



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 03:37 pm GMT

PDB ID : 3V3Y
Title : Photosynthetic Reaction Center From Rhodobacter Sphaeroides strain RV
Authors : Gabdulkhakov, A.G.; Fufina, T.Y.; Vasilieva, L.G.; Shuvalov, V.A.
Deposited on : 2011-12-14
Resolution : 2.80 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

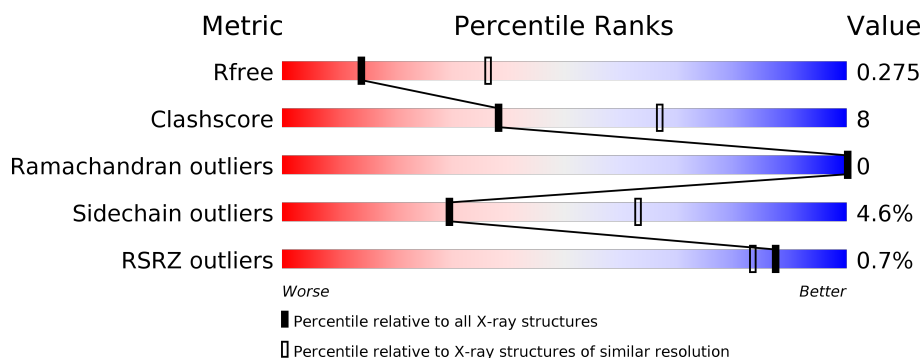
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	111664	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (2.80-2.80)

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	H	241	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>18%</div> </div> </div>
2	L	281	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>21%</div> <div>.</div> </div> </div>
3	M	302	<div> <div></div> <div> <div></div> <div>82%</div> <div>16%</div> <div>.</div> </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
6	BPH	L	402	X	-	-	-
6	BPH	M	401	X	-	-	-
7	U10	L	502	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 7270 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 H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	241	Total	C	N	O	S	0	0	0
			1840	1178	315	338	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	0	0
			2233	1508	355	362	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	178	THR	SER	SEE REMARK 999	UNP P0C0Y8

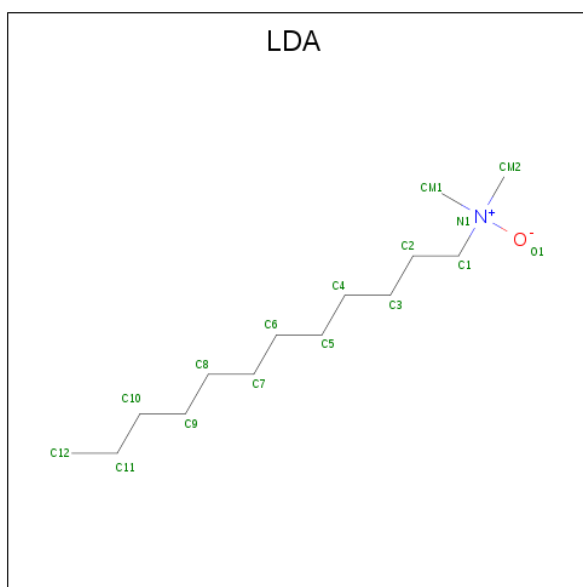
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	0	0
			2409	1608	394	397	10			

There is a discrepancy between the modelled and reference sequences:

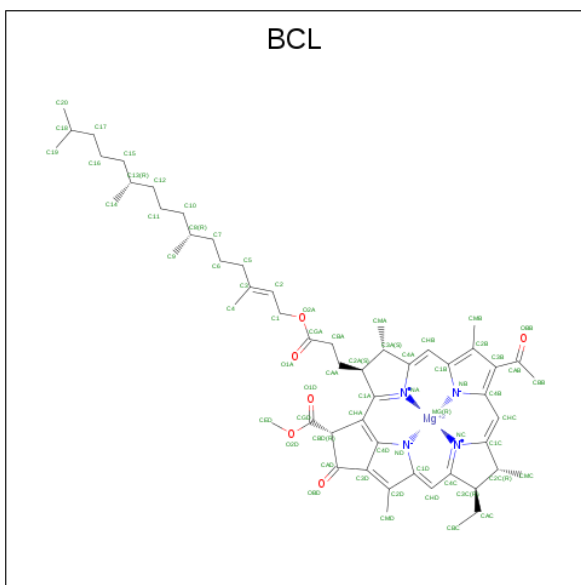
Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	SEE REMARK 999	UNP P0C0Y9

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).



