



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:15 PM GMT

PDB ID : 2HHK
Title : Reaction centre from Rhodobacter sphaeroides strain R-26.1 complexed with dibrominated phosphatidylglycerol
Authors : Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.
Deposited on : 2006-06-28
Resolution : 2.50 Å(reported)

This is a full wwPDB validation 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>

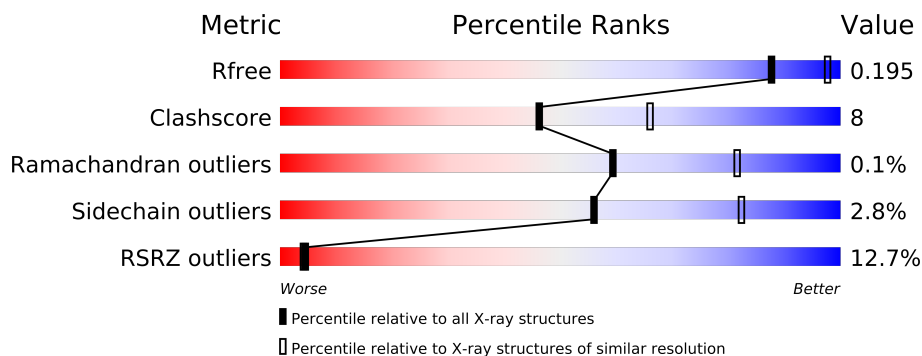
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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	L	281	
2	M	307	
3	H	260	

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

Mol	Type	Chain	Res	Geometry	Electron density
10	U10	L	502	-	X
11	CDL	M	800	-	X
12	PGT	H	801[A]	-	X
12	PGT	H	801[B]	-	X
13	PGK	M	802	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
14	LDA	H	901	-	X
14	LDA	H	903	-	X
14	LDA	H	904	-	X
14	LDA	M	902	-	X
14	LDA	M	907	-	X
14	LDA	M	920	-	X
15	GOL	H	706	-	X
15	GOL	L	707	-	X
15	GOL	L	708	-	X
15	GOL	L	709	-	X
7	PO4	M	705	-	X

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 7824 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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	1	0
			2235	1510	356	361	8			

- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	10	0
			2448	1633	402	402	11			

- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	241	Total	C	N	O	S	0	8	0
			1862	1189	323	339	11			

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Fe	0	0
			1	1		

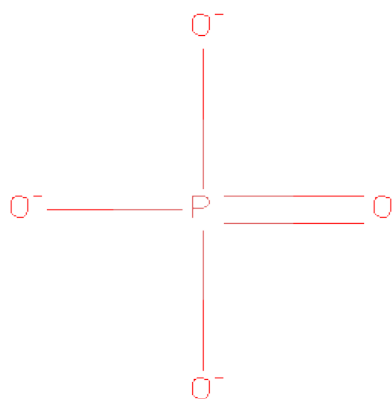
- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	K	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

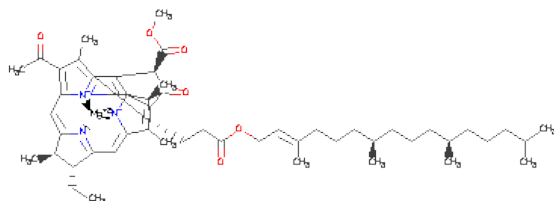
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	1	Total	Cl	0	0
			1	1		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



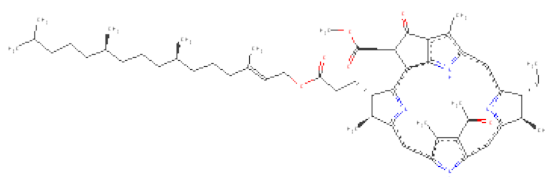
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	O	P	0	0
			5	4	1		
7	M	1	Total	O	P	0	0
			5	4	1		
7	H	1	Total	O	P	0	0
			5	4	1		
7	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



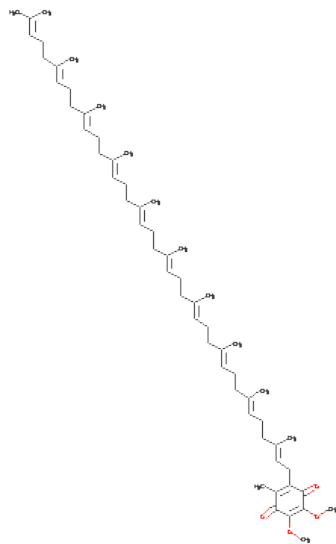
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 9 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



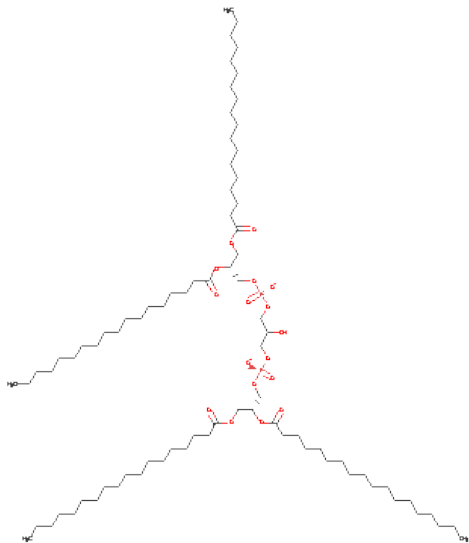
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	N	O	0	0
			65	55	4	6		
9	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 10 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	C	O	0	0
			48	44	4		
10	L	1	Total	C	O	0	0
			48	44	4		

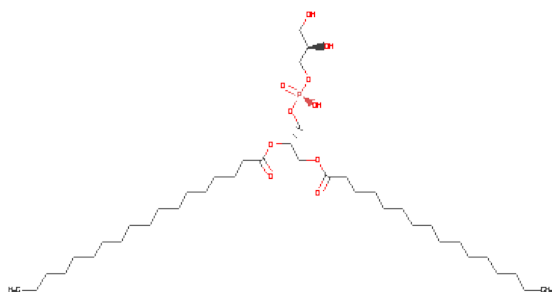
- Molecule 11 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	M	1	Total	C	O	P	0	0
			81	62	17	2		

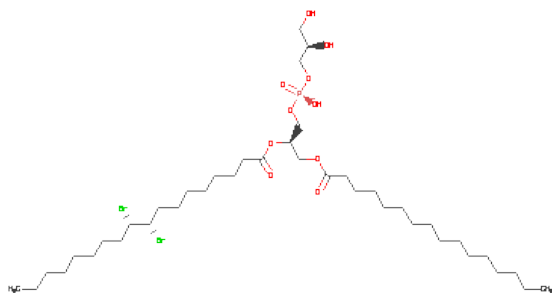
- Molecule 12 is (1S)-2-{{[[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSP

HORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYLSTEARATE (three-letter code: PGT) (formula: $C_{40}H_{79}O_{10}P$).



