



wwPDB X-ray Structure Validation Summary Report

Jun 17, 2014 – 05:43 AM BST

PDB ID : 4V8K
Title : Crystal structure of the LH1-RC complex from Thermochromatium tepidum
in P21 form
Authors : Niwa, S.; Takeda, K.; Wang-Otomo, Z.-Y.; Miki, K.
Deposited on : 2013-11-22
Resolution : 3.01 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>

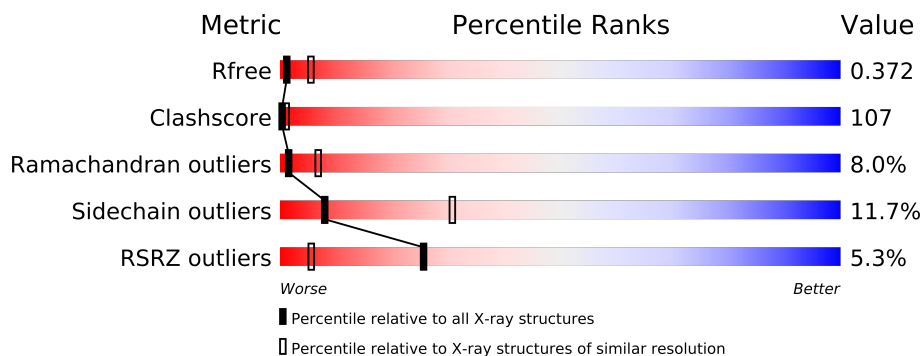
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
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) : stable23397

1 Overall quality at a glance

The reported resolution of this entry is 3.01 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	AC	404	
1	BC	404	
2	AL	281	
2	BL	281	
3	AM	325	
3	BM	325	
4	AH	259	
4	BH	259	
5	A1	61	
5	A3	61	
5	A5	61	
5	A7	61	
5	A9	61	
5	AA	61	

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Mol	Chain	Length	Quality of chain
5	AD	61	
5	AF	61	
5	AI	61	
5	AK	61	
5	AO	61	
5	AQ	61	
5	AS	61	
5	AU	61	
5	AW	61	
5	AY	61	
5	B1	61	
5	B3	61	
5	B5	61	
5	B7	61	
5	B9	61	
5	BA	61	
5	BD	61	
5	BF	61	
5	BI	61	
5	BK	61	
5	BO	61	
5	BQ	61	
5	BS	61	
5	BU	61	
5	BW	61	
5	BY	61	
6	A0	47	
6	A2	47	
6	A4	47	
6	A6	47	
6	A8	47	
6	AB	47	
6	AE	47	
6	AG	47	
6	AJ	47	
6	AN	47	
6	AP	47	
6	AR	47	
6	AT	47	
6	AV	47	
6	AX	47	
6	AZ	47	

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Mol	Chain	Length	Quality of chain
6	B0	47	
6	B2	47	
6	B4	47	
6	B6	47	
6	B8	47	
6	BB	47	
6	BE	47	
6	BG	47	
6	BJ	47	
6	BN	47	
6	BP	47	
6	BR	47	
6	BT	47	
6	BV	47	
6	BX	47	
6	BZ	47	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
13	MQ8	AM	405	-	X
13	MQ8	BM	405	-	X
14	CRT	A0	101	-	X
14	CRT	A1	103	-	X
14	CRT	A2	102	-	X
14	CRT	A5	103	-	X
14	CRT	A7	102	-	X
14	CRT	AA	102	-	X
14	CRT	AB	102	-	X
14	CRT	AG	102	-	X
14	CRT	AJ	102	-	X
14	CRT	AN	102	-	X
14	CRT	AP	102	-	X
14	CRT	AR	102	-	X
14	CRT	AS	104	-	X
14	CRT	AT	102	-	X
14	CRT	AW	102	-	X
14	CRT	AX	102	-	X
14	CRT	B0	101	-	X
14	CRT	B1	103	-	X
14	CRT	B2	102	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
14	CRT	B5	103	-	X
14	CRT	B7	102	-	X
14	CRT	BA	102	-	X
14	CRT	BB	102	-	X
14	CRT	BF	103	-	X
14	CRT	BG	102	-	X
14	CRT	BN	102	-	X
14	CRT	BO	103	-	X
14	CRT	BP	102	-	X
14	CRT	BS	103	-	X
14	CRT	BU	103	-	X
14	CRT	BV	102	-	X
14	CRT	BW	103	-	X
15	PEF	AM	407	-	X
15	PEF	AM	409	-	X
15	PEF	AS	101	-	X
15	PEF	BM	407	-	X
15	PEF	BQ	101	-	X
9	BCL	A3	103	-	X
9	BCL	AI	102	-	X
9	BCL	AQ	102	-	X
9	BCL	AS	103	-	X
9	BCL	AU	102	-	X
9	BCL	AW	101	-	X
9	BCL	B0	102	-	X
9	BCL	B7	103	-	X
9	BCL	B9	102	-	X
9	BCL	BD	102	-	X
9	BCL	BK	102	-	X
9	BCL	BM	402	-	X
9	BCL	BN	101	-	X
9	BCL	BQ	103	-	X

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 50862 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 Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AC	317	Total	C	N	O	S	0	0	0
			2458	1551	430	460	17			
1	BC	317	Total	C	N	O	S	0	0	0
			2458	1551	430	460	17			

- Molecule 2 is a protein called Photosynthetic reaction center L subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AL	280	Total	C	N	O	S	0	0	0
			2231	1501	359	361	10			
2	BL	280	Total	C	N	O	S	0	0	0
			2231	1501	359	361	10			

- Molecule 3 is a protein called Photosynthetic reaction center M subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AM	319	Total	C	N	O	S	0	0	0
			2551	1713	417	410	11			
3	BM	319	Total	C	N	O	S	0	0	0
			2551	1713	417	410	11			

- Molecule 4 is a protein called Photosynthetic reaction center H subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AH	258	Total	C	N	O	S	0	0	0
			1982	1275	339	363	5			
4	BH	258	Total	C	N	O	S	0	0	0
			1982	1275	339	363	5			

- Molecule 5 is a protein called LH1 alpha polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AA	48	Total	C	N	O	S	0	0	0
			392	265	62	64	1			
5	AD	57	Total	C	N	O	S	0	0	0
			447	295	74	77	1			
5	AF	59	Total	C	N	O	S	0	0	0
			462	304	76	80	2			
5	AI	59	Total	C	N	O	S	0	0	0
			462	304	76	80	2			
5	AK	58	Total	C	N	O	S	0	0	0
			455	300	75	78	2			
5	AO	59	Total	C	N	O	S	0	0	0
			462	304	76	80	2			
5	AQ	57	Total	C	N	O	S	0	0	0
			447	295	74	77	1			
5	AS	59	Total	C	N	O	S	0	0	0
			462	304	76	80	2			
5	AU	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	AW	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	AY	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	A1	58	Total	C	N	O	S	0	0	0
			455	300	75	78	2			
5	A3	57	Total	C	N	O	S	0	0	0
			447	295	74	77	1			
5	A5	56	Total	C	N	O	S	0	0	0
			444	294	73	75	2			
5	A7	51	Total	C	N	O	S	0	0	0
			417	279	67	69	2			
5	A9	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	BA	55	Total	C	N	O	S	0	0	0
			448	299	72	75	2			
5	BD	45	Total	C	N	O	S	0	0	0
			370	250	59	60	1			
5	BF	56	Total	C	N	O	S	0	0	0
			444	294	73	75	2			
5	BI	50	Total	C	N	O	S	0	0	0
			409	274	66	68	1			
5	BK	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	BO	59	Total	C	N	O	S	0	0	0
			462	304	76	80	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	BQ	59	Total	C	N	O	S	0	0	0
			467	310	76	79	2			
5	BS	59	Total	C	N	O	S	0	0	0
			462	304	76	80	2			
5	BU	58	Total	C	N	O	S	0	0	0
			462	307	75	78	2			
5	BW	58	Total	C	N	O	S	0	0	0
			455	300	75	78	2			
5	BY	54	Total	C	N	O	S	0	0	0
			426	284	69	72	1			
5	B1	54	Total	C	N	O	S	0	0	0
			426	284	69	72	1			
5	B3	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	B5	51	Total	C	N	O	S	0	0	0
			417	279	67	69	2			
5	B7	54	Total	C	N	O	S	0	0	0
			426	284	69	72	1			
5	B9	51	Total	C	N	O	S	0	0	0
			417	279	67	69	2			

- Molecule 6 is a protein called LH1 beta polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AB	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	AE	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	AG	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	AJ	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	AN	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	AP	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	AR	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	AT	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	AV	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			

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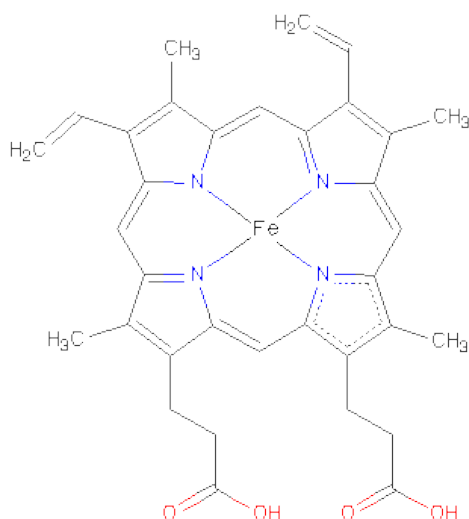
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AX	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	AZ	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	A2	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	A4	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	A6	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	A8	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	A0	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	BB	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	BE	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	BG	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	BJ	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	BN	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	BP	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	BR	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	BT	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	BV	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	BX	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	BZ	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	B2	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	B4	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	B6	40	Total 337	C 228	N 52	O 55	S 2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B8	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	B0	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	AC	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	AC	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	AC	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	AC	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	BC	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	BC	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	BC	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

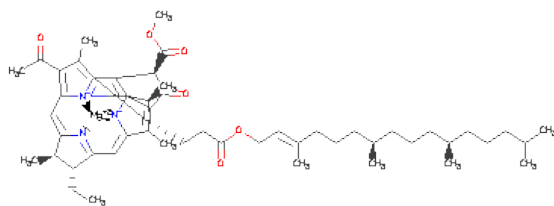
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	BA	1	Total Ca 1 1	0	0
8	AK	1	Total Ca 1 1	0	0
8	B1	1	Total Ca 1 1	0	0
8	BI	1	Total Ca 1 1	0	0
8	AS	1	Total Ca 1 1	0	0
8	B5	1	Total Ca 1 1	0	0
8	B9	1	Total Ca 1 1	0	0
8	BF	1	Total Ca 1 1	0	0
8	AV	1	Total Ca 1 1	0	0
8	AA	1	Total Ca 1 1	0	0
8	BQ	1	Total Ca 1 1	0	0
8	A5	1	Total Ca 1 1	0	0
8	BC	1	Total Ca 1 1	0	0
8	BU	1	Total Ca 1 1	0	0
8	A1	1	Total Ca 1 1	0	0
8	AD	1	Total Ca 1 1	0	0
8	AI	1	Total Ca 1 1	0	0
8	BY	1	Total Ca 1 1	0	0
8	B3	1	Total Ca 1 1	0	0
8	BK	1	Total Ca 1 1	0	0
8	AU	1	Total Ca 1 1	0	0
8	B7	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A9	1	Total	Ca	0	0
			1	1		
8	BO	1	Total	Ca	0	0
			1	1		
8	AQ	1	Total	Ca	0	0
			1	1		
8	AC	1	Total	Ca	0	0
			1	1		
8	BS	1	Total	Ca	0	0
			1	1		
8	A7	1	Total	Ca	0	0
			1	1		
8	BD	1	Total	Ca	0	0
			1	1		
8	AO	1	Total	Ca	0	0
			1	1		
8	BW	1	Total	Ca	0	0
			1	1		
8	AY	1	Total	Ca	0	0
			1	1		
8	A3	1	Total	Ca	0	0
			1	1		
8	AF	1	Total	Ca	0	0
			1	1		

- Molecule 9 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	AL	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AL	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AM	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AM	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AA	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AB	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AD	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AE	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AF	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AG	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AI	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AJ	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AK	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AN	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AO	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AP	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AQ	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AR	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AS	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AT	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AU	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AV	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	AW	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AX	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AY	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AZ	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	A1	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	A2	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	A3	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	A3	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	A5	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	A6	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	A7	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	A8	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	A9	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	A0	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BL	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BL	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BM	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BM	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BA	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BB	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BD	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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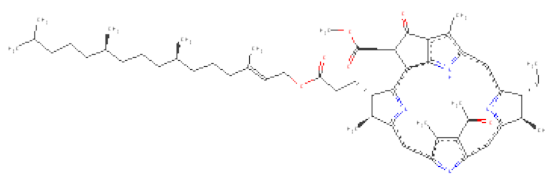
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	BE	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BF	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BG	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BI	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BJ	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BK	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BN	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BO	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BP	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BQ	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BQ	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BS	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BT	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BU	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BV	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BW	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BX	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BY	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BZ	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	B1	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	B2	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B3	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	B4	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	B5	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	B6	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	B7	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	B8	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	B9	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	B0	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 10 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



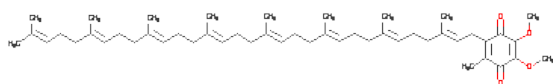
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	AL	1	Total	C	N	O	0	0
			65	55	4	6		
10	AM	1	Total	C	N	O	0	0
			65	55	4	6		
10	BL	1	Total	C	N	O	0	0
			65	55	4	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	BM	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 11 is Ubiquinone-8 (three-letter code: UQ8) (formula: C₄₉H₇₄O₄).

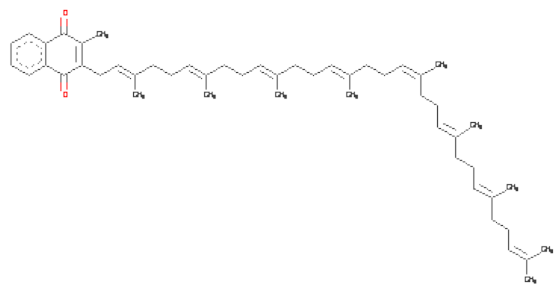


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	AL	1	Total	C	O	0	0
			53	49	4		
11	BL	1	Total	C	O	0	0
			53	49	4		

- Molecule 12 is FE (III) ION (three-letter code: FE) (formula: Fe).

