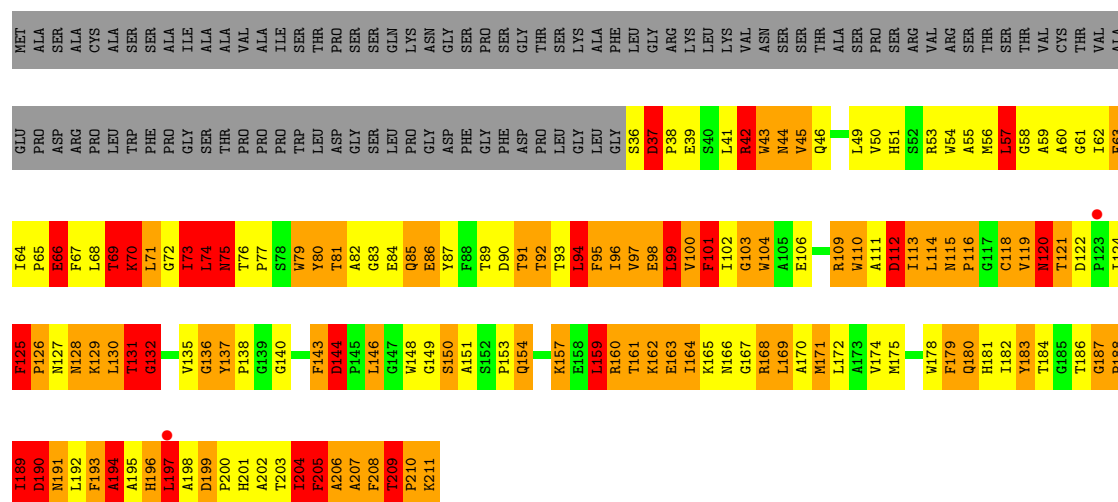
• Molecule 1: AT3G54890

Chain 1: 



• Molecule 2: TYPE II CHLOROPHYLL A/B BINDING PROTEIN FROM PHOTOSYSTEM I

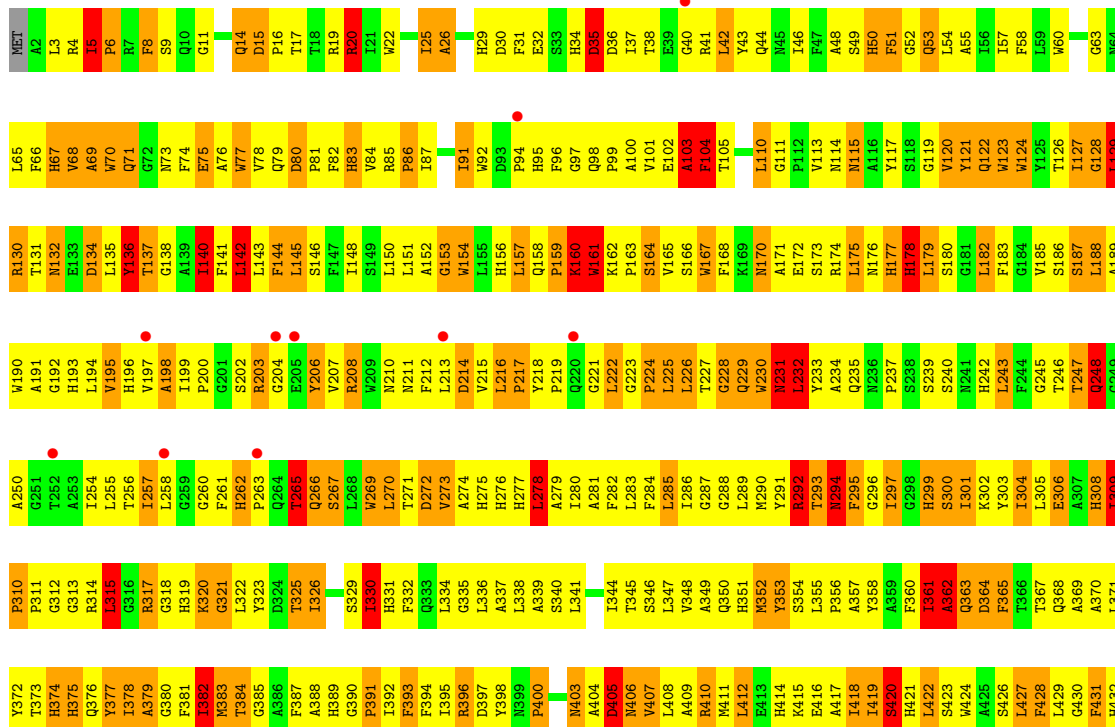
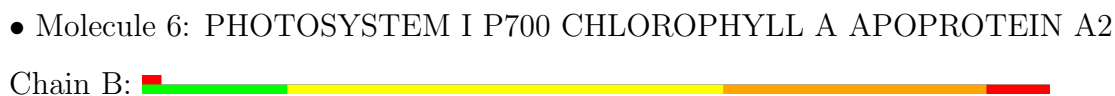
Chain 2: 

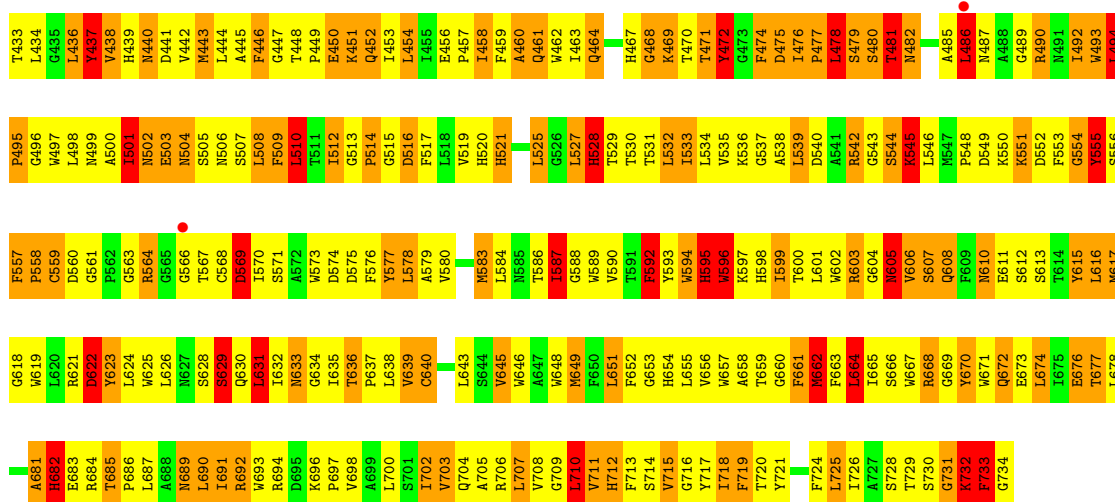


• Molecule 3: LHCA3

Chain 3: 

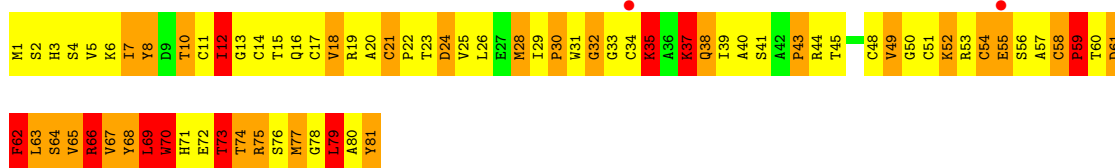






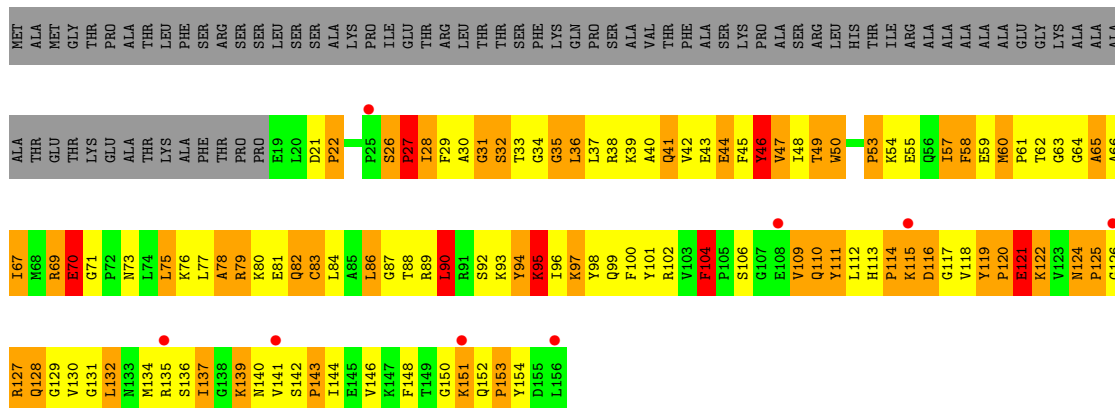
- Molecule 7: PHOTOSYSTEM I IRON-SULFUR CENTER

Chain C:



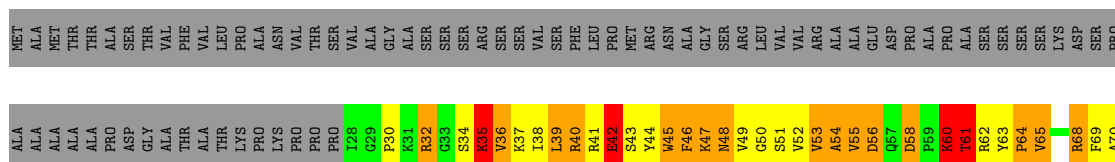
- Molecule 8: PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC

Chain D:



● Molecule 9: PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC

Chain E: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.20Å 190.20Å 130.30Å 90.00° 91.53° 90.00°	Depositor
Resolution (Å)	50.00 – 3.48 49.46 – 3.47	Depositor EDS
% Data completeness (in resolution range)	96.4 (50.00-3.48) 96.2 (49.46-3.47)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.391 , 0.425 0.388 , 0.390	Depositor DCC
R_{free} test set	1456 reflections (2.05%)	DCC
Wilson B-factor (Å ²)	81.0	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.09 , -10.0	EDS
Estimated twinning fraction	0.016 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 72533 reflections	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	36033	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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: SUC, SF4, CLA, PQN, LMU, UNL, BCR, LMG

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	1	0.55	1/1303 (0.1%)	0.73	1/1774 (0.1%)
2	2	0.67	0/1420	1.10	7/1943 (0.4%)
3	3	0.60	0/1221	0.91	2/1642 (0.1%)
4	4	0.77	0/1359	1.12	10/1851 (0.5%)
5	A	0.61	1/5938 (0.0%)	0.88	9/8104 (0.1%)
6	B	0.58	0/6058	0.86	8/8278 (0.1%)
7	C	0.78	0/632	1.05	1/856 (0.1%)
8	D	0.71	0/1122	0.91	0/1514
9	E	0.70	0/530	0.95	1/718 (0.1%)
10	F	0.67	0/1250	0.88	0/1687
11	G	0.84	1/760 (0.1%)	1.20	7/1031 (0.7%)
12	H	0.70	0/543	1.02	0/741
13	I	0.62	0/235	0.80	0/320
14	J	0.65	0/349	0.91	0/475
15	K	0.65	1/599 (0.2%)	0.88	1/810 (0.1%)
16	L	0.69	1/1251 (0.1%)	0.94	2/1709 (0.1%)
17	N	0.89	0/699	1.22	5/936 (0.5%)
All	All	0.65	5/25269 (0.0%)	0.93	54/34389 (0.2%)