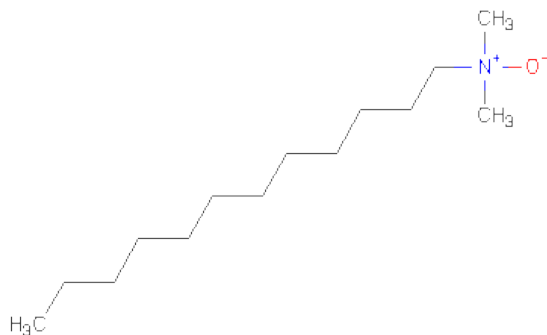
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
12	H	1	102	80	20	2	0	1

- Molecule 13 is (1R)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL(9S,10S)-9,10-DIBROMOOCTADECANOATE (three-letter code: PGK) (formula: $C_{40}H_{77}Br_2O_{10}P$).



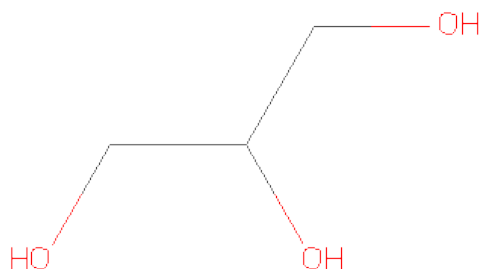
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	M	1	Total	Br	C	O	P	0	0
			53	2	40	10	1		

- Molecule 14 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	H	1	Total	C	N	O	0	0
			16	14	1	1		
14	M	1	Total	C	N	O	0	0
			16	14	1	1		
14	H	1	Total	C	N	O	0	0
			16	14	1	1		
14	H	1	Total	C	N	O	0	0
			16	14	1	1		
14	M	1	Total	C	N	O	0	0
			16	14	1	1		
14	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 15 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	H	1	Total	C	O	0	0
			6	3	3		
15	L	1	Total	C	O	0	0
			6	3	3		
15	L	1	Total	C	O	0	0
			6	3	3		
15	L	1	Total	C	O	0	0
			6	3	3		

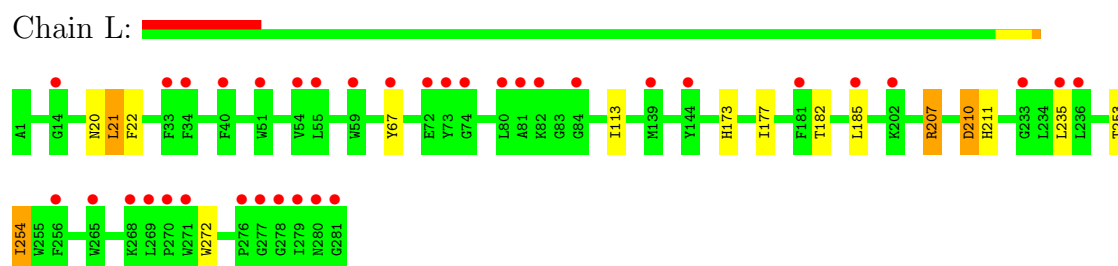
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	H	199	Total	O	0	0
			199	199		
16	L	92	Total	O	0	0
			92	92		
16	M	119	Total	O	0	0
			119	119		

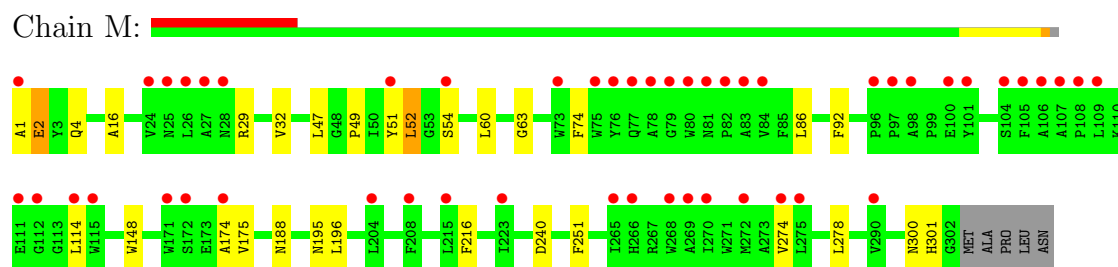
3 Residue-property plots

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.

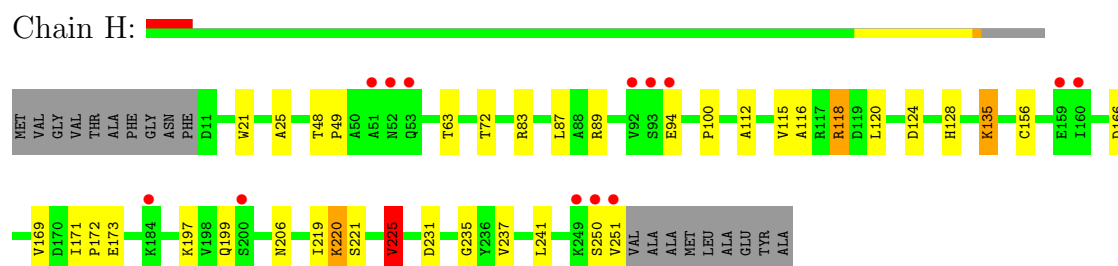
- Molecule 1: Reaction center protein L chain



- Molecule 2: Reaction center protein M chain



- Molecule 3: Reaction center protein H chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.42Å 139.42Å 183.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.00 – 2.50 45.63 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.00-2.50) 99.5 (45.63-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.172 , 0.197 0.173 , 0.195	Depositor DCC
R_{free} test set	3546 reflections (4.97%)	DCC
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 67.4	EDS
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 71469 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7824	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, GOL, LDA, CL, CDL, BPH, K, PGK, PGT, FE, U10, 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	L	0.88	0/2328	0.73	1/3186 (0.0%)
2	M	0.87	0/2592	0.78	1/3536 (0.0%)
3	H	0.93	5/1953 (0.3%)	0.82	4/2652 (0.2%)
All	All	0.89	5/6873 (0.1%)	0.78	6/9374 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	M	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	173	GLU	CD-OE2	5.32	1.31	1.25
3	H	237	VAL	CB-CG2	5.12	1.63	1.52
3	H	221[A]	SER	CB-OG	5.07	1.48	1.42
3	H	221[B]	SER	CB-OG	5.07	1.48	1.42
3	H	94	GLU	CG-CD	5.05	1.59	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	210	ASP	CB-CG-OD1	6.50	124.15	118.30
3	H	124	ASP	CB-CG-OD1	6.31	123.98	118.30
3	H	225	VAL	CB-CA-C	-5.53	100.90	111.40
3	H	89	ARG	NE-CZ-NH2	-5.40	117.60	120.30
2	M	240	ASP	CB-CG-OD1	5.20	122.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	83	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	1	ALA	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	L	2235	0	2196	10	0
2	M	2448	0	2367	26	0
3	H	1862	0	1883	25	0
4	M	1	0	0	0	0
5	H	1	0	0	0	0
6	M	1	0	0	0	0
7	H	5	0	0	0	0
7	M	15	0	0	1	0
8	L	132	0	148	6	0
8	M	132	0	148	20	0
9	L	65	0	75	0	0
9	M	65	0	76	4	0
10	L	48	0	63	4	0
10	M	48	0	63	1	0
11	M	81	0	106	3	0
12	H	102	0	156	20	0
13	M	53	0	74	11	0
14	H	48	0	93	25	0
14	M	48	0	93	12	0
15	H	6	0	8	0	0
15	L	18	0	24	5	0
16	H	199	0	0	4	0
16	L	92	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	M	119	0	0	2	0
All	All	7824	0	7573	123	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 8.