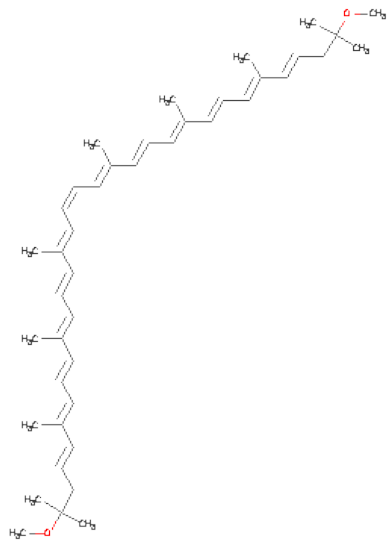
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	BM	1	Total	Fe	0	0
			1	1		
12	AM	1	Total	Fe	0	0
			1	1		

- Molecule 13 is MENAQUINONE 8 (three-letter code: MQ8) (formula: C₅₁H₇₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	AM	1	Total	C	O	0	0
			53	51	2		
13	BM	1	Total	C	O	0	0
			53	51	2		

- Molecule 14 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: C₄₂H₆₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	AM	1	Total	C	O	0	0
			44	42	2		
14	AA	1	Total	C	O	0	0
			44	42	2		

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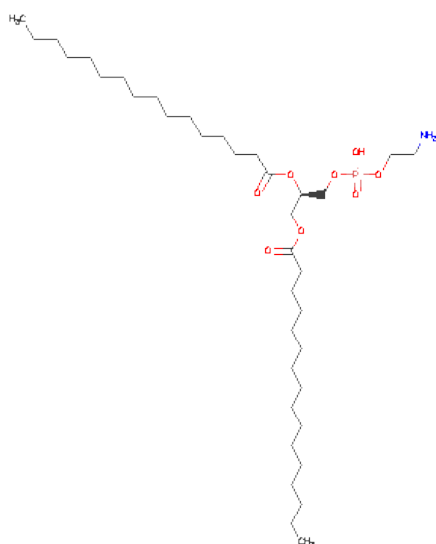
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	AB	1	Total	C	O	0	0
			44	42	2		
14	AG	1	Total	C	O	0	0
			44	42	2		
14	AJ	1	Total	C	O	0	0
			44	42	2		
14	AN	1	Total	C	O	0	0
			44	42	2		
14	AP	1	Total	C	O	0	0
			44	42	2		
14	AR	1	Total	C	O	0	0
			44	42	2		
14	AS	1	Total	C	O	0	0
			44	42	2		
14	AT	1	Total	C	O	0	0
			44	42	2		
14	AW	1	Total	C	O	0	0
			44	42	2		
14	AX	1	Total	C	O	0	0
			44	42	2		
14	A1	1	Total	C	O	0	0
			44	42	2		
14	A2	1	Total	C	O	0	0
			44	42	2		
14	A5	1	Total	C	O	0	0
			44	42	2		
14	A7	1	Total	C	O	0	0
			44	42	2		
14	A0	1	Total	C	O	0	0
			44	42	2		
14	BM	1	Total	C	O	0	0
			44	42	2		
14	BA	1	Total	C	O	0	0
			44	42	2		
14	BB	1	Total	C	O	0	0
			44	42	2		
14	BF	1	Total	C	O	0	0
			44	42	2		
14	BG	1	Total	C	O	0	0
			44	42	2		
14	BN	1	Total	C	O	0	0
			44	42	2		

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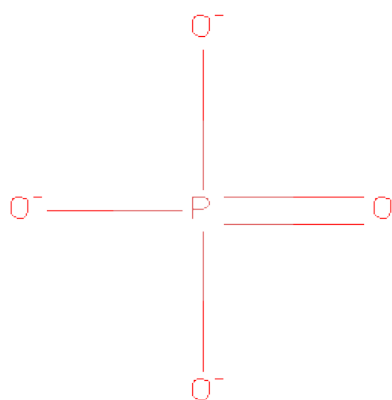
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	BO	1	Total	C	O	0	0
			44	42	2		
14	BP	1	Total	C	O	0	0
			44	42	2		
14	BS	1	Total	C	O	0	0
			44	42	2		
14	BU	1	Total	C	O	0	0
			44	42	2		
14	BV	1	Total	C	O	0	0
			44	42	2		
14	BW	1	Total	C	O	0	0
			44	42	2		
14	B1	1	Total	C	O	0	0
			44	42	2		
14	B2	1	Total	C	O	0	0
			44	42	2		
14	B5	1	Total	C	O	0	0
			44	42	2		
14	B7	1	Total	C	O	0	0
			44	42	2		
14	B0	1	Total	C	O	0	0
			44	42	2		

- Molecule 15 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: $C_{37}H_{74}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	AM	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
15	AM	1	Total	C	N	O	P	0	0
			14	6	1	6	1		
15	AM	1	Total	C	N	O	P	0	0
			47	37	1	8	1		
15	AH	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
15	AS	1	Total	C	N	O	P	0	0
			47	37	1	8	1		
15	BM	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
15	BQ	1	Total	C	N	O	P	0	0
			47	37	1	8	1		

- Molecule 16 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	AM	1	Total	O	P	0	0
			5	4	1		
16	AH	1	Total	O	P	0	0
			5	4	1		
16	A3	1	Total	O	P	0	0
			5	4	1		
16	BH	1	Total	O	P	0	0
			5	4	1		

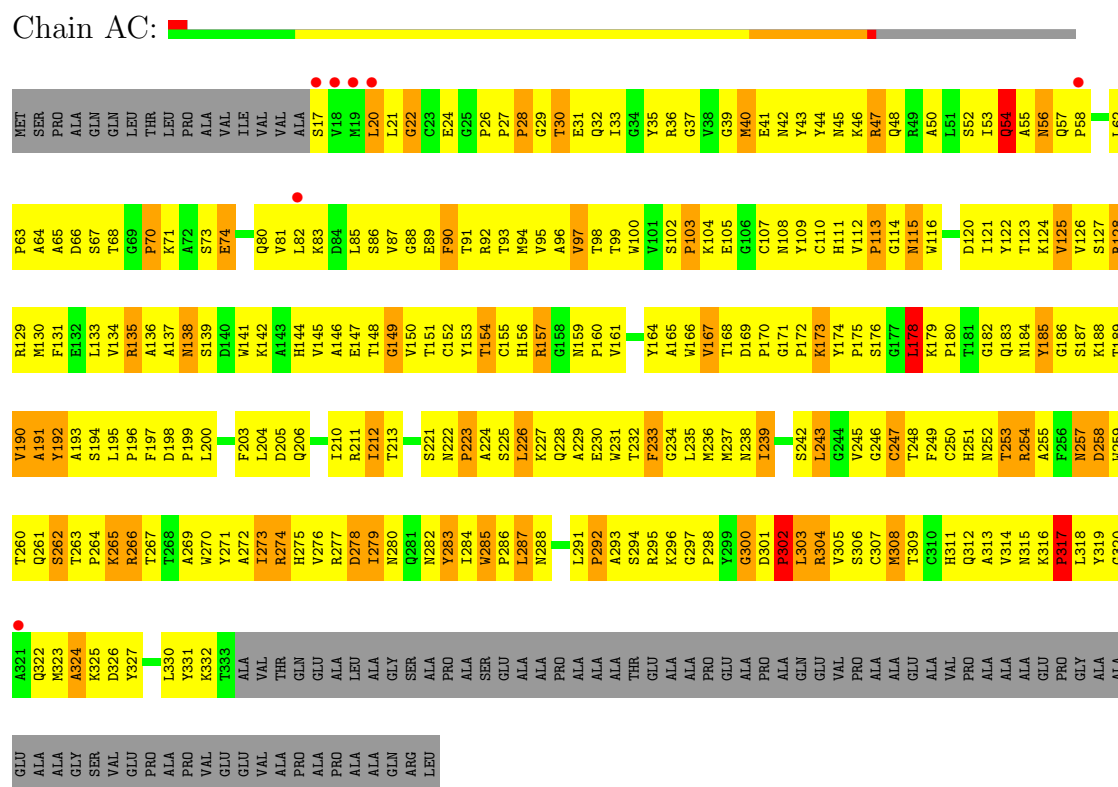
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	AC	1	Total 1	O 1	0	0
17	AL	3	Total 3	O 3	0	0
17	AM	3	Total 3	O 3	0	0
17	AH	2	Total 2	O 2	0	0
17	AA	1	Total 1	O 1	0	0
17	AI	1	Total 1	O 1	0	0
17	AW	1	Total 1	O 1	0	0
17	BC	1	Total 1	O 1	0	0
17	BL	3	Total 3	O 3	0	0
17	BM	3	Total 3	O 3	0	0
17	BH	1	Total 1	O 1	0	0
17	B1	1	Total 1	O 1	0	0

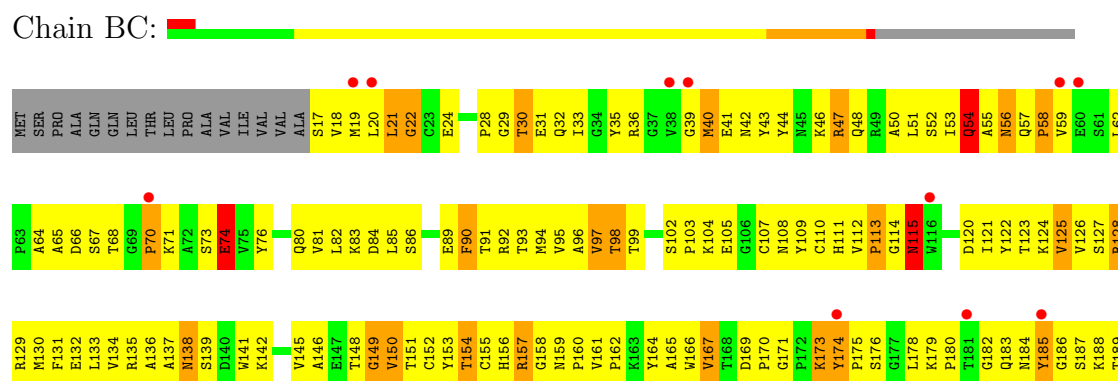
3 Residue-property plots

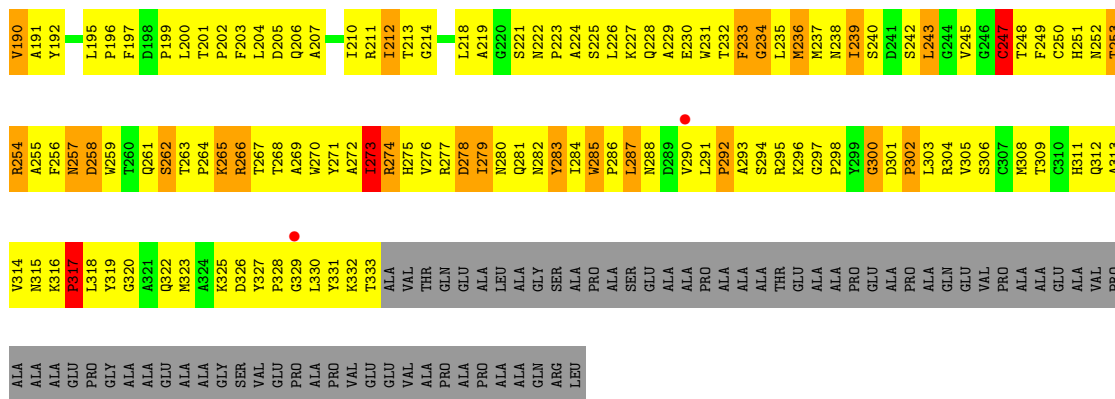
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Photosynthetic reaction center cytochrome c subunit



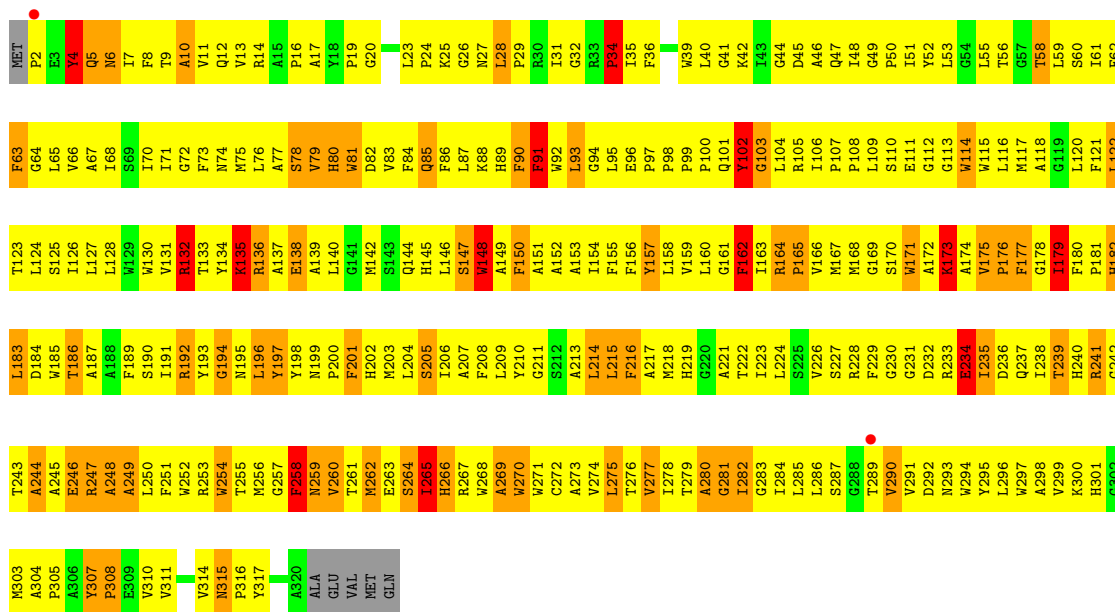
- Molecule 1: Photosynthetic reaction center cytochrome c subunit





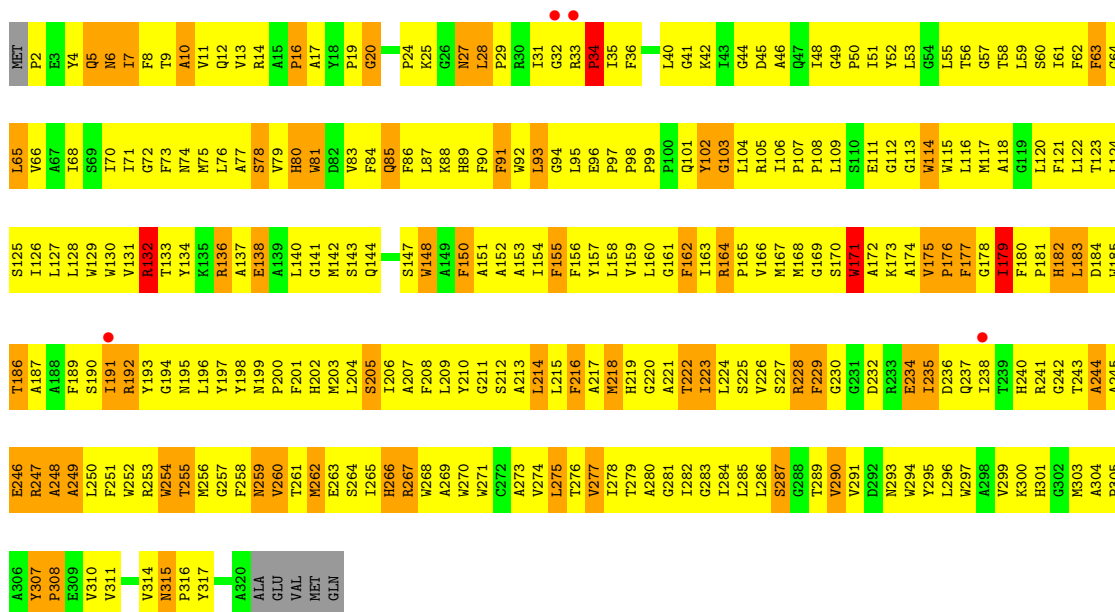
● Molecule 3: Photosynthetic reaction center M subunit

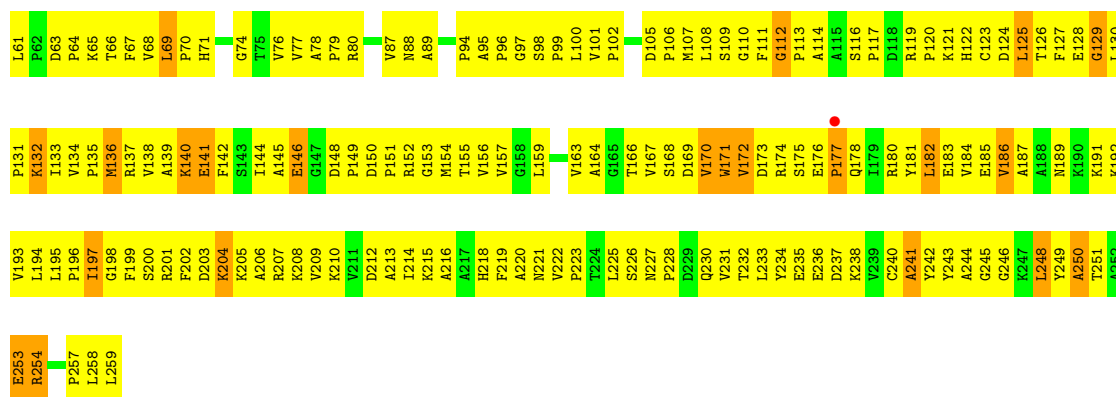
Chain AM:



● Molecule 3: Photosynthetic reaction center M subunit

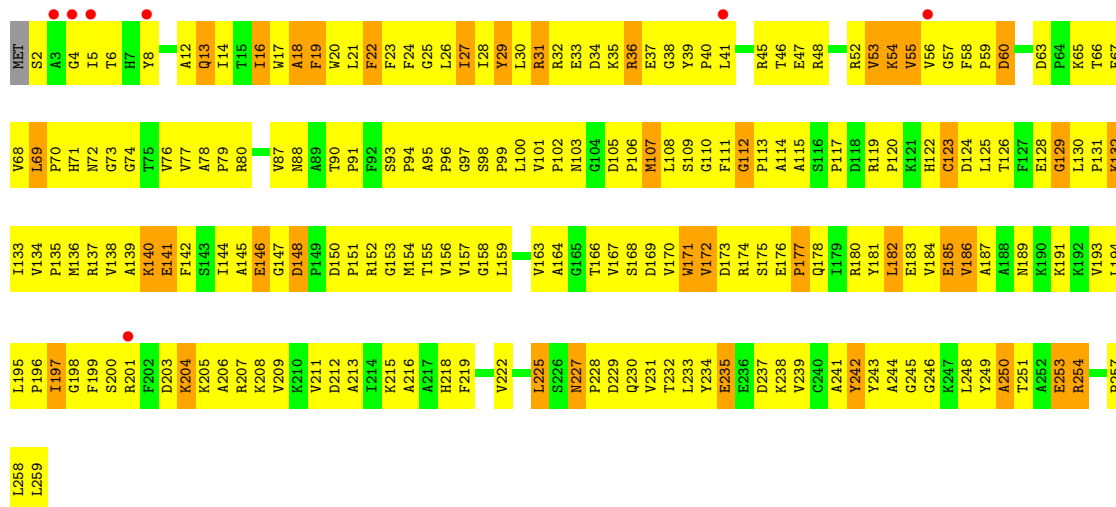
Chain BM:





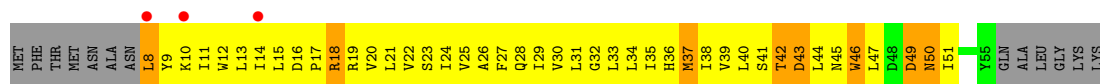
• Molecule 4: Photosynthetic reaction center H subunit

Chain BH:



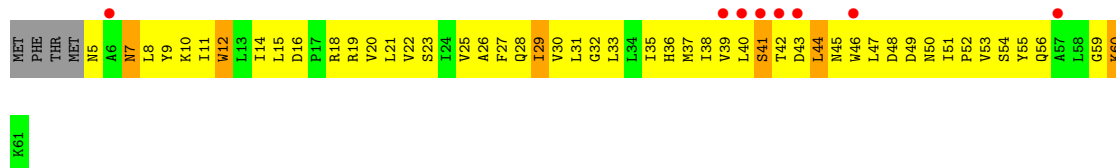
• Molecule 5: LH1 alpha polypeptide

Chain AA:



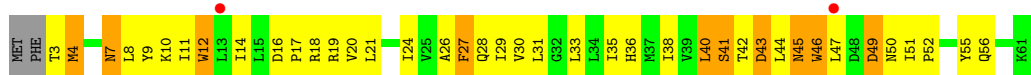
• Molecule 5: LH1 alpha polypeptide

Chain AD:



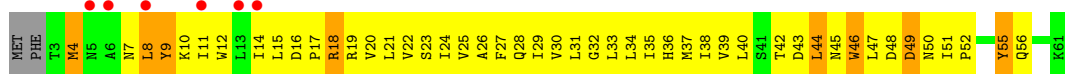
• Molecule 5: LH1 alpha polypeptide

Chain AF:



- Molecule 5: LH1 alpha polypeptide

Chain AI:



- Molecule 5: LH1 alpha polypeptide

Chain AK:



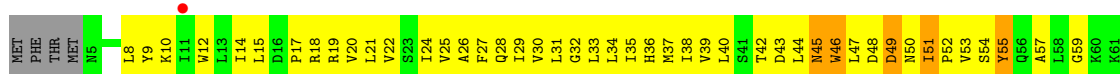
- Molecule 5: LH1 alpha polypeptide

Chain AO:



- Molecule 5: LH1 alpha polypeptide

Chain AQ:



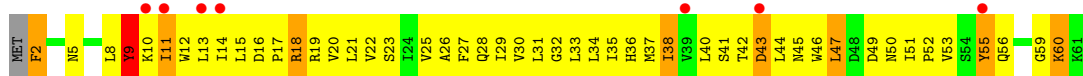
- Molecule 5: LH1 alpha polypeptide

Chain AS:



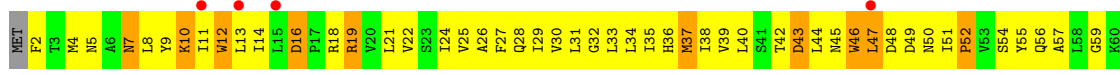
- Molecule 5: LH1 alpha polypeptide

Chain AU:



- Molecule 5: LH1 alpha polypeptide

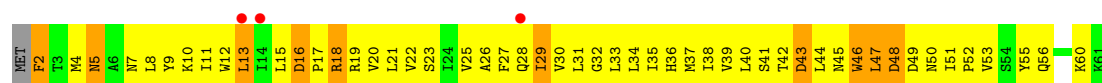
Chain AW:



K61

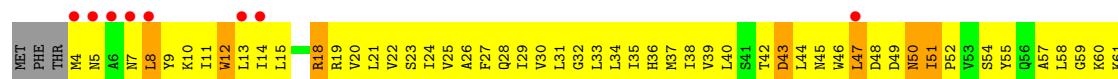
- Molecule 5: LH1 alpha polypeptide

Chain AY: 



- Molecule 5: LH1 alpha polypeptide

Chain A1: 



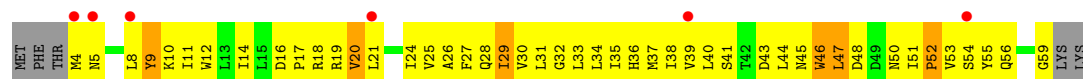
- Molecule 5: LH1 alpha polypeptide

Chain A3: 



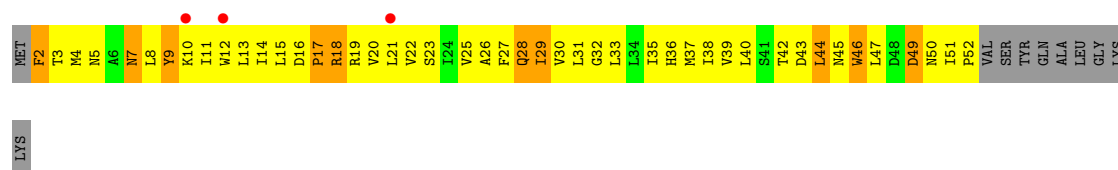
- Molecule 5: LH1 alpha polypeptide

Chain A5: 



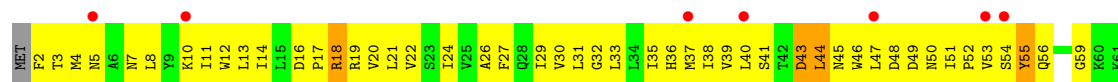
- Molecule 5: LH1 alpha polypeptide

Chain A7: 



- Molecule 5: LH1 alpha polypeptide

Chain A9: 



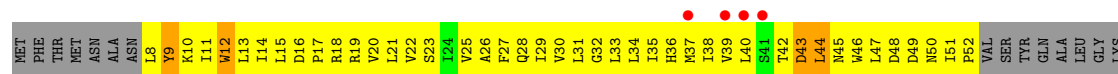
- Molecule 5: LH1 alpha polypeptide

Chain BA: 



- Molecule 5: LH1 alpha polypeptide

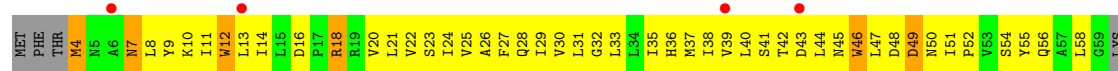
Chain BD: 



LYS

- Molecule 5: LH1 alpha polypeptide

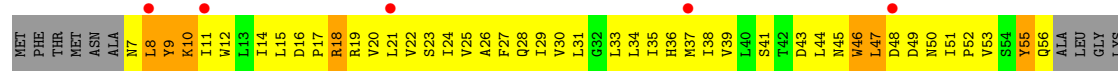
Chain BF:



LYS

- Molecule 5: LH1 alpha polypeptide

Chain BI:



LYS

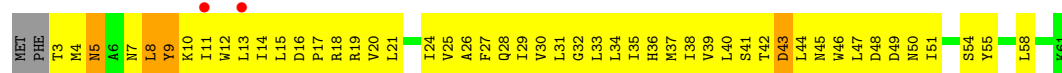
- Molecule 5: LH1 alpha polypeptide

Chain BK:



- Molecule 5: LH1 alpha polypeptide

Chain BO:



- Molecule 5: LH1 alpha polypeptide

Chain BQ:

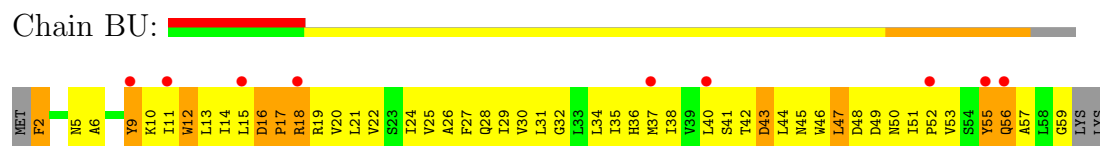


- Molecule 5: LH1 alpha polypeptide

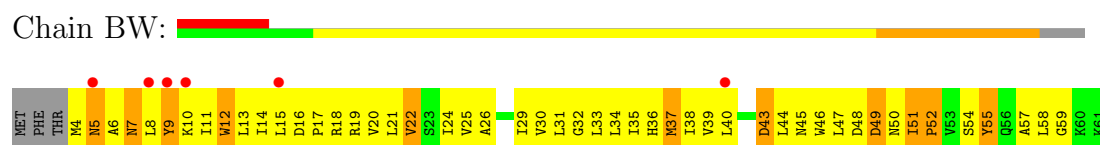
Chain BS:



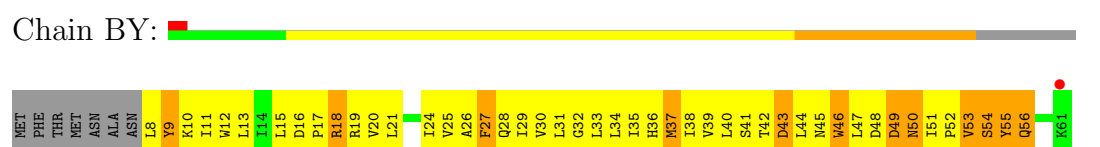
- Molecule 5: LH1 alpha polypeptide



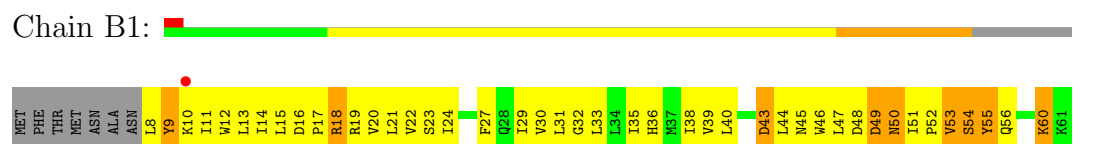
- Molecule 5: LH1 alpha polypeptide



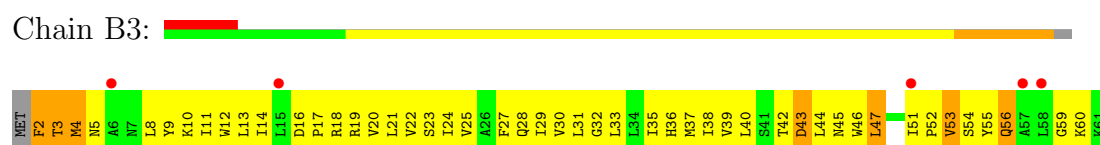
- Molecule 5: LH1 alpha polypeptide



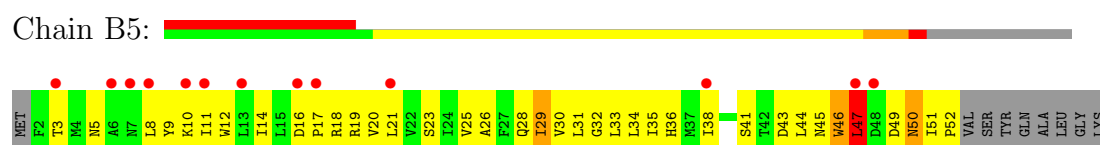
- Molecule 5: LH1 alpha polypeptide



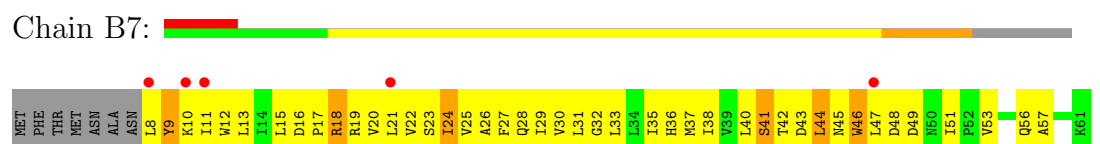
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide

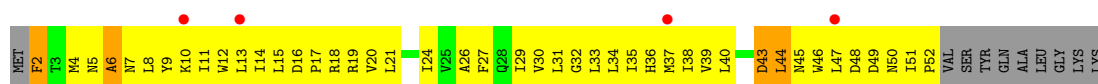


- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide





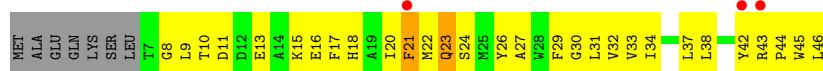
- Molecule 6: LH1 beta polypeptide

Chain AB:



- Molecule 6: LH1 beta polypeptide

Chain AE:



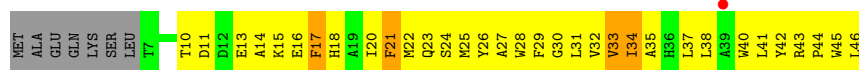
- Molecule 6: LH1 beta polypeptide

Chain AG:



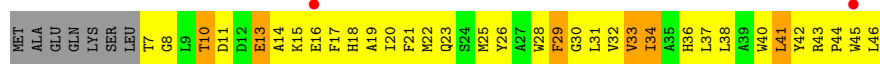
- Molecule 6: LH1 beta polypeptide

Chain AJ:



- Molecule 6: LH1 beta polypeptide

Chain AN:



- Molecule 6: LH1 beta polypeptide

Chain AP:



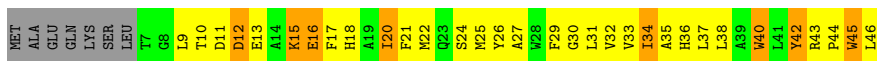
- Molecule 6: LH1 beta polypeptide

Chain AR:



- Molecule 6: LH1 beta polypeptide

Chain AT:



- Molecule 6: LH1 beta polypeptide

Chain AV:



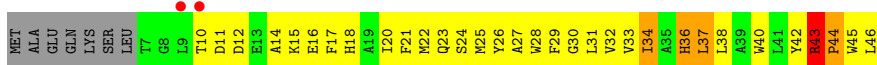
- Molecule 6: LH1 beta polypeptide

Chain AX:



- Molecule 6: LH1 beta polypeptide

Chain AZ:



- Molecule 6: LH1 beta polypeptide

Chain A2:



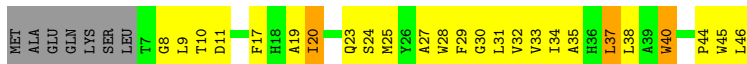
- Molecule 6: LH1 beta polypeptide

Chain A4:



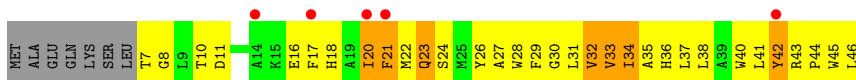
- Molecule 6: LH1 beta polypeptide

Chain A6:



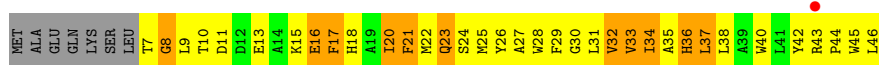
- Molecule 6: LH1 beta polypeptide

Chain A8:



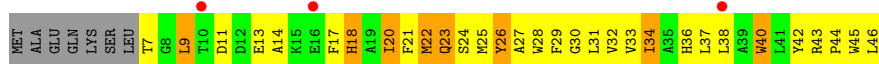
- Molecule 6: LH1 beta polypeptide

Chain A0:



- Molecule 6: LH1 beta polypeptide

Chain BB:



- Molecule 6: LH1 beta polypeptide

Chain BE:



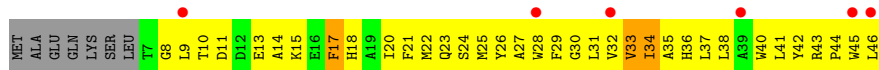
- Molecule 6: LH1 beta polypeptide

Chain BG:



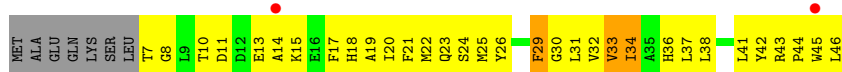
- Molecule 6: LH1 beta polypeptide

Chain BJ:



- Molecule 6: LH1 beta polypeptide

Chain BN:



- Molecule 6: LH1 beta polypeptide

Chain BP:



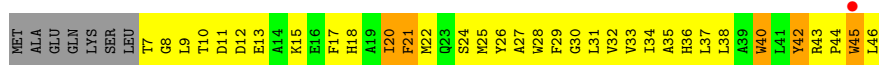
- Molecule 6: LH1 beta polypeptide

Chain BR:



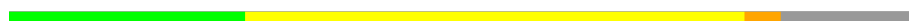
- Molecule 6: LH1 beta polypeptide

Chain BT:



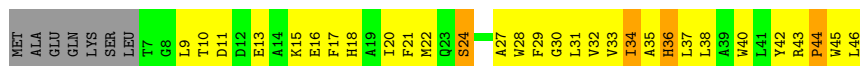
- Molecule 6: LH1 beta polypeptide

Chain BV:



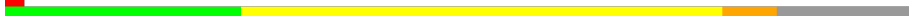
- Molecule 6: LH1 beta polypeptide

Chain BX:



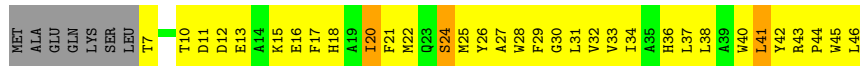
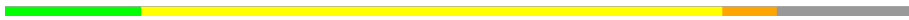
- Molecule 6: LH1 beta polypeptide

Chain BZ:



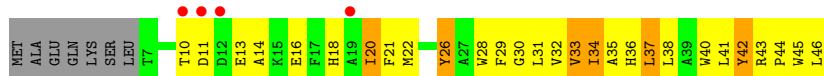
- Molecule 6: LH1 beta polypeptide

Chain B2:



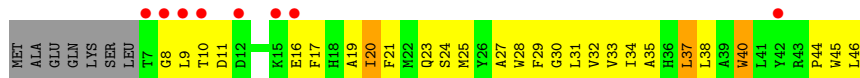
- Molecule 6: LH1 beta polypeptide

Chain B4:



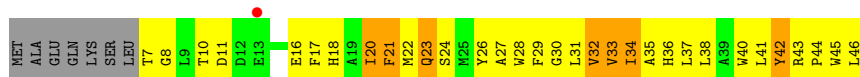
- Molecule 6: LH1 beta polypeptide

Chain B6:



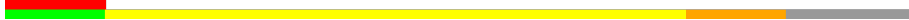
- Molecule 6: LH1 beta polypeptide

Chain B8:



- Molecule 6: LH1 beta polypeptide

Chain B0:



MET	ALA	GLU	GLN	LYS	SER	LEU	T7	G8	L9	T10	D11	D12	E13	A14	K15	E16	F17	H18	A19	I20	F21	N22	Q23	S24	M25	Y26	A27	W28	F29	G30	L31	V32	V33	I34	A35	H36	L37	L38	W40	L41	Y42	R43	P44	W45	L46
-----	-----	-----	-----	-----	-----	-----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	167.16Å 145.43Å 210.53Å 90.00° 108.50° 90.00°	Depositor
Resolution (Å)	43.79 – 3.01 43.79 – 3.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.79-3.01) 69.3 (43.79-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.335 , 0.356 0.372 , 0.372	Depositor DCC
R_{free} test set	8241 reflections (5.17%)	DCC
Wilson B-factor (Å ²)	55.8	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 56.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Outliers	8 of 167610 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	50862	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.99% 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: BCL, CRT, BPH, CA, UQ8, FE, MQ8, HEM, PEF, PO4

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	AC	0.61	0/2528	0.81	2/3451 (0.1%)
1	BC	0.59	1/2528 (0.0%)	0.79	1/3451 (0.0%)
2	AL	0.39	0/2318	0.63	0/3167
2	BL	0.36	0/2318	0.60	0/3167
3	AM	0.37	0/2651	0.63	0/3628
3	BM	0.36	0/2651	0.61	0/3628
4	AH	0.34	0/2037	0.57	0/2776
4	BH	0.33	0/2037	0.58	0/2776
5	A1	0.38	0/464	0.70	0/634
5	A3	0.30	0/456	0.64	0/624
5	A5	0.34	0/453	0.66	0/620
5	A7	0.30	0/426	0.61	0/583
5	A9	0.33	0/483	0.67	0/660
5	AA	0.31	0/401	0.57	0/550
5	AD	0.30	0/456	0.58	0/624
5	AF	0.30	0/471	0.62	0/644
5	AI	0.39	0/471	0.67	0/644
5	AK	0.28	0/464	0.57	0/634
5	AO	0.45	0/471	0.80	0/644
5	AQ	0.30	0/456	0.62	0/624
5	AS	0.32	0/471	0.65	0/644
5	AU	0.34	0/483	0.64	0/660
5	AW	0.34	0/483	0.61	0/660
5	AY	0.34	0/483	0.70	0/660
5	B1	0.32	0/435	0.58	0/595
5	B3	0.33	0/483	0.60	0/660
5	B5	0.32	0/426	0.68	0/583
5	B7	0.31	0/435	0.57	0/595
5	B9	0.35	0/426	0.65	0/583
5	BA	0.31	0/458	0.61	0/627
5	BD	0.41	0/378	0.67	0/518
5	BF	0.37	0/453	0.64	0/620

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	BI	0.33	0/418	0.61	0/573
5	BK	0.29	0/483	0.56	0/660
5	BO	0.37	0/471	0.71	0/644
5	BQ	0.29	0/477	0.58	0/653
5	BS	0.29	0/471	0.58	0/644
5	BU	0.42	1/472 (0.2%)	0.62	1/646 (0.2%)
5	BW	0.34	0/464	0.60	0/634
5	BY	0.31	0/435	0.58	0/595
6	A0	0.46	0/350	0.58	0/476
6	A2	0.33	0/350	0.52	0/476
6	A4	0.43	0/350	0.61	0/476
6	A6	0.34	0/350	0.57	0/476
6	A8	0.47	0/350	0.61	0/476
6	AB	0.40	0/350	0.53	0/476
6	AE	0.40	0/350	0.51	0/476
6	AG	0.46	0/350	0.59	0/476
6	AJ	0.45	0/350	0.57	0/476
6	AN	0.43	0/350	0.54	0/476
6	AP	0.41	0/350	0.56	0/476
6	AR	0.37	0/350	0.53	0/476
6	AT	0.35	0/350	0.52	0/476
6	AV	0.40	0/350	0.65	0/476
6	AX	0.39	0/350	0.56	0/476
6	AZ	0.52	1/350 (0.3%)	0.68	1/476 (0.2%)
6	B0	0.44	0/350	0.62	0/476
6	B2	0.40	0/350	0.59	0/476
6	B4	0.42	0/350	0.64	0/476
6	B6	0.33	0/350	0.55	0/476
6	B8	0.47	0/350	0.61	0/476
6	BB	0.43	0/350	0.59	0/476
6	BE	0.37	0/350	0.56	0/476
6	BG	0.49	0/350	0.76	1/476 (0.2%)
6	BJ	0.42	0/350	0.57	0/476
6	BN	0.45	0/350	0.60	0/476
6	BP	0.42	0/350	0.57	0/476
6	BR	0.38	0/350	0.57	0/476
6	BT	0.42	0/350	0.63	0/476
6	BV	0.37	0/350	0.71	0/476
6	BX	0.36	0/350	0.60	0/476
6	BZ	0.40	0/350	0.53	0/476
All	All	0.40	3/44845 (0.0%)	0.64	6/61215 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	BU	17	PRO	N-CD	5.25	1.55	1.47
6	AZ	44	PRO	N-CD	5.16	1.55	1.47
1	BC	247	CYS	CB-SG	-5.11	1.73	1.81

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	AZ	43	ARG	C-N-CD	5.83	140.64	128.40
1	AC	178	LEU	N-CA-C	5.77	126.58	111.00
5	BU	16	ASP	C-N-CD	5.61	140.17	128.40
6	BG	21	PHE	CB-CG-CD2	-5.49	116.95	120.80
1	BC	186	GLY	N-CA-C	-5.10	100.35	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AC	2458	0	2377	475	0
1	BC	2458	0	2377	488	0
2	AL	2231	0	2192	644	0
2	BL	2231	0	2192	563	0
3	AM	2551	0	2526	741	0
3	BM	2551	0	2526	662	0
4	AH	1982	0	1981	399	0
4	BH	1982	0	1981	373	0
5	A1	455	0	460	165	0
5	A3	447	0	451	135	0
5	A5	444	0	456	138	0
5	A7	417	0	441	159	0
5	A9	473	0	476	126	0
5	AA	392	0	412	138	0
5	AD	447	0	451	124	0
5	AF	462	0	467	153	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AI	462	0	467	147	0
5	AK	455	0	460	91	0
5	AO	462	0	467	153	0
5	AQ	447	0	451	118	0
5	AS	462	0	467	187	0
5	AU	473	0	476	150	0
5	AW	473	0	476	184	0
5	AY	473	0	476	165	0
5	B1	426	0	434	137	0
5	B3	473	0	476	134	0
5	B5	417	0	441	92	0
5	B7	426	0	434	133	0
5	B9	417	0	441	137	0
5	BA	448	0	462	154	0
5	BD	370	0	399	134	0
5	BF	444	0	456	146	0
5	BI	409	0	426	108	0
5	BK	473	0	476	102	0
5	BO	462	0	467	145	0
5	BQ	467	0	474	121	0
5	BS	462	0	467	111	0
5	BU	462	0	472	174	0
5	BW	455	0	460	159	0
5	BY	426	0	434	149	0
6	A0	337	0	323	111	0
6	A2	337	0	323	106	0
6	A4	337	0	323	82	0
6	A6	337	0	323	57	0
6	A8	337	0	323	105	0
6	AB	337	0	321	89	0
6	AE	337	0	323	69	0
6	AG	337	0	323	89	0
6	AJ	337	0	323	94	0
6	AN	337	0	323	86	0
6	AP	337	0	323	105	0
6	AR	337	0	323	73	0
6	AT	337	0	323	79	0
6	AV	337	0	323	98	0
6	AX	337	0	323	82	0
6	AZ	337	0	323	99	0
6	B0	337	0	323	123	0
6	B2	337	0	323	132	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B4	337	0	323	70	0
6	B6	337	0	323	51	0
6	B8	337	0	323	71	0
6	BB	337	0	323	97	0
6	BE	337	0	323	72	0
6	BG	337	0	323	78	0
6	BJ	337	0	323	91	0
6	BN	337	0	323	66	0
6	BP	337	0	323	91	0
6	BR	337	0	323	68	0
6	BT	337	0	323	64	0
6	BV	337	0	323	107	0
6	BX	337	0	323	71	0
6	BZ	337	0	323	80	0
7	AC	172	0	120	35	0
7	BC	172	0	120	33	0
8	A1	1	0	0	0	0
8	A3	1	0	0	0	0
8	A5	1	0	0	0	0
8	A7	1	0	0	0	0
8	A9	1	0	0	0	0
8	AA	1	0	0	0	0
8	AC	1	0	0	0	0
8	AD	1	0	0	0	0
8	AF	1	0	0	0	0
8	AI	1	0	0	0	0
8	AK	1	0	0	0	0
8	AO	1	0	0	0	0
8	AQ	1	0	0	0	0
8	AS	1	0	0	0	0
8	AU	1	0	0	0	0
8	AV	1	0	0	0	0
8	AY	1	0	0	0	0
8	B1	1	0	0	0	0
8	B3	1	0	0	0	0
8	B5	1	0	0	0	0
8	B7	1	0	0	0	0
8	B9	1	0	0	0	0
8	BA	1	0	0	0	0
8	BC	1	0	0	0	0
8	BD	1	0	0	0	0
8	BF	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	BI	1	0	0	0	0
8	BK	1	0	0	0	0
8	BO	1	0	0	0	0
8	BQ	1	0	0	0	0
8	BS	1	0	0	0	0
8	BU	1	0	0	0	0
8	BW	1	0	0	0	0
8	BY	1	0	0	0	0
9	A0	66	0	72	71	0
9	A1	66	0	74	55	0
9	A2	66	0	74	31	0
9	A3	132	0	148	69	0
9	A5	66	0	74	40	0
9	A6	66	0	74	31	0
9	A7	66	0	74	51	0
9	A8	66	0	74	46	0
9	A9	66	0	74	35	0
9	AA	66	0	74	41	0
9	AB	66	0	74	33	0
9	AD	66	0	74	29	0
9	AE	66	0	74	32	0
9	AF	66	0	74	38	0
9	AG	66	0	74	37	0
9	AI	66	0	74	41	0
9	AJ	66	0	74	44	0
9	AK	66	0	74	67	0
9	AL	132	0	148	58	0
9	AM	132	0	148	61	0
9	AN	66	0	74	57	0
9	AO	66	0	74	50	0
9	AP	66	0	74	41	0
9	AQ	66	0	74	26	0
9	AR	66	0	74	34	0
9	AS	66	0	74	32	0
9	AT	66	0	74	25	0
9	AU	66	0	73	46	0
9	AV	66	0	74	28	0
9	AW	66	0	72	40	0
9	AX	66	0	74	36	0
9	AY	66	0	74	47	0
9	AZ	66	0	72	41	0
9	B0	66	0	74	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B1	66	0	74	40	0
9	B2	66	0	74	45	0
9	B3	66	0	74	51	0
9	B4	66	0	74	24	0
9	B5	66	0	74	25	0
9	B6	66	0	74	26	0
9	B7	66	0	74	41	0
9	B8	66	0	74	37	0
9	B9	66	0	74	35	0
9	BA	66	0	74	37	0
9	BB	66	0	74	51	0
9	BD	66	0	74	38	0
9	BE	66	0	74	48	0
9	BF	66	0	74	41	0
9	BG	66	0	74	44	0
9	BI	66	0	74	50	0
9	BJ	66	0	74	30	0
9	BK	66	0	74	32	0
9	BL	132	0	148	51	0
9	BM	132	0	148	54	0
9	BN	66	0	74	31	0
9	BO	66	0	74	50	0
9	BP	66	0	74	40	0
9	BQ	132	0	148	53	0
9	BS	66	0	74	25	0
9	BT	66	0	74	19	0
9	BU	66	0	74	41	0
9	BV	66	0	74	25	0
9	BW	66	0	74	44	0
9	BX	66	0	74	37	0
9	BY	66	0	74	37	0
9	BZ	66	0	74	30	0
10	AL	65	0	76	17	0
10	AM	65	0	76	14	0
10	BL	65	0	76	11	0
10	BM	65	0	76	9	0
11	AL	53	0	74	8	0
11	BL	53	0	74	12	0
12	AM	1	0	0	0	0
12	BM	1	0	0	0	0
13	AM	53	0	72	9	0
13	BM	53	0	72	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A0	44	0	60	27	0
14	A1	44	0	60	29	0
14	A2	44	0	60	51	0
14	A5	44	0	60	29	0
14	A7	44	0	60	45	0
14	AA	44	0	60	24	0
14	AB	44	0	60	45	0
14	AG	44	0	60	11	0
14	AJ	44	0	60	21	0
14	AM	44	0	60	13	0
14	AN	44	0	60	14	0
14	AP	44	0	60	24	0
14	AR	44	0	60	20	0
14	AS	44	0	60	77	0
14	AT	44	0	60	17	0
14	AW	44	0	60	32	0
14	AX	44	0	60	46	0
14	B0	44	0	60	42	0
14	B1	44	0	60	40	0
14	B2	44	0	60	75	0
14	B5	44	0	60	21	0
14	B7	44	0	60	39	0
14	BA	44	0	60	26	0
14	BB	44	0	60	27	0
14	BF	44	0	60	19	0
14	BG	44	0	60	14	0
14	BM	44	0	60	8	0
14	BN	44	0	60	15	0
14	BO	44	0	60	14	0
14	BP	44	0	60	28	0
14	BS	44	0	60	11	0
14	BU	44	0	60	61	0
14	BV	44	0	60	59	0
14	BW	44	0	60	21	0
15	AH	19	0	11	8	0
15	AM	80	0	92	23	0
15	AS	47	0	73	37	0
15	BM	19	0	11	2	0
15	BQ	47	0	73	12	0
16	A3	5	0	0	0	0
16	AH	5	0	0	1	0
16	AM	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	BH	5	0	0	1	0
17	AA	1	0	0	0	0
17	AC	1	0	0	0	0
17	AH	2	0	0	0	0
17	AI	1	0	0	0	0
17	AL	3	0	0	2	0
17	AM	3	0	0	2	0
17	AW	1	0	0	1	0
17	B1	1	0	0	0	0
17	BC	1	0	0	0	0
17	BH	1	0	0	0	0
17	BL	3	0	0	3	0
17	BM	3	0	0	0	0
All	All	50862	0	51516	10984	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 107.