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	1	0	3
2	2	0	17
3	3	0	17
4	4	0	20
5	A	0	20
6	B	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	C	0	1
8	D	0	1
9	E	0	3
10	F	0	7
11	G	1	13
12	H	0	9
15	K	0	6
16	L	0	2
17	N	0	22
18	R	0	16
All	All	1	169

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	165	TYR	CE2-CZ	-6.04	1.30	1.38
11	G	15	SER	CB-OG	5.83	1.49	1.42
1	1	185	TRP	CB-CG	-5.34	1.40	1.50
15	K	41	GLU	CG-CD	5.15	1.59	1.51
5	A	22	VAL	CA-CB	-5.05	1.44	1.54

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	180	LYS	C-N-CA	-10.34	95.85	121.70
11	G	46	ALA	N-CA-C	-10.20	83.47	111.00
6	B	731	GLY	N-CA-C	-7.75	93.73	113.10
11	G	16	LEU	CA-CB-CG	7.25	131.98	115.30
6	B	315	LEU	CA-CB-CG	7.00	131.41	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	G	21	PHE	CA

5 of 169 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	184	PRO	Peptide
1	1	185	TRP	Peptide
1	1	72	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	2	42	ARG	Peptide
2	2	73	ILE	Peptide

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	1	1264	0	1229	137	3
2	2	1374	0	1331	301	2
3	3	1186	0	1147	291	6
4	4	1319	0	1282	609	3
5	A	5745	0	5597	1350	0
6	B	5848	0	5655	1211	5
7	C	619	0	608	204	0
8	D	1095	0	1112	189	0
9	E	520	0	528	128	0
10	F	1221	0	1249	201	0
11	G	740	0	708	190	1
12	H	529	0	514	106	0
13	I	229	0	252	55	0
14	J	338	0	340	64	0
15	K	593	0	619	110	0
16	L	1215	0	1222	311	3
17	N	685	0	668	320	1
18	R	265	0	68	78	0
19	1	1072	0	710	174	1
19	2	596	0	409	136	0
19	3	604	0	376	84	0
19	4	759	0	514	177	0
19	A	2610	0	2341	814	0
19	B	2157	0	1981	654	0
19	F	130	0	86	17	0
19	G	51	0	40	4	0
19	H	163	0	140	43	0
19	I	60	0	58	12	0
19	J	61	0	60	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	L	97	0	72	36	0
19	R	122	0	123	14	0
20	2	35	0	46	29	0
20	4	35	0	46	1	0
20	A	1503	0	1967	302	18
20	B	25	0	23	1	0
20	L	35	0	46	1	0
20	R	35	0	46	9	1
21	2	22	0	19	10	0
21	3	23	0	22	6	0
21	B	229	0	217	35	17
21	H	23	0	22	14	0
22	A	33	0	46	7	0
22	B	33	0	46	28	0
23	A	279	0	375	178	0
23	B	280	0	378	155	0
23	I	40	0	54	38	0
23	L	40	0	54	36	0
24	B	49	0	71	17	0
25	B	8	0	0	17	0
25	C	16	0	0	5	0
26	B	23	0	0	1	0
All	All	36033	0	34517	7355	31

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 104.

The worst 5 of 7355 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:4:160:MET:CE	19:4:1201:CLA:HBB2	1.18	1.65
4:4:69:ILE:HD11	4:4:175:LYS:CB	1.26	1.65
3:3:97:PHE:CD2	3:3:98:ILE:HG23	1.33	1.62
1:1:185:TRP:CH2	19:1:1199:CLA:H12	1.38	1.59
3:3:97:PHE:CE2	3:3:98:ILE:HD13	1.42	1.55

The worst 5 of 31 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	Distance(Å)	Clash(Å)
20:A:7008:LMU:C5B	21:B:8062:SUC:O1[1_654]	0.08	2.12
3:3:180:LYS:CD	6:B:490:ARG:CZ[1_556]	0.31	1.89
3:3:180:LYS:NZ	6:B:490:ARG:CD[1_556]	0.56	1.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:7008:LMU:O4'	21:B:8062:SUC:O2[1.654]	1.01	1.19
3:3:180:LYS:CG	6:B:490:ARG:NE[1.556]	1.05	1.15

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	1	161/241 (67%)	84 (52%)	39 (24%)	38 (24%)	0	1
2	2	174/269 (65%)	67 (38%)	51 (29%)	56 (32%)	0	0
3	3	145/276 (52%)	76 (52%)	36 (25%)	33 (23%)	0	1
4	4	164/251 (65%)	57 (35%)	44 (27%)	63 (38%)	0	0
5	A	726/758 (96%)	366 (50%)	187 (26%)	173 (24%)	0	1
6	B	731/734 (100%)	379 (52%)	204 (28%)	148 (20%)	0	2
7	C	79/81 (98%)	23 (29%)	31 (39%)	25 (32%)	0	0
8	D	136/212 (64%)	47 (35%)	48 (35%)	41 (30%)	0	0
9	E	63/143 (44%)	30 (48%)	15 (24%)	18 (29%)	0	0
10	F	152/231 (66%)	71 (47%)	40 (26%)	41 (27%)	0	1
11	G	93/167 (56%)	38 (41%)	27 (29%)	28 (30%)	0	0
12	H	67/144 (46%)	30 (45%)	16 (24%)	21 (31%)	0	0
13	I	28/40 (70%)	11 (39%)	10 (36%)	7 (25%)	0	1
14	J	40/44 (91%)	19 (48%)	11 (28%)	10 (25%)	0	1
15	K	82/131 (63%)	50 (61%)	13 (16%)	19 (23%)	0	1
16	L	160/216 (74%)	72 (45%)	49 (31%)	39 (24%)	0	1
17	N	83/170 (49%)	21 (25%)	19 (23%)	43 (52%)	0	0
All	All	3084/4108 (75%)	1441 (47%)	840 (27%)	803 (26%)	0	1

5 of 803 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	25	ASP

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Mol	Chain	Res	Type
1	1	30	GLY
1	1	35	ASN
1	1	58	LEU
1	1	73	GLU

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	1	127/190 (67%)	100 (79%)	27 (21%)	1	8
2	2	140/216 (65%)	81 (58%)	59 (42%)	0	1
3	3	112/215 (52%)	76 (68%)	36 (32%)	0	3
4	4	138/201 (69%)	85 (62%)	53 (38%)	0	1
5	A	592/618 (96%)	410 (69%)	182 (31%)	0	4
6	B	598/600 (100%)	397 (66%)	201 (34%)	0	2
7	C	70/70 (100%)	41 (59%)	29 (41%)	0	1
8	D	118/173 (68%)	82 (70%)	36 (30%)	0	4
9	E	56/114 (49%)	38 (68%)	18 (32%)	0	3
10	F	127/190 (67%)	80 (63%)	47 (37%)	0	2
11	G	79/144 (55%)	53 (67%)	26 (33%)	0	3
12	H	57/115 (50%)	30 (53%)	27 (47%)	0	0
13	I	26/36 (72%)	22 (85%)	4 (15%)	4	23
14	J	36/39 (92%)	25 (69%)	11 (31%)	0	4
15	K	61/102 (60%)	43 (70%)	18 (30%)	0	4
16	L	125/169 (74%)	88 (70%)	37 (30%)	0	4
17	N	74/139 (53%)	43 (58%)	31 (42%)	0	1
All	All	2536/3331 (76%)	1694 (67%)	842 (33%)	0	3

5 of 842 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	121	TYR

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Mol	Chain	Res	Type
6	B	438	VAL
16	L	14	LEU
6	B	142	LEU
6	B	278	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	67	HIS
6	B	333	GLN
15	K	80	ASN
6	B	71	GLN
6	B	193	HIS

