



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2018 – 11:01 PM EST

PDB ID : 2HG3
Title : Reaction centre from Rhodobacter sphaeroides strain R-26.1 complexed with brominated phosphatidylcholine
Authors : Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.
Deposited on : 2006-06-26
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

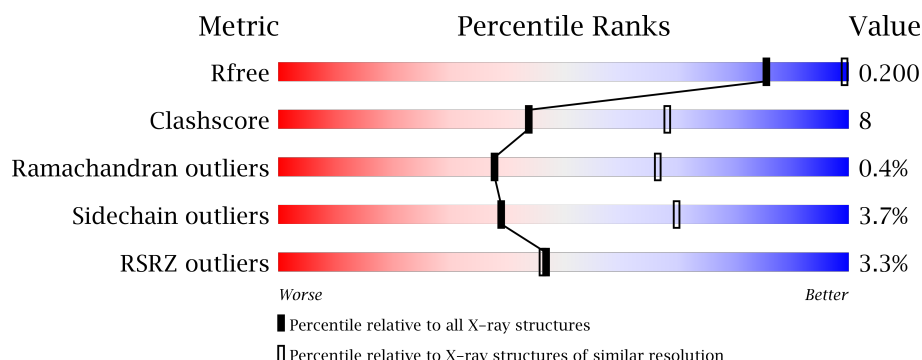
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	L	281	<div> <div>3%</div> <div>91%</div> <div>9%</div> <div>.</div> </div>
2	M	307	<div> <div>4%</div> <div>84%</div> <div>14%</div> <div>..</div> </div>
3	H	260	<div> <div>2%</div> <div>82%</div> <div>9%</div> <div>.</div> <div>8%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	GOL	H	706	-	-	-	X
10	GOL	L	707	-	-	-	X
10	GOL	L	708	-	-	-	X
12	CDL	M	800	-	-	-	X
13	PC9	M	801	-	-	-	X
13	PC9	M	802	-	-	-	X
4	PO4	L	701	-	-	-	X
4	PO4	M	703	-	-	X	-
7	U10	L	502	-	-	-	X
8	HTO	L	705	-	-	-	X
9	LDA	H	903	-	-	-	X
9	LDA	L	905	-	-	-	X
9	LDA	L	906	-	-	-	X
9	LDA	L	908	-	-	-	X
9	LDA	L	909	-	-	-	X
9	LDA	M	907	-	-	-	X
9	LDA	M	920	-	-	-	X

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 7921 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	4	0
			2246	1516	357	365	8			

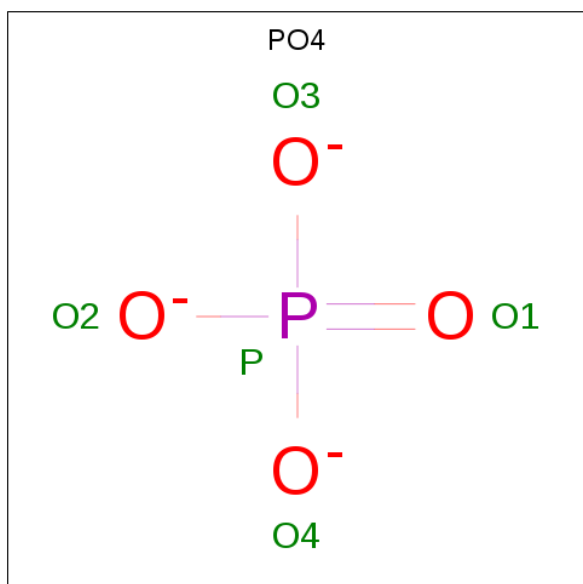
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	14	0
			2477	1654	405	407	11			

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

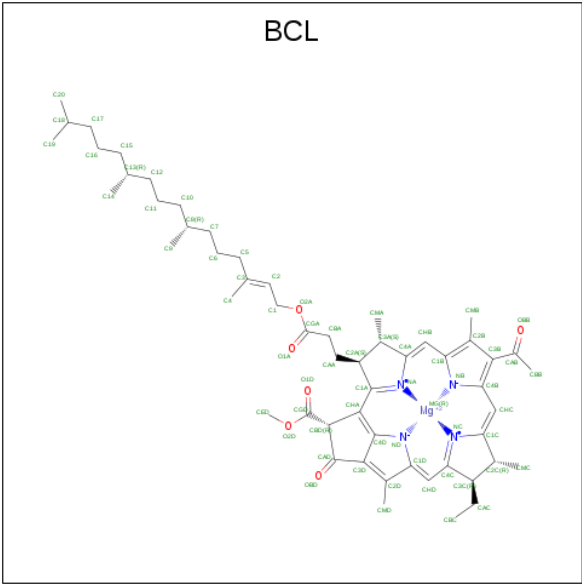
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	8	0
			1851	1181	321	338	11			

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



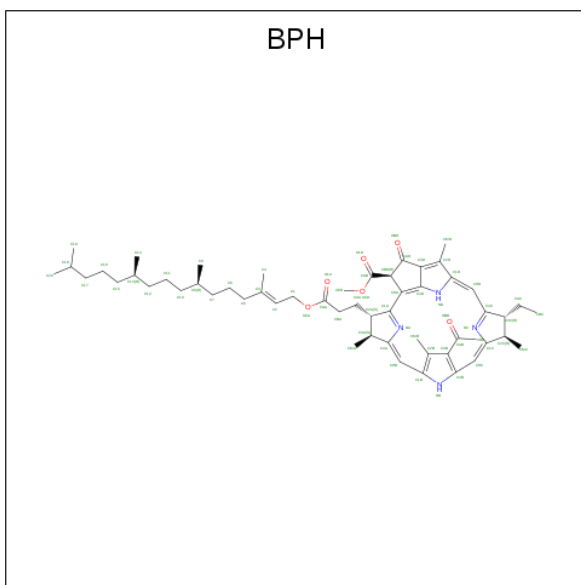
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total O P 5 4 1	0	0
4	L	1	Total O P 5 4 1	0	0
4	M	1	Total O P 5 4 1	0	0
4	M	1	Total O P 5 4 1	0	0

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



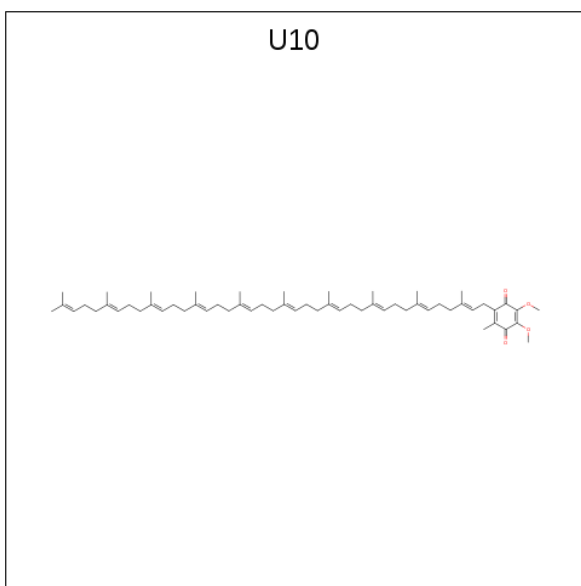
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total C Mg N O 66 55 1 4 6	0	0
5	L	1	Total C Mg N O 66 55 1 4 6	0	0
5	M	1	Total C Mg N O 66 55 1 4 6	0	0
5	M	1	Total C Mg N O 66 55 1 4 6	0	0

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆).