The worst 5 of 10984 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:A7:102:CRT:C22	14:A7:102:CRT:C21	1.82	1.56
14:AS:104:CRT:C9	6:AV:20:ILE:HD12	1.38	1.54
5:AS:30:VAL:HG22	15:AS:101:PEF:C41	1.47	1.44
5:AS:30:VAL:CG2	15:AS:101:PEF:H412	1.46	1.43
9:AW:101:BCL:O2A	9:AW:101:BCL:C1	1.65	1.42

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	AC	315/404 (78%)	195 (62%)	75 (24%)	45 (14%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BC	315/404 (78%)	192 (61%)	87 (28%)	36 (11%)	1	3
2	AL	278/281 (99%)	137 (49%)	97 (35%)	44 (16%)	0	1
2	BL	278/281 (99%)	149 (54%)	97 (35%)	32 (12%)	1	3
3	AM	317/325 (98%)	162 (51%)	94 (30%)	61 (19%)	0	0
3	BM	317/325 (98%)	188 (59%)	85 (27%)	44 (14%)	0	2
4	AH	256/259 (99%)	162 (63%)	73 (28%)	21 (8%)	1	6
4	BH	256/259 (99%)	166 (65%)	66 (26%)	24 (9%)	1	5
5	A1	56/61 (92%)	43 (77%)	9 (16%)	4 (7%)	2	9
5	A3	55/61 (90%)	45 (82%)	7 (13%)	3 (6%)	3	16
5	A5	54/61 (88%)	42 (78%)	10 (18%)	2 (4%)	5	28
5	A7	49/61 (80%)	35 (71%)	11 (22%)	3 (6%)	2	14
5	A9	58/61 (95%)	47 (81%)	10 (17%)	1 (2%)	14	54
5	AA	46/61 (75%)	33 (72%)	11 (24%)	2 (4%)	4	23
5	AD	55/61 (90%)	40 (73%)	12 (22%)	3 (6%)	3	16
5	AF	57/61 (93%)	41 (72%)	13 (23%)	3 (5%)	3	18
5	AI	57/61 (93%)	47 (82%)	6 (10%)	4 (7%)	2	9
5	AK	56/61 (92%)	44 (79%)	10 (18%)	2 (4%)	5	29
5	AO	57/61 (93%)	46 (81%)	6 (10%)	5 (9%)	1	5
5	AQ	55/61 (90%)	36 (66%)	17 (31%)	2 (4%)	5	29
5	AS	57/61 (93%)	46 (81%)	7 (12%)	4 (7%)	2	9
5	AU	58/61 (95%)	43 (74%)	11 (19%)	4 (7%)	2	9
5	AW	58/61 (95%)	45 (78%)	8 (14%)	5 (9%)	1	5
5	AY	58/61 (95%)	43 (74%)	11 (19%)	4 (7%)	2	9
5	B1	52/61 (85%)	34 (65%)	11 (21%)	7 (14%)	0	2
5	B3	58/61 (95%)	38 (66%)	16 (28%)	4 (7%)	2	9
5	B5	49/61 (80%)	35 (71%)	10 (20%)	4 (8%)	1	6
5	B7	52/61 (85%)	40 (77%)	10 (19%)	2 (4%)	5	27
5	B9	49/61 (80%)	33 (67%)	14 (29%)	2 (4%)	4	24
5	BA	53/61 (87%)	29 (55%)	20 (38%)	4 (8%)	2	8
5	BD	43/61 (70%)	32 (74%)	8 (19%)	3 (7%)	2	9
5	BF	54/61 (88%)	42 (78%)	11 (20%)	1 (2%)	12	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	BI	48/61 (79%)	32 (67%)	13 (27%)	3 (6%)	2	12
5	BK	58/61 (95%)	43 (74%)	12 (21%)	3 (5%)	3	18
5	BO	57/61 (93%)	46 (81%)	11 (19%)	0	100	100
5	BQ	57/61 (93%)	41 (72%)	14 (25%)	2 (4%)	6	30
5	BS	57/61 (93%)	45 (79%)	9 (16%)	3 (5%)	3	18
5	BU	56/61 (92%)	43 (77%)	12 (21%)	1 (2%)	13	53
5	BW	56/61 (92%)	38 (68%)	14 (25%)	4 (7%)	2	9
5	BY	52/61 (85%)	30 (58%)	16 (31%)	6 (12%)	1	3
6	A0	38/47 (81%)	30 (79%)	7 (18%)	1 (3%)	8	39
6	A2	38/47 (81%)	29 (76%)	8 (21%)	1 (3%)	8	39
6	A4	38/47 (81%)	31 (82%)	6 (16%)	1 (3%)	8	39
6	A6	38/47 (81%)	35 (92%)	3 (8%)	0	100	100
6	A8	38/47 (81%)	27 (71%)	10 (26%)	1 (3%)	8	39
6	AB	38/47 (81%)	33 (87%)	5 (13%)	0	100	100
6	AE	38/47 (81%)	33 (87%)	5 (13%)	0	100	100
6	AG	38/47 (81%)	32 (84%)	5 (13%)	1 (3%)	8	39
6	AJ	38/47 (81%)	29 (76%)	9 (24%)	0	100	100
6	AN	38/47 (81%)	35 (92%)	3 (8%)	0	100	100
6	AP	38/47 (81%)	28 (74%)	10 (26%)	0	100	100
6	AR	38/47 (81%)	31 (82%)	7 (18%)	0	100	100
6	AT	38/47 (81%)	30 (79%)	5 (13%)	3 (8%)	1	7
6	AV	38/47 (81%)	35 (92%)	2 (5%)	1 (3%)	8	39
6	AX	38/47 (81%)	32 (84%)	6 (16%)	0	100	100
6	AZ	38/47 (81%)	29 (76%)	9 (24%)	0	100	100
6	B0	38/47 (81%)	30 (79%)	8 (21%)	0	100	100
6	B2	38/47 (81%)	31 (82%)	7 (18%)	0	100	100
6	B4	38/47 (81%)	32 (84%)	6 (16%)	0	100	100
6	B6	38/47 (81%)	35 (92%)	3 (8%)	0	100	100
6	B8	38/47 (81%)	27 (71%)	10 (26%)	1 (3%)	8	39
6	BB	38/47 (81%)	33 (87%)	5 (13%)	0	100	100
6	BE	38/47 (81%)	32 (84%)	6 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	BG	38/47 (81%)	32 (84%)	6 (16%)	0	100	100
6	BJ	38/47 (81%)	29 (76%)	9 (24%)	0	100	100
6	BN	38/47 (81%)	35 (92%)	3 (8%)	0	100	100
6	BP	38/47 (81%)	25 (66%)	12 (32%)	1 (3%)	8	39
6	BR	38/47 (81%)	31 (82%)	7 (18%)	0	100	100
6	BT	38/47 (81%)	30 (79%)	5 (13%)	3 (8%)	1	7
6	BV	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	BX	38/47 (81%)	32 (84%)	6 (16%)	0	100	100
6	BZ	38/47 (81%)	31 (82%)	7 (18%)	0	100	100
All	All	5285/5994 (88%)	3628 (69%)	1236 (23%)	421 (8%)	1	7

5 of 421 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AC	64	ALA
1	AC	70	PRO
1	AC	97	VAL
1	AC	138	ASN
1	AC	154	THR

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	AC	265/317 (84%)	239 (90%)	26 (10%)	12	41
1	BC	265/317 (84%)	238 (90%)	27 (10%)	11	38
2	AL	228/229 (100%)	199 (87%)	29 (13%)	6	27
2	BL	228/229 (100%)	206 (90%)	22 (10%)	12	43
3	AM	256/261 (98%)	217 (85%)	39 (15%)	4	20
3	BM	256/261 (98%)	219 (86%)	37 (14%)	5	22
4	AH	210/211 (100%)	194 (92%)	16 (8%)	19	57
4	BH	210/211 (100%)	189 (90%)	21 (10%)	11	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	A1	48/56 (86%)	45 (94%)	3 (6%)	25	66
5	A3	47/56 (84%)	41 (87%)	6 (13%)	6	27
5	A5	48/56 (86%)	44 (92%)	4 (8%)	16	52
5	A7	48/56 (86%)	40 (83%)	8 (17%)	3	16
5	A9	50/56 (89%)	46 (92%)	4 (8%)	17	53
5	AA	44/56 (79%)	38 (86%)	6 (14%)	5	24
5	AD	47/56 (84%)	44 (94%)	3 (6%)	25	66
5	AF	49/56 (88%)	42 (86%)	7 (14%)	5	22
5	AI	49/56 (88%)	45 (92%)	4 (8%)	17	52
5	AK	48/56 (86%)	42 (88%)	6 (12%)	7	28
5	AO	49/56 (88%)	43 (88%)	6 (12%)	7	29
5	AQ	47/56 (84%)	43 (92%)	4 (8%)	15	51
5	AS	49/56 (88%)	44 (90%)	5 (10%)	11	38
5	AU	50/56 (89%)	43 (86%)	7 (14%)	5	23
5	AW	50/56 (89%)	45 (90%)	5 (10%)	11	39
5	AY	50/56 (89%)	43 (86%)	7 (14%)	5	23
5	B1	45/56 (80%)	43 (96%)	2 (4%)	39	82
5	B3	50/56 (89%)	46 (92%)	4 (8%)	17	53
5	B5	48/56 (86%)	45 (94%)	3 (6%)	25	66
5	B7	45/56 (80%)	41 (91%)	4 (9%)	14	48
5	B9	48/56 (86%)	46 (96%)	2 (4%)	40	83
5	BA	50/56 (89%)	45 (90%)	5 (10%)	11	39
5	BD	43/56 (77%)	42 (98%)	1 (2%)	63	93
5	BF	48/56 (86%)	43 (90%)	5 (10%)	10	37
5	BI	46/56 (82%)	40 (87%)	6 (13%)	6	26
5	BK	50/56 (89%)	44 (88%)	6 (12%)	7	30
5	BO	49/56 (88%)	45 (92%)	4 (8%)	17	52
5	BQ	50/56 (89%)	46 (92%)	4 (8%)	17	53
5	BS	49/56 (88%)	46 (94%)	3 (6%)	26	68
5	BU	50/56 (89%)	43 (86%)	7 (14%)	5	23
5	BW	48/56 (86%)	41 (85%)	7 (15%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	BY	45/56 (80%)	39 (87%)	6 (13%)	6	25
6	A0	33/39 (85%)	23 (70%)	10 (30%)	0	2
6	A2	33/39 (85%)	29 (88%)	4 (12%)	7	29
6	A4	33/39 (85%)	26 (79%)	7 (21%)	1	8
6	A6	33/39 (85%)	30 (91%)	3 (9%)	14	46
6	A8	33/39 (85%)	26 (79%)	7 (21%)	1	8
6	AB	33/39 (85%)	27 (82%)	6 (18%)	2	13
6	AE	33/39 (85%)	31 (94%)	2 (6%)	26	68
6	AG	33/39 (85%)	25 (76%)	8 (24%)	1	5
6	AJ	33/39 (85%)	28 (85%)	5 (15%)	4	20
6	AN	33/39 (85%)	27 (82%)	6 (18%)	2	13
6	AP	33/39 (85%)	28 (85%)	5 (15%)	4	20
6	AR	33/39 (85%)	28 (85%)	5 (15%)	4	20
6	AT	33/39 (85%)	28 (85%)	5 (15%)	4	20
6	AV	33/39 (85%)	28 (85%)	5 (15%)	4	20
6	AX	33/39 (85%)	29 (88%)	4 (12%)	7	29
6	AZ	33/39 (85%)	29 (88%)	4 (12%)	7	29
6	B0	33/39 (85%)	27 (82%)	6 (18%)	2	13
6	B2	33/39 (85%)	30 (91%)	3 (9%)	14	46
6	B4	33/39 (85%)	27 (82%)	6 (18%)	2	13
6	B6	33/39 (85%)	30 (91%)	3 (9%)	14	46
6	B8	33/39 (85%)	25 (76%)	8 (24%)	1	5
6	BB	33/39 (85%)	24 (73%)	9 (27%)	0	3
6	BE	33/39 (85%)	29 (88%)	4 (12%)	7	29
6	BG	33/39 (85%)	30 (91%)	3 (9%)	14	46
6	BJ	33/39 (85%)	30 (91%)	3 (9%)	14	46
6	BN	33/39 (85%)	29 (88%)	4 (12%)	7	29
6	BP	33/39 (85%)	31 (94%)	2 (6%)	26	68
6	BR	33/39 (85%)	27 (82%)	6 (18%)	2	13
6	BT	33/39 (85%)	30 (91%)	3 (9%)	14	46
6	BV	33/39 (85%)	31 (94%)	2 (6%)	26	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	BX	33/39 (85%)	29 (88%)	4 (12%)	7	29
6	BZ	33/39 (85%)	30 (91%)	3 (9%)	14	46
All	All	4511/5076 (89%)	3985 (88%)	526 (12%)	8	31

5 of 526 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A3	56	GLN
1	BC	190	VAL
5	B1	18	ARG
6	A4	42	TYR
5	A9	18	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 114 such sidechains are listed below:

Mol	Chain	Res	Type
6	A4	23	GLN
1	BC	80	GLN
6	BZ	23	GLN
5	A5	56	GLN
5	A9	7	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 169 ligands modelled in this entry, 36 are monoatomic - leaving 133 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$
14	CRT	A0	101	-	43,43,43	1.63	6 (13%)	54,54,54	1.98	16 (29%)
9	BCL	A0	102	-	74,74,74	2.20	16 (21%)	98,115,115	3.41	30 (30%)
9	BCL	A1	102	-	74,74,74	2.67	22 (29%)	98,115,115	2.36	29 (29%)
14	CRT	A1	103	-	43,43,43	1.53	10 (23%)	54,54,54	2.34	18 (33%)
9	BCL	A2	101	-	74,74,74	1.97	16 (21%)	98,115,115	2.58	26 (26%)
14	CRT	A2	102	-	43,43,43	1.87	8 (18%)	54,54,54	1.76	13 (24%)
16	PO4	A3	101	-	4,4,4	0.92	0	6,6,6	0.29	0
9	BCL	A3	103	-	74,74,74	2.16	18 (24%)	98,115,115	2.15	27 (27%)
9	BCL	A3	104	-	74,74,74	2.00	18 (24%)	98,115,115	3.20	28 (28%)
9	BCL	A5	102	-	74,74,74	2.10	18 (24%)	98,115,115	2.73	30 (30%)
14	CRT	A5	103	-	43,43,43	1.45	8 (18%)	54,54,54	1.71	14 (25%)
9	BCL	A6	101	-	74,74,74	2.24	18 (24%)	98,115,115	2.33	29 (29%)
14	CRT	A7	102	-	43,43,43	3.25	10 (23%)	54,54,54	3.35	14 (25%)
9	BCL	A7	103	-	74,74,74	2.31	18 (24%)	98,115,115	2.44	31 (31%)
9	BCL	A8	101	-	74,74,74	2.14	22 (29%)	98,115,115	2.99	28 (28%)
9	BCL	A9	102	-	74,74,74	1.97	19 (25%)	98,115,115	2.90	29 (29%)
9	BCL	AA	101	-	74,74,74	1.93	18 (24%)	98,115,115	2.08	23 (23%)
14	CRT	AA	102	-	43,43,43	1.57	4 (9%)	54,54,54	1.64	14 (25%)
9	BCL	AB	101	-	74,74,74	1.92	18 (24%)	98,115,115	2.27	26 (26%)
14	CRT	AB	102	-	43,43,43	1.31	5 (11%)	54,54,54	1.86	20 (37%)
7	HEM	AC	501	1	50,50,50	2.47	15 (30%)	46,82,82	1.48	8 (17%)
7	HEM	AC	502	1	50,50,50	2.31	15 (30%)	46,82,82	1.48	9 (19%)
7	HEM	AC	503	1	50,50,50	2.13	13 (26%)	46,82,82	1.43	7 (15%)
7	HEM	AC	504	1	50,50,50	2.29	14 (28%)	46,82,82	1.42	7 (15%)
9	BCL	AD	102	-	74,74,74	1.93	15 (20%)	98,115,115	2.17	24 (24%)
9	BCL	AE	101	-	74,74,74	2.06	17 (22%)	98,115,115	2.34	28 (28%)
9	BCL	AF	102	-	74,74,74	1.97	16 (21%)	98,115,115	2.12	25 (25%)
9	BCL	AG	101	-	74,74,74	1.98	17 (22%)	98,115,115	2.13	28 (28%)
14	CRT	AG	102	-	43,43,43	1.46	6 (13%)	54,54,54	1.74	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	PEF	AH	301	-	16,18,46	4.43	6 (37%)	19,23,51	1.99	6 (31%)
16	PO4	AH	302	-	4,4,4	0.89	0	6,6,6	0.28	0
9	BCL	AI	102	-	74,74,74	1.94	15 (20%)	98,115,115	2.16	24 (24%)
9	BCL	AJ	101	-	74,74,74	1.92	16 (21%)	98,115,115	2.23	26 (26%)
14	CRT	AJ	102	-	43,43,43	1.56	5 (11%)	54,54,54	1.89	16 (29%)
9	BCL	AK	102	-	74,74,74	1.81	16 (21%)	98,115,115	2.21	26 (26%)
9	BCL	AL	301	-	74,74,74	1.89	16 (21%)	98,115,115	2.07	27 (27%)
10	BPH	AL	302	-	70,70,70	0.98	4 (5%)	94,101,101	1.19	9 (9%)
9	BCL	AL	303	-	74,74,74	1.63	12 (16%)	98,115,115	2.16	26 (26%)
11	UQ8	AL	304	-	53,53,53	1.39	2 (3%)	67,67,67	1.80	17 (25%)
9	BCL	AM	401	-	74,74,74	1.69	13 (17%)	98,115,115	2.18	24 (24%)
9	BCL	AM	402	-	74,74,74	1.70	13 (17%)	98,115,115	2.24	25 (25%)
10	BPH	AM	403	-	70,70,70	0.99	4 (5%)	94,101,101	1.06	4 (4%)
13	MQ8	AM	405	-	54,54,54	1.04	3 (5%)	69,69,69	1.58	15 (21%)
14	CRT	AM	406	-	43,43,43	1.66	7 (16%)	54,54,54	1.55	10 (18%)
15	PEF	AM	407	-	16,18,46	4.43	6 (37%)	19,23,51	1.99	6 (31%)
15	PEF	AM	408	-	10,13,46	4.52	4 (40%)	10,16,51	1.24	1 (10%)
15	PEF	AM	409	-	46,46,46	2.12	6 (13%)	51,51,51	1.36	7 (13%)
16	PO4	AM	410	-	4,4,4	0.92	0	6,6,6	0.29	0
9	BCL	AN	101	-	74,74,74	2.04	19 (25%)	98,115,115	2.28	28 (28%)
14	CRT	AN	102	-	43,43,43	1.43	8 (18%)	54,54,54	1.79	19 (35%)
9	BCL	AO	102	-	74,74,74	1.82	15 (20%)	98,115,115	2.20	26 (26%)
9	BCL	AP	101	-	74,74,74	1.94	20 (27%)	98,115,115	2.33	31 (31%)
14	CRT	AP	102	-	43,43,43	1.83	9 (20%)	54,54,54	1.73	17 (31%)
9	BCL	AQ	102	-	74,74,74	1.79	17 (22%)	98,115,115	2.15	25 (25%)
9	BCL	AR	101	-	74,74,74	1.91	17 (22%)	98,115,115	2.18	24 (24%)
14	CRT	AR	102	-	43,43,43	1.42	7 (16%)	54,54,54	1.78	16 (29%)
15	PEF	AS	101	-	46,46,46	2.12	6 (13%)	51,51,51	1.44	7 (13%)
9	BCL	AS	103	-	74,74,74	2.03	18 (24%)	98,115,115	2.21	27 (27%)
14	CRT	AS	104	-	43,43,43	1.55	5 (11%)	54,54,54	2.07	17 (31%)
9	BCL	AT	101	-	74,74,74	2.02	19 (25%)	98,115,115	2.15	31 (31%)
14	CRT	AT	102	-	43,43,43	1.60	7 (16%)	54,54,54	1.75	14 (25%)
9	BCL	AU	102	-	74,74,74	2.11	20 (27%)	98,115,115	2.81	36 (36%)
9	BCL	AV	102	-	74,74,74	2.10	20 (27%)	98,115,115	2.07	30 (30%)
9	BCL	AW	101	-	74,74,74	2.02	17 (22%)	98,115,115	3.79	29 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CRT	AW	102	-	43,43,43	1.84	11 (25%)	54,54,54	1.73	18 (33%)
9	BCL	AX	101	-	74,74,74	2.32	17 (22%)	98,115,115	2.87	29 (29%)
14	CRT	AX	102	-	43,43,43	2.11	10 (23%)	54,54,54	2.09	14 (25%)
9	BCL	AY	102	-	74,74,74	2.10	17 (22%)	98,115,115	2.32	28 (28%)
9	BCL	AZ	101	-	74,74,74	2.57	19 (25%)	98,115,115	3.14	27 (27%)
14	CRT	B0	101	-	43,43,43	2.12	9 (20%)	54,54,54	1.89	14 (25%)
9	BCL	B0	102	-	74,74,74	1.81	18 (24%)	98,115,115	2.25	30 (30%)
9	BCL	B1	102	-	74,74,74	1.90	14 (18%)	98,115,115	2.16	26 (26%)
14	CRT	B1	103	-	43,43,43	1.37	6 (13%)	54,54,54	1.95	20 (37%)
9	BCL	B2	101	-	74,74,74	1.82	17 (22%)	98,115,115	2.22	29 (29%)
14	CRT	B2	102	-	43,43,43	2.46	12 (27%)	54,54,54	1.93	17 (31%)
9	BCL	B3	102	-	74,74,74	1.77	13 (17%)	98,115,115	2.14	25 (25%)
9	BCL	B4	101	-	74,74,74	1.94	21 (28%)	98,115,115	2.30	30 (30%)
9	BCL	B5	102	-	74,74,74	1.97	16 (21%)	98,115,115	2.11	25 (25%)
14	CRT	B5	103	-	43,43,43	1.55	4 (9%)	54,54,54	1.65	12 (22%)
9	BCL	B6	101	-	74,74,74	1.98	14 (18%)	98,115,115	2.23	31 (31%)
14	CRT	B7	102	-	43,43,43	1.98	8 (18%)	54,54,54	1.86	12 (22%)
9	BCL	B7	103	-	74,74,74	2.02	16 (21%)	98,115,115	2.22	26 (26%)
9	BCL	B8	101	-	74,74,74	1.94	16 (21%)	98,115,115	2.42	30 (30%)
9	BCL	B9	102	-	74,74,74	1.96	15 (20%)	98,115,115	2.22	27 (27%)
9	BCL	BA	101	-	74,74,74	1.85	16 (21%)	98,115,115	2.11	23 (23%)
14	CRT	BA	102	-	43,43,43	1.57	4 (9%)	54,54,54	1.62	12 (22%)
9	BCL	BB	101	-	74,74,74	2.06	15 (20%)	98,115,115	2.38	31 (31%)
14	CRT	BB	102	-	43,43,43	1.48	7 (16%)	54,54,54	1.85	18 (33%)
7	HEM	BC	501	1	50,50,50	2.34	14 (28%)	46,82,82	1.54	11 (23%)
7	HEM	BC	502	1	50,50,50	2.24	11 (22%)	46,82,82	1.50	9 (19%)
7	HEM	BC	503	1	50,50,50	2.29	12 (24%)	46,82,82	1.44	7 (15%)
7	HEM	BC	504	1	50,50,50	2.36	13 (26%)	46,82,82	1.43	8 (17%)
9	BCL	BD	102	-	74,74,74	2.18	20 (27%)	98,115,115	2.18	28 (28%)
9	BCL	BE	101	-	74,74,74	2.11	23 (31%)	98,115,115	2.05	25 (25%)
9	BCL	BF	102	-	74,74,74	2.12	18 (24%)	98,115,115	2.23	29 (29%)
14	CRT	BF	103	-	43,43,43	1.55	8 (18%)	54,54,54	2.19	17 (31%)
9	BCL	BG	101	-	74,74,74	1.98	18 (24%)	98,115,115	2.20	27 (27%)
14	CRT	BG	102	-	43,43,43	1.49	6 (13%)	54,54,54	1.69	16 (29%)
16	PO4	BH	301	-	4,4,4	0.88	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	BI	102	-	74,74,74	1.82	19 (25%)	98,115,115	2.20	25 (25%)
9	BCL	BJ	101	-	74,74,74	1.81	19 (25%)	98,115,115	2.14	25 (25%)
9	BCL	BK	102	-	74,74,74	1.93	17 (22%)	98,115,115	2.14	23 (23%)
9	BCL	BL	301	-	74,74,74	1.90	17 (22%)	98,115,115	2.06	27 (27%)
10	BPH	BL	302	-	70,70,70	1.00	5 (7%)	94,101,101	1.09	8 (8%)
9	BCL	BL	303	-	74,74,74	1.64	13 (17%)	98,115,115	2.13	24 (24%)
11	UQ8	BL	304	-	53,53,53	1.35	2 (3%)	67,67,67	1.66	17 (25%)
9	BCL	BM	401	-	74,74,74	1.68	13 (17%)	98,115,115	2.18	25 (25%)
9	BCL	BM	402	-	74,74,74	1.78	15 (20%)	98,115,115	2.31	25 (25%)
10	BPH	BM	403	-	70,70,70	1.00	4 (5%)	94,101,101	1.16	7 (7%)
13	MQ8	BM	405	-	54,54,54	1.10	5 (9%)	69,69,69	1.42	12 (17%)
14	CRT	BM	406	-	43,43,43	1.56	8 (18%)	54,54,54	1.58	12 (22%)
15	PEF	BM	407	-	16,18,46	4.41	6 (37%)	19,23,51	1.98	6 (31%)
9	BCL	BN	101	-	74,74,74	1.85	15 (20%)	98,115,115	2.12	27 (27%)
14	CRT	BN	102	-	43,43,43	1.62	9 (20%)	54,54,54	1.82	15 (27%)
9	BCL	BO	102	-	74,74,74	1.84	15 (20%)	98,115,115	2.19	23 (23%)
14	CRT	BO	103	-	43,43,43	1.41	7 (16%)	54,54,54	1.79	16 (29%)
9	BCL	BP	101	-	74,74,74	2.07	20 (27%)	98,115,115	2.33	33 (33%)
14	CRT	BP	102	-	43,43,43	1.97	9 (20%)	54,54,54	1.63	14 (25%)
15	PEF	BQ	101	-	46,46,46	2.12	6 (13%)	51,51,51	1.43	7 (13%)
9	BCL	BQ	103	-	74,74,74	1.86	19 (25%)	98,115,115	2.16	24 (24%)
9	BCL	BQ	104	-	74,74,74	1.92	19 (25%)	98,115,115	2.16	29 (29%)
9	BCL	BS	102	-	74,74,74	1.67	14 (18%)	98,115,115	2.25	26 (26%)
14	CRT	BS	103	-	43,43,43	1.51	5 (11%)	54,54,54	1.69	15 (27%)
9	BCL	BT	101	-	74,74,74	1.90	19 (25%)	98,115,115	2.22	33 (33%)
9	BCL	BU	102	-	74,74,74	1.96	16 (21%)	98,115,115	2.20	25 (25%)
14	CRT	BU	103	-	43,43,43	1.91	11 (25%)	54,54,54	2.27	18 (33%)
9	BCL	BV	101	-	74,74,74	1.80	16 (21%)	98,115,115	2.14	29 (29%)
14	CRT	BV	102	-	43,43,43	2.06	12 (27%)	54,54,54	1.73	14 (25%)
9	BCL	BW	102	-	74,74,74	1.90	20 (27%)	98,115,115	2.22	27 (27%)
14	CRT	BW	103	-	43,43,43	1.79	8 (18%)	54,54,54	1.65	14 (25%)
9	BCL	BX	101	-	74,74,74	2.07	21 (28%)	98,115,115	2.29	25 (25%)
9	BCL	BY	102	-	74,74,74	1.98	16 (21%)	98,115,115	2.18	23 (23%)
9	BCL	BZ	101	-	74,74,74	1.86	15 (20%)	98,115,115	2.18	30 (30%)