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 257 ligands modelled in this entry, 1 is unknown - leaving 256 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
19	CLA	1	1014	-	59,59,73	3.01	17 (28%)	77,96,113	4.41	33 (42%)
19	CLA	1	1142	-	53,54,73	3.06	14 (26%)	71,90,113	4.72	28 (39%)
19	CLA	1	1143	-	58,58,73	2.98	16 (27%)	75,95,113	4.56	31 (41%)
19	CLA	1	1145	-	62,63,73	2.82	16 (25%)	81,101,113	4.72	39 (48%)
19	CLA	1	1146	-	58,58,73	3.11	17 (29%)	75,95,113	4.58	35 (46%)
19	CLA	1	1148	-	62,63,73	2.90	14 (22%)	81,101,113	4.37	32 (39%)
19	CLA	1	1149	-	52,54,73	2.12	14 (26%)	68,90,113	4.04	38 (55%)
19	CLA	1	1187	1	53,54,73	3.08	16 (30%)	71,90,113	4.71	38 (53%)
19	CLA	1	1188	-	48,49,73	3.09	13 (27%)	64,84,113	4.66	31 (48%)
19	CLA	1	1189	-	54,55,73	3.30	19 (35%)	72,91,113	4.98	33 (45%)
19	CLA	1	1190	-	53,54,73	3.36	20 (37%)	71,90,113	4.89	36 (50%)
19	CLA	1	1191	-	41,44,73	2.18	11 (26%)	51,78,113	3.79	23 (45%)
19	CLA	1	1192	-	69,69,73	2.74	15 (21%)	89,108,113	3.83	34 (38%)
19	CLA	1	1193	-	59,59,73	3.02	18 (30%)	77,96,113	4.51	36 (46%)
19	CLA	1	1194	-	23,32,73	6.62	14 (60%)	12,54,113	3.95	7 (58%)
19	CLA	1	1195	-	23,32,73	6.52	14 (60%)	12,54,113	3.68	8 (66%)
19	CLA	1	1196	1	41,44,73	2.11	11 (26%)	51,78,113	3.54	24 (47%)
19	CLA	1	1197	-	59,59,73	3.26	18 (30%)	77,96,113	5.07	39 (50%)
19	CLA	1	1198	-	23,32,73	6.28	15 (65%)	12,54,113	4.13	7 (58%)
19	CLA	1	1199	-	59,59,73	3.34	23 (38%)	77,96,113	4.89	35 (45%)
19	CLA	1	1200	-	23,32,73	6.04	14 (60%)	12,54,113	4.30	8 (66%)
19	CLA	1	1307	-	23,32,73	6.49	14 (60%)	12,54,113	3.86	7 (58%)
19	CLA	1	1308	-	55,56,73	3.06	14 (25%)	73,92,113	4.48	29 (39%)
19	CLA	1	1309	-	23,32,73	6.66	13 (56%)	12,54,113	4.15	8 (66%)
19	CLA	1	1505	-	62,63,73	2.75	14 (22%)	81,101,113	4.50	34 (41%)
19	CLA	2	1212	-	59,59,73	3.25	19 (32%)	77,96,113	4.66	32 (41%)
19	CLA	2	1213	-	65,66,73	3.05	18 (27%)	85,104,113	4.57	37 (43%)
19	CLA	2	1214	-	23,32,73	5.62	14 (60%)	12,54,113	4.45	7 (58%)
19	CLA	2	1215	-	58,58,73	2.88	14 (24%)	75,95,113	4.17	31 (41%)
19	CLA	2	1216	-	23,32,73	5.49	14 (60%)	12,54,113	4.42	6 (50%)
19	CLA	2	1217	-	73,73,73	2.68	15 (20%)	95,113,113	3.83	31 (32%)
19	CLA	2	1218	-	23,32,73	5.70	13 (56%)	12,54,113	4.65	7 (58%)
19	CLA	2	1219	-	41,44,73	2.13	10 (24%)	51,78,113	3.70	24 (47%)
19	CLA	2	1220	-	23,32,73	5.93	13 (56%)	12,54,113	4.08	6 (50%)
19	CLA	2	1221	2	58,58,73	3.30	20 (34%)	75,95,113	4.61	33 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	2	1222	-	58,58,73	2.91	14 (24%)	75,95,113	4.59	31 (41%)
19	CLA	2	1223	-	69,69,73	2.88	17 (24%)	89,108,113	4.36	41 (46%)
20	LMU	2	1224	-	36,36,36	0.50	0	47,47,47	1.70	6 (12%)
21	SUC	2	1225	-	22,23,24	0.75	1 (4%)	33,35,36	1.45	6 (18%)
19	CLA	2	2006	-	58,58,73	3.13	16 (27%)	75,95,113	4.58	31 (41%)
19	CLA	2	2010	-	23,32,73	5.98	15 (65%)	12,54,113	4.35	7 (58%)
19	CLA	3	1212	-	23,32,73	6.47	13 (56%)	12,54,113	4.20	8 (66%)
19	CLA	3	1213	-	41,44,73	2.15	8 (19%)	51,78,113	3.82	24 (47%)
19	CLA	3	1214	-	23,32,73	5.93	15 (65%)	12,54,113	4.70	9 (75%)
19	CLA	3	1215	-	23,32,73	6.02	14 (60%)	12,54,113	4.46	7 (58%)
19	CLA	3	1216	-	23,32,73	6.68	15 (65%)	12,54,113	4.33	7 (58%)
19	CLA	3	1217	-	50,50,73	3.31	19 (38%)	66,85,113	5.10	33 (50%)
19	CLA	3	1218	-	64,64,73	3.02	18 (28%)	83,102,113	4.25	32 (38%)
19	CLA	3	1219	-	23,32,73	6.10	14 (60%)	12,54,113	4.15	9 (75%)
19	CLA	3	1220	-	23,32,73	6.73	14 (60%)	12,54,113	4.38	9 (75%)
19	CLA	3	1221	-	73,73,73	2.82	15 (20%)	95,113,113	3.93	38 (40%)
19	CLA	3	1222	-	73,73,73	2.66	15 (20%)	95,113,113	4.05	33 (34%)
21	SUC	3	1223	-	24,24,24	0.51	0	36,36,36	1.45	5 (13%)
19	CLA	3	3001	-	23,32,73	6.71	13 (56%)	12,54,113	4.04	8 (66%)
19	CLA	3	3008	-	58,58,73	2.83	13 (22%)	75,95,113	4.28	31 (41%)
19	CLA	3	3011	-	73,73,73	2.72	19 (26%)	95,113,113	4.61	36 (37%)
19	CLA	3	3014	-	23,32,73	6.34	14 (60%)	12,54,113	4.32	7 (58%)
19	CLA	3	3015	-	23,32,73	5.75	14 (60%)	12,54,113	4.24	8 (66%)
19	CLA	4	1196	-	62,63,73	2.91	15 (24%)	81,101,113	4.35	31 (38%)
19	CLA	4	1197	-	41,44,73	2.37	13 (31%)	51,78,113	3.74	24 (47%)
19	CLA	4	1198	-	73,73,73	2.78	20 (27%)	95,113,113	4.13	41 (43%)
19	CLA	4	1199	-	62,63,73	2.80	15 (24%)	81,101,113	4.01	34 (41%)
19	CLA	4	1200	-	58,58,73	3.09	16 (27%)	75,95,113	4.60	31 (41%)
19	CLA	4	1201	-	60,60,73	3.27	21 (35%)	79,97,113	4.74	42 (53%)
19	CLA	4	1202	-	23,32,73	6.18	16 (69%)	12,54,113	3.82	8 (66%)
19	CLA	4	1203	-	23,32,73	6.12	13 (56%)	12,54,113	4.08	8 (66%)
19	CLA	4	1204	-	23,32,73	6.50	13 (56%)	12,54,113	4.25	8 (66%)
19	CLA	4	1205	-	58,58,73	3.03	17 (29%)	75,95,113	4.15	28 (37%)
19	CLA	4	1206	-	73,73,73	2.92	18 (24%)	95,113,113	4.13	32 (33%)
19	CLA	4	1207	-	23,32,73	5.96	14 (60%)	12,54,113	4.54	7 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	4	1208	-	23,32,73	6.34	15 (65%)	12,54,113	4.05	7 (58%)
19	CLA	4	1209	4	41,44,73	2.07	11 (26%)	51,78,113	3.67	24 (47%)
19	CLA	4	1210	4	23,32,73	6.93	14 (60%)	12,54,113	3.98	6 (50%)
19	CLA	4	1211	-	53,54,73	3.12	16 (30%)	71,90,113	4.30	33 (46%)
20	LMU	4	1212	-	36,36,36	0.70	1 (2%)	47,47,47	1.13	3 (6%)
19	CLA	4	4007	-	60,60,73	3.16	17 (28%)	79,97,113	4.70	38 (48%)
19	CLA	4	4014	-	54,55,73	3.19	17 (31%)	72,91,113	4.89	38 (52%)
19	CLA	A	1759	-	53,54,73	3.52	16 (30%)	71,90,113	4.60	33 (46%)
19	CLA	A	1760	19	62,63,73	2.94	15 (24%)	81,101,113	4.08	34 (41%)
19	CLA	A	1761	-	62,62,73	2.75	16 (25%)	80,99,113	3.82	33 (41%)
19	CLA	A	1762	-	64,64,73	2.74	17 (26%)	83,102,113	4.23	32 (38%)
19	CLA	A	1763	-	53,54,73	3.04	15 (28%)	71,90,113	4.62	34 (47%)
19	CLA	A	1764	5	67,68,73	2.89	19 (28%)	87,107,113	3.86	34 (39%)
19	CLA	A	1765	-	60,60,73	2.94	15 (25%)	79,97,113	4.28	35 (44%)
19	CLA	A	1766	-	51,53,73	3.11	16 (31%)	68,89,113	4.63	30 (44%)
19	CLA	A	1767	19,5	73,73,73	2.65	15 (20%)	95,113,113	3.84	33 (34%)
19	CLA	A	1768	5	62,62,73	2.70	15 (24%)	80,99,113	4.31	31 (38%)
19	CLA	A	1769	-	58,58,73	2.88	15 (25%)	75,95,113	4.20	31 (41%)
19	CLA	A	1770	-	23,32,73	6.67	14 (60%)	12,54,113	4.10	8 (66%)
19	CLA	A	1771	-	58,58,73	2.89	16 (27%)	75,95,113	4.40	35 (46%)
19	CLA	A	1772	-	62,62,73	2.99	18 (29%)	80,99,113	4.22	35 (43%)
19	CLA	A	1773	-	60,60,73	2.99	14 (23%)	79,97,113	4.48	33 (41%)
19	CLA	A	1774	-	67,68,73	3.23	18 (26%)	87,107,113	3.75	37 (42%)
19	CLA	A	1775	-	41,44,73	2.15	12 (29%)	51,78,113	3.80	23 (45%)
19	CLA	A	1776	-	65,66,73	2.75	16 (24%)	85,104,113	4.29	32 (37%)
19	CLA	A	1777	-	59,59,73	3.15	16 (27%)	77,96,113	4.29	29 (37%)
19	CLA	A	1778	5	50,50,73	3.07	15 (30%)	66,85,113	4.50	29 (43%)
19	CLA	A	1779	-	58,58,73	2.89	16 (27%)	75,95,113	4.21	29 (38%)
19	CLA	A	1780	-	65,66,73	2.75	15 (23%)	85,104,113	3.77	34 (40%)
19	CLA	A	1781	-	67,67,73	2.86	14 (20%)	86,105,113	4.15	33 (38%)
19	CLA	A	1782	-	73,73,73	2.57	15 (20%)	95,113,113	3.49	28 (29%)
19	CLA	A	1783	-	73,73,73	2.71	15 (20%)	95,113,113	4.22	33 (34%)
19	CLA	A	1784	5	62,63,73	2.88	16 (25%)	81,101,113	4.13	35 (43%)
19	CLA	A	1785	-	73,73,73	2.54	15 (20%)	95,113,113	3.59	31 (32%)
19	CLA	A	1786	-	58,58,73	2.94	15 (25%)	75,95,113	4.38	30 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	1787	5	67,68,73	2.74	14 (20%)	87,107,113	3.96	31 (35%)
19	CLA	A	1788	-	73,73,73	2.61	15 (20%)	95,113,113	3.94	28 (29%)
19	CLA	A	1789	5	73,73,73	2.63	19 (26%)	95,113,113	4.40	38 (40%)
19	CLA	A	1790	5	58,58,73	2.89	16 (27%)	75,95,113	4.45	33 (44%)
19	CLA	A	1791	19,5	51,53,73	3.08	15 (29%)	68,89,113	4.82	34 (50%)
19	CLA	A	1792	-	53,54,73	3.15	15 (28%)	71,90,113	4.49	31 (43%)
19	CLA	A	1793	-	73,73,73	2.84	18 (24%)	95,113,113	4.00	37 (38%)
19	CLA	A	1794	-	54,55,73	3.11	16 (29%)	72,91,113	4.21	28 (38%)
19	CLA	A	1795	-	59,59,73	3.05	17 (28%)	77,96,113	4.46	34 (44%)
19	CLA	A	1796	-	73,73,73	2.63	16 (21%)	95,113,113	3.81	36 (37%)
19	CLA	A	1797	19	66,67,73	3.17	20 (30%)	83,105,113	4.27	39 (46%)
19	CLA	A	1798	-	62,63,73	2.77	15 (24%)	81,101,113	4.36	34 (41%)
19	CLA	A	1799	-	23,32,73	6.87	14 (60%)	12,54,113	4.30	7 (58%)
19	CLA	A	1800	-	73,73,73	2.61	14 (19%)	95,113,113	3.92	35 (36%)
19	CLA	A	1801	-	62,63,73	2.88	13 (20%)	81,101,113	4.21	33 (40%)
22	PQN	A	1802	-	34,34,34	1.46	2 (5%)	45,45,45	1.14	4 (8%)
23	BCR	A	1803	-	41,41,41	1.97	3 (7%)	56,56,56	5.38	22 (39%)
23	BCR	A	1804	-	41,41,41	2.04	3 (7%)	56,56,56	5.48	21 (37%)
23	BCR	A	1805	-	41,41,41	2.03	4 (9%)	56,56,56	5.60	26 (46%)