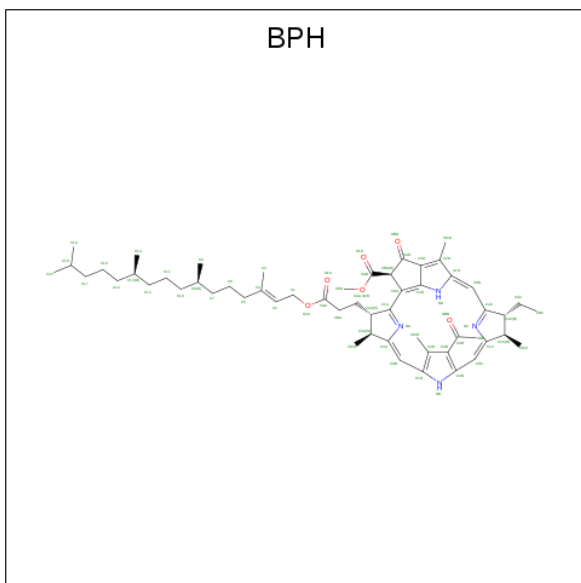
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



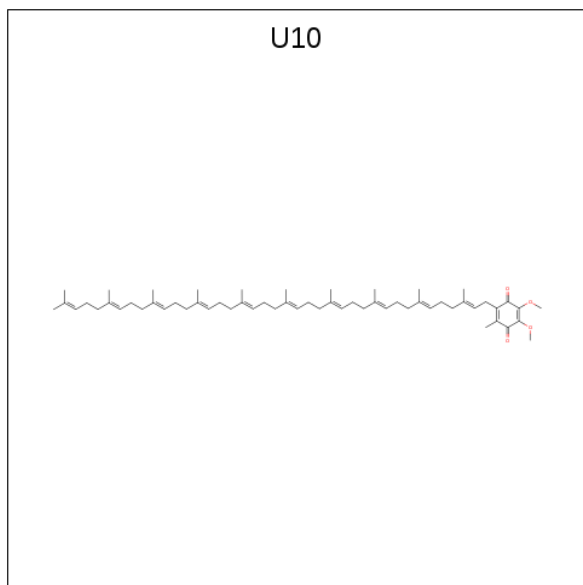
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $\text{C}_{55}\text{H}_{76}\text{N}_4\text{O}_6$).



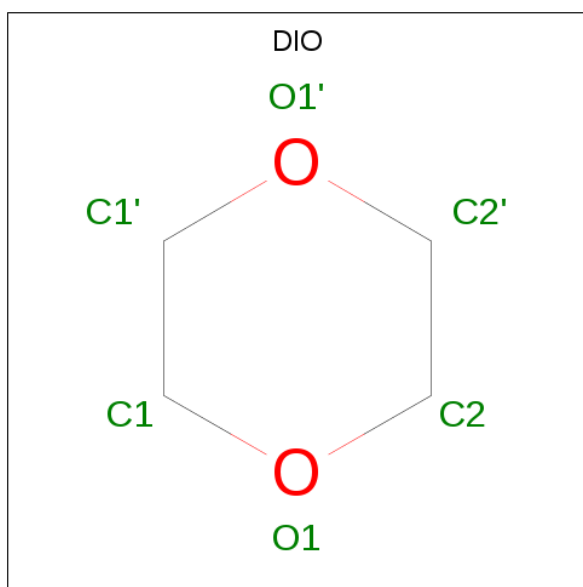
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			65	55	4	6		
6	M	1	Total	C	N	O	0	0
			65	55	4	6		

- 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 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).

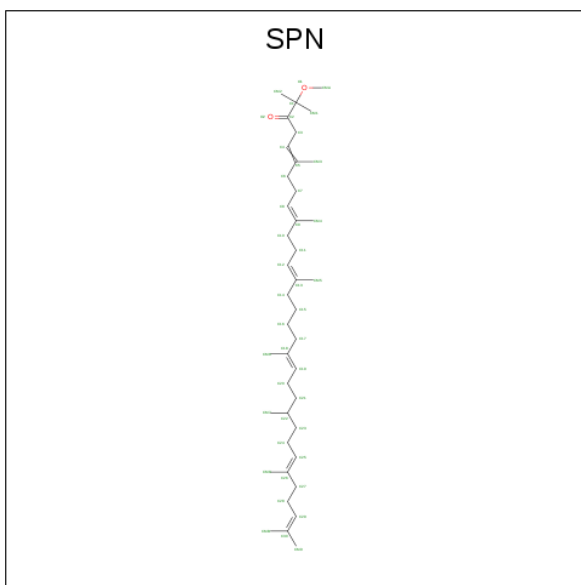


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			6	4	2		
8	L	1	Total	C	O	0	0
			6	4	2		
8	M	1	Total	C	O	0	0
			6	4	2		

- Molecule 9 is FE (III) ION (three-letter code: FE) (formula: Fe).