All (123) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:301[A]:HIS:HE1	16:M:1031:HOH:O	1.41	1.03
8:M:311:BCL:C9	8:M:311:BCL:H41	1.91	0.99
8:M:311:BCL:C7	8:M:311:BCL:H41	1.92	0.98
14:M:902:LDA:C12	14:H:903:LDA:C12	2.43	0.96
14:M:902:LDA:C12	14:H:903:LDA:H123	1.96	0.95
8:M:311:BCL:C4	8:M:311:BCL:H92	1.98	0.94
14:M:902:LDA:H122	14:H:903:LDA:C12	1.98	0.93
14:M:902:LDA:H122	14:H:903:LDA:H123	1.49	0.93
8:M:311:BCL:H92	8:M:311:BCL:H41	1.48	0.92
15:L:709:GOL:H2	3:H:241:LEU:HD13	1.54	0.89
12:H:801[A]:PGT:C44	14:H:901:LDA:H121	2.05	0.86
12:H:801[A]:PGT:C43	14:H:901:LDA:H121	2.05	0.85
8:M:313:BCL:H201	13:M:802:PGK:H252	1.59	0.84
8:M:311:BCL:HBB2	8:M:311:BCL:HMB1	1.63	0.81
8:M:311:BCL:CBB	8:M:311:BCL:HMB1	2.13	0.79
8:M:311:BCL:H41	8:M:311:BCL:H71	1.64	0.77
14:M:902:LDA:H123	14:H:903:LDA:C12	2.15	0.77
3:H:250:SER:O	3:H:251:VAL:HG23	1.85	0.76
10:L:502:U10:H153	13:M:802:PGK:H482	1.69	0.74
12:H:801[A]:PGT:H442	14:H:901:LDA:C12	2.20	0.71
8:M:311:BCL:C8	8:M:311:BCL:H41	2.20	0.71
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.73	0.69
1:L:254:ILE:C	1:L:254:ILE:HD12	2.13	0.69
8:L:314:BCL:HBB2	8:L:314:BCL:HMB1	1.74	0.68
12:H:801[B]:PGT:C32	12:H:801[B]:PGT:H12	2.22	0.68
12:H:801[A]:PGT:H362	12:H:801[A]:PGT:H321	1.75	0.68
1:L:182:THR:OG1	8:M:311:BCL:H2	1.94	0.68
12:H:801[A]:PGT:H442	14:H:901:LDA:H121	1.72	0.68
3:H:220[B]:LYS:NZ	16:H:1209:HOH:O	2.25	0.67
10:L:502:U10:H153	13:M:802:PGK:C48	2.25	0.66
3:H:219:ILE:HG21	3:H:225:VAL:HG13	1.78	0.66
12:H:801[B]:PGT:C43	14:H:901:LDA:H121	2.24	0.66
12:H:801[B]:PGT:C44	14:H:901:LDA:H121	2.26	0.65
8:M:313:BCL:C20	13:M:802:PGK:H252	2.26	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:M:311:BCL:C4	8:M:311:BCL:C9	2.63	0.64
12:H:801[A]:PGT:H412	14:H:903:LDA:H111	1.82	0.62
12:H:801[A]:PGT:H432	14:H:901:LDA:H121	1.81	0.62
14:M:902:LDA:H122	14:H:903:LDA:H122	1.80	0.62
11:M:800:CDL:H231	14:H:904:LDA:HM12	1.82	0.60
2:M:174:ALA:HB1	14:M:920:LDA:H121	1.83	0.60
2:M:175:VAL:H	14:M:920:LDA:H123	1.66	0.60
8:M:311:BCL:H191	13:M:802:PGK:BR2	2.57	0.60
8:M:311:BCL:H42	8:M:311:BCL:H92	1.84	0.60
3:H:118[B]:ARG:HE	3:H:120:LEU:HD12	1.68	0.57
14:M:902:LDA:C12	14:H:903:LDA:H122	2.33	0.57
8:M:311:BCL:C4	8:M:311:BCL:H71	2.33	0.57
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.40	0.57
3:H:21:TRP:CD1	12:H:801[B]:PGT:H5	2.41	0.56
8:L:314:BCL:CBB	8:L:314:BCL:HMB1	2.37	0.55
11:M:800:CDL:C23	14:H:904:LDA:HM12	2.37	0.54
8:M:311:BCL:H8	13:M:802:PGK:H471	1.91	0.52
2:M:60[A]:LEU:HD23	9:M:401:BPH:H4C1	1.92	0.52
12:H:801[B]:PGT:H322	12:H:801[B]:PGT:H12	1.92	0.52
15:L:709:GOL:H2	3:H:241:LEU:CD1	2.35	0.51
2:M:278[B]:LEU:HD11	11:M:800:CDL:H811	1.91	0.51
3:H:197[A]:LYS:NZ	3:H:199:GLN:HE21	2.09	0.51
10:L:502:U10:C15	13:M:802:PGK:H482	2.41	0.50
12:H:801[B]:PGT:H431	14:H:901:LDA:H121	1.90	0.50
2:M:175:VAL:N	14:M:920:LDA:H123	2.26	0.50
3:H:169:VAL:HG23	3:H:171:ILE:HD13	1.93	0.50
2:M:51:TYR:O	2:M:52:LEU:HD23	2.11	0.50
3:H:87:LEU:HD23	3:H:100:PRO:HA	1.93	0.50
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.47	0.50
8:L:312:BCL:CBB	8:L:312:BCL:HMB1	2.43	0.48
2:M:188[B]:ASN:ND2	16:M:1077:HOH:O	2.43	0.48
3:H:220[B]:LYS:NZ	16:H:1100:HOH:O	2.41	0.48
2:M:175:VAL:H	14:M:920:LDA:C12	2.27	0.47
2:M:54:SER:OG	7:M:703:PO4:O2	2.32	0.47
12:H:801[A]:PGT:H442	14:H:901:LDA:H123	1.96	0.47
10:L:502:U10:H4M3	10:L:502:U10:H3M2	1.96	0.47
12:H:801[A]:PGT:C41	14:H:903:LDA:H111	2.44	0.47
2:M:29:ARG:O	13:M:802:PGK:H42	2.15	0.47
1:L:113:ILE:O	15:L:709:GOL:H11	2.15	0.47
2:M:175:VAL:HB	14:M:920:LDA:H123	1.97	0.47
8:M:313:BCL:HMB1	8:M:313:BCL:CBB	2.45	0.46
1:L:113:ILE:O	15:L:709:GOL:C1	2.63	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:L:312:BCL:HHC	8:L:312:BCL:OBB	2.15	0.46
3:H:63:THR:CG2	3:H:72:THR:HB	2.46	0.46
1:L:207:ARG:HG2	1:L:211:HIS:CG	2.51	0.46
15:L:709:GOL:C2	3:H:241:LEU:HD13	2.36	0.46
3:H:156[A]:CYS:HB3	3:H:206:ASN:O	2.16	0.45
3:H:156[B]:CYS:HB3	3:H:206:ASN:O	2.16	0.45
8:M:313:BCL:HBD	8:M:313:BCL:HAA2	1.99	0.45
2:M:148:TRP:HA	2:M:148:TRP:HE3	1.81	0.45
13:M:802:PGK:H121	13:M:802:PGK:H31	1.53	0.45
9:M:401:BPH:CBC	9:M:401:BPH:HHD	2.47	0.45
3:H:128[B]:HIS:HE1	16:H:1109:HOH:O	1.99	0.45
1:L:21:LEU:HD13	1:L:22:PHE:CE1	2.52	0.44
12:H:801[A]:PGT:H362	12:H:801[A]:PGT:C32	2.46	0.44
3:H:135:LYS:HB3	3:H:135:LYS:HE3	1.57	0.44
2:M:63:GLY:HA3	9:M:401:BPH:H5C2	1.99	0.44
8:L:312:BCL:HMB1	8:L:312:BCL:HBB3	1.99	0.44
2:M:47:LEU:HD22	13:M:802:PGK:BR2	2.73	0.43
12:H:801[B]:PGT:H322	12:H:801[B]:PGT:H351	1.58	0.43
12:H:801[A]:PGT:H432	14:H:903:LDA:H112	2.00	0.43
2:M:196:LEU:HD12	2:M:196:LEU:HA	1.91	0.43
3:H:128[B]:HIS:HD2	16:H:1280:HOH:O	2.01	0.42
1:L:67:TYR:HB3	16:L:1167:HOH:O	2.19	0.42
8:M:313:BCL:H201	13:M:802:PGK:C25	2.40	0.42
1:L:253:THR:OG1	1:L:254:ILE:N	2.51	0.42
3:H:135:LYS:HB3	3:H:166:ASP:OD2	2.20	0.42
2:M:74:PHE:CD1	2:M:92:PHE:HB3	2.54	0.42
3:H:48:THR:HB	3:H:49:PRO:HD2	2.02	0.42
3:H:25:ALA:HB2	14:H:903:LDA:H52	2.01	0.42
12:H:801[A]:PGT:C44	14:H:901:LDA:C12	2.81	0.42
2:M:2:GLU:HG3	2:M:2:GLU:H	1.53	0.42
2:M:2:GLU:O	2:M:4:GLN:NE2	2.52	0.42
14:H:901:LDA:H22	14:H:901:LDA:HM11	1.80	0.42
2:M:32:VAL:HG12	2:M:49:PRO:HD3	2.02	0.42
3:H:115:VAL:HG12	3:H:116:ALA:N	2.35	0.42
10:M:501:U10:H322	10:M:501:U10:H28	1.80	0.41
12:H:801[B]:PGT:C41	14:H:903:LDA:H111	2.50	0.41
3:H:112:ALA:HA	3:H:235:GLY:O	2.20	0.41
1:L:20:ASN:ND2	16:L:1300:HOH:O	2.52	0.41
8:L:312:BCL:CGA	8:L:314:BCL:HBC1	2.51	0.41
3:H:118[B]:ARG:NE	3:H:120:LEU:HD12	2.35	0.41
3:H:171:ILE:HB	3:H:172:PRO:HD3	2.01	0.41
2:M:251:PHE:CD1	2:M:251:PHE:C	2.94	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:52:LEU:HD11	2:M:60[A]:LEU:HD12	2.02	0.41
9:M:401:BPH:HBC3	9:M:401:BPH:HHD	2.02	0.40
8:M:311:BCL:HMB1	8:M:311:BCL:HBB3	2.00	0.40