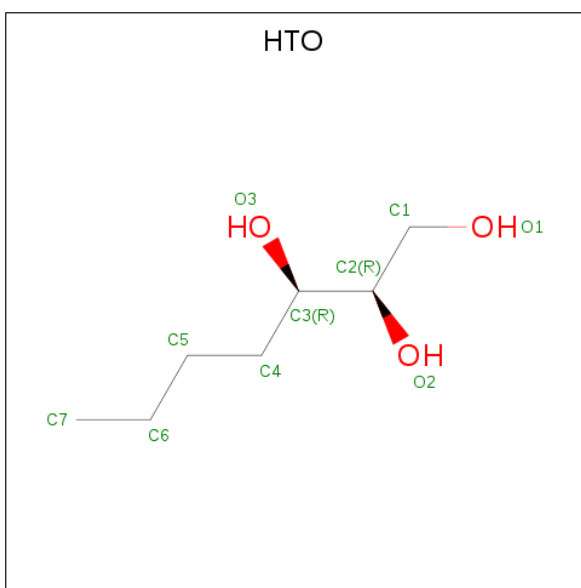
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			65	55	4	6		
6	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



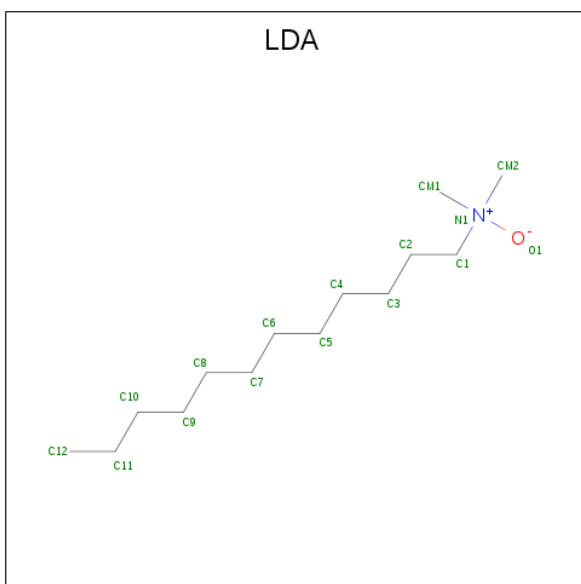
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			48	44	4		
7	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 8 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



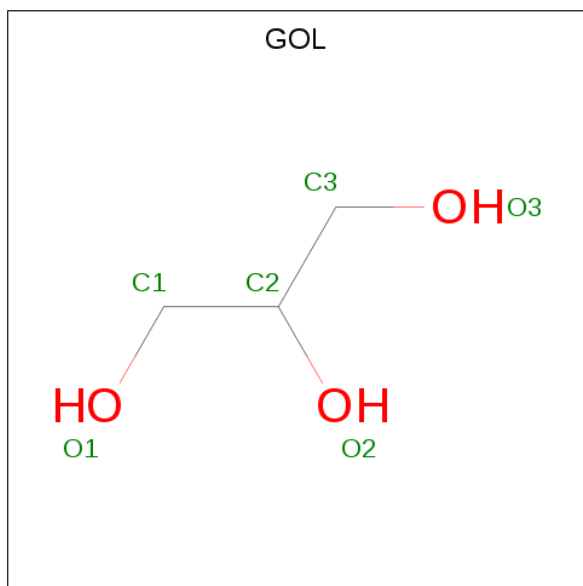
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	L	1	Total	C	N	O	0	0
			16	14	1	1		

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

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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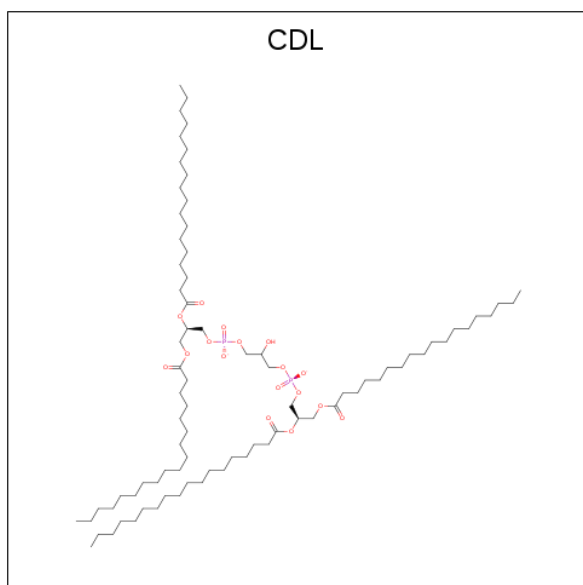
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).

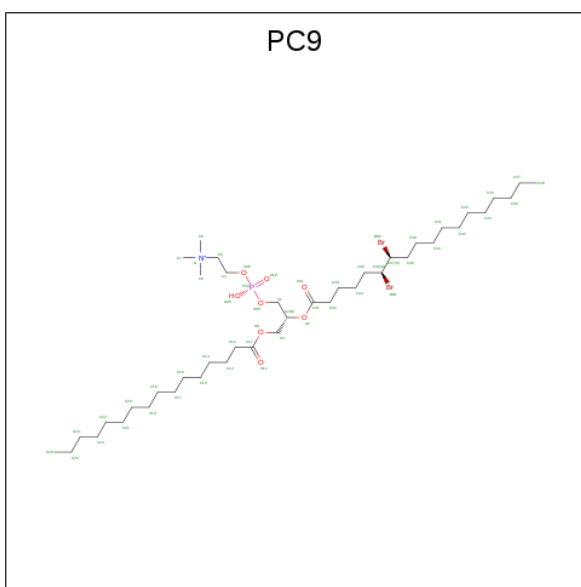
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

- Molecule 12 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 13 is (7R,14S)-14,15-DIBROMO-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: PC9) (formula: $C_{42}H_{83}Br_2NO_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	M	1	Total	Br	C	N	O	P	0	0
			54	2	42	1	8	1		
13	M	1	Total	Br	C	N	O	P	0	0
			54	2	42	1	8	1		

- Molecule 14 is POTASSIUM ION (three-letter code: K) (formula: K).