23	BCR	A	1806	-	41,41,41	1.94	3 (7%)	56,56,56	5.44	18 (32%)
23	BCR	A	1807	-	40,40,41	1.80	5 (12%)	49,53,56	4.45	20 (40%)
23	BCR	A	1808	-	41,41,41	2.54	6 (14%)	56,56,56	5.98	21 (37%)
23	BCR	A	1809	-	41,41,41	1.98	3 (7%)	56,56,56	5.58	21 (37%)
20	LMU	A	1810	-	36,36,36	0.68	0	47,47,47	1.32	7 (14%)
20	LMU	A	1811	-	36,36,36	0.66	1 (2%)	47,47,47	1.49	8 (17%)
20	LMU	A	1812	-	36,36,36	0.47	0	47,47,47	0.88	3 (6%)
19	CLA	A	1813	-	73,73,73	2.57	15 (20%)	95,113,113	4.28	34 (35%)
19	CLA	A	1814	-	73,73,73	2.69	16 (21%)	95,113,113	4.24	35 (36%)
19	CLA	A	1815	-	73,73,73	2.80	17 (23%)	95,113,113	4.06	34 (35%)
19	CLA	A	1816	-	62,62,73	2.92	17 (27%)	80,99,113	4.39	35 (43%)
19	CLA	A	1817	-	73,73,73	2.67	16 (21%)	95,113,113	4.00	33 (34%)
20	LMU	A	7001	-	36,36,36	0.66	0	47,47,47	1.65	9 (19%)
20	LMU	A	7003	-	36,36,36	0.48	0	47,47,47	0.75	1 (2%)
20	LMU	A	7004	-	36,36,36	0.45	0	47,47,47	1.45	6 (12%)
20	LMU	A	7005	-	36,36,36	0.43	0	47,47,47	1.17	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	LMU	A	7006	-	36,36,36	0.55	0	47,47,47	0.70	0
20	LMU	A	7008	21	36,36,36	1.07	2 (5%)	47,47,47	2.20	11 (23%)
20	LMU	A	7009	20	35,35,36	1.06	3 (8%)	46,46,47	1.87	11 (23%)
20	LMU	A	7010	-	36,36,36	0.53	0	47,47,47	0.89	2 (4%)
20	LMU	A	7011	-	36,36,36	0.46	0	47,47,47	1.54	6 (12%)
20	LMU	A	7013	20	36,36,36	0.55	0	47,47,47	1.02	2 (4%)
20	LMU	A	7014	-	36,36,36	0.83	1 (2%)	47,47,47	2.15	12 (25%)
20	LMU	A	7015	-	36,36,36	0.67	0	47,47,47	1.35	4 (8%)
20	LMU	A	7016	-	36,36,36	0.49	0	47,47,47	1.49	6 (12%)
20	LMU	A	7017	-	36,36,36	0.62	0	47,47,47	1.92	14 (29%)
20	LMU	A	7019	-	36,36,36	0.74	1 (2%)	47,47,47	1.34	9 (19%)
20	LMU	A	7020	-	36,36,36	0.56	0	47,47,47	1.55	9 (19%)
20	LMU	A	7021	-	36,36,36	0.69	0	47,47,47	1.52	7 (14%)
20	LMU	A	7022	-	36,36,36	0.56	0	47,47,47	1.33	5 (10%)
20	LMU	A	7023	-	36,36,36	0.50	0	47,47,47	1.35	7 (14%)
20	LMU	A	7024	-	36,36,36	0.72	1 (2%)	47,47,47	1.46	8 (17%)
20	LMU	A	7025	-	36,36,36	0.51	0	47,47,47	1.27	5 (10%)
20	LMU	A	7026	-	36,36,36	0.83	1 (2%)	47,47,47	2.17	14 (29%)
20	LMU	A	7027	-	36,36,36	0.80	1 (2%)	47,47,47	1.63	11 (23%)
20	LMU	A	7028	-	36,36,36	0.50	0	47,47,47	1.05	3 (6%)
20	LMU	A	7030	-	36,36,36	0.59	0	47,47,47	1.68	8 (17%)
20	LMU	A	7031	-	36,36,36	0.45	0	47,47,47	1.28	4 (8%)
20	LMU	A	7032	-	36,36,36	0.70	1 (2%)	47,47,47	1.70	8 (17%)
20	LMU	A	7033	-	36,36,36	0.68	0	47,47,47	1.68	8 (17%)
20	LMU	A	7034	-	36,36,36	0.45	0	47,47,47	1.50	8 (17%)
20	LMU	A	7035	-	36,36,36	0.63	0	47,47,47	1.44	9 (19%)
20	LMU	A	7036	-	35,35,36	1.03	2 (5%)	46,46,47	1.39	5 (10%)
20	LMU	A	7037	-	36,36,36	0.60	0	47,47,47	1.92	13 (27%)
20	LMU	A	7038	-	36,36,36	0.69	0	47,47,47	1.78	11 (23%)
20	LMU	A	7039	-	36,36,36	0.60	0	47,47,47	1.65	8 (17%)
20	LMU	A	7040	-	36,36,36	0.65	1 (2%)	47,47,47	1.72	12 (25%)
20	LMU	A	7041	-	36,36,36	0.37	0	47,47,47	1.06	3 (6%)
20	LMU	A	7042	-	36,36,36	0.51	0	47,47,47	1.33	7 (14%)
20	LMU	A	7043	-	36,36,36	0.59	1 (2%)	47,47,47	1.62	11 (23%)
20	LMU	A	7047	-	36,36,36	0.79	1 (2%)	47,47,47	1.24	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	LMU	A	7049	20	36,36,36	0.49	0	47,47,47	0.97	2 (4%)
19	CLA	B	1735	-	73,73,73	2.71	16 (21%)	95,113,113	3.84	32 (33%)
19	CLA	B	1736	-	51,53,73	3.14	18 (35%)	68,89,113	4.41	26 (38%)
19	CLA	B	1737	-	69,69,73	2.94	17 (24%)	89,108,113	3.88	35 (39%)
19	CLA	B	1738	-	73,73,73	2.84	17 (23%)	95,113,113	4.02	35 (36%)
19	CLA	B	1739	-	67,68,73	2.83	16 (23%)	87,107,113	4.10	36 (41%)
19	CLA	B	1740	6	23,32,73	6.79	15 (65%)	12,54,113	3.82	6 (50%)
19	CLA	B	1741	6	60,62,73	2.37	17 (28%)	77,100,113	3.34	28 (36%)
19	CLA	B	1742	6	62,63,73	2.62	14 (22%)	81,101,113	4.20	33 (40%)
19	CLA	B	1743	-	73,73,73	2.73	14 (19%)	95,113,113	4.08	31 (32%)
19	CLA	B	1744	-	67,68,73	2.80	15 (22%)	87,107,113	3.82	31 (35%)
19	CLA	B	1745	6	67,68,73	2.64	13 (19%)	87,107,113	3.77	32 (36%)
19	CLA	B	1746	-	53,54,73	2.94	13 (24%)	71,90,113	4.06	31 (43%)
19	CLA	B	1747	-	60,61,73	2.83	14 (23%)	79,98,113	4.22	32 (40%)
19	CLA	B	1748	-	48,49,73	3.55	19 (39%)	64,84,113	5.08	30 (46%)
19	CLA	B	1749	-	69,69,73	2.67	14 (20%)	89,108,113	4.30	36 (40%)
19	CLA	B	1750	-	58,58,73	2.89	14 (24%)	75,95,113	4.48	29 (38%)
19	CLA	B	1751	-	53,54,73	2.92	14 (26%)	71,90,113	4.88	29 (40%)
19	CLA	B	1752	6	62,63,73	2.97	15 (24%)	81,101,113	4.35	33 (40%)
19	CLA	B	1753	-	73,73,73	3.03	22 (30%)	95,113,113	4.03	33 (34%)
19	CLA	B	1754	-	62,62,73	3.02	15 (24%)	80,99,113	4.30	33 (41%)
19	CLA	B	1755	-	65,66,73	2.93	15 (23%)	85,104,113	4.21	31 (36%)
19	CLA	B	1756	6	73,73,73	2.68	16 (21%)	95,113,113	4.02	34 (35%)
19	CLA	B	1757	-	73,73,73	2.71	16 (21%)	95,113,113	4.04	32 (33%)
19	CLA	B	1758	-	73,73,73	2.70	15 (20%)	95,113,113	3.60	36 (37%)
19	CLA	B	1759	-	73,73,73	2.61	17 (23%)	95,113,113	3.56	31 (32%)
19	CLA	B	1760	-	58,58,73	2.97	15 (25%)	75,95,113	4.16	33 (44%)
19	CLA	B	1761	10,6	58,58,73	3.15	18 (31%)	75,95,113	4.60	33 (44%)
19	CLA	B	1762	6	67,67,73	2.91	16 (23%)	86,105,113	4.20	32 (37%)
19	CLA	B	1763	6	58,58,73	3.03	16 (27%)	75,95,113	4.22	33 (44%)
19	CLA	B	1764	19	51,53,73	3.23	16 (31%)	68,89,113	4.68	26 (38%)
19	CLA	B	1765	19	51,53,73	3.30	15 (29%)	68,89,113	4.44	29 (42%)
19	CLA	B	1766	-	59,59,73	3.15	18 (30%)	77,96,113	4.40	32 (41%)
19	CLA	B	1767	-	67,68,73	2.78	14 (20%)	87,107,113	4.07	31 (35%)
19	CLA	B	1768	6	73,73,73	2.64	15 (20%)	95,113,113	3.65	31 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	1769	-	54,55,73	3.41	20 (37%)	72,91,113	4.83	33 (45%)
19	CLA	B	1770	-	73,73,73	2.53	16 (21%)	95,113,113	3.61	29 (30%)
19	CLA	B	1771	-	73,73,73	2.61	15 (20%)	95,113,113	3.63	30 (31%)
19	CLA	B	1772	-	41,44,73	2.18	11 (26%)	51,78,113	3.64	25 (49%)
22	PQN	B	1773	-	34,34,34	1.41	2 (5%)	45,45,45	1.27	6 (13%)
23	BCR	B	1774	-	41,41,41	1.89	3 (7%)	56,56,56	5.62	18 (32%)
23	BCR	B	1775	-	41,41,41	1.87	3 (7%)	56,56,56	5.13	24 (42%)
23	BCR	B	1776	-	41,41,41	1.77	3 (7%)	56,56,56	4.69	18 (32%)
23	BCR	B	1777	-	41,41,41	1.99	4 (9%)	56,56,56	5.46	22 (39%)
23	BCR	B	1778	-	41,41,41	2.03	3 (7%)	56,56,56	5.36	19 (33%)
23	BCR	B	1779	-	41,41,41	2.17	5 (12%)	56,56,56	5.64	23 (41%)
23	BCR	B	1780	-	41,41,41	1.96	3 (7%)	56,56,56	5.34	14 (25%)
24	LMG	B	1781	-	49,49,55	1.20	3 (6%)	57,57,63	1.07	2 (3%)
20	LMU	B	1782	-	26,26,36	1.24	2 (7%)	36,37,47	1.38	6 (16%)
25	SF4	B	1783	5,6	12,12,12	78.96	12 (100%)	0,24,24	0.00	-
19	CLA	B	1784	-	73,73,73	2.61	16 (21%)	95,113,113	3.84	33 (34%)
21	SUC	B	8051	-	24,24,24	0.44	0	36,36,36	1.21	2 (5%)
21	SUC	B	8052	-	24,24,24	0.34	0	36,36,36	0.95	0
21	SUC	B	8053	-	22,23,24	0.73	1 (4%)	33,35,36	1.38	5 (15%)
21	SUC	B	8054	-	24,24,24	0.56	0	36,36,36	0.99	2 (5%)
21	SUC	B	8055	-	24,24,24	0.45	0	36,36,36	1.26	4 (11%)
21	SUC	B	8056	-	24,24,24	0.49	0	36,36,36	1.20	6 (16%)
21	SUC	B	8059	-	24,24,24	0.51	0	36,36,36	1.22	2 (5%)
21	SUC	B	8060	-	24,24,24	0.47	0	36,36,36	0.96	2 (5%)
21	SUC	B	8061	-	24,24,24	0.51	0	36,36,36	1.63	9 (25%)
21	SUC	B	8062	20	24,24,24	1.05	2 (8%)	36,36,36	2.12	11 (30%)
25	SF4	C	1082	7	12,12,12	37.10	12 (100%)	0,24,24	0.00	-
25	SF4	C	1083	7	12,12,12	95.20	12 (100%)	0,24,24	0.00	-
19	CLA	F	1155	-	41,44,73	2.26	13 (31%)	51,78,113	3.91	24 (47%)
19	CLA	F	1156	19	48,49,73	3.21	14 (29%)	64,84,113	4.78	27 (42%)
19	CLA	F	1157	19	60,61,73	3.20	22 (36%)	79,98,113	4.51	33 (41%)
19	CLA	G	1099	-	59,59,73	3.06	19 (32%)	77,96,113	4.19	30 (38%)
19	CLA	H	1079	-	65,66,73	3.18	20 (30%)	85,104,113	4.10	36 (42%)
19	CLA	H	1080	-	62,63,73	2.77	13 (20%)	81,101,113	4.31	33 (40%)
19	CLA	H	1081	16	58,58,73	2.87	14 (24%)	75,95,113	4.43	32 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	SUC	H	1082	-	24,24,24	0.43	0	36,36,36	0.90	1 (2%)
19	CLA	I	1031	-	67,68,73	2.76	13 (19%)	87,107,113	4.26	29 (33%)
23	BCR	I	1032	-	41,41,41	2.14	5 (12%)	56,56,56	6.04	27 (48%)
19	CLA	J	1043	-	69,69,73	2.90	16 (23%)	89,108,113	4.15	32 (35%)
19	CLA	L	1167	-	54,55,73	3.06	14 (25%)	72,91,113	4.65	32 (44%)
19	CLA	L	1168	-	58,58,73	3.00	16 (27%)	75,95,113	4.82	33 (44%)
23	BCR	L	1169	-	41,41,41	2.02	4 (9%)	56,56,56	5.53	18 (32%)
20	LMU	L	1170	-	36,36,36	0.69	0	47,47,47	1.33	5 (10%)
19	CLA	R	1054	-	65,65,73	2.73	14 (21%)	85,103,113	4.38	34 (40%)
19	CLA	R	1055	-	73,73,73	2.57	12 (16%)	95,113,113	3.96	35 (36%)
20	LMU	R	1056	20	36,36,36	0.48	0	47,47,47	0.87	1 (2%)