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	L	280/281 (100%)	274 (98%)	6 (2%)	0	100	100
2	M	310/307 (101%)	298 (96%)	11 (4%)	1 (0%)	50	73
3	H	247/260 (95%)	242 (98%)	5 (2%)	0	100	100
All	All	837/848 (99%)	814 (97%)	22 (3%)	1 (0%)	59	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	195	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	221/220 (100%)	214 (97%)	7 (3%)	51	77
2	M	246/240 (102%)	240 (98%)	6 (2%)	61	86
3	H	204/208 (98%)	197 (97%)	7 (3%)	49	75
All	All	671/668 (100%)	651 (97%)	20 (3%)	56	80

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	21	LEU
1	L	185	LEU
1	L	207	ARG
1	L	210	ASP
1	L	235	LEU
1	L	254	ILE
1	L	272	TRP
2	M	2	GLU
2	M	52	LEU
2	M	86	LEU
2	M	114	LEU
2	M	216	PHE
2	M	274	VAL
3	H	118[A]	ARG
3	H	118[B]	ARG
3	H	135	LYS
3	H	220[A]	LYS
3	H	220[B]	LYS
3	H	225	VAL
3	H	231	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	28	ASN
3	H	199	GLN

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 29 ligands modelled in this entry, 3 are monoatomic - leaving 26 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$
7	PO4	H	704	-	4,4,4	0.30	0	6,6,6	0.31	0
15	GOL	H	706	-	5,5,5	0.23	0	5,5,5	0.82	0
12	PGT	H	801[A]	-	50,50,50	0.70	0	56,56,56	0.94	3 (5%)
12	PGT	H	801[B]	-	50,50,50	0.84	1 (2%)	56,56,56	1.07	5 (8%)
14	LDA	H	901	-	15,15,15	3.28	2 (13%)	17,17,17	1.07	1 (5%)
14	LDA	H	903	-	15,15,15	3.51	2 (13%)	17,17,17	0.95	2 (11%)
14	LDA	H	904	-	15,15,15	3.77	2 (13%)	17,17,17	0.88	2 (11%)
8	BCL	L	312	1	74,74,74	1.43	10 (13%)	97,115,115	1.53	16 (16%)
8	BCL	L	314	1	74,74,74	1.42	12 (16%)	97,115,115	1.52	18 (18%)
9	BPH	L	402	-	70,70,70	1.34	8 (11%)	94,101,101	1.22	13 (13%)
10	U10	L	502	-	48,48,63	1.17	5 (10%)	59,61,79	1.76	11 (18%)
15	GOL	L	707	-	5,5,5	0.30	0	5,5,5	0.52	0
15	GOL	L	708	-	5,5,5	0.45	0	5,5,5	0.64	0
15	GOL	L	709	-	5,5,5	0.55	0	5,5,5	0.75	0
8	BCL	M	311	2	74,74,74	1.33	9 (12%)	97,115,115	1.85	25 (25%)
8	BCL	M	313	2	74,74,74	1.36	10 (13%)	97,115,115	1.87	26 (26%)
9	BPH	M	401	-	70,70,70	1.36	6 (8%)	94,101,101	1.45	13 (13%)
10	U10	M	501	-	48,48,63	1.18	5 (10%)	59,61,79	1.60	9 (15%)
7	PO4	M	702	-	4,4,4	0.27	0	6,6,6	0.31	0
7	PO4	M	703	-	4,4,4	0.33	0	6,6,6	0.37	0
7	PO4	M	705	-	4,4,4	0.27	0	6,6,6	0.33	0
11	CDL	M	800	-	80,80,99	1.51	8 (10%)	92,92,111	1.48	14 (15%)
13	PGK	M	802	-	52,52,52	0.83	2 (3%)	60,60,60	1.41	6 (10%)
14	LDA	M	902	-	15,15,15	3.53	1 (6%)	17,17,17	0.81	0
14	LDA	M	907	-	15,15,15	3.76	1 (6%)	17,17,17	1.05	2 (11%)
14	LDA	M	920	-	15,15,15	3.41	2 (13%)	17,17,17	1.52	2 (11%)