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

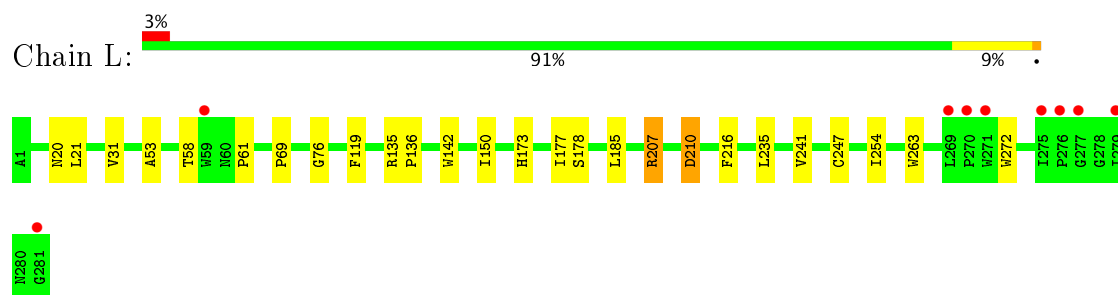
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	L	104	Total	O	0	0
			104	104		
15	M	141	Total	O	0	0
			141	141		
15	H	207	Total	O	0	0
			207	207		

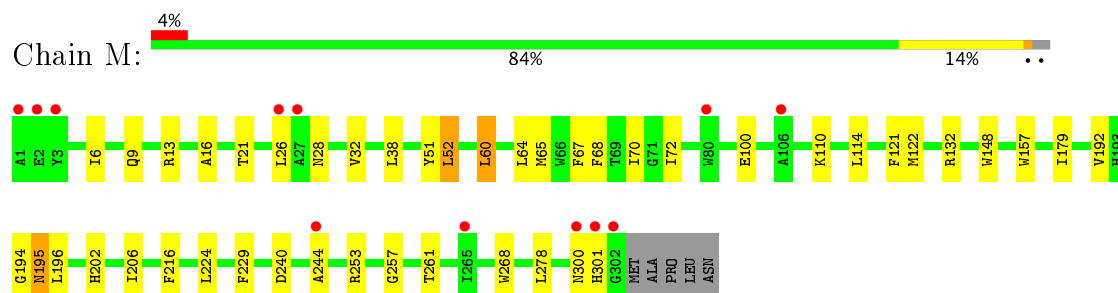
3 Residue-property plots [i](#)

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

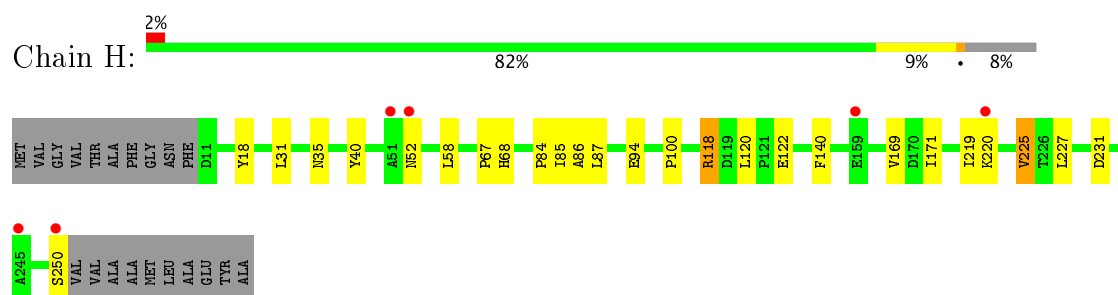
- Molecule 1: Reaction center protein L chain