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
19	CLA	1	1014	-	1/1/17/25	0/21/119/135	0/0/9/9
19	CLA	1	1142	-	-	2/15/113/135	0/0/9/9
19	CLA	1	1143	-	-	0/19/117/135	0/0/9/9
19	CLA	1	1145	-	2/2/18/25	0/25/123/135	0/0/9/9
19	CLA	1	1146	-	-	0/19/117/135	0/0/9/9
19	CLA	1	1148	-	1/1/18/25	0/25/123/135	0/0/9/9
19	CLA	1	1149	-	2/2/16/25	0/16/112/135	0/0/9/9
19	CLA	1	1187	1	-	1/15/113/135	0/0/9/9
19	CLA	1	1188	-	-	0/8/106/135	0/0/9/9
19	CLA	1	1189	-	-	1/16/114/135	0/0/9/9
19	CLA	1	1190	-	-	1/15/113/135	0/0/9/9
19	CLA	1	1191	-	-	0/0/96/135	0/0/9/9
19	CLA	1	1192	-	1/1/19/25	0/33/131/135	0/0/9/9
19	CLA	1	1193	-	1/1/17/25	0/21/119/135	0/0/9/9
19	CLA	1	1194	-	-	0/0/66/135	0/0/8/9
19	CLA	1	1195	-	-	0/0/66/135	0/0/8/9
19	CLA	1	1196	1	-	0/0/96/135	0/0/9/9
19	CLA	1	1197	-	1/1/17/25	0/21/119/135	0/0/9/9
19	CLA	1	1198	-	-	0/0/66/135	0/0/8/9
19	CLA	1	1199	-	2/2/17/25	0/21/119/135	0/0/9/9
19	CLA	1	1200	-	-	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	1	1307	-	-	0/0/66/135	0/0/8/9
19	CLA	1	1308	-	-	0/17/115/135	0/0/9/9
19	CLA	1	1309	-	-	0/0/66/135	0/0/8/9
19	CLA	1	1505	-	1/1/18/25	0/25/123/135	0/0/9/9
19	CLA	2	1212	-	-	0/21/119/135	0/0/9/9
19	CLA	2	1213	-	1/1/18/25	0/29/127/135	0/0/9/9
19	CLA	2	1214	-	-	0/0/66/135	0/0/8/9
19	CLA	2	1215	-	-	0/19/117/135	0/0/9/9
19	CLA	2	1216	-	-	0/0/66/135	0/0/8/9
19	CLA	2	1217	-	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	2	1218	-	-	0/0/66/135	0/0/8/9
19	CLA	2	1219	-	-	0/0/96/135	0/0/9/9
19	CLA	2	1220	-	-	0/0/66/135	0/0/8/9
19	CLA	2	1221	2	-	0/19/117/135	0/0/9/9
19	CLA	2	1222	-	-	0/19/117/135	0/0/9/9
19	CLA	2	1223	-	1/1/19/25	0/33/131/135	0/0/9/9
20	LMU	2	1224	-	-	0/21/61/61	0/2/2/2
21	SUC	2	1225	-	1/1/9/9	0/10/49/51	0/2/2/2
19	CLA	2	2006	-	-	1/19/117/135	0/0/9/9
19	CLA	2	2010	-	-	0/0/66/135	0/0/8/9
19	CLA	3	1212	-	-	0/0/66/135	0/0/8/9
19	CLA	3	1213	-	-	0/0/96/135	0/0/9/9
19	CLA	3	1214	-	-	0/0/66/135	0/0/8/9
19	CLA	3	1215	-	-	0/0/66/135	0/0/8/9
19	CLA	3	1216	-	-	0/0/66/135	0/0/8/9
19	CLA	3	1217	-	-	0/10/108/135	0/0/9/9
19	CLA	3	1218	-	1/1/18/25	0/27/125/135	0/0/9/9
19	CLA	3	1219	-	-	0/0/66/135	0/0/8/9
19	CLA	3	1220	-	-	0/0/66/135	0/0/8/9
19	CLA	3	1221	-	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	3	1222	-	1/1/20/25	0/37/135/135	0/0/9/9
21	SUC	3	1223	-	1/1/9/9	0/12/51/51	0/2/2/2
19	CLA	3	3001	-	-	0/0/66/135	0/0/8/9
19	CLA	3	3008	-	-	0/19/117/135	0/0/9/9
19	CLA	3	3011	-	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	3	3014	-	-	0/0/66/135	0/0/8/9
19	CLA	3	3015	-	-	0/0/66/135	0/0/8/9
19	CLA	4	1196	-	1/1/18/25	0/25/123/135	0/0/9/9
19	CLA	4	1197	-	-	0/0/96/135	0/0/9/9
19	CLA	4	1198	-	2/2/20/25	0/37/135/135	0/0/9/9
19	CLA	4	1199	-	1/1/18/25	0/25/123/135	0/0/9/9
19	CLA	4	1200	-	-	0/19/117/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	4	1201	-	1/1/17/25	0/22/120/135	0/0/9/9
19	CLA	4	1202	-	-	0/0/66/135	0/0/8/9
19	CLA	4	1203	-	-	0/0/66/135	0/0/8/9
19	CLA	4	1204	-	-	0/0/66/135	0/0/8/9
19	CLA	4	1205	-	-	0/19/117/135	0/0/9/9
19	CLA	4	1206	-	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	4	1207	-	-	0/0/66/135	0/0/8/9
19	CLA	4	1208	-	-	0/0/66/135	0/0/8/9
19	CLA	4	1209	4	-	0/0/96/135	0/0/9/9
19	CLA	4	1210	4	-	0/0/66/135	0/0/8/9
19	CLA	4	1211	-	-	0/15/113/135	0/0/9/9
20	LMU	4	1212	-	-	0/21/61/61	0/2/2/2
19	CLA	4	4007	-	-	0/22/120/135	0/0/9/9
19	CLA	4	4014	-	-	0/16/114/135	0/0/9/9
19	CLA	A	1759	-	-	0/15/113/135	0/0/9/9
19	CLA	A	1760	19	1/1/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1761	-	-	0/23/122/135	0/0/9/9
19	CLA	A	1762	-	1/1/18/25	0/27/125/135	0/0/9/9
19	CLA	A	1763	-	-	1/15/113/135	0/0/9/9
19	CLA	A	1764	5	1/1/19/25	0/31/129/135	0/0/9/9
19	CLA	A	1765	-	-	0/22/120/135	0/0/9/9
19	CLA	A	1766	-	-	0/11/111/135	0/0/9/9
19	CLA	A	1767	19,5	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1768	5	-	0/23/122/135	0/0/9/9
19	CLA	A	1769	-	-	0/19/117/135	0/0/9/9
19	CLA	A	1770	-	-	0/0/66/135	0/0/8/9
19	CLA	A	1771	-	-	0/19/117/135	0/0/9/9
19	CLA	A	1772	-	-	0/23/122/135	0/0/9/9
19	CLA	A	1773	-	-	0/22/120/135	0/0/9/9
19	CLA	A	1774	-	1/1/19/25	0/31/129/135	0/0/9/9
19	CLA	A	1775	-	-	0/0/96/135	0/0/9/9
19	CLA	A	1776	-	1/1/18/25	0/29/127/135	0/0/9/9
19	CLA	A	1777	-	-	0/21/119/135	0/0/9/9
19	CLA	A	1778	5	-	0/10/108/135	0/0/9/9
19	CLA	A	1779	-	-	0/19/117/135	0/0/9/9
19	CLA	A	1780	-	1/1/18/25	0/29/127/135	0/0/9/9
19	CLA	A	1781	-	1/1/18/25	1/29/128/135	0/0/9/9
19	CLA	A	1782	-	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1783	-	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1784	5	1/1/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1785	-	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1786	-	-	0/19/117/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1787	5	1/1/19/25	0/31/129/135	0/0/9/9
19	CLA	A	1788	-	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1789	5	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1790	5	-	0/19/117/135	0/0/9/9
19	CLA	A	1791	19,5	-	0/11/111/135	0/0/9/9
19	CLA	A	1792	-	-	0/15/113/135	0/0/9/9
19	CLA	A	1793	-	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1794	-	-	0/16/114/135	0/0/9/9
19	CLA	A	1795	-	-	0/21/119/135	0/0/9/9
19	CLA	A	1796	-	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1797	19	1/1/18/25	0/29/127/135	0/0/9/9
19	CLA	A	1798	-	1/1/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1799	-	-	0/0/66/135	0/0/8/9
19	CLA	A	1800	-	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1801	-	1/1/18/25	0/25/123/135	0/0/9/9
22	PQN	A	1802	-	1/1/8/9	0/23/43/43	0/0/2/2
23	BCR	A	1803	-	-	0/29/63/63	0/2/2/2
23	BCR	A	1804	-	-	0/29/63/63	0/2/2/2
23	BCR	A	1805	-	-	0/29/63/63	0/2/2/2
23	BCR	A	1806	-	-	0/29/63/63	0/2/2/2
23	BCR	A	1807	-	-	0/29/60/63	0/2/2/2
23	BCR	A	1808	-	-	0/29/63/63	0/2/2/2
23	BCR	A	1809	-	-	1/29/63/63	0/2/2/2
20	LMU	A	1810	-	-	0/21/61/61	0/2/2/2
20	LMU	A	1811	-	-	0/21/61/61	0/2/2/2
20	LMU	A	1812	-	-	0/21/61/61	0/2/2/2
19	CLA	A	1813	-	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1814	-	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1815	-	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1816	-	-	0/23/122/135	0/0/9/9
19	CLA	A	1817	-	1/1/20/25	0/37/135/135	0/0/9/9
20	LMU	A	7001	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7003	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7004	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7005	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7006	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7008	21	-	0/21/61/61	0/2/2/2
20	LMU	A	7009	20	-	0/20/60/61	0/2/2/2
20	LMU	A	7010	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7011	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7013	20	-	0/21/61/61	0/2/2/2
20	LMU	A	7014	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LMU	A	7015	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7016	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7017	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7019	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7020	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7021	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7022	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7023	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7024	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7025	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7026	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7027	-	-	1/21/61/61	0/2/2/2
20	LMU	A	7028	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7030	-	-	1/21/61/61	0/2/2/2
20	LMU	A	7031	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7032	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7033	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7034	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7035	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7036	-	-	0/20/60/61	0/2/2/2
20	LMU	A	7037	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7038	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7039	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7040	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7041	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7042	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7043	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7047	-	-	0/21/61/61	0/2/2/2
20	LMU	A	7049	20	-	0/21/61/61	0/2/2/2
19	CLA	B	1735	-	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1736	-	-	0/11/111/135	0/0/9/9
19	CLA	B	1737	-	1/1/19/25	0/33/131/135	0/0/9/9
19	CLA	B	1738	-	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1739	-	1/1/19/25	0/31/129/135	0/0/9/9
19	CLA	B	1740	6	-	0/0/66/135	0/0/8/9
19	CLA	B	1741	6	1/1/18/25	0/25/121/135	0/0/9/9
19	CLA	B	1742	6	1/1/18/25	0/25/123/135	0/0/9/9
19	CLA	B	1743	-	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1744	-	1/1/19/25	0/31/129/135	0/0/9/9
19	CLA	B	1745	6	1/1/19/25	0/31/129/135	0/0/9/9
19	CLA	B	1746	-	-	0/15/113/135	0/0/9/9
19	CLA	B	1747	-	-	0/23/121/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	1748	-	-	0/8/106/135	0/0/9/9
19	CLA	B	1749	-	1/1/19/25	0/33/131/135	0/0/9/9
19	CLA	B	1750	-	-	0/19/117/135	0/0/9/9
19	CLA	B	1751	-	-	0/15/113/135	0/0/9/9
19	CLA	B	1752	6	1/1/18/25	0/25/123/135	0/0/9/9
19	CLA	B	1753	-	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1754	-	-	0/23/122/135	0/0/9/9
19	CLA	B	1755	-	1/1/18/25	0/29/127/135	0/0/9/9
19	CLA	B	1756	6	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1757	-	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1758	-	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1759	-	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1760	-	-	0/19/117/135	0/0/9/9
19	CLA	B	1761	10,6	-	0/19/117/135	0/0/9/9
19	CLA	B	1762	6	1/1/18/25	0/29/128/135	0/0/9/9
19	CLA	B	1763	6	-	0/19/117/135	0/0/9/9
19	CLA	B	1764	19	-	0/11/111/135	0/0/9/9
19	CLA	B	1765	19	-	0/11/111/135	0/0/9/9
19	CLA	B	1766	-	-	0/21/119/135	0/0/9/9
19	CLA	B	1767	-	1/1/19/25	0/31/129/135	0/0/9/9
19	CLA	B	1768	6	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1769	-	-	0/16/114/135	0/0/9/9
19	CLA	B	1770	-	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1771	-	1/1/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1772	-	-	0/0/96/135	0/0/9/9
22	PQN	B	1773	-	1/1/8/9	0/23/43/43	0/0/2/2
23	BCR	B	1774	-	-	2/29/63/63	0/2/2/2
23	BCR	B	1775	-	-	0/29/63/63	0/2/2/2
23	BCR	B	1776	-	-	0/29/63/63	0/2/2/2
23	BCR	B	1777	-	-	0/29/63/63	0/2/2/2
23	BCR	B	1778	-	-	0/29/63/63	0/2/2/2
23	BCR	B	1779	-	-	0/29/63/63	0/2/2/2
23	BCR	B	1780	-	-	2/29/63/63	0/2/2/2
24	LMG	B	1781	-	-	0/44/64/70	1/1/1/1
20	LMU	B	1782	-	-	0/11/51/61	0/2/2/2
25	SF4	B	1783	5,6	-	0/0/48/48	0/0/5/5
19	CLA	B	1784	-	1/1/20/25	0/37/135/135	0/0/9/9
21	SUC	B	8051	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8052	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8053	-	1/1/9/9	0/10/49/51	0/2/2/2
21	SUC	B	8054	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8055	-	1/1/9/9	0/12/51/51	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	SUC	B	8056	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8059	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8060	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8061	-	1/1/9/9	0/12/51/51	0/2/2/2
21	SUC	B	8062	20	1/1/9/9	0/12/51/51	0/2/2/2
25	SF4	C	1082	7	-	0/0/48/48	0/0/5/5
25	SF4	C	1083	7	-	0/0/48/48	0/0/5/5
19	CLA	F	1155	-	-	0/0/96/135	0/0/9/9
19	CLA	F	1156	19	-	0/8/106/135	0/0/9/9
19	CLA	F	1157	19	3/3/17/25	1/23/121/135	0/0/9/9
19	CLA	G	1099	-	-	0/21/119/135	0/0/9/9
19	CLA	H	1079	-	1/1/18/25	0/29/127/135	0/0/9/9
19	CLA	H	1080	-	1/1/18/25	0/25/123/135	0/0/9/9
19	CLA	H	1081	16	-	0/19/117/135	0/0/9/9
21	SUC	H	1082	-	1/1/9/9	0/12/51/51	0/2/2/2
19	CLA	I	1031	-	1/1/19/25	0/31/129/135	0/0/9/9
23	BCR	I	1032	-	-	0/29/63/63	0/2/2/2
19	CLA	J	1043	-	1/1/19/25	0/33/131/135	0/0/9/9
19	CLA	L	1167	-	-	0/16/114/135	0/0/9/9
19	CLA	L	1168	-	1/1/17/25	0/19/117/135	0/0/9/9
23	BCR	L	1169	-	-	0/29/63/63	0/2/2/2
20	LMU	L	1170	-	-	0/21/61/61	0/2/2/2
19	CLA	R	1054	-	1/1/18/25	0/28/126/135	0/0/9/9
19	CLA	R	1055	-	1/1/20/25	0/37/135/135	0/0/9/9
20	LMU	R	1056	20	-	0/21/61/61	0/2/2/2