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
7	PO4	H	704	-	-	0/0/0/0	0/0/0/0
15	GOL	H	706	-	-	0/4/4/4	0/0/0/0
12	PGT	H	801[A]	-	-	0/55/55/55	0/0/0/0
12	PGT	H	801[B]	-	-	0/55/55/55	0/0/0/0
14	LDA	H	901	-	-	0/13/13/13	0/0/0/0
14	LDA	H	903	-	-	0/13/13/13	0/0/0/0
14	LDA	H	904	-	-	0/13/13/13	0/0/0/0
8	BCL	L	312	1	-	0/41/137/137	0/0/9/9
8	BCL	L	314	1	-	0/41/137/137	0/0/9/9
9	BPH	L	402	-	2/2/18/22	0/49/105/105	0/0/6/6
10	U10	L	502	-	-	0/45/69/87	0/1/1/1
15	GOL	L	707	-	-	0/4/4/4	0/0/0/0
15	GOL	L	708	-	-	0/4/4/4	0/0/0/0
15	GOL	L	709	-	-	0/4/4/4	0/0/0/0
8	BCL	M	311	2	-	0/41/137/137	0/0/9/9
8	BCL	M	313	2	-	0/41/137/137	0/0/9/9
9	BPH	M	401	-	2/2/18/22	0/49/105/105	0/0/6/6
10	U10	M	501	-	-	0/45/69/87	0/1/1/1
7	PO4	M	702	-	-	0/0/0/0	0/0/0/0
7	PO4	M	703	-	-	0/0/0/0	0/0/0/0
7	PO4	M	705	-	-	0/0/0/0	0/0/0/0
11	CDL	M	800	-	1/1/9/9	0/91/91/110	0/0/0/0
13	PGK	M	802	-	-	0/60/60/60	0/0/0/0
14	LDA	M	902	-	-	0/13/13/13	0/0/0/0
14	LDA	M	907	-	-	0/13/13/13	0/0/0/0
14	LDA	M	920	-	-	0/13/13/13	0/0/0/0

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	907	LDA	O1-N1	-14.36	1.25	1.39
14	H	904	LDA	O1-N1	-14.22	1.26	1.39
14	M	902	LDA	O1-N1	-13.48	1.26	1.39
14	H	903	LDA	O1-N1	-13.33	1.26	1.39
14	M	920	LDA	O1-N1	-12.89	1.27	1.39
14	H	901	LDA	O1-N1	-12.31	1.27	1.39
9	M	401	BPH	C1D-CHD	6.31	1.42	1.35
9	L	402	BPH	C1D-CHD	6.26	1.42	1.35
11	M	800	CDL	OA8-CA7	5.06	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	800	CDL	C43-C42	-5.04	1.53	1.55
8	L	314	BCL	C1B-C2B	4.79	1.46	1.40
11	M	800	CDL	C58-C57	-4.69	1.53	1.55
8	L	312	BCL	MG-NB	4.62	2.15	2.05
11	M	800	CDL	OB6-CB5	4.29	1.47	1.34
8	M	311	BCL	C1B-C2B	4.28	1.45	1.40
8	M	313	BCL	MG-NA	4.28	2.19	2.07
11	M	800	CDL	C84-C83	-4.16	1.53	1.55
10	M	501	U10	O3-C3	4.09	1.47	1.36
8	M	311	BCL	C3B-C4B	4.07	1.46	1.40
8	L	312	BCL	MG-NA	4.07	2.19	2.07
11	M	800	CDL	OB8-CB7	4.05	1.46	1.33
11	M	800	CDL	OA6-CA5	4.04	1.46	1.34
9	L	402	BPH	C3B-C4B	4.04	1.46	1.40
10	L	502	U10	O3-C3	4.04	1.47	1.36
8	L	312	BCL	C1B-C2B	3.91	1.45	1.40
8	L	312	BCL	C3B-C4B	3.90	1.46	1.40
8	M	313	BCL	C1A-NA	3.89	1.40	1.32
8	M	313	BCL	C3B-C4B	3.86	1.46	1.40
8	M	311	BCL	C1A-NA	3.81	1.40	1.32
9	M	401	BPH	C3B-C4B	3.68	1.45	1.40
8	M	311	BCL	MG-NA	3.68	2.18	2.07
8	M	311	BCL	C1B-NB	3.62	1.39	1.34
8	L	312	BCL	C1A-NA	3.44	1.39	1.32
10	L	502	U10	C13-C14	3.42	1.39	1.32
8	L	314	BCL	MG-NA	3.25	2.16	2.07
8	L	314	BCL	C3B-C4B	3.23	1.45	1.40
8	L	314	BCL	C4C-NC	3.20	1.39	1.32
8	L	314	BCL	C1A-NA	3.17	1.39	1.32
8	M	311	BCL	MG-NB	3.14	2.12	2.05
8	L	312	BCL	C1B-NB	3.10	1.38	1.34
12	H	801[B]	PGT	C1-C2	3.09	1.59	1.50
8	M	313	BCL	C4B-NB	3.05	1.38	1.34
13	M	802	PGK	P-O1P	2.99	1.62	1.51
10	M	501	U10	O4-C4	2.98	1.44	1.36
9	M	401	BPH	C1B-NB	2.95	1.39	1.36
8	M	313	BCL	C1C-NC	-2.95	1.32	1.39
9	M	401	BPH	CHA-C1A	-2.93	1.34	1.45
8	L	312	BCL	C4-C3	2.90	1.58	1.50
8	L	314	BCL	MG-NB	2.86	2.11	2.05
14	H	901	LDA	C1-N1	-2.78	1.46	1.51
8	M	313	BCL	C4C-NC	2.75	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	502	U10	C33-C34	2.66	1.38	1.32
8	L	314	BCL	MG-NC	-2.55	1.99	2.07
8	M	313	BCL	CHB-C4A	2.54	1.42	1.36
8	L	312	BCL	C4C-NC	2.54	1.37	1.32
8	M	313	BCL	C4A-NA	-2.52	1.33	1.39
10	L	502	U10	O4-C4	2.52	1.43	1.36
8	L	314	BCL	C1C-NC	-2.48	1.33	1.39
8	M	311	BCL	C4C-NC	2.43	1.37	1.32
8	L	314	BCL	C4A-NA	-2.42	1.33	1.39
14	H	904	LDA	C1-N1	-2.42	1.46	1.51
9	M	401	BPH	C4B-CHC	-2.42	1.36	1.46
8	L	312	BCL	C4B-NB	2.41	1.37	1.34
14	M	920	LDA	C1-N1	-2.37	1.46	1.51
10	M	501	U10	C41-C39	2.34	1.53	1.40
9	L	402	BPH	C4C-NC	2.32	1.40	1.34
8	M	313	BCL	MG-ND	2.30	2.10	2.05
8	M	311	BCL	C1C-NC	-2.30	1.34	1.39
14	H	903	LDA	C1-N1	-2.28	1.47	1.51
10	M	501	U10	C13-C14	2.26	1.37	1.32
9	L	402	BPH	C1C-NC	-2.25	1.33	1.38
9	L	402	BPH	C1D-ND	2.24	1.40	1.38
8	L	312	BCL	C4A-NA	-2.24	1.34	1.39
9	L	402	BPH	CHA-C1A	-2.23	1.37	1.45
8	L	314	BCL	C1B-NB	2.22	1.37	1.34
8	L	314	BCL	CHB-C4A	2.16	1.41	1.36
8	M	311	BCL	C4A-NA	-2.15	1.34	1.39
8	L	314	BCL	C2A-C1A	-2.13	1.48	1.52
13	M	802	PGK	O2-C2	-2.13	1.41	1.46
10	L	502	U10	C41-C39	2.12	1.52	1.40
9	L	402	BPH	C4D-ND	-2.10	1.35	1.38
9	M	401	BPH	C1C-NC	-2.08	1.34	1.38
10	M	501	U10	C8-C9	2.04	1.37	1.32
11	M	800	CDL	PA1-OA3	-2.04	1.43	1.48
9	L	402	BPH	C1B-CHB	-2.03	1.38	1.46
8	M	313	BCL	C2C-C1C	-2.01	1.46	1.51