- 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	139.84Å 139.84Å 184.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.35 – 2.70 34.35 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.35-2.70) 99.7 (34.35-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.164 , 0.199 0.169 , 0.200	Depositor DCC
R_{free} test set	2852 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	53.8	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 78.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7921	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, GOL, LDA, PC9, CDL, BPH, K, HTO, 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	0.85	0/2351	0.77	3/3217 (0.1%)
2	M	0.88	0/2628	0.79	1/3584 (0.0%)
3	H	0.96	2/1945 (0.1%)	0.83	0/2642
All	All	0.89	2/6924 (0.0%)	0.79	4/9443 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	94	GLU	CG-CD	6.36	1.61	1.51
3	H	94	GLU	CD-OE2	6.10	1.32	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	210	ASP	CB-CG-OD1	6.91	124.52	118.30
1	L	207	ARG	NE-CZ-NH2	5.59	123.10	120.30
1	L	207	ARG	NE-CZ-NH1	-5.51	117.54	120.30
2	M	240	ASP	CB-CG-OD1	5.16	122.95	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2246	0	2207	14	0
2	M	2477	0	2389	39	0
3	H	1851	0	1866	16	0
4	L	10	0	0	0	0
4	M	10	0	0	2	0
5	L	132	0	148	5	0
5	M	132	0	148	14	0
6	L	65	0	76	3	0
6	M	65	0	76	4	0
7	L	48	0	63	8	0
7	M	48	0	63	1	0
8	L	10	0	16	0	0
9	H	64	0	124	7	0
9	L	64	0	124	10	0
9	M	32	0	62	7	0
10	H	12	0	16	0	0
10	L	12	0	16	0	0
11	M	1	0	0	0	0
12	M	81	0	106	3	0
13	M	108	0	160	23	0
14	H	1	0	0	0	0
15	H	207	0	0	0	0
15	L	104	0	0	0	0
15	M	141	0	0	5	0
All	All	7921	0	7660	116	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (116) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:801:PC9:H261	9:H:903:LDA:H121	1.33	1.05
2:M:257:GLY:O	13:M:801:PC9:H32	1.64	0.98
5:M:311:BCL:H41	13:M:802:PC9:H441	1.45	0.97
3:H:118[B]:ARG:HD3	3:H:120:LEU:HD12	1.65	0.79
3:H:84:PRO:O	3:H:85:ILE:HD13	1.85	0.76
5:L:312:BCL:CBB	5:L:312:BCL:HMB1	2.18	0.74
12:M:800:CDL:HB4	12:M:800:CDL:HA61	1.66	0.74
2:M:122:MET:SD	9:M:920:LDA:H123	2.28	0.74
2:M:253[B]:ARG:NH2	13:M:801:PC9:O2	2.24	0.71
5:M:311:BCL:H41	13:M:802:PC9:C44	2.19	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:801:PC9:H141	13:M:801:PC9:H31	1.72	0.70
13:M:801:PC9:H261	9:H:903:LDA:C12	2.16	0.70
5:M:311:BCL:CBB	5:M:311:BCL:HMB1	2.22	0.69
7:L:502:U10:H303	5:M:311:BCL:C14	2.25	0.66
5:L:312:BCL:HMB1	5:L:312:BCL:HBB3	1.76	0.66
2:M:65[A]:MET:HE2	2:M:121:PHE:CZ	2.32	0.65
2:M:52:LEU:HD21	2:M:60[A]:LEU:HD21	1.78	0.65
2:M:70:ILE:HD13	9:M:920:LDA:HM22	1.78	0.65
13:M:801:PC9:C4	3:H:52:ASN:HD21	2.10	0.64
13:M:801:PC9:C26	9:H:903:LDA:H121	2.20	0.63
5:M:311:BCL:C4	13:M:802:PC9:H441	2.25	0.62
1:L:61:PRO:O	1:L:150:ILE:HD13	1.99	0.62
2:M:70:ILE:HG21	9:M:920:LDA:HM23	1.80	0.62
2:M:157:TRP:HE1	9:M:920:LDA:H122	1.65	0.61
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.84	0.59
13:M:802:PC9:H121	13:M:802:PC9:H162	1.84	0.59
3:H:118[B]:ARG:CD	3:H:120:LEU:HD12	2.31	0.59
5:M:313:BCL:H191	13:M:802:PC9:C26	2.33	0.58
1:L:178:SER:OG	7:L:502:U10:H302	2.03	0.58
5:M:311:BCL:HBB2	5:M:311:BCL:HMB1	1.86	0.58
12:M:800:CDL:HB4	12:M:800:CDL:CA6	2.33	0.58
2:M:21:THR:HG23	2:M:26:LEU:HD21	1.85	0.57
6:M:401:BPH:CB	6:M:401:BPH:HH	2.35	0.57
5:L:314:BCL:HBB2	5:L:314:BCL:HMB1	1.86	0.56
9:L:906:LDA:HM22	9:L:908:LDA:H52	1.88	0.56
3:H:18:TYR:CD1	9:H:903:LDA:O1	2.59	0.55
7:L:502:U10:H303	5:M:311:BCL:H143	1.88	0.55
9:H:903:LDA:H62	9:H:904:LDA:CM2	2.37	0.55
3:H:67:PRO:HB2	3:H:68:HIS:CD2	2.42	0.55
2:M:301[A]:HIS:CE1	15:M:1031:HOH:O	2.60	0.54
6:L:402:BPH:HBB3	6:L:402:BPH:CMB	2.38	0.54
2:M:67[B]:PHE:HZ	5:M:313:BCL:H203	1.73	0.54
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.42	0.54
2:M:60[A]:LEU:HD12	6:M:401:BPH:H4C1	1.89	0.53
1:L:119:PHE:CD2	9:L:908:LDA:H111	2.42	0.53
2:M:65[A]:MET:HE3	2:M:121:PHE:CE2	2.44	0.53
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.92	0.52
2:M:110:LYS:NZ	15:M:1431:HOH:O	2.43	0.52
5:M:313:BCL:H191	13:M:802:PC9:H263	1.90	0.52
9:L:906:LDA:H32	9:L:906:LDA:HM11	1.91	0.51
13:M:801:PC9:H41	3:H:52:ASN:HD21	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:802:PC9:H51	13:M:802:PC9:O11	2.11	0.51
13:M:802:PC9:H412	13:M:802:PC9:H451	1.93	0.51
7:L:502:U10:H351	7:L:502:U10:H38	1.92	0.50
1:L:76:GLY:HA3	9:L:909:LDA:HM13	1.94	0.50
7:M:501:U10:H23	13:M:801:PC9:H191	1.94	0.50
9:H:903:LDA:H62	9:H:904:LDA:HM21	1.93	0.50
7:L:502:U10:H351	7:L:502:U10:C38	2.42	0.49
6:M:401:BPH:HBC2	6:M:401:BPH:HH2	1.94	0.49
9:L:906:LDA:CM2	9:L:908:LDA:H52	2.42	0.49
2:M:157:TRP:NE1	9:M:920:LDA:H122	2.26	0.49
2:M:65[A]:MET:CE	2:M:121:PHE:CE2	2.95	0.49
2:M:70:ILE:HD13	9:M:920:LDA:CM2	2.42	0.48
3:H:40:TYR:HB3	3:H:58:LEU:HD21	1.96	0.48
1:L:241:VAL:HG21	6:L:402:BPH:HAC1	1.95	0.48
4:M:703:PO4:O3	15:M:1448:HOH:O	2.20	0.48
9:M:920:LDA:HM11	9:M:920:LDA:H22	1.56	0.48
5:M:313:BCL:HMB1	5:M:313:BCL:CBB	2.43	0.47
3:H:87:LEU:HD23	3:H:100:PRO:HA	1.95	0.47
3:H:219:ILE:HG21	3:H:225:VAL:HG13	1.95	0.47
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.49	0.47
1:L:263:TRP:HH2	7:L:502:U10:H352	1.80	0.46
13:M:801:PC9:H2	13:M:801:PC9:O1P	2.16	0.46
2:M:52:LEU:HD21	2:M:60[A]:LEU:CD2	2.46	0.46
13:M:801:PC9:H141	13:M:801:PC9:C3	2.42	0.46
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.98	0.46
13:M:802:PC9:C12	13:M:802:PC9:H162	2.46	0.45
2:M:6:ILE:CD1	2:M:224:LEU:HD13	2.46	0.45
2:M:13:ARG:O	3:H:140:PHE:HA	2.16	0.45
5:M:311:BCL:HMB1	5:M:311:BCL:HBB3	1.98	0.45
2:M:28:ASN:HB2	2:M:51:TYR:CE2	2.52	0.45
5:L:312:BCL:CGA	5:L:314:BCL:HBC1	2.47	0.45
13:M:801:PC9:BR1	9:H:902:LDA:H102	2.72	0.44
9:L:908:LDA:C3	9:L:908:LDA:HM11	2.46	0.44
1:L:263:TRP:CH2	7:L:502:U10:H352	2.52	0.44
9:L:906:LDA:HM21	9:L:906:LDA:H22	1.71	0.44
2:M:68[A]:PHE:CE1	2:M:72:ILE:HD11	2.52	0.44
13:M:801:PC9:H222	13:M:801:PC9:H252	1.31	0.44
2:M:194:GLY:O	2:M:195:ASN:HB3	2.17	0.44
3:H:122:GLU:HB2	3:H:227:LEU:HD21	1.99	0.43
6:L:402:BPH:CMB	6:L:402:BPH:CBB	2.95	0.43
1:L:53:ALA:HB1	1:L:58:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:314:BCL:CBB	5:L:314:BCL:HMB1	2.49	0.43
6:M:401:BPH:CBC	6:M:401:BPH:CHD	2.95	0.43
2:M:229:PHE:HB2	2:M:244:ALA:HB2	2.00	0.43
2:M:65[A]:MET:CE	2:M:121:PHE:CZ	3.02	0.43
2:M:261:THR:HG23	3:H:35:ASN:O	2.19	0.42
4:M:703:PO4:P	15:M:1448:HOH:O	2.77	0.42
2:M:268:TRP:CE3	3:H:31:LEU:HD13	2.54	0.42
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.54	0.42
2:M:68[A]:PHE:O	2:M:72:ILE:HD13	2.18	0.42
2:M:253[B]:ARG:HH21	13:M:801:PC9:H12	1.85	0.42
1:L:216:PHE:CD2	7:L:502:U10:H102	2.55	0.42
2:M:301[A]:HIS:HE1	15:M:1031:HOH:O	1.99	0.42
9:L:908:LDA:C3	9:L:908:LDA:CM1	2.97	0.42
1:L:119:PHE:CE2	9:L:908:LDA:H111	2.55	0.42
2:M:179:ILE:HG23	5:M:311:BCL:HED1	2.02	0.42
2:M:6:ILE:HD13	2:M:224:LEU:HD13	2.02	0.41
1:L:76:GLY:CA	9:L:909:LDA:HM13	2.51	0.41
5:M:311:BCL:H61	5:M:313:BCL:H193	2.01	0.41
3:H:169:VAL:HG23	3:H:171:ILE:HD13	2.01	0.41
3:H:84:PRO:C	3:H:85:ILE:HD13	2.41	0.41
2:M:148:TRP:CD1	12:M:800:CDL:OB6	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	283/281 (101%)	272 (96%)	10 (4%)	1 (0%)	38	66
2	M	314/307 (102%)	298 (95%)	15 (5%)	1 (0%)	44	73
3	H	246/260 (95%)	240 (98%)	5 (2%)	1 (0%)	38	66
All	All	843/848 (99%)	810 (96%)	30 (4%)	3 (0%)	38	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	195	ASN
3	H	86	ALA
1	L	31	VAL