The worst 5 of 2801 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	1083	SF4	S3-FE1	186.27	3.58	2.33
25	C	1083	SF4	S4-FE3	183.47	3.56	2.33
25	C	1083	SF4	S1-FE4	175.15	3.51	2.33
25	B	1783	SF4	S3-FE2	-87.63	1.74	2.33
25	B	1783	SF4	S1-FE3	-83.60	1.77	2.33

The worst 5 of 5600 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1774	BCR	C20-C21-C22	35.93	179.07	127.29
23	L	1169	BCR	C20-C21-C22	35.46	178.38	127.29
23	A	1805	BCR	C20-C21-C22	35.22	178.03	127.29
23	A	1806	BCR	C20-C21-C22	35.14	177.93	127.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1777	BCR	C20-C21-C22	35.07	177.82	127.29

5 of 98 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A	1785	CLA	C8
19	B	1739	CLA	C8
19	B	1770	CLA	C8
19	A	1760	CLA	C8
19	3	1218	CLA	C8

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	1	1142	CLA	C1-O2A-CGA-CBA
19	A	1763	CLA	C1-O2A-CGA-CBA
19	2	2006	CLA	CED-O2D-CGD-CBD
20	A	7030	LMU	C1'-O1'-C1-C2
19	A	1781	CLA	CED-O2D-CGD-CBD