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	313	BCL	CMB-C2B-C1B	-6.01	119.38	128.62
11	M	800	CDL	OB6-CB5-C51	5.26	123.09	111.56
8	M	311	BCL	C4-C3-C2	-5.15	113.32	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	311	BCL	OBB-CAB-C3B	5.10	127.73	120.07
10	L	502	U10	C25-C24-C26	5.05	123.07	115.39
8	M	313	BCL	CAC-C3C-C2C	-4.96	102.49	113.89
8	M	311	BCL	C2B-C1B-NB	-4.87	105.73	109.41
13	M	802	PGK	C3-C2-C1	-4.81	100.90	111.86
13	M	802	PGK	BR1-C39-C40	-4.78	100.39	110.23
8	M	313	BCL	CMB-C2B-C3B	4.77	132.48	124.97
8	L	312	BCL	CMB-C2B-C1B	-4.68	121.41	128.62
8	L	314	BCL	CAA-C2A-C3A	-4.58	102.21	113.04
8	M	313	BCL	CMD-C2D-C3D	4.57	132.16	124.97
8	L	312	BCL	CMB-C2B-C3B	4.56	132.16	124.97
9	M	401	BPH	C1-C2-C3	-4.35	118.45	126.19
11	M	800	CDL	OB8-CB6-CB4	4.23	119.91	108.83
8	M	313	BCL	C3B-C4B-NB	-4.23	104.53	108.64
11	M	800	CDL	CA4-OA6-CA5	-4.20	107.55	117.92
10	M	501	U10	C17-C18-C19	-4.18	118.77	127.80
8	M	311	BCL	C4B-NB-C1B	4.07	112.13	106.76
12	H	801[A]	PGT	O2-C31-C32	4.07	120.47	111.56
13	M	802	PGK	O2-C31-C32	4.06	120.45	111.56
9	M	401	BPH	O2D-CGD-CBD	4.06	119.59	111.33
10	L	502	U10	O2-C2-C3	-4.01	112.07	120.96
8	L	314	BCL	CAC-C3C-C2C	-3.95	104.81	113.89
9	M	401	BPH	CAA-C2A-C3A	-3.91	103.80	113.04
8	M	311	BCL	CMB-C2B-C1B	-3.90	122.63	128.62
10	M	501	U10	C22-C23-C24	-3.89	119.41	127.80
12	H	801[B]	PGT	O2-C31-C32	3.89	120.08	111.56
10	L	502	U10	C12-C13-C14	-3.87	119.44	127.80
11	M	800	CDL	OA6-CA5-C11	3.84	119.98	111.56
14	M	920	LDA	C2-C1-N1	-3.80	107.24	113.80
8	M	313	BCL	C4B-NB-C1B	3.76	111.72	106.76
10	L	502	U10	C25-C24-C23	-3.72	116.15	123.52
8	L	312	BCL	CAA-C2A-C3A	-3.71	104.27	113.04
8	M	313	BCL	O2A-C1-C2	3.61	116.36	108.55
8	M	311	BCL	C1-O2A-CGA	3.57	126.97	116.98
8	M	311	BCL	O2D-CGD-CBD	3.55	118.56	111.33
10	M	501	U10	C7-C6-C5	-3.55	114.90	118.75
8	M	311	BCL	C2C-C1C-NC	3.49	115.20	110.95
12	H	801[B]	PGT	C2-O2-C31	-3.49	109.30	117.92
10	L	502	U10	C30-C29-C31	3.48	120.68	115.39
8	M	311	BCL	CED-O2D-CGD	-3.48	107.73	116.02
8	L	314	BCL	C2B-C1B-NB	-3.47	106.79	109.41
10	M	501	U10	C26-C27-C28	-3.46	101.73	111.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	311	BCL	C5-C3-C2	3.44	127.70	121.08
8	M	313	BCL	C2A-C1A-NA	3.43	115.05	111.24
10	M	501	U10	C15-C14-C16	3.43	120.61	115.39
9	M	401	BPH	CAC-C3C-C4C	3.39	122.03	112.68
10	M	501	U10	C32-C33-C34	-3.38	120.50	127.80
9	L	402	BPH	CMB-C2B-C1B	-3.37	123.52	128.65
10	M	501	U10	C30-C29-C31	3.36	120.50	115.39
10	L	502	U10	C3M-O3-C3	3.36	127.91	116.48
10	L	502	U10	C7-C6-C5	-3.32	115.15	118.75
14	M	920	LDA	CM2-N1-CM1	-3.30	105.07	108.85
10	L	502	U10	C22-C23-C24	-3.27	120.75	127.80
9	M	401	BPH	OBD-CAD-CBD	-3.26	121.02	125.94
8	L	314	BCL	C5-C3-C2	-3.21	114.92	121.08
9	M	401	BPH	CMB-C2B-C1B	-3.16	123.83	128.65
8	L	312	BCL	CHA-C1A-NA	-3.14	119.78	126.22
8	L	312	BCL	C2C-C1C-NC	3.13	114.76	110.95
8	L	314	BCL	C4B-NB-C1B	3.12	110.87	106.76
11	M	800	CDL	OA8-CA7-C31	3.11	121.72	111.94
8	M	311	BCL	C1D-C2D-C3D	-3.09	104.25	106.78
8	M	313	BCL	C4-C3-C5	3.08	120.06	115.39
8	L	312	BCL	C2C-C3C-C4C	3.08	105.31	101.05
9	M	401	BPH	C4-C3-C2	-3.07	117.43	123.52
8	L	314	BCL	O2D-CGD-CBD	3.04	117.53	111.33
10	M	501	U10	C37-C38-C39	-3.03	121.29	128.63
9	L	402	BPH	C1-C2-C3	-3.01	120.84	126.19
8	L	312	BCL	CGD-CBD-CHA	2.99	121.12	110.96
8	L	312	BCL	C4B-NB-C1B	2.94	110.64	106.76
11	M	800	CDL	OB8-CB7-C71	2.92	121.12	111.94
8	L	314	BCL	C2C-C3C-C4C	2.90	105.08	101.05
8	M	313	BCL	C2C-C1C-CHC	-2.89	118.32	124.33
14	H	901	LDA	O1-N1-CM1	2.87	112.88	109.01
8	M	311	BCL	CHA-C1A-NA	-2.87	120.33	126.22
13	M	802	PGK	C2-O2-C31	-2.86	110.85	117.92
8	M	311	BCL	CAA-C2A-C3A	-2.82	106.38	113.04
9	L	402	BPH	CMB-C2B-C3B	2.82	129.41	124.97
11	M	800	CDL	OA2-CA2-C1	2.82	117.46	108.62
9	L	402	BPH	CAC-C3C-C2C	2.78	120.26	113.89
8	L	314	BCL	CAA-CBA-CGA	2.75	122.13	113.27
8	M	313	BCL	CHA-C1A-NA	-2.73	120.61	126.22