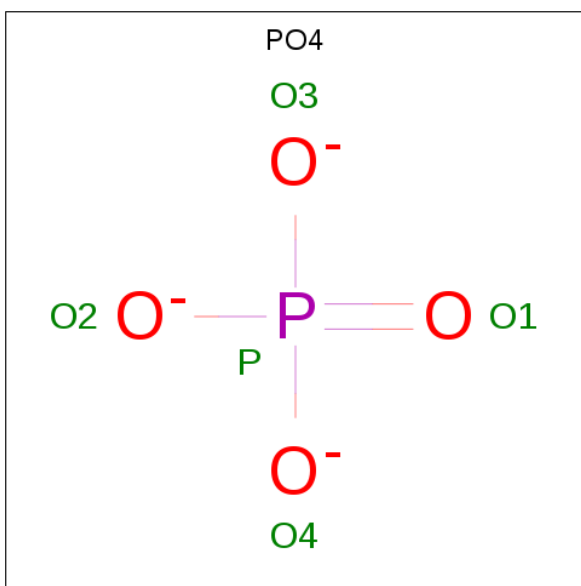
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	1	Total	Fe	0	0
			1	1		

- Molecule 10 is SPEROIDENONE (three-letter code: SPN) (formula: C₄₁H₇₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	C	O	0	0
			43	41	2		

- Molecule 11 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

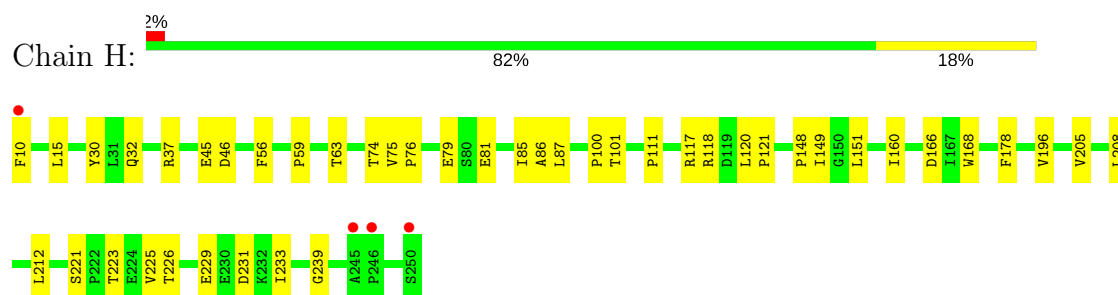
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	H	40	Total	O	0	0
			40	40		
13	L	21	Total	O	0	0
			21	21		
13	M	31	Total	O	0	0
			31	31		

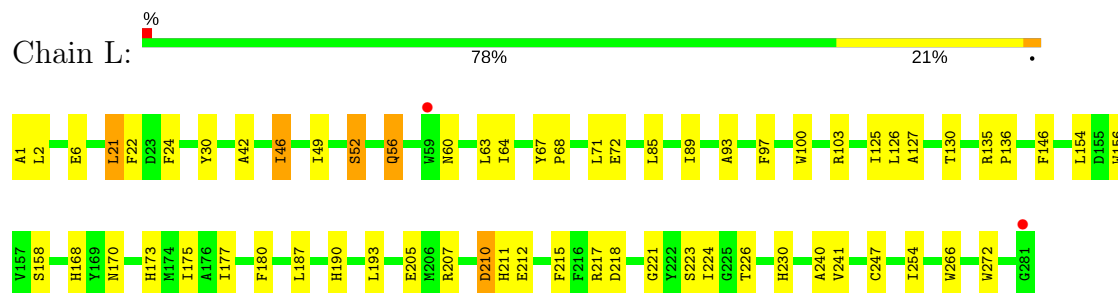
3 Residue-property plots [i](#)

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.

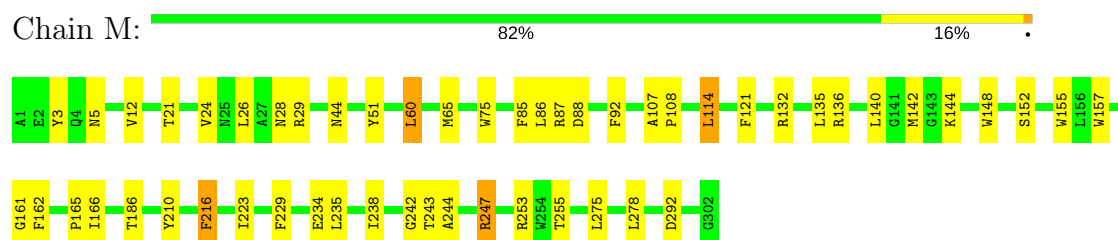
• Molecule 1: Reaction center protein H chain