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	1781	LMG	C1-C2-C3-C4-C5-O6

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	1	165/241 (68%)	0.58	7 (4%) 35 14	21, 24, 25, 25	0
2	2	176/269 (65%)	0.31	2 (1%) 77 42	21, 23, 24, 25	0
3	3	153/276 (55%)	0.52	7 (4%) 31 13	49, 78, 110, 112	0
4	4	166/251 (66%)	0.14	0 100 100	21, 23, 24, 25	0
5	A	730/758 (96%)	0.25	7 (0%) 79 46	20, 22, 23, 25	0
6	B	733/734 (99%)	0.30	12 (1%) 68 34	20, 22, 24, 25	0
7	C	81/81 (100%)	0.42	2 (2%) 54 24	21, 22, 23, 23	0
8	D	138/212 (65%)	0.52	8 (5%) 22 9	21, 23, 24, 25	0
9	E	65/143 (45%)	0.21	0 100 100	21, 22, 24, 24	0
10	F	154/231 (66%)	0.27	5 (3%) 45 20	21, 22, 23, 24	0
11	G	95/167 (56%)	0.43	2 (2%) 60 28	21, 23, 24, 25	0
12	H	69/144 (47%)	0.38	2 (2%) 49 22	21, 23, 24, 25	0
13	I	30/40 (75%)	0.19	0 100 100	21, 22, 23, 23	0
14	J	42/44 (95%)	0.15	0 100 100	21, 23, 23, 24	0
15	K	84/131 (64%)	0.63	5 (5%) 21 9	21, 24, 24, 26	0
16	L	162/216 (75%)	0.24	2 (1%) 75 41	20, 23, 24, 25	0
17	N	85/170 (50%)	0.29	2 (2%) 56 25	22, 23, 24, 25	0
18	R	0/53	-	-	-	-
All	All	3128/4161 (75%)	0.32	63 (2%) 62 29	20, 23, 25, 112	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	K	16	THR	4.7
3	3	40	SER	4.7
6	B	258	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	1	88	PRO	3.4
15	K	63	CYS	3.4