8	L	314	BCL	C4-C3-C5	2.72	119.52	115.39
8	M	311	BCL	C3B-C4B-NB	-2.70	106.02	108.64
8	M	311	BCL	CMB-C2B-C3B	2.69	129.21	124.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	313	BCL	O2D-CGD-O1D	-2.68	118.34	123.79
9	M	401	BPH	CMB-C2B-C3B	2.68	129.18	124.97
8	M	313	BCL	C4D-CHA-CBD	-2.66	103.10	109.37
8	M	313	BCL	C2C-C3C-C4C	2.64	104.70	101.05
8	M	313	BCL	CBD-CHA-C1A	2.64	132.22	128.77
9	M	401	BPH	O2D-CGD-O1D	-2.63	118.44	123.79
8	L	314	BCL	CMB-C2B-C1B	-2.63	124.58	128.62
12	H	801[B]	PGT	O3-C11-C12	2.60	120.11	111.94
8	L	312	BCL	C3B-C4B-NB	-2.59	106.12	108.64
10	M	501	U10	C40-C39-C38	-2.59	117.42	123.62
8	L	312	BCL	C4-C3-C5	2.57	119.30	115.39
9	L	402	BPH	C1D-C2D-C3D	-2.56	104.69	106.89
9	L	402	BPH	CAA-C2A-C3A	-2.55	107.02	113.04
8	M	313	BCL	C3B-C4B-CHC	2.55	130.83	126.00
8	L	312	BCL	CAC-C3C-C2C	-2.55	108.05	113.89
12	H	801[A]	PGT	O3-C3-C2	2.55	115.50	108.83
11	M	800	CDL	CA6-OA8-CA7	2.54	124.57	117.13
8	M	313	BCL	C2C-C1C-NC	2.54	114.04	110.95
9	L	402	BPH	O2D-CGD-CBD	2.53	116.48	111.33
8	M	313	BCL	C1D-C2D-C3D	-2.50	104.74	106.78
8	L	314	BCL	C2C-C1C-NC	2.48	113.97	110.95
8	L	312	BCL	OBD-CAD-CBD	-2.47	122.21	125.94
8	L	314	BCL	O1D-CGD-CBD	-2.46	119.38	124.42
8	M	313	BCL	C2B-C1B-NB	-2.45	107.56	109.41
8	L	312	BCL	C2A-C1A-NA	2.45	113.96	111.24
11	M	800	CDL	OA5-PA1-OA2	-2.43	97.86	104.53
8	L	314	BCL	OBB-CAB-C3B	2.43	123.71	120.07
8	M	313	BCL	C4B-CHC-C1C	-2.36	125.15	130.06
9	L	402	BPH	CMA-C3A-C2A	-2.36	104.01	114.14
8	M	311	BCL	C4-C3-C5	2.36	118.97	115.39
8	M	311	BCL	CAA-CBA-CGA	2.34	120.82	113.27
8	M	313	BCL	C1-C2-C3	-2.33	122.04	126.19
8	L	312	BCL	C3A-C4A-NA	2.32	113.78	110.95
14	M	907	LDA	O1-N1-CM2	-2.32	105.88	109.01
8	L	314	BCL	CAC-C3C-C4C	-2.32	107.43	112.58
8	M	313	BCL	CHC-C1C-NC	2.32	127.32	124.58
11	M	800	CDL	C74-C73-C72	-2.32	102.08	114.61
14	M	907	LDA	CM2-N1-CM1	-2.32	106.20	108.85
14	H	903	LDA	C2-C1-N1	-2.30	109.83	113.80
9	L	402	BPH	CMD-C2D-C3D	2.30	128.59	124.97
8	M	313	BCL	CMA-C3A-C4A	2.29	118.41	111.76
11	M	800	CDL	C72-C71-CB7	-2.29	104.53	113.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	314	BCL	CMC-C2C-C3C	-2.29	104.31	114.14
9	L	402	BPH	CAC-C3C-C4C	2.28	118.96	112.68
13	M	802	PGK	BR2-C40-C39	-2.28	105.55	110.23
9	L	402	BPH	O2D-CGD-O1D	-2.28	119.17	123.79
9	M	401	BPH	O2A-C1-C2	-2.28	103.62	108.55
11	M	800	CDL	OB8-CB7-OB9	-2.27	117.23	123.43
10	L	502	U10	C37-C38-C39	-2.27	123.13	128.63
8	M	311	BCL	C1D-CHD-C4C	2.26	129.44	125.55
12	H	801[A]	PGT	O3-C11-C12	2.26	119.05	111.94
8	M	313	BCL	C16-C15-C13	-2.24	108.70	115.14
12	H	801[B]	PGT	O3-C3-C2	2.19	114.58	108.83
9	L	402	BPH	C4D-C3D-C2D	2.19	110.01	107.37
9	M	401	BPH	CAA-C2A-C1A	-2.18	106.98	112.72
10	L	502	U10	C1M-C1-C6	-2.17	119.88	124.20
9	L	402	BPH	C4B-C3B-C2B	2.16	109.17	107.60
8	M	311	BCL	C6-C5-C3	-2.16	107.65	112.78
14	H	903	LDA	CM2-N1-CM1	-2.15	106.39	108.85
13	M	802	PGK	C3-O3-C11	-2.15	110.82	117.13
9	M	401	BPH	CMA-C3A-C2A	-2.15	104.88	114.14
14	H	904	LDA	O1-N1-CM1	-2.14	106.13	109.01
8	M	311	BCL	CMD-C2D-C3D	2.14	128.34	124.97
12	H	801[B]	PGT	O2-C31-O31	-2.13	117.94	123.65
8	M	311	BCL	OB D-CAD-C3D	2.13	131.88	127.91
11	M	800	CDL	OA6-CA5-OA7	-2.11	118.01	123.65
8	L	312	BCL	CMA-C3A-C2A	-2.11	105.08	114.14
9	M	401	BPH	C3C-C4C-CHD	2.09	126.18	121.83
11	M	800	CDL	CB6-CB4-CB3	-2.09	107.10	111.86
8	M	311	BCL	OB D-CAD-CBD	-2.09	122.78	125.94
8	L	314	BCL	CHB-C4A-NA	2.08	127.04	124.58
8	M	311	BCL	C2A-C1A-CHA	2.08	127.43	123.83
10	L	502	U10	C27-C28-C29	-2.07	123.34	127.80
8	L	314	BCL	C4D-CHA-CBD	-2.06	104.52	109.37
14	H	904	LDA	CM2-N1-CM1	2.06	111.20	108.85
8	M	313	BCL	CHB-C1B-NB	2.06	128.01	124.58
8	L	314	BCL	CMA-C3A-C2A	-2.05	105.33	114.14
8	L	312	BCL	C2C-C1C-CHC	-2.05	120.07	124.33
8	M	311	BCL	C4D-CHA-CBD	-2.03	104.60	109.37
8	M	313	BCL	C3C-C4C-NC	-2.02	109.00	111.60
8	M	311	BCL	C2C-C3C-C4C	2.00	103.83	101.05