• Molecule 2: Reaction center protein L chain



• Molecule 3: Reaction center protein M chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.75Å 139.75Å 185.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.94 – 2.80 26.60 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.94-2.80) 99.2 (26.60-2.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.244 , 0.284 0.239 , 0.275	Depositor DCC
R_{free} test set	2645 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7270	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, LDA, DIO, CL, BPH, PO4, FE, SPN, U10

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	H	0.48	0/1889	0.67	0/2569
2	L	0.47	0/2321	0.61	0/3177
3	M	0.48	0/2501	0.60	0/3415
All	All	0.48	0/6711	0.62	0/9161

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	H	1840	0	1845	24	0
2	L	2233	0	2189	40	0
3	M	2409	0	2323	40	0
4	H	48	0	93	5	0
4	M	80	0	155	3	0
5	L	66	0	74	4	0
5	M	198	0	222	13	0
6	L	65	0	76	6	0
6	M	65	0	76	5	0
7	L	48	0	63	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	48	0	63	1	0
8	L	12	0	16	2	0
8	M	6	0	8	0	0
9	M	1	0	0	0	0
10	M	43	0	70	6	0
11	M	15	0	0	0	0
12	M	1	0	0	0	0
13	H	40	0	0	0	0
13	L	21	0	0	0	0
13	M	31	0	0	1	0
All	All	7270	0	7273	119	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 (119) 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)
5:M:303:BCL:H62	5:M:304:BCL:H202	1.62	0.82
1:H:81:GLU:HG3	1:H:85:ILE:HD11	1.66	0.78
1:H:63:THR:HG1	1:H:74:THR:HG1	1.33	0.77
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.72	0.72
2:L:30:TYR:O	2:L:103:ARG:NH2	2.26	0.69
6:L:402:BPH:HHB3	6:L:402:BPH:HBB3	1.76	0.68
6:L:402:BPH:HBB2	3:M:210:TYR:HB3	1.78	0.65
2:L:190:HIS:HD1	7:L:502:U10:H4M1	1.61	0.65
4:H:702:LDA:HM22	3:M:253:ARG:HH22	1.62	0.64
1:H:111:PRO:O	3:M:247:ARG:NH2	2.31	0.64
3:M:234:GLU:O	3:M:238:ILE:HG13	1.99	0.63
1:H:30:TYR:CZ	4:H:704:LDA:H12	2.34	0.62
1:H:111:PRO:HB2	1:H:239:GLY:HA2	1.82	0.61
3:M:136:ARG:NH2	13:M:336:HOH:O	2.33	0.61
2:L:49:ILE:HG12	2:L:89:ILE:HD13	1.83	0.60
5:M:304:BCL:H192	6:M:401:BPH:H7C2	1.84	0.60
2:L:71:LEU:H	2:L:71:LEU:HD12	1.69	0.58
1:H:120:LEU:N	1:H:226:THR:HB	2.19	0.57
3:M:161:GLY:HA3	10:M:600:SPN:H201	1.86	0.57
2:L:266:TRP:CG	8:L:900:DIO:H21	2.42	0.55
1:H:120:LEU:H	1:H:226:THR:HB	1.72	0.55
2:L:60:ASN:O	2:L:64:ILE:HG13	2.07	0.55
5:L:302:BCL:HBB2	5:M:304:BCL:NA	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:401:BPH:HHC	6:M:401:BPH:HBB3	1.88	0.55
5:L:302:BCL:NA	5:M:304:BCL:HBB2	2.23	0.53
3:M:157:TRP:CD1	10:M:600:SPN:H202	2.43	0.53
2:L:97:PHE:HB3	2:L:125:ILE:HG12	1.90	0.53
6:L:402:BPH:HHC	6:L:402:BPH:CBB	2.39	0.53
3:M:243:THR:O	3:M:247:ARG:HG2	2.09	0.53