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
14	CRT	A0	101	-	-	0/51/51/51	0/0/0/0
9	BCL	A0	102	-	-	0/41/137/137	0/0/9/9
9	BCL	A1	102	-	-	0/41/137/137	0/0/9/9
14	CRT	A1	103	-	-	0/51/51/51	0/0/0/0
9	BCL	A2	101	-	-	0/41/137/137	0/0/9/9
14	CRT	A2	102	-	-	0/51/51/51	0/0/0/0
16	PO4	A3	101	-	-	0/0/0/0	0/0/0/0
9	BCL	A3	103	-	-	0/41/137/137	0/0/9/9
9	BCL	A3	104	-	-	0/41/137/137	0/0/9/9
9	BCL	A5	102	-	-	0/41/137/137	0/0/9/9
14	CRT	A5	103	-	-	0/51/51/51	0/0/0/0
9	BCL	A6	101	-	-	0/41/137/137	0/0/9/9
14	CRT	A7	102	-	-	0/51/51/51	0/0/0/0
9	BCL	A7	103	-	-	0/41/137/137	0/0/9/9
9	BCL	A8	101	-	-	0/41/137/137	0/0/9/9
9	BCL	A9	102	-	-	0/41/137/137	0/0/9/9
9	BCL	AA	101	-	-	0/41/137/137	0/0/9/9
14	CRT	AA	102	-	-	0/51/51/51	0/0/0/0
9	BCL	AB	101	-	-	0/41/137/137	0/0/9/9
14	CRT	AB	102	-	-	0/51/51/51	0/0/0/0
7	HEM	AC	501	1	-	0/14/114/114	0/0/8/8
7	HEM	AC	502	1	-	0/14/114/114	0/0/8/8
7	HEM	AC	503	1	-	0/14/114/114	0/0/8/8
7	HEM	AC	504	1	-	0/14/114/114	0/0/8/8
9	BCL	AD	102	-	-	0/41/137/137	0/0/9/9
9	BCL	AE	101	-	-	0/41/137/137	0/0/9/9
9	BCL	AF	102	-	-	0/41/137/137	0/0/9/9
9	BCL	AG	101	-	-	0/41/137/137	0/0/9/9
14	CRT	AG	102	-	-	0/51/51/51	0/0/0/0
15	PEF	AH	301	-	-	1/20/20/50	0/0/0/0
16	PO4	AH	302	-	-	0/0/0/0	0/0/0/0
9	BCL	AI	102	-	-	0/41/137/137	0/0/9/9
9	BCL	AJ	101	-	-	0/41/137/137	0/0/9/9
14	CRT	AJ	102	-	-	0/51/51/51	0/0/0/0
9	BCL	AK	102	-	-	0/41/137/137	0/0/9/9
9	BCL	AL	301	-	-	0/41/137/137	0/0/9/9
10	BPH	AL	302	-	2/2/18/22	0/51/105/105	0/1/6/6
9	BCL	AL	303	-	-	0/41/137/137	0/0/9/9
11	UQ8	AL	304	-	-	0/51/75/75	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	AM	401	-	-	0/41/137/137	0/0/9/9
9	BCL	AM	402	-	-	0/41/137/137	0/0/9/9
10	BPH	AM	403	-	2/2/18/22	0/51/105/105	0/1/6/6
13	MQ8	AM	405	-	-	0/47/67/67	0/2/2/2
14	CRT	AM	406	-	-	0/51/51/51	0/0/0/0
15	PEF	AM	407	-	-	0/20/20/50	0/0/0/0
15	PEF	AM	408	-	-	0/11/13/50	0/0/0/0
15	PEF	AM	409	-	-	0/50/50/50	0/0/0/0
16	PO4	AM	410	-	-	0/0/0/0	0/0/0/0
9	BCL	AN	101	-	-	0/41/137/137	0/0/9/9
14	CRT	AN	102	-	-	0/51/51/51	0/0/0/0
9	BCL	AO	102	-	-	0/41/137/137	0/0/9/9
9	BCL	AP	101	-	-	0/41/137/137	0/0/9/9
14	CRT	AP	102	-	-	0/51/51/51	0/0/0/0
9	BCL	AQ	102	-	-	0/41/137/137	0/0/9/9
9	BCL	AR	101	-	-	0/41/137/137	0/0/9/9
14	CRT	AR	102	-	-	0/51/51/51	0/0/0/0
15	PEF	AS	101	-	-	0/50/50/50	0/0/0/0
9	BCL	AS	103	-	-	0/41/137/137	0/0/9/9
14	CRT	AS	104	-	-	0/51/51/51	0/0/0/0
9	BCL	AT	101	-	-	0/41/137/137	0/0/9/9
14	CRT	AT	102	-	-	0/51/51/51	0/0/0/0
9	BCL	AU	102	-	-	0/41/137/137	0/0/9/9
9	BCL	AV	102	-	-	0/41/137/137	0/0/9/9
9	BCL	AW	101	-	-	0/41/137/137	0/0/9/9
14	CRT	AW	102	-	-	0/51/51/51	0/0/0/0
9	BCL	AX	101	-	-	0/41/137/137	0/0/9/9
14	CRT	AX	102	-	-	0/51/51/51	0/0/0/0
9	BCL	AY	102	-	-	0/41/137/137	0/0/9/9
9	BCL	AZ	101	-	-	0/41/137/137	0/0/9/9
14	CRT	B0	101	-	-	0/51/51/51	0/0/0/0
9	BCL	B0	102	-	-	0/41/137/137	0/0/9/9
9	BCL	B1	102	-	-	0/41/137/137	0/0/9/9
14	CRT	B1	103	-	-	0/51/51/51	0/0/0/0
9	BCL	B2	101	-	-	0/41/137/137	0/0/9/9
14	CRT	B2	102	-	-	0/51/51/51	0/0/0/0
9	BCL	B3	102	-	-	0/41/137/137	0/0/9/9
9	BCL	B4	101	-	-	0/41/137/137	0/0/9/9
9	BCL	B5	102	-	-	0/41/137/137	0/0/9/9
14	CRT	B5	103	-	-	0/51/51/51	0/0/0/0
9	BCL	B6	101	-	-	0/41/137/137	0/0/9/9
14	CRT	B7	102	-	-	0/51/51/51	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	B7	103	-	-	0/41/137/137	0/0/9/9
9	BCL	B8	101	-	-	0/41/137/137	0/0/9/9
9	BCL	B9	102	-	-	0/41/137/137	0/0/9/9
9	BCL	BA	101	-	-	0/41/137/137	0/0/9/9
14	CRT	BA	102	-	-	0/51/51/51	0/0/0/0
9	BCL	BB	101	-	-	0/41/137/137	0/0/9/9
14	CRT	BB	102	-	-	0/51/51/51	0/0/0/0
7	HEM	BC	501	1	-	0/14/114/114	0/0/8/8
7	HEM	BC	502	1	-	0/14/114/114	0/0/8/8
7	HEM	BC	503	1	-	0/14/114/114	0/0/8/8
7	HEM	BC	504	1	-	0/14/114/114	0/0/8/8
9	BCL	BD	102	-	-	0/41/137/137	0/0/9/9
9	BCL	BE	101	-	-	0/41/137/137	0/0/9/9
9	BCL	BF	102	-	-	0/41/137/137	0/0/9/9
14	CRT	BF	103	-	-	0/51/51/51	0/0/0/0
9	BCL	BG	101	-	-	0/41/137/137	0/0/9/9
14	CRT	BG	102	-	-	0/51/51/51	0/0/0/0
16	PO4	BH	301	-	-	0/0/0/0	0/0/0/0
9	BCL	BI	102	-	-	0/41/137/137	0/0/9/9
9	BCL	BJ	101	-	-	0/41/137/137	0/0/9/9
9	BCL	BK	102	-	-	0/41/137/137	0/0/9/9
9	BCL	BL	301	-	-	0/41/137/137	0/0/9/9
10	BPH	BL	302	-	2/2/18/22	0/51/105/105	0/1/6/6
9	BCL	BL	303	-	-	0/41/137/137	0/0/9/9
11	UQ8	BL	304	-	-	0/51/75/75	0/1/1/1
9	BCL	BM	401	-	-	0/41/137/137	0/0/9/9
9	BCL	BM	402	-	-	0/41/137/137	0/0/9/9
10	BPH	BM	403	-	2/2/18/22	0/51/105/105	0/1/6/6
13	MQ8	BM	405	-	-	0/47/67/67	0/2/2/2
14	CRT	BM	406	-	-	0/51/51/51	0/0/0/0
15	PEF	BM	407	-	-	1/20/20/50	0/0/0/0
9	BCL	BN	101	-	-	0/41/137/137	0/0/9/9
14	CRT	BN	102	-	-	0/51/51/51	0/0/0/0
9	BCL	BO	102	-	-	0/41/137/137	0/0/9/9
14	CRT	BO	103	-	-	0/51/51/51	0/0/0/0
9	BCL	BP	101	-	-	0/41/137/137	0/0/9/9
14	CRT	BP	102	-	-	0/51/51/51	0/0/0/0
15	PEF	BQ	101	-	-	0/50/50/50	0/0/0/0
9	BCL	BQ	103	-	-	0/41/137/137	0/0/9/9
9	BCL	BQ	104	-	-	0/41/137/137	0/0/9/9
9	BCL	BS	102	-	-	0/41/137/137	0/0/9/9
14	CRT	BS	103	-	-	0/51/51/51	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	BT	101	-	-	0/41/137/137	0/0/9/9
9	BCL	BU	102	-	-	0/41/137/137	0/0/9/9
14	CRT	BU	103	-	-	0/51/51/51	0/0/0/0
9	BCL	BV	101	-	-	0/41/137/137	0/0/9/9
14	CRT	BV	102	-	-	0/51/51/51	0/0/0/0
9	BCL	BW	102	-	-	0/41/137/137	0/0/9/9
14	CRT	BW	103	-	-	0/51/51/51	0/0/0/0
9	BCL	BX	101	-	-	0/41/137/137	0/0/9/9
9	BCL	BY	102	-	-	0/41/137/137	0/0/9/9
9	BCL	BZ	101	-	-	0/41/137/137	0/0/9/9

The worst 5 of 1665 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	AZ	101	BCL	O2A-C1	-14.96	0.97	1.46
14	A7	102	CRT	C21-C20	13.96	1.71	1.35
9	A1	102	BCL	O2A-C1	13.08	1.89	1.46
14	A7	102	CRT	C21-C22	12.26	1.82	1.43
15	AM	407	PEF	O4-C10	11.80	1.47	1.22

The worst 5 of 2679 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AW	101	BCL	O2A-C1-C2	29.87	176.53	108.12
9	A0	102	BCL	O2A-C1-C2	25.22	165.88	108.12
9	A3	104	BCL	O2A-C1-C2	22.17	158.90	108.12
9	AZ	101	BCL	O2A-C1-C2	18.26	149.94	108.12
9	A8	101	BCL	O2A-C1-C2	17.41	147.99	108.12

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	BM	403	BPH	C8
10	BM	403	BPH	C13
10	BL	302	BPH	C8
10	BL	302	BPH	C13
10	AL	302	BPH	C8

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	BM	407	PEF	C3-O3-C30-C31

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Mol	Chain	Res	Type	Atoms
15	AH	301	PEF	C3-O3-C30-C31

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AC	317/404 (78%)	0.10	7 (2%) 59 12	41, 84, 141, 197	1 (0%)
1	BC	317/404 (78%)	0.17	13 (4%) 35 7	58, 91, 139, 165	1 (0%)
2	AL	280/281 (99%)	-0.04	5 (1%) 65 14	21, 58, 119, 145	0
2	BL	280/281 (99%)	0.05	7 (2%) 54 11	33, 77, 136, 156	0
3	AM	319/325 (98%)	-0.03	2 (0%) 86 32	19, 65, 107, 121	0
3	BM	319/325 (98%)	0.01	4 (1%) 74 19	37, 80, 125, 184	0
4	AH	258/259 (99%)	0.20	10 (3%) 37 7	46, 95, 149, 183	0
4	BH	258/259 (99%)	0.19	7 (2%) 52 10	57, 104, 164, 183	0
5	A1	58/61 (95%)	0.45	8 (13%) 4 1	73, 163, 300, 305	0
5	A3	57/61 (93%)	0.34	2 (3%) 42 8	117, 162, 318, 320	0
5	A5	56/61 (91%)	0.81	6 (10%) 6 2	70, 165, 320, 321	0
5	A7	51/61 (83%)	0.35	3 (5%) 22 5	111, 148, 234, 251	0
5	A9	60/61 (98%)	0.49	7 (11%) 5 2	96, 151, 319, 319	0
5	AA	48/61 (78%)	0.44	3 (6%) 19 5	92, 144, 241, 257	0
5	AD	57/61 (93%)	0.50	8 (14%) 3 1	97, 145, 222, 239	0
5	AF	59/61 (96%)	0.21	2 (3%) 43 8	99, 130, 226, 235	0
5	AI	59/61 (96%)	0.52	6 (10%) 7 2	81, 143, 236, 267	0
5	AK	58/61 (95%)	0.04	2 (3%) 43 8	81, 140, 227, 261	0
5	AO	59/61 (96%)	0.54	8 (13%) 4 1	88, 158, 258, 262	0
5	AQ	57/61 (93%)	0.09	1 (1%) 65 14	56, 135, 277, 280	0
5	AS	59/61 (96%)	0.31	4 (6%) 17 4	86, 158, 300, 309	0
5	AU	60/61 (98%)	0.64	7 (11%) 5 2	144, 167, 252, 254	0
5	AW	60/61 (98%)	0.16	4 (6%) 17 4	68, 135, 239, 250	0
5	AY	60/61 (98%)	0.44	3 (5%) 28 6	128, 152, 278, 284	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	B1	54/61 (88%)	0.17	1 (1%) 64 13	88, 126, 237, 238	0
5	B3	60/61 (98%)	0.41	5 (8%) 11 3	103, 151, 262, 263	0
5	B5	51/61 (83%)	0.97	13 (25%) 1 1	131, 174, 234, 237	0
5	B7	54/61 (88%)	0.42	5 (9%) 9 2	120, 191, 255, 261	0
5	B9	51/61 (83%)	0.36	4 (7%) 13 3	101, 150, 240, 241	0
5	BA	55/61 (90%)	0.48	3 (5%) 24 5	112, 161, 261, 269	0
5	BD	45/61 (73%)	0.70	4 (8%) 10 3	135, 140, 226, 247	0
5	BF	56/61 (91%)	0.41	4 (7%) 16 4	135, 168, 237, 251	0
5	BI	50/61 (81%)	0.35	5 (10%) 8 2	107, 134, 223, 229	0
5	BK	60/61 (98%)	0.61	4 (6%) 17 4	152, 166, 314, 318	0
5	BO	59/61 (96%)	0.29	2 (3%) 43 8	76, 129, 292, 295	0
5	BQ	59/61 (96%)	0.65	8 (13%) 4 1	150, 168, 266, 274	0
5	BS	59/61 (96%)	0.66	7 (11%) 5 1	91, 159, 250, 253	0
5	BU	58/61 (95%)	0.84	9 (15%) 3 1	109, 150, 280, 282	0
5	BW	58/61 (95%)	0.54	6 (10%) 7 2	49, 114, 230, 232	0
5	BY	54/61 (88%)	0.20	1 (1%) 64 13	46, 95, 222, 230	0
6	A0	40/47 (85%)	0.02	1 (2%) 54 11	166, 177, 205, 220	0
6	A2	40/47 (85%)	0.32	6 (15%) 3 1	122, 146, 202, 211	0
6	A4	40/47 (85%)	-0.06	0 100 100	147, 151, 221, 222	0
6	A6	40/47 (85%)	-0.12	0 100 100	140, 155, 199, 213	0
6	A8	40/47 (85%)	0.43	5 (12%) 5 1	129, 187, 225, 229	0
6	AB	40/47 (85%)	0.23	1 (2%) 54 11	122, 162, 189, 190	0
6	AE	40/47 (85%)	0.32	3 (7%) 14 3	120, 145, 169, 184	0
6	AG	40/47 (85%)	-0.05	0 100 100	74, 116, 140, 145	0
6	AJ	40/47 (85%)	0.07	1 (2%) 54 11	118, 129, 154, 159	0
6	AN	40/47 (85%)	-0.01	2 (5%) 28 6	101, 121, 155, 161	0
6	AP	40/47 (85%)	0.12	1 (2%) 54 11	106, 142, 245, 248	0
6	AR	40/47 (85%)	0.49	4 (10%) 8 2	122, 157, 194, 199	0
6	AT	40/47 (85%)	0.04	0 100 100	119, 148, 198, 205	0
6	AV	40/47 (85%)	0.37	4 (10%) 8 2	130, 167, 222, 225	0
6	AX	40/47 (85%)	0.15	1 (2%) 54 11	157, 167, 194, 199	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
6	AZ	40/47 (85%)	0.36	2 (5%) 28 6	111, 137, 238, 240	0
6	B0	40/47 (85%)	0.47	5 (12%) 5 1	197, 208, 220, 221	0
6	B2	40/47 (85%)	-0.05	0 100 100	116, 127, 158, 162	0
6	B4	40/47 (85%)	0.37	4 (10%) 8 2	134, 156, 191, 199	0
6	B6	40/47 (85%)	0.57	8 (20%) 2 1	115, 152, 213, 215	0
6	B8	40/47 (85%)	0.36	1 (2%) 54 11	123, 199, 232, 234	0
6	BB	40/47 (85%)	0.39	3 (7%) 14 3	155, 164, 229, 231	0
6	BE	40/47 (85%)	0.22	3 (7%) 14 3	148, 170, 194, 212	0
6	BG	40/47 (85%)	0.47	4 (10%) 8 2	185, 204, 218, 220	0
6	BJ	40/47 (85%)	0.56	6 (15%) 3 1	199, 204, 208, 209	0
6	BN	40/47 (85%)	0.19	2 (5%) 28 6	152, 160, 194, 201	0
6	BP	40/47 (85%)	0.11	4 (10%) 8 2	124, 149, 226, 230	0
6	BR	40/47 (85%)	0.34	3 (7%) 14 3	138, 171, 206, 213	0
6	BT	40/47 (85%)	0.16	1 (2%) 54 11	132, 157, 227, 233	0
6	BV	40/47 (85%)	-0.07	0 100 100	91, 143, 170, 174	0
6	BX	40/47 (85%)	-0.09	0 100 100	100, 127, 169, 172	0
6	BZ	40/47 (85%)	0.23	1 (2%) 54 11	121, 135, 178, 186	0
All	All	5429/5994 (90%)	0.23	286 (5%) 25 5	19, 123, 237, 321	2 (0%)