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
19	CLA	1	1307	25/65	0.46	36.14	2,48,60,60	0
19	CLA	A	1799	25/65	0.31	16.13	2,43,60,60	0
19	CLA	3	3014	25/65	0.51	13.21	2,47,60,60	0
19	CLA	1	1197	51/65	0.57	5.79	2,42,60,60	0
23	BCR	A	1803	40/40	0.48	3.80	2,45,60,60	0
20	LMU	A	7033	35/35	0.25	3.15	2,46,60,60	0
23	BCR	A	1804	40/40	0.41	2.55	2,34,60,60	0
19	CLA	4	1200	50/65	0.45	2.52	2,21,60,60	0
20	LMU	A	7010	35/35	0.43	2.37	2,39,60,60	0
23	BCR	A	1806	40/40	0.37	2.34	2,31,60,60	0
19	CLA	A	1801	55/65	0.39	2.29	2,44,60,60	0
19	CLA	A	1775	36/65	0.38	2.28	2,51,60,60	0
19	CLA	A	1798	55/65	0.35	2.18	2,44,60,60	0
19	CLA	2	1220	25/65	0.48	2.16	2,34,60,60	0
19	CLA	4	1210	25/65	0.29	2.00	2,35,60,60	0
20	LMU	A	7047	35/35	0.32	1.99	2,40,60,60	0
20	LMU	2	1224	35/35	0.24	1.93	2,21,60,60	0
23	BCR	L	1169	40/40	0.46	1.91	2,18,60,60	0
19	CLA	4	1202	25/65	0.43	1.90	2,39,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	CLA	A	1776	58/65	0.33	1.88	2,20,60,60	0
23	BCR	B	1774	40/40	0.47	1.85	2,33,60,60	0
23	BCR	A	1807	39/40	0.33	1.72	2,8,60,60	0
23	BCR	I	1032	40/40	0.39	1.67	2,38,60,60	0
19	CLA	A	1780	58/65	0.35	1.62	2,18,60,60	0
19	CLA	4	1199	55/65	0.43	1.51	4,39,60,60	0
19	CLA	4	1203	25/65	0.30	1.51	2,29,60,60	0
19	CLA	A	1792	46/65	0.37	1.43	2,20,60,60	0
19	CLA	1	1187	46/65	0.26	1.27	2,56,60,60	0
19	CLA	2	1214	25/65	0.48	1.26	2,27,60,60	0
19	CLA	2	1222	50/65	0.31	1.15	2,25,60,60	0
23	BCR	B	1775	40/40	0.30	1.11	2,5,60,60	0
19	CLA	4	1207	25/65	0.26	1.03	2,15,60,60	0
19	CLA	1	1199	51/65	0.34	1.02	2,39,60,60	0
21	SUC	2	1225	22/23	0.36	1.02	2,35,60,60	0
19	CLA	B	1746	46/65	0.41	0.96	2,28,60,60	0
19	CLA	B	1749	61/65	0.32	0.91	2,16,60,60	0
19	CLA	A	1774	60/65	0.32	0.91	2,11,52,60	0
19	CLA	F	1157	53/65	0.31	0.87	2,22,60,60	0
19	CLA	G	1099	51/65	0.39	0.87	2,44,60,60	0
23	BCR	B	1776	40/40	0.42	0.86	2,21,60,60	0
24	LMG	B	1781	49/55	0.34	0.86	2,20,60,60	0
23	BCR	A	1805	40/40	0.34	0.75	2,5,44,60	0
19	CLA	A	1777	51/65	0.29	0.72	2,44,60,60	0
19	CLA	A	1764	60/65	0.30	0.71	2,10,60,60	0
19	CLA	A	1773	52/65	0.33	0.69	2,33,60,60	0
20	LMU	L	1170	35/35	0.30	0.65	2,22,60,60	0
19	CLA	H	1080	55/65	0.33	0.61	2,33,60,60	0
23	BCR	B	1777	40/40	0.33	0.57	2,11,60,60	0
19	CLA	B	1772	36/65	0.35	0.56	2,52,60,60	0
19	CLA	A	1766	45/65	0.34	0.55	2,38,60,60	0
19	CLA	A	1782	65/65	0.31	0.52	2,16,60,60	0
19	CLA	A	1783	65/65	0.30	0.51	2,2,50,60	0
19	CLA	A	1786	50/65	0.27	0.50	2,32,60,60	0
19	CLA	A	1787	60/65	0.28	0.48	2,18,60,60	0
19	CLA	B	1736	45/65	0.27	0.45	2,14,56,60	0
19	CLA	A	1759	46/65	0.34	0.41	2,14,49,60	0
19	CLA	A	1790	50/65	0.25	0.40	2,18,56,60	0
19	CLA	A	1800	65/65	0.31	0.37	2,22,60,60	0
19	CLA	B	1745	60/65	0.42	0.36	2,40,60,60	0
20	LMU	A	1810	35/35	0.24	0.35	2,26,60,60	0
19	CLA	1	1505	55/65	0.49	0.34	2,49,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	CLA	F	1156	41/65	0.32	0.33	2,41,60,60	0
19	CLA	4	1197	36/65	0.32	0.32	2,26,60,60	0
19	CLA	4	1209	36/65	0.23	0.32	2,21,60,60	0
19	CLA	B	1739	60/65	0.30	0.30	2,2,60,60	0
19	CLA	B	1754	54/65	0.30	0.30	2,15,60,60	0
19	CLA	4	1196	55/65	0.28	0.29	2,33,60,60	0
23	BCR	B	1780	40/40	0.33	0.28	2,10,60,60	0
19	CLA	1	1191	36/65	0.31	0.25	2,52,60,60	0
19	CLA	B	1763	50/65	0.27	0.25	2,11,53,60	0
19	CLA	A	1779	50/65	0.25	0.24	2,7,60,60	0
19	CLA	2	1215	50/65	0.28	0.22	2,48,60,60	0
19	CLA	I	1031	60/65	0.33	0.17	2,18,60,60	0
19	CLA	B	1757	65/65	0.30	0.16	2,10,56,60	0
19	CLA	H	1079	58/65	0.31	0.15	2,15,60,60	0
19	CLA	B	1735	65/65	0.29	0.14	2,11,60,60	0
19	CLA	1	1192	61/65	0.30	0.13	2,35,60,60	0
19	CLA	B	1771	65/65	0.29	0.12	2,2,55,60	0
19	CLA	4	1198	65/65	0.35	0.10	2,32,60,60	0
19	CLA	B	1744	60/65	0.35	0.09	2,19,60,60	0
19	CLA	4	1201	52/65	0.28	0.07	2,26,60,60	0
19	CLA	B	1784	65/65	0.28	0.05	2,2,55,60	0
19	CLA	A	1817	65/65	0.32	0.05	2,14,56,60	0
19	CLA	B	1762	59/65	0.26	0.04	2,6,60,60	0
19	CLA	B	1748	41/65	0.31	0.04	2,5,40,60	0
19	CLA	B	1742	55/65	0.29	0.03	2,28,60,60	0
23	BCR	A	1808	40/40	0.26	0.02	2,4,50,60	0
19	CLA	B	1770	65/65	0.28	0.02	2,11,60,60	0
19	CLA	A	1781	59/65	0.28	0.02	2,25,60,60	0
22	PQN	A	1802	33/33	0.31	-0.04	2,4,59,60	0
19	CLA	B	1750	50/65	0.26	-0.05	2,37,60,60	0
19	CLA	A	1795	51/65	0.30	-0.05	2,12,60,60	0
19	CLA	L	1168	50/65	0.26	-0.06	2,18,60,60	0
23	BCR	B	1778	40/40	0.27	-0.07	2,2,60,60	0
19	CLA	2	2010	25/65	0.25	-0.10	2,36,60,60	0
19	CLA	B	1760	50/65	0.30	-0.11	2,12,60,60	0
19	CLA	A	1760	55/65	0.30	-0.12	2,11,60,60	0
19	CLA	B	1764	45/65	0.26	-0.13	2,16,60,60	0
19	CLA	A	1785	65/65	0.29	-0.14	2,12,60,60	0
19	CLA	B	1751	46/65	0.32	-0.18	2,34,60,60	0
19	CLA	2	1221	50/65	0.31	-0.20	2,18,60,60	0
19	CLA	L	1167	47/65	0.24	-0.20	2,13,45,60	0
19	CLA	B	1761	50/65	0.26	-0.21	2,7,51,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	CLA	4	1205	50/65	0.24	-0.21	2,20,60,60	0
19	CLA	B	1765	45/65	0.36	-0.22	12,37,60,60	0
19	CLA	A	1767	65/65	0.33	-0.22	2,15,60,60	0
19	CLA	1	1200	25/65	0.26	-0.23	5,42,60,60	0
19	CLA	B	1767	60/65	0.30	-0.23	2,2,60,60	0
19	CLA	A	1784	55/65	0.27	-0.24	2,12,60,60	0
19	CLA	A	1778	42/65	0.26	-0.24	2,46,60,60	0
19	CLA	H	1081	50/65	0.28	-0.24	2,27,60,60	0
20	LMU	B	1782	25/35	0.21	-0.24	2,36,60,60	0
19	CLA	B	1741	54/65	0.24	-0.27	2,17,60,60	0
19	CLA	A	1796	65/65	0.30	-0.29	2,8,60,60	0
19	CLA	A	1814	65/65	0.25	-0.30	2,4,48,60	0
19	CLA	B	1747	53/65	0.27	-0.34	2,14,60,60	0
19	CLA	1	1188	41/65	0.26	-0.35	2,41,60,60	0
19	CLA	3	1212	25/65	0.32	-0.36	15,54,60,60	0
19	CLA	A	1788	65/65	0.25	-0.36	2,9,59,60	0
19	CLA	F	1155	36/65	0.24	-0.37	2,17,60,60	0
19	CLA	B	1740	25/65	0.32	-0.38	2,2,60,60	0
19	CLA	A	1769	50/65	0.26	-0.38	2,29,60,60	0
19	CLA	B	1756	65/65	0.32	-0.39	2,15,60,60	0
19	CLA	3	1218	56/65	0.33	-0.40	2,36,60,60	0
19	CLA	A	1761	54/65	0.26	-0.42	2,10,60,60	0
19	CLA	B	1758	65/65	0.25	-0.43	2,11,46,60	0
19	CLA	A	1762	56/65	0.27	-0.43	2,2,54,60	0
19	CLA	B	1752	55/65	0.26	-0.43	2,30,60,60	0
19	CLA	B	1753	65/65	0.25	-0.45	2,17,60,60	0
20	LMU	A	7023	35/35	0.27	-0.45	2,32,60,60	0
19	CLA	A	1768	54/65	0.27	-0.45	2,28,60,60	0
19	CLA	B	1738	65/65	0.24	-0.46	2,2,53,60	0
19	CLA	A	1763	46/65	0.27	-0.49	2,20,60,60	0
19	CLA	A	1815	65/65	0.26	-0.51	2,2,60,60	0
19	CLA	B	1768	65/65	0.24	-0.51	2,7,60,60	0
19	CLA	B	1755	58/65	0.30	-0.52	2,13,60,60	0
19	CLA	B	1737	61/65	0.26	-0.53	2,9,48,60	0
19	CLA	A	1772	54/65	0.27	-0.54	2,31,60,60	0
19	CLA	B	1766	51/65	0.32	-0.55	2,45,60,60	0
19	CLA	3	1213	36/65	0.28	-0.56	2,53,60,60	0
20	LMU	A	1811	35/35	0.24	-0.57	2,27,60,60	0
19	CLA	B	1743	65/65	0.25	-0.59	2,13,60,60	0
19	CLA	A	1771	50/65	0.30	-0.59	2,21,60,60	0
19	CLA	B	1759	65/65	0.24	-0.60	2,6,53,60	0
19	CLA	3	1215	25/65	0.26	-0.61	17,42,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	CLA	1	1196	36/65	0.28	-0.61	2,35,60,60	0
19	CLA	1	1195	25/65	0.30	-0.62	11,37,60,60	0
19	CLA	A	1791	45/65	0.27	-0.63	2,37,60,60	0
22	PQN	B	1773	33/33	0.29	-0.64	2,2,46,51	0
19	CLA	J	1043	61/65	0.24	-0.66	2,19,60,60	0
19	CLA	2	2006	50/65	0.31	-0.66	2,33,60,60	0
19	CLA	A	1765	52/65	0.22	-0.68	2,10,60,60	0
19	CLA	A	1789	65/65	0.24	-0.69	2,14,60,60	0
19	CLA	3	1216	25/65	0.26	-0.69	2,56,60,60	0
19	CLA	A	1813	65/65	0.26	-0.74	2,2,48,60	0
19	CLA	1	1143	50/65	0.29	-0.74	2,28,60,60	0
19	CLA	4	1208	25/65	0.21	-0.80	2,2,26,32	0
21	SUC	H	1082	23/23	0.24	-0.81	3,33,60,60	0
19	CLA	3	1221	65/65	0.31	-0.86	2,26,60,60	0
19	CLA	3	1220	25/65	0.26	-0.89	2,47,60,60	0
19	CLA	1	1198	25/65	0.23	-0.91	2,42,60,60	0
20	LMU	A	7040	35/35	0.29	-0.93	2,37,60,60	0
23	BCR	B	1779	40/40	0.21	-0.96	2,6,60,60	0
19	CLA	A	1770	25/65	0.28	-0.98	2,31,60,60	0
19	CLA	1	1190	46/65	0.26	-1.00	2,35,60,60	0
19	CLA	A	1797	59/65	0.29	-1.01	2,30,60,60	0
19	CLA	A	1793	65/65	0.28	-1.04	2,6,60,60	0
19	CLA	B	1769	47/65	0.24	-1.05	2,5,55,60	0
19	CLA	A	1794	47/65	0.23	-1.08	2,8,50,60	0
19	CLA	2	1213	58/65	0.20	-1.08	2,22,60,60	0
19	CLA	2	1223	61/65	0.23	-1.09	2,34,60,60	0
19	CLA	3	3011	65/65	0.33	-1.10	2,33,60,60	0
19	CLA	1	1189	47/65	0.23	-1.19	2,17,60,60	0
19	CLA	A	1816	54/65	0.24	-1.20	2,6,45,60	0
19	CLA	3	1214	25/65	0.21	-1.20	2,28,60,60	0
20	LMU	A	7035	35/35	0.25	-1.36	2,29,60,60	0
19	CLA	2	1218	25/65	0.21	-1.69	2,12,60,60	0
19	CLA	2	1212	51/65	0.23	-1.71	2,33,60,60	0
19	CLA	3	1219	25/65	0.22	-1.84	2,37,60,60	0
20	LMU	A	7001	35/35	0.22	-1.89	2,37,60,60	0
25	SF4	C	1083	8/8	0.09	-2.15	12,19,20,24	0
25	SF4	C	1082	8/8	0.08	-2.30	18,22,26,32	0
25	SF4	B	1783	8/8	0.05	-3.06	23,24,24,25	0
19	CLA	2	1216	25/65	0.23	-3.08	2,57,60,60	0
20	LMU	A	7039	35/35	0.24	-10.14	2,33,60,60	0
21	SUC	B	8051	23/23	0.33	-	2,44,60,60	0
20	LMU	A	7013	35/35	0.21	-	2,44,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
20	LMU	A	7028	35/35	0.24	-	2,23,60,60	0
20	LMU	A	7026	35/35	0.30	-	2,15,60,60	0
19	CLA	1	1149	46/65	0.40	-	2,43,60,60	0
20	LMU	A	7009	34/35	0.22	-	2,22,60,60	0
20	LMU	A	7037	35/35	0.27	-	2,30,60,60	0
20	LMU	A	7036	34/35	0.27	-	2,23,60,60	0
21	SUC	B	8056	23/23	0.18	-	2,31,56,60	0
21	SUC	B	8060	23/23	0.24	-	6,40,60,60	0
20	LMU	A	7032	35/35	0.18	-	2,31,60,60	0
19	CLA	1	1146	50/65	0.29	-	2,60,60,60	0
20	LMU	A	7019	35/35	0.32	-	2,43,60,60	0
19	CLA	3	1222	65/65	0.40	-	2,46,60,60	0
20	LMU	A	7016	35/35	0.39	-	2,45,60,60	0
21	SUC	B	8059	23/23	0.29	-	2,29,60,60	0
20	LMU	A	7008	35/35	0.24	-	2,34,60,60	0
19	CLA	2	1219	36/65	0.32	-	2,34,60,60	0
20	LMU	A	7021	35/35	0.31	-	2,35,60,60	0
20	LMU	A	7006	35/35	0.21	-	2,25,60,60	0
20	LMU	A	7004	35/35	0.24	-	2,11,50,60	0
20	LMU	A	7015	35/35	0.43	-	2,35,60,60	0
19	CLA	R	1054	57/65	0.27	-	2,38,60,60	0
19	CLA	3	3015	25/65	0.33	-	2,42,60,60	0
20	LMU	A	7014	35/35	0.36	-	2,45,60,60	0
20	LMU	A	7011	35/35	0.25	-	2,12,50,57	0
19	CLA	4	1206	65/65	0.26	-	2,15,60,60	0
20	LMU	A	7030	35/35	0.25	-	2,16,60,60	0
19	CLA	1	1145	55/65	0.37	-	2,47,60,60	0
19	CLA	1	1014	51/65	0.37	-	2,51,60,60	0
21	SUC	B	8061	23/23	0.34	-	2,52,60,60	0
20	LMU	A	7031	35/35	0.32	-	2,40,60,60	0
20	LMU	4	1212	35/35	0.32	-	2,37,60,60	0
19	CLA	3	3008	50/65	0.32	-	2,56,60,60	0
20	LMU	A	7043	35/35	0.27	-	2,41,60,60	0
19	CLA	4	4007	52/65	0.41	-	2,34,60,60	0
21	SUC	B	8062	23/23	0.26	-	2,34,60,60	0
21	SUC	3	1223	23/23	0.21	-	2,27,60,60	0
20	LMU	A	7025	35/35	0.24	-	2,27,60,60	0
26	UNL	B	8057	23/-	0.19	-	2,31,60,60	0
20	LMU	A	7027	35/35	0.29	-	2,29,60,60	0
19	CLA	2	1217	65/65	0.24	-	2,24,60,60	0
19	CLA	3	1217	42/65	0.24	-	2,53,60,60	0
19	CLA	R	1055	65/65	0.32	-	2,35,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	CLA	4	1204	25/65	0.45	-	2,40,60,60	0
19	CLA	1	1142	46/65	0.24	-	2,51,60,60	0
19	CLA	4	1211	46/65	0.30	-	2,45,60,60	0
20	LMU	R	1056	35/35	0.23	-	2,21,60,60	0
19	CLA	1	1308	48/65	0.27	-	2,34,60,60	0
19	CLA	1	1194	25/65	0.26	-	2,31,60,60	0
20	LMU	A	7024	35/35	0.28	-	2,35,60,60	0
20	LMU	A	1812	35/35	0.27	-	2,45,60,60	0
20	LMU	A	7020	35/35	0.24	-	2,38,60,60	0
20	LMU	A	7034	35/35	0.27	-	2,21,55,60	0
21	SUC	B	8054	23/23	0.29	-	2,30,60,60	0
19	CLA	1	1193	51/65	0.27	-	2,36,60,60	0
20	LMU	A	7049	35/35	0.27	-	2,51,60,60	0
20	LMU	A	7003	35/35	0.35	-	2,44,60,60	0
19	CLA	3	3001	25/65	0.60	-	2,30,60,60	0
21	SUC	B	8053	22/23	0.39	-	6,52,60,60	0
19	CLA	4	4014	47/65	0.30	-	2,37,60,60	0
19	CLA	1	1309	25/65	0.65	-	2,42,60,60	0
21	SUC	B	8055	23/23	0.27	-	2,41,60,60	0
20	LMU	A	7041	35/35	0.23	-	2,38,60,60	0
20	LMU	A	7042	35/35	0.30	-	2,38,60,60	0
20	LMU	A	7005	35/35	0.18	-	2,28,59,60	0
20	LMU	A	7017	35/35	0.21	-	2,31,60,60	0
20	LMU	A	7038	35/35	0.36	-	2,34,60,60	0
19	CLA	1	1148	55/65	0.48	-	2,46,60,60	0
23	BCR	A	1809	40/40	0.42	-	2,32,60,60	0
21	SUC	B	8052	23/23	0.33	-	9,40,60,60	0
20	LMU	A	7022	35/35	0.20	-	2,36,60,60	0

6.5 Other polymers ⓘ

There are no such residues in this entry.