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	224/220 (102%)	215 (96%)	9 (4%)	36	67
2	M	250/240 (104%)	239 (96%)	11 (4%)	33	63
3	H	203/208 (98%)	197 (97%)	6 (3%)	46	76
All	All	677/668 (101%)	651 (96%)	26 (4%)	39	68

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	20	ASN
1	L	21	LEU
1	L	185	LEU
1	L	207	ARG
1	L	210	ASP
1	L	235	LEU
1	L	247	CYS
1	L	254	ILE
1	L	272	TRP
2	M	38	LEU
2	M	52	LEU
2	M	60[A]	LEU
2	M	60[B]	LEU
2	M	100	GLU
2	M	114	LEU
2	M	132	ARG
2	M	192	VAL
2	M	196	LEU

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Mol	Chain	Res	Type
2	M	216	PHE
2	M	278	LEU
3	H	118[A]	ARG
3	H	118[B]	ARG
3	H	220	LYS
3	H	225	VAL
3	H	231	ASP
3	H	250	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	274	ASN
2	M	28	ASN
3	H	68	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 2 are monoatomic - leaving 30 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
10	GOL	H	706	-	5,5,5	0.33	0	5,5,5	0.89	0
10	GOL	H	709	-	5,5,5	0.53	0	5,5,5	0.22	0
9	LDA	H	901	-	13,15,15	2.30	1 (7%)	14,17,17	0.59	0
9	LDA	H	902	-	13,15,15	2.28	1 (7%)	14,17,17	0.84	1 (7%)
9	LDA	H	903	-	13,15,15	2.32	1 (7%)	14,17,17	0.53	0
9	LDA	H	904	-	13,15,15	2.41	2 (15%)	14,17,17	0.65	0
5	BCL	L	312	1	55,74,74	1.34	2 (3%)	65,115,115	1.20	6 (9%)
5	BCL	L	314	1	55,74,74	1.29	2 (3%)	65,115,115	1.65	15 (23%)
6	BPH	L	402	-	65,70,70	0.79	1 (1%)	75,101,101	1.41	10 (13%)
7	U10	L	502	-	48,48,63	1.29	7 (14%)	58,61,79	1.79	13 (22%)
4	PO4	L	701	-	4,4,4	0.83	0	6,6,6	0.60	0
4	PO4	L	702	-	4,4,4	4.24	2 (50%)	6,6,6	1.09	0
8	HTO	L	705	-	9,9,9	0.61	0	9,10,10	0.72	0
10	GOL	L	707	-	5,5,5	0.68	0	5,5,5	0.96	0
10	GOL	L	708	-	5,5,5	0.53	0	5,5,5	0.32	0
9	LDA	L	905	-	13,15,15	2.28	1 (7%)	14,17,17	0.63	0
9	LDA	L	906	-	13,15,15	1.97	1 (7%)	14,17,17	0.67	0
9	LDA	L	908	-	13,15,15	2.23	1 (7%)	14,17,17	0.57	0
9	LDA	L	909	-	13,15,15	2.29	1 (7%)	14,17,17	0.95	1 (7%)
5	BCL	M	311	2	55,74,74	1.34	3 (5%)	65,115,115	1.82	19 (29%)
5	BCL	M	313	2	55,74,74	1.36	4 (7%)	65,115,115	1.44	11 (16%)
6	BPH	M	401	-	65,70,70	1.01	4 (6%)	75,101,101	1.88	20 (26%)
7	U10	M	501	-	48,48,63	1.05	2 (4%)	58,61,79	1.73	13 (22%)
4	PO4	M	703	-	4,4,4	0.72	0	6,6,6	0.41	0
4	PO4	M	704	-	4,4,4	2.12	1 (25%)	6,6,6	1.01	0
12	CDL	M	800	-	80,80,99	1.28	4 (5%)	82,92,111	1.46	10 (12%)
13	PC9	M	801	-	53,53,53	1.11	6 (11%)	58,63,63	1.57	9 (15%)
13	PC9	M	802	-	53,53,53	1.01	4 (7%)	58,63,63	1.49	6 (10%)
9	LDA	M	907	-	13,15,15	2.16	1 (7%)	14,17,17	1.08	2 (14%)
9	LDA	M	920	-	13,15,15	2.03	1 (7%)	14,17,17	0.99	1 (7%)

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
10	GOL	H	706	-	-	0/4/4/4	0/0/0/0
10	GOL	H	709	-	-	0/4/4/4	0/0/0/0
9	LDA	H	901	-	-	0/13/13/13	0/0/0/0
9	LDA	H	902	-	-	0/13/13/13	0/0/0/0
9	LDA	H	903	-	-	0/13/13/13	0/0/0/0
9	LDA	H	904	-	-	0/13/13/13	0/0/0/0
5	BCL	L	312	1	-	0/37/137/137	0/0/9/9
5	BCL	L	314	1	-	0/37/137/137	0/0/9/9
6	BPH	L	402	-	-	0/54/105/105	0/1/6/6
7	U10	L	502	-	-	0/45/69/87	0/1/1/1
4	PO4	L	701	-	-	0/0/0/0	0/0/0/0
4	PO4	L	702	-	-	0/0/0/0	0/0/0/0
8	HTO	L	705	-	-	0/10/10/10	0/0/0/0
10	GOL	L	707	-	-	0/4/4/4	0/0/0/0
10	GOL	L	708	-	-	0/4/4/4	0/0/0/0
9	LDA	L	905	-	-	0/13/13/13	0/0/0/0
9	LDA	L	906	-	-	0/13/13/13	0/0/0/0
9	LDA	L	908	-	-	0/13/13/13	0/0/0/0
9	LDA	L	909	-	-	0/13/13/13	0/0/0/0
5	BCL	M	311	2	-	0/37/137/137	0/0/9/9
5	BCL	M	313	2	-	0/37/137/137	0/0/9/9
6	BPH	M	401	-	-	0/54/105/105	0/1/6/6
7	U10	M	501	-	-	0/45/69/87	0/1/1/1
4	PO4	M	703	-	-	0/0/0/0	0/0/0/0
4	PO4	M	704	-	-	0/0/0/0	0/0/0/0
12	CDL	M	800	-	-	0/91/91/110	0/0/0/0
13	PC9	M	801	-	-	0/60/60/60	0/0/0/0
13	PC9	M	802	-	-	0/60/60/60	0/0/0/0
9	LDA	M	907	-	-	0/13/13/13	0/0/0/0
9	LDA	M	920	-	-	0/13/13/13	0/0/0/0