The worst 5 of 286 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AC	17	SER	9.3
5	A5	5	ASN	9.3
4	AH	51	GLY	9.2
5	BW	8	LEU	8.8
4	AH	52	ARG	8.8

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
14	CRT	B2	102	44/44	1.58	12.08	132,151,166,171	0
14	CRT	AP	102	44/44	1.46	7.93	137,140,147,148	0
14	CRT	BO	103	44/44	1.58	7.88	179,182,185,186	0
14	CRT	AG	102	44/44	1.02	7.40	126,127,135,138	0
14	CRT	AX	102	44/44	1.84	7.35	218,225,227,229	0
14	CRT	AT	102	44/44	1.22	7.11	200,205,209,210	0
13	MQ8	AM	405	53/53	0.58	6.42	76,93,128,137	0
14	CRT	BU	103	44/44	1.53	6.30	161,173,176,176	0
14	CRT	B1	103	44/44	1.21	5.93	205,224,238,240	0
14	CRT	AB	102	44/44	1.29	5.90	170,172,177,178	0
14	CRT	AS	104	44/44	1.04	5.89	165,170,177,180	0
14	CRT	B0	101	44/44	1.77	5.31	202,220,238,242	0
15	PEF	AM	409	47/47	0.72	5.27	129,183,183,183	0
14	CRT	BA	102	44/44	1.10	5.24	143,157,171,174	0
14	CRT	AW	102	44/44	1.33	5.16	127,136,144,147	0
14	CRT	BS	103	44/44	1.50	4.48	193,197,199,200	0
14	CRT	BP	102	44/44	1.04	4.40	149,151,153,154	0
14	CRT	B5	103	44/44	1.75	4.26	178,198,221,226	0
14	CRT	AR	102	44/44	1.25	4.16	189,193,200,201	0
14	CRT	BN	102	44/44	0.96	4.06	134,135,140,141	0
15	PEF	AS	101	47/47	0.51	4.01	178,225,225,225	0
13	MQ8	BM	405	53/53	0.49	3.81	68,99,166,168	0
14	CRT	BF	103	44/44	1.03	3.77	134,141,147,149	0
14	CRT	A1	103	44/44	1.12	3.76	110,123,135,138	0
14	CRT	A0	101	44/44	0.71	3.47	179,184,194,195	0
14	CRT	BV	102	44/44	0.99	3.33	208,214,218,220	0
15	PEF	BQ	101	47/47	1.03	3.28	121,145,161,161	0
14	CRT	AA	102	44/44	1.16	3.26	164,164,167,167	0
14	CRT	A5	103	44/44	1.62	3.09	167,174,185,187	0
15	PEF	BM	407	19/47	0.45	2.95	102,136,173,178	0
14	CRT	BB	102	44/44	1.28	2.92	169,185,201,205	0
14	CRT	AJ	102	44/44	0.87	2.87	138,140,144,147	0
15	PEF	AM	407	19/47	0.45	2.58	114,165,177,177	0
14	CRT	B7	102	44/44	0.87	2.49	173,194,212,217	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
14	CRT	A2	102	44/44	1.05	2.41	107,117,146,149	0
14	CRT	BG	102	44/44	0.69	2.38	122,130,143,145	0
9	BCL	BM	402	66/66	0.39	2.24	41,58,73,79	0
14	CRT	BW	103	44/44	1.04	2.15	129,145,156,161	0
9	BCL	BN	101	66/66	0.58	2.03	153,170,192,193	0
14	CRT	A7	102	44/44	0.74	2.01	126,137,150,152	0
11	UQ8	BL	304	53/53	0.49	1.94	66,137,159,166	0
14	CRT	BM	406	44/44	0.46	1.91	69,74,96,109	0
9	BCL	AQ	102	66/66	0.55	1.88	187,198,210,221	0
9	BCL	BA	101	66/66	0.50	1.83	206,224,237,238	0
9	BCL	BK	102	66/66	0.58	1.69	194,257,267,269	0
9	BCL	AU	102	66/66	0.62	1.64	161,175,231,234	0
9	BCL	AG	101	66/66	0.41	1.59	105,132,177,178	0
9	BCL	AO	102	66/66	0.48	1.58	199,207,214,219	0
9	BCL	AI	102	66/66	0.53	1.56	148,163,190,191	0
9	BCL	BV	101	66/66	0.48	1.54	172,194,218,220	0
9	BCL	AS	103	66/66	0.68	1.54	206,220,229,233	0
14	CRT	AN	102	44/44	0.92	1.52	133,135,140,140	0
9	BCL	B0	102	66/66	0.52	1.44	198,202,205,207	0
9	BCL	BQ	103	66/66	0.54	1.42	168,191,225,226	0
9	BCL	B2	101	66/66	0.44	1.40	136,152,203,204	0
10	BPH	BM	403	65/65	0.28	1.39	72,96,164,176	0
10	BPH	AM	403	65/65	0.29	1.37	43,61,150,153	0
9	BCL	A3	103	66/66	0.52	1.35	127,137,178,178	0
9	BCL	AJ	101	66/66	0.48	1.24	134,165,191,193	0
10	BPH	AL	302	65/65	0.29	1.22	31,54,75,84	0
9	BCL	B7	103	66/66	0.55	1.20	232,250,259,260	0
9	BCL	AW	101	66/66	0.54	1.16	143,191,243,243	0
9	BCL	BX	101	66/66	0.37	1.15	126,139,204,205	0
9	BCL	AT	101	66/66	0.39	1.13	187,198,247,248	0
9	BCL	AY	102	66/66	0.50	1.07	133,140,195,196	0
9	BCL	BT	101	66/66	0.48	1.00	176,191,253,254	0
9	BCL	B9	102	66/66	0.56	0.96	205,229,236,237	0
9	BCL	AA	101	66/66	0.44	0.95	235,252,257,260	0
14	CRT	AM	406	44/44	0.42	0.95	58,70,105,107	0
9	BCL	B1	102	66/66	0.40	0.94	87,118,185,186	0
9	BCL	AL	303	66/66	0.28	0.93	19,34,93,96	0
9	BCL	AP	101	66/66	0.39	0.90	107,127,189,190	0
9	BCL	BP	101	66/66	0.43	0.90	156,173,208,209	0
9	BCL	AX	101	66/66	0.44	0.90	157,171,252,255	0
9	BCL	AL	301	66/66	0.29	0.89	38,50,92,96	0
9	BCL	B8	101	66/66	0.42	0.86	226,245,252,258	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	BCL	BD	102	66/66	0.50	0.85	147,182,237,238	0
9	BCL	A3	104	66/66	0.41	0.83	151,177,223,224	0
9	BCL	BF	102	66/66	0.48	0.81	143,168,206,210	0
9	BCL	AN	101	66/66	0.35	0.80	106,126,157,171	0
9	BCL	BO	102	66/66	0.40	0.80	153,180,189,193	0
9	BCL	BU	102	66/66	0.43	0.79	144,161,240,240	0
9	BCL	AM	402	66/66	0.28	0.79	40,48,81,101	0
11	UQ8	AL	304	53/53	0.39	0.78	74,107,143,151	0
9	BCL	B3	102	66/66	0.41	0.76	104,112,169,170	0
9	BCL	AK	102	66/66	0.43	0.75	142,154,184,184	0
9	BCL	BY	102	66/66	0.40	0.75	110,129,169,169	0
10	BPH	BL	302	65/65	0.27	0.74	36,63,98,116	0
9	BCL	BW	102	66/66	0.43	0.64	129,145,213,213	0
9	BCL	B6	101	66/66	0.42	0.63	238,251,261,264	0
9	BCL	B4	101	66/66	0.46	0.57	149,166,212,214	0
9	BCL	A5	102	66/66	0.45	0.56	152,159,199,200	0
9	BCL	A2	101	66/66	0.41	0.55	122,133,201,203	0
9	BCL	BB	101	66/66	0.46	0.54	187,209,245,245	0
9	BCL	AF	102	66/66	0.42	0.54	156,175,222,222	0
9	BCL	A1	102	66/66	0.44	0.54	96,135,194,194	0
9	BCL	AD	102	66/66	0.48	0.53	179,196,260,263	0
9	BCL	A9	102	66/66	0.47	0.52	213,227,251,252	0
9	BCL	A7	103	66/66	0.39	0.45	239,243,267,268	0
9	BCL	A6	101	66/66	0.37	0.44	238,254,268,272	0
7	HEM	AC	503	43/43	0.29	0.40	71,84,106,112	0
9	BCL	BS	102	66/66	0.43	0.40	152,193,231,231	0
9	BCL	AR	101	66/66	0.37	0.39	187,200,230,231	0
9	BCL	BZ	101	66/66	0.33	0.37	125,139,192,193	0
9	BCL	BL	301	66/66	0.25	0.28	36,53,94,100	0
7	HEM	BC	502	43/43	0.31	0.27	50,80,94,103	0
9	BCL	BI	102	66/66	0.43	0.26	131,159,208,208	0
9	BCL	AZ	101	66/66	0.38	0.25	120,142,217,218	0
7	HEM	AC	502	43/43	0.29	0.24	53,68,81,88	0
7	HEM	AC	504	43/43	0.27	0.24	39,76,101,104	0
9	BCL	BQ	104	66/66	0.40	0.19	181,191,253,254	0
9	BCL	BJ	101	66/66	0.44	0.14	202,204,207,208	0
9	BCL	A8	101	66/66	0.29	0.11	201,214,245,247	0
7	HEM	AC	501	43/43	0.32	0.11	86,86,86,96	0
9	BCL	BL	303	66/66	0.24	0.11	33,56,137,146	0
9	BCL	BE	101	66/66	0.40	0.10	146,170,225,227	0
16	PO4	AM	410	5/5	0.25	0.10	83,84,84,84	0
9	BCL	A0	102	66/66	0.31	0.09	199,210,239,240	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	CA	AO	101	1/1	0.43	0.09	267,267,267,267	0
9	BCL	AV	102	66/66	0.43	0.02	183,194,249,250	0
9	BCL	AM	401	66/66	0.24	0.02	32,54,95,104	0
9	BCL	BG	101	66/66	0.36	-0.01	201,207,214,217	0
7	HEM	BC	504	43/43	0.23	-0.04	55,78,92,106	0
7	HEM	BC	503	43/43	0.26	-0.05	84,110,135,146	0
7	HEM	BC	501	43/43	0.27	-0.07	52,60,117,131	0
9	BCL	B5	102	66/66	0.31	-0.13	154,171,221,221	0
9	BCL	AE	101	66/66	0.33	-0.16	135,156,211,212	0
9	BCL	BM	401	66/66	0.22	-0.18	39,55,82,90	0
9	BCL	AB	101	66/66	0.31	-0.21	124,158,224,224	0
8	CA	BY	101	1/1	0.20	-0.43	148,148,148,148	0
15	PEF	AH	301	19/47	0.23	-0.52	128,144,161,167	0
15	PEF	AM	408	14/47	0.24	-0.53	12,90,119,125	0
8	CA	B9	101	1/1	0.28	-0.83	150,150,150,150	0
16	PO4	AH	302	5/5	0.16	-0.87	102,103,104,104	0
16	PO4	BH	301	5/5	0.15	-0.90	108,109,109,110	0
8	CA	BO	101	1/1	0.14	-0.99	238,238,238,238	0
8	CA	AF	101	1/1	0.14	-1.06	254,254,254,254	0
8	CA	AU	101	1/1	0.14	-1.09	223,223,223,223	0
8	CA	B5	101	1/1	0.15	-1.09	226,226,226,226	0
8	CA	BU	101	1/1	0.12	-1.12	237,237,237,237	0
8	CA	AD	101	1/1	0.07	-1.13	238,238,238,238	0
8	CA	B3	101	1/1	0.10	-1.19	222,222,222,222	0
16	PO4	A3	101	5/5	0.21	-1.24	153,154,154,154	0
8	CA	BK	101	1/1	0.21	-1.25	275,275,275,275	0
8	CA	B1	101	1/1	0.10	-1.27	184,184,184,184	0
8	CA	A5	101	1/1	0.10	-1.31	255,255,255,255	0
8	CA	A9	101	1/1	0.08	-1.33	268,268,268,268	0
8	CA	AS	102	1/1	0.12	-1.45	190,190,190,190	0
8	CA	AY	101	1/1	0.16	-1.49	197,197,197,197	0
8	CA	AC	505	1/1	0.10	-1.52	30,30,30,30	0
8	CA	AA	103	1/1	0.14	-1.54	275,275,275,275	0
8	CA	B7	101	1/1	0.14	-1.55	259,259,259,259	0
8	CA	A1	101	1/1	0.06	-1.55	212,212,212,212	0
8	CA	A7	101	1/1	0.10	-1.58	213,213,213,213	0
8	CA	BI	101	1/1	0.11	-1.61	236,236,236,236	0
8	CA	A3	102	1/1	0.10	-1.63	256,256,256,256	0
8	CA	AV	101	1/1	0.10	-1.64	168,168,168,168	0
8	CA	BF	101	1/1	0.07	-1.72	276,276,276,276	0
8	CA	BQ	102	1/1	0.07	-1.77	249,249,249,249	0
8	CA	AI	101	1/1	0.08	-1.84	224,224,224,224	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	CA	AQ	101	1/1	0.05	-1.84	207,207,207,207	0
8	CA	BS	101	1/1	0.10	-1.89	222,222,222,222	0
8	CA	BW	101	1/1	0.08	-1.91	204,204,204,204	0
8	CA	AK	101	1/1	0.09	-1.98	216,216,216,216	0
12	FE	BM	404	1/1	0.06	-2.20	44,44,44,44	0
8	CA	BD	101	1/1	0.06	-2.24	236,236,236,236	0
12	FE	AM	404	1/1	0.11	-2.57	47,47,47,47	0
8	CA	BA	103	1/1	0.09	-2.84	283,283,283,283	0
8	CA	BC	505	1/1	0.13	-3.19	69,69,69,69	0

6.5 Other polymers

There are no such residues in this entry.