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	M	800	CDL	CA4
9	L	402	BPH	C8
9	L	402	BPH	C13
9	M	401	BPH	C8
9	M	401	BPH	C13

There are no torsion outliers.

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	L	281/281 (100%)	0.79	36 (12%) 4 4	54, 62, 73, 80	0
2	M	302/307 (98%)	0.82	50 (16%) 2 2	54, 62, 73, 94	0
3	H	241/260 (92%)	0.34	13 (5%) 25 25	54, 62, 73, 100	0
All	All	824/848 (97%)	0.67	99 (12%) 4 5	54, 62, 73, 100	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	277	GLY	6.8
3	H	251	VAL	5.5
2	M	80	TRP	5.2
1	L	281	GLY	5.0
1	L	278	GLY	4.9
1	L	271	TRP	4.8
2	M	97	PRO	4.8
2	M	75	TRP	4.6
1	L	269	LEU	4.6
2	M	28	ASN	4.5
1	L	279	ILE	4.4
2	M	105	PHE	4.4
2	M	101	TYR	4.3
1	L	80	LEU	4.2
3	H	250	SER	4.0
1	L	59	TRP	4.0
2	M	1	ALA	3.9
3	H	52	ASN	3.9
2	M	26	LEU	3.8
1	L	276	PRO	3.7
1	L	33	PHE	3.7
1	L	40	PHE	3.7
2	M	98	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
2	M	82	PRO	3.6
2	M	275	LEU	3.6
1	L	202	LYS	3.6
2	M	171	TRP	3.6
2	M	265	ILE	3.6
2	M	100[A]	GLU	3.5
1	L	73	TYR	3.5
1	L	270	PRO	3.5
1	L	268	LYS	3.4
3	H	249	LYS	3.4
2	M	114	LEU	3.4
3	H	51	ALA	3.4
1	L	280	ASN	3.3
2	M	106	ALA	3.3
2	M	79	GLY	3.2
2	M	27	ALA	3.2
2	M	208	PHE	3.2
2	M	111	GLU	3.2
2	M	104	SER	3.1
2	M	83	ALA	3.1
1	L	236	LEU	3.1
3	H	160	ILE	3.0
1	L	256	PHE	3.0
2	M	109	LEU	2.9
2	M	274	VAL	2.9
2	M	270	ILE	2.9
3	H	93	SER	2.9
2	M	174	ALA	2.9
2	M	76	TYR	2.9
2	M	78	ALA	2.8
1	L	72	GLU	2.8
2	M	51	TYR	2.7
3	H	94	GLU	2.7
1	L	139	MET	2.7
1	L	185	LEU	2.7
2	M	204	LEU	2.7
2	M	108	PRO	2.7
2	M	268	TRP	2.6
2	M	77	GLN	2.6
1	L	51	TRP	2.6
2	M	269	ALA	2.6
2	M	290	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	M	272	MET	2.6
2	M	96	PRO	2.5
2	M	73	TRP	2.5
2	M	54	SER	2.5
3	H	53	GLN	2.5
2	M	107	ALA	2.5
3	H	92	VAL	2.5
1	L	34	PHE	2.5
1	L	235	LEU	2.5
2	M	266	HIS	2.4
2	M	84	VAL	2.4
1	L	233	GLY	2.4
1	L	14	GLY	2.3
2	M	112	GLY	2.3
1	L	67	TYR	2.3
1	L	55	LEU	2.3
2	M	81	ASN	2.3
3	H	159	GLU	2.3
1	L	81	ALA	2.2
2	M	215	LEU	2.2
3	H	200	SER	2.2
1	L	74	GLY	2.2
1	L	265	TRP	2.2
2	M	115	TRP	2.2
1	L	82	LYS	2.2
2	M	25	ASN	2.1
1	L	54	VAL	2.1
1	L	181	PHE	2.1
1	L	144	TYR	2.1
1	L	84	GLY	2.1
2	M	223	ILE	2.1
2	M	172	SER	2.1
2	M	24	VAL	2.0
3	H	184	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
14	LDA	H	903	16/16	1.40	26.02	73,75,78,78	16
14	LDA	M	907	16/16	0.48	15.70	69,72,77,77	16
14	LDA	M	902	16/16	0.81	15.33	66,71,75,79	16
14	LDA	H	904	16/16	0.72	14.40	76,79,86,86	16
12	PGT	H	801[A]	51/51	1.22	12.49	45,73,81,82	51
12	PGT	H	801[B]	51/51	1.22	12.47	47,76,84,85	51
15	GOL	L	709	6/6	0.68	8.36	65,66,68,70	6
15	GOL	H	706	6/6	0.54	6.68	72,72,73,74	6
10	U10	L	502	48/63	0.60	6.20	53,68,86,90	48
14	LDA	M	920	16/16	0.53	5.79	41,60,78,80	16
15	GOL	L	708	6/6	0.33	4.83	60,66,68,68	6
13	PGK	M	802	53/53	0.62	4.23	61,67,76,77	53
11	CDL	M	800	81/100	0.43	3.98	49,74,88,90	81
14	LDA	H	901	16/16	0.40	3.29	72,77,86,88	16
7	PO4	M	705	5/5	0.26	2.31	63,64,65,65	5
15	GOL	L	707	6/6	0.42	2.12	65,67,68,68	6
7	PO4	H	704	5/5	0.25	1.92	61,61,63,63	5
10	U10	M	501	48/63	0.32	1.87	56,69,90,93	0
7	PO4	M	702	5/5	0.28	1.25	69,71,74,77	5
8	BCL	L	314	66/66	0.23	1.24	50,59,75,80	0
6	CL	M	701	1/1	0.21	0.97	73,73,73,73	1
8	BCL	M	313	66/66	0.19	0.77	51,59,84,95	0
8	BCL	M	311	66/66	0.23	0.73	55,62,119,120	0
8	BCL	L	312	66/66	0.19	0.34	49,59,70,78	0
9	BPH	M	401	65/65	0.20	0.26	56,62,116,118	0
9	BPH	L	402	65/65	0.18	0.21	50,62,66,68	0
4	FE	M	500	1/1	0.20	-0.84	59,59,59,59	0
7	PO4	M	703	5/5	0.18	-1.63	59,59,63,64	5
5	K	H	700	1/1	0.09	-2.19	58,58,58,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.