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	H	904	LDA	O1-N1	-8.28	1.25	1.42
9	H	903	LDA	O1-N1	-8.22	1.26	1.42
9	H	901	LDA	O1-N1	-8.05	1.26	1.42
9	L	909	LDA	O1-N1	-7.97	1.26	1.42
9	L	905	LDA	O1-N1	-7.95	1.26	1.42
9	H	902	LDA	O1-N1	-7.94	1.26	1.42
9	L	908	LDA	O1-N1	-7.79	1.26	1.42
9	M	907	LDA	O1-N1	-7.42	1.27	1.42
9	M	920	LDA	O1-N1	-7.04	1.28	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	906	LDA	O1-N1	-6.79	1.28	1.42
5	M	313	BCL	C3C-C4C	-3.27	1.47	1.51
6	M	401	BPH	OBD-CAD	-2.97	1.18	1.22
13	M	802	PC9	O2-C2	-2.73	1.39	1.46
13	M	801	PC9	BR1-C36	-2.51	1.91	1.97
9	H	904	LDA	C1-N1	-2.28	1.46	1.51
5	M	313	BCL	CBA-CGA	-2.22	1.44	1.50
7	L	502	U10	C3-C2	-2.18	1.42	1.48
6	M	401	BPH	C3D-CAD	-2.06	1.42	1.47
7	L	502	U10	C13-C14	2.06	1.38	1.33
7	L	502	U10	C38-C39	2.11	1.38	1.32
13	M	801	PC9	O2-C2	2.12	1.52	1.46
13	M	801	PC9	C32-C31	2.12	1.56	1.50
6	L	402	BPH	C4-C3	2.21	1.56	1.50
6	M	401	BPH	C5-C3	2.22	1.56	1.51
7	L	502	U10	C26-C24	2.26	1.56	1.51
5	M	311	BCL	OBD-CAD	2.27	1.25	1.22
13	M	802	PC9	O3-C11	2.30	1.40	1.33
13	M	801	PC9	O3-C3	2.50	1.50	1.45
7	L	502	U10	C28-C29	2.52	1.39	1.33
6	M	401	BPH	CHC-C1C	2.54	1.41	1.36
13	M	802	PC9	O3-C3	2.75	1.51	1.45
4	L	702	PO4	P-O2	2.78	1.64	1.54
13	M	802	PC9	P-O1P	2.81	1.61	1.50
7	M	501	U10	O4-C4	2.99	1.44	1.36
13	M	801	PC9	C1-C2	3.08	1.59	1.50
13	M	801	PC9	P-O1P	3.14	1.62	1.50
7	M	501	U10	O3-C3	3.40	1.45	1.36
7	L	502	U10	O4-C4	3.81	1.46	1.36
4	M	704	PO4	P-O1	4.13	1.59	1.50
12	M	800	CDL	OB8-CB7	4.23	1.45	1.33
5	M	313	BCL	CHC-C1C	4.29	1.39	1.33
7	L	502	U10	O3-C3	4.35	1.47	1.36
12	M	800	CDL	OA6-CA5	4.60	1.47	1.34
5	M	311	BCL	CHB-C4A	4.68	1.39	1.33
5	L	314	BCL	CHB-C4A	5.24	1.40	1.33
12	M	800	CDL	OB6-CB5	5.35	1.49	1.34
12	M	800	CDL	OA8-CA7	5.48	1.49	1.33
5	L	312	BCL	CHB-C4A	5.57	1.40	1.33
5	L	314	BCL	CHC-C1C	5.76	1.40	1.33
5	L	312	BCL	CHC-C1C	5.82	1.40	1.33
5	M	313	BCL	CHB-C4A	6.27	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	311	BCL	CHC-C1C	6.28	1.41	1.33
4	L	702	PO4	P-O1	7.80	1.67	1.50

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	401	BPH	C4D-C3D-CAD	-5.96	104.37	107.78
6	L	402	BPH	C1-C2-C3	-4.82	117.07	125.96
6	M	401	BPH	OBD-CAD-CBD	-4.53	119.09	125.94
5	M	311	BCL	CMB-C2B-C1B	-4.22	121.98	128.46
5	L	314	BCL	CAA-C2A-C3A	-4.16	101.40	112.81
7	M	501	U10	C17-C18-C19	-4.15	117.25	127.68
7	L	502	U10	C7-C8-C9	-4.12	119.81	126.71
5	L	314	BCL	CMB-C2B-C1B	-4.03	122.27	128.46
6	M	401	BPH	C1-C2-C3	-4.02	118.56	125.96
7	M	501	U10	C32-C33-C34	-3.92	117.82	127.68
5	M	313	BCL	CAC-C3C-C2C	-3.83	104.61	114.24
13	M	802	PC9	C3-C2-C1	-3.75	103.39	111.86
13	M	801	PC9	C2-O2-C31	-3.73	109.06	117.88
7	L	502	U10	C12-C13-C14	-3.63	118.56	127.68
6	M	401	BPH	C1C-NC-C4C	-3.59	107.31	110.54
5	L	314	BCL	CAC-C3C-C2C	-3.55	105.33	114.24
12	M	800	CDL	CA4-OA6-CA5	-3.45	109.73	117.88
7	L	502	U10	O2-C2-C3	-3.42	113.67	120.95
7	L	502	U10	C25-C24-C23	-3.39	114.65	123.69
7	M	501	U10	C11-C9-C8	-3.38	114.19	121.10
7	M	501	U10	C26-C27-C28	-3.37	100.39	111.97
5	M	311	BCL	OBD-CAD-CBD	-3.31	120.95	125.94
5	M	313	BCL	CMB-C2B-C1B	-3.24	123.48	128.46
5	M	313	BCL	OBD-CAD-CBD	-3.24	121.05	125.94
5	M	313	BCL	CHA-C1A-NA	-3.20	118.74	126.18
12	M	800	CDL	OA6-CA5-OA7	-3.07	116.03	123.68
7	M	501	U10	C31-C29-C28	-3.03	114.90	121.10
5	M	311	BCL	C6-C5-C3	-3.02	105.81	112.66
6	M	401	BPH	CAA-C2A-C3A	-2.99	104.62	112.81
9	M	907	LDA	CM2-N1-CM1	-2.97	105.30	110.99
7	M	501	U10	C7-C6-C5	-2.97	114.67	118.47
5	L	312	BCL	CAA-C2A-C3A	-2.97	104.67	112.81
13	M	802	PC9	O2-C2-C3	-2.94	97.75	108.44
13	M	801	PC9	BR2-C37-C38	-2.90	103.99	108.92
9	L	909	LDA	CM2-N1-CM1	-2.86	105.52	110.99
5	M	313	BCL	C1-C2-C3	-2.85	120.71	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	402	BPH	O2D-CGD-O1D	-2.75	118.29	123.82
7	L	502	U10	C6-C1-C2	-2.75	117.42	120.29
5	L	314	BCL	C5-C3-C2	-2.74	115.48	121.10
7	M	501	U10	C26-C24-C23	-2.72	115.55	121.10
7	M	501	U10	C16-C14-C13	-2.71	115.56	121.10
6	M	401	BPH	C4-C3-C2	-2.62	116.71	123.69
5	L	312	BCL	CAA-C2A-C1A	-2.60	103.45	111.97
5	M	311	BCL	CAA-C2A-C3A	-2.58	105.73	112.81
6	L	402	BPH	CAA-C2A-C1A	-2.53	105.74	112.28
12	M	800	CDL	OB8-CB7-OB9	-2.53	117.27	123.55
5	M	311	BCL	C4-C3-C5	-2.53	110.90	115.29
13	M	801	PC9	O2-C31-O31	-2.51	117.42	123.68
9	H	902	LDA	CM2-N1-CM1	-2.44	106.31	110.99
5	L	314	BCL	CAC-C3C-C4C	-2.44	107.18	112.58
6	M	401	BPH	CMA-C3A-C4A	-2.42	105.10	112.37
5	L	314	BCL	O1D-CGD-CBD	-2.41	120.27	124.60
5	M	311	BCL	CHA-C1A-NA	-2.41	120.59	126.18
13	M	802	PC9	BR2-C37-C36	-2.39	105.60	110.28
6	M	401	BPH	O2D-CGD-O1D	-2.36	119.07	123.82
6	L	402	BPH	CAA-C2A-C3A	-2.34	106.38	112.81
6	M	401	BPH	C4B-C3B-CAB	-2.32	121.54	130.09
13	M	801	PC9	C13-C12-C11	-2.32	105.13	113.58
7	L	502	U10	C12-C11-C9	-2.29	105.17	112.93
5	L	312	BCL	CHA-C1A-NA	-2.28	120.88	126.18
5	L	312	BCL	OBD-CAD-CBD	-2.26	122.53	125.94
5	M	313	BCL	CMC-C2C-C3C	-2.24	104.67	113.77
7	L	502	U10	C22-C23-C24	-2.24	122.05	127.68
12	M	800	CDL	OA8-CA7-OA9	-2.24	118.00	123.55
5	M	311	BCL	OBB-CAB-CBB	-2.23	115.08	120.16
13	M	801	PC9	BR1-C36-C37	-2.22	105.93	110.28
6	L	402	BPH	OBD-CAD-CBD	-2.21	122.60	125.94
5	M	313	BCL	O2D-CGD-O1D	-2.13	119.53	123.82
7	L	502	U10	O5-C5-C6	-2.12	117.92	121.82
5	M	311	BCL	C1B-CHB-C4A	-2.11	125.93	130.12
5	M	311	BCL	CMA-C3A-C4A	-2.11	106.09	111.77
5	L	314	BCL	OBB-CAB-CBB	-2.11	115.35	120.16
5	L	314	BCL	CHA-C1A-NA	-2.10	121.29	126.18
5	M	313	BCL	OBB-CAB-CBB	-2.10	115.38	120.16
7	L	502	U10	C35-C34-C33	-2.05	118.21	123.69
5	M	311	BCL	CMA-C3A-C2A	-2.04	105.49	113.77
7	M	501	U10	C22-C23-C24	-2.04	122.56	127.68
6	M	401	BPH	CMA-C3A-C2A	-2.03	105.52	113.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	311	BCL	C6-C7-C8	2.01	122.32	115.73
5	M	313	BCL	O1D-CGD-CBD	2.01	128.21	124.60
6	L	402	BPH	C1B-NB-C4B	2.05	110.58	106.52
6	M	401	BPH	CMD-C2D-C3D	2.07	128.73	124.89
5	L	314	BCL	OBB-CAB-C3B	2.13	124.00	119.95
6	M	401	BPH	CAA-CBA-CGA	2.14	119.80	113.35
9	M	907	LDA	O1-N1-C1	2.17	114.60	109.27
13	M	801	PC9	BR2-C37-C36	2.21	114.61	110.28
5	L	312	BCL	C4-C3-C5	2.23	119.16	115.29
7	M	501	U10	C10-C9-C11	2.24	119.17	115.29
5	L	314	BCL	C4-C3-C5	2.26	119.21	115.29
5	M	311	BCL	C2C-C3C-C4C	2.27	104.74	101.34
12	M	800	CDL	OB6-CB4-CB6	2.31	116.82	108.44
6	L	402	BPH	CAC-C3C-C4C	2.32	118.63	112.67
5	L	314	BCL	C2C-C3C-C4C	2.34	104.84	101.34
6	M	401	BPH	C5-C3-C2	2.34	125.89	121.10
7	M	501	U10	C35-C34-C36	2.34	119.35	115.29
6	L	402	BPH	C3A-C2A-C1A	2.36	104.47	101.68
9	M	920	LDA	O1-N1-C1	2.39	115.13	109.27
7	L	502	U10	O4-C4-C5	2.43	124.14	116.60
5	M	311	BCL	C1-C2-C3	2.57	130.69	125.96
5	M	313	BCL	C2A-C1A-CHA	2.59	128.50	123.92
5	M	311	BCL	OBB-CAB-C3B	2.63	124.96	119.95
5	L	314	BCL	CBC-CAC-C3C	2.63	119.47	113.51
6	M	401	BPH	C2C-C3C-C4C	2.71	105.40	101.34
5	L	314	BCL	CMB-C2B-C3B	2.73	129.96	124.89
5	L	312	BCL	C1-O2A-CGA	2.74	123.34	116.77
12	M	800	CDL	OB8-CB6-CB4	2.77	115.62	108.66
5	L	314	BCL	CAA-CBA-CGA	2.81	121.82	113.35
13	M	802	PC9	O3-C3-C2	2.83	115.78	108.66
5	M	311	BCL	CMB-C2B-C3B	2.85	130.18	124.89
5	M	311	BCL	OBD-CAD-C3D	2.87	133.31	128.03
6	M	401	BPH	C7-C6-C5	2.91	121.21	113.11
7	L	502	U10	C36-C34-C33	2.92	127.08	121.10
7	L	502	U10	C3M-O3-C3	3.04	127.32	116.44
7	M	501	U10	C15-C14-C16	3.10	120.67	115.29
5	L	314	BCL	O2D-CGD-CBD	3.19	117.00	111.30
6	L	402	BPH	C3C-C4C-NC	3.22	111.00	107.97
6	M	401	BPH	C3C-C4C-NC	3.29	111.07	107.97
6	L	402	BPH	O2D-CGD-CBD	3.41	117.39	111.30
5	M	311	BCL	O2D-CGD-CBD	3.43	117.43	111.30
6	M	401	BPH	CMC-C2C-C1C	3.44	121.70	112.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	802	PC9	O3-C11-C12	3.46	121.95	111.90
13	M	801	PC9	O3-C3-C2	3.56	117.60	108.66
5	M	313	BCL	CMD-C2D-C3D	3.61	131.60	124.89
6	M	401	BPH	C1-O2A-CGA	3.74	125.75	116.77
12	M	800	CDL	OA8-CA7-C31	3.93	123.34	111.90
6	M	401	BPH	CAC-C3C-C4C	3.96	122.85	112.67
13	M	801	PC9	O2-C2-C1	3.97	122.88	108.44
12	M	800	CDL	OA6-CA5-C11	4.18	120.24	111.55
12	M	800	CDL	OB8-CB7-C71	4.35	124.57	111.90
5	M	311	BCL	C5-C3-C2	4.57	130.46	121.10
6	M	401	BPH	O2D-CGD-CBD	4.66	119.62	111.30
7	M	501	U10	C30-C29-C31	4.80	123.63	115.29
13	M	801	PC9	O2-C31-C32	5.54	123.06	111.55
5	M	311	BCL	C1-O2A-CGA	5.66	130.35	116.77
7	L	502	U10	C25-C24-C26	5.86	125.46	115.29
12	M	800	CDL	OB6-CB5-C51	6.13	124.28	111.55
13	M	802	PC9	O2-C31-C32	6.18	124.38	111.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	H	902	LDA	1	0
9	H	903	LDA	6	0
9	H	904	LDA	2	0
5	L	312	BCL	3	0
5	L	314	BCL	3	0
6	L	402	BPH	3	0
7	L	502	U10	8	0
9	L	906	LDA	4	0
9	L	908	LDA	6	0
9	L	909	LDA	2	0
5	M	311	BCL	10	0
5	M	313	BCL	5	0
6	M	401	BPH	4	0
7	M	501	U10	1	0
4	M	703	PO4	2	0
12	M	800	CDL	3	0
13	M	801	PC9	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	802	PC9	9	0
9	M	920	LDA	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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%)	-0.45	9 (3%)	48	48	42, 51, 63, 72	0
2	M	302/307 (98%)	-0.15	12 (3%)	39	37	40, 51, 61, 88	1 (0%)
3	H	240/260 (92%)	-0.30	6 (2%)	58	58	39, 51, 59, 83	0
All	All	823/848 (97%)	-0.30	27 (3%)	47	46	39, 51, 62, 88	1 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	250	SER	4.7
1	L	271	TRP	4.2
2	M	1	ALA	3.8
1	L	270	PRO	3.6
2	M	2[A]	GLU	3.1
1	L	275	ILE	3.1
1	L	269	LEU	3.1
2	M	302	GLY	3.1
1	L	276[A]	PRO	2.8
1	L	59	TRP	2.7
1	L	281	GLY	2.7
2	M	301[A]	HIS	2.7
3	H	51	ALA	2.7
2	M	80	TRP	2.6
3	H	52	ASN	2.6
1	L	279	ILE	2.5
1	L	277	GLY	2.5
3	H	245	ALA	2.4
2	M	300[A]	ASN	2.4
2	M	27	ALA	2.4
2	M	3	TYR	2.3
3	H	220	LYS	2.3
3	H	159	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	M	26	LEU	2.2
2	M	244	ALA	2.1
2	M	265	ILE	2.1
2	M	106	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
9	LDA	M	920	16/16	0.66	0.70	23.67	49,53,65,66	16
9	LDA	L	906	16/16	0.72	0.45	20.73	51,55,69,70	16
8	HTO	L	705	10/10	0.88	0.41	19.96	56,60,62,65	10
9	LDA	L	905	16/16	0.26	1.20	18.71	61,66,70,71	16
10	GOL	L	708	6/6	0.95	0.27	11.26	49,57,59,60	0
13	PC9	M	802	54/54	0.66	0.52	6.79	42,54,70,73	54
7	U10	L	502	48/63	0.73	0.45	5.63	37,56,66,67	48
9	LDA	L	909	16/16	0.50	0.45	5.18	50,54,71,73	16
12	CDL	M	800	81/100	0.74	0.38	4.99	50,69,80,87	81
13	PC9	M	801	54/54	0.71	0.48	4.75	30,52,79,80	54
10	GOL	H	706	6/6	0.95	0.45	4.55	59,62,63,65	6
9	LDA	H	903	16/16	0.54	0.47	3.91	49,55,63,63	16
4	PO4	L	701	5/5	0.88	0.32	3.21	65,65,66,67	5
9	LDA	M	907	16/16	0.82	0.30	2.96	60,64,70,71	16
10	GOL	L	707	6/6	0.85	0.28	2.24	58,61,62,66	6
5	BCL	M	311	66/66	0.96	0.21	1.51	41,51,103,104	0
6	BPH	M	401	65/65	0.90	0.20	1.14	44,52,96,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	LDA	L	908	16/16	0.75	0.44	1.05	51,59,72,73	16
7	U10	M	501	48/63	0.91	0.22	0.68	46,54,80,83	0
6	BPH	L	402	65/65	0.97	0.12	0.21	42,49,55,56	0
5	BCL	L	312	66/66	0.97	0.12	0.12	40,48,55,59	0
14	K	H	700	1/1	0.98	0.13	-0.07	52,52,52,52	0
5	BCL	M	313	66/66	0.97	0.14	-0.18	41,48,72,80	0
5	BCL	L	314	66/66	0.97	0.11	-0.33	38,46,66,73	0
4	PO4	L	702	5/5	0.93	0.16	-0.85	64,65,66,68	5
4	PO4	M	704	5/5	0.96	0.19	-0.87	54,54,56,58	5
11	FE	M	500	1/1	1.00	0.14	-1.57	52,52,52,52	0
9	LDA	H	904	16/16	0.80	0.44	-	60,62,66,66	16
10	GOL	H	709	6/6	0.70	0.24	-	50,51,52,53	6
9	LDA	H	901	16/16	0.56	0.49	-	52,55,66,66	16
9	LDA	H	902	16/16	0.56	0.59	-	64,66,72,72	16
4	PO4	M	703	5/5	0.75	0.38	-	64,65,66,67	5

6.5 Other polymers [i](#)

There are no such residues in this entry.