1:H:196:VAL:HG12	1:H:205:VAL:HG22	1.91	0.52
2:L:210:ASP:OD1	2:L:210:ASP:N	2.43	0.52
1:H:117:ARG:HD2	3:M:242:GLY:HA2	1.92	0.52
3:M:275:LEU:HD23	3:M:278:LEU:HD23	1.93	0.51
2:L:266:TRP:CD2	8:L:900:DIO:H21	2.47	0.50
2:L:180:PHE:CE2	2:L:240:ALA:HB1	2.47	0.49
5:M:305:BCL:HMB1	5:M:305:BCL:HBB2	1.95	0.48
2:L:127:ALA:O	2:L:130:THR:HB	2.12	0.48
7:L:502:U10:H122	7:L:502:U10:H101	1.52	0.48
3:M:28:ASN:HB2	3:M:51:TYR:CE2	2.49	0.48
5:M:303:BCL:H111	5:M:303:BCL:H142	1.69	0.48
1:H:149:ILE:HD13	1:H:166:ASP:HA	1.95	0.48
2:L:187:LEU:HD13	3:M:216:PHE:CG	2.49	0.48
2:L:193:LEU:HG	2:L:212:GLU:HG2	1.96	0.48
3:M:21:THR:HG23	3:M:26:LEU:HD21	1.95	0.47
1:H:86:ALA:HB1	1:H:101:THR:OG1	2.13	0.47
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.97	0.47
2:L:224:ILE:HG22	7:L:502:U10:C2	2.44	0.47
5:M:303:BCL:C4B	10:M:600:SPN:H152	2.45	0.47
1:H:87:LEU:HD23	1:H:100:PRO:HA	1.96	0.47
1:H:37:ARG:HB3	1:H:75:VAL:HB	1.97	0.46
2:L:175:ILE:HG12	7:L:502:U10:H261	1.97	0.46
2:L:103:ARG:NH1	3:M:255:THR:O	2.42	0.46
5:M:303:BCL:CAB	10:M:600:SPN:H162	2.46	0.46
4:M:703:LDA:H11	4:M:703:LDA:H41	1.60	0.46
2:L:170:ASN:O	2:L:173:HIS:HB3	2.15	0.46
2:L:1:ALA:C	2:L:2:LEU:HD23	2.37	0.45
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.98	0.45
5:M:303:BCL:H2	6:M:401:BPH:CMB	2.46	0.45
3:M:60:LEU:HA	6:M:401:BPH:H4C2	1.98	0.45
3:M:85:PHE:HD2	3:M:86:LEU:HD12	1.81	0.45
1:H:121:PRO:HB3	1:H:225:VAL:O	2.17	0.45
2:L:180:PHE:CD2	2:L:240:ALA:HB1	2.52	0.44
5:L:302:BCL:CGA	5:M:305:BCL:HBC1	2.48	0.44
1:H:81:GLU:HG3	1:H:85:ILE:CD1	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:107:ALA:HA	3:M:108:PRO:HD3	1.86	0.44
3:M:75:TRP:HE1	10:M:600:SPN:HMA2	1.82	0.44
2:L:205:GLU:O	2:L:207:ARG:NH1	2.51	0.43
2:L:215:PHE:HB2	3:M:142:MET:HE1	2.00	0.43
2:L:217:ARG:O	2:L:221:GLY:HA2	2.18	0.43
3:M:114:LEU:HD13	3:M:114:LEU:HA	1.80	0.43
3:M:162:PHE:O	3:M:166:ILE:HG12	2.18	0.43
2:L:223:SER:O	3:M:44:ASN:ND2	2.48	0.43
3:M:223:ILE:HD13	3:M:223:ILE:HA	1.87	0.43
1:H:32:GLN:HG2	1:H:56:PHE:CE2	2.53	0.43
7:L:502:U10:H72	7:L:502:U10:H1M1	1.81	0.43
3:M:65:MET:HB3	3:M:121:PHE:CD2	2.54	0.43
3:M:235:LEU:HD23	3:M:235:LEU:HA	1.75	0.43
1:H:59:PRO:HG2	1:H:76:PRO:HD3	2.00	0.43
4:H:704:LDA:HM11	4:H:704:LDA:H22	1.79	0.43
2:L:218:ASP:OD1	3:M:29:ARG:HD3	2.19	0.43
2:L:93:ALA:HB2	6:L:402:BPH:H122	2.01	0.43
3:M:3:TYR:CZ	3:M:5:ASN:HA	2.53	0.43
5:M:304:BCL:HHC	5:M:304:BCL:OBB	2.19	0.43
2:L:146:PHE:HB3	2:L:156:TRP:CD2	2.54	0.42
2:L:230:HIS:CD2	3:M:223:ILE:HG13	2.55	0.42
1:H:168:TRP:HB2	1:H:178:PHE:HB2	2.01	0.42
1:H:229:GLU:O	1:H:233:ILE:HG13	2.20	0.42
1:H:118:ARG:HD3	1:H:120:LEU:HD12	2.02	0.42
2:L:22:PHE:HA	2:L:24:PHE:CE2	2.55	0.42
2:L:42:ALA:O	2:L:46:ILE:HB	2.19	0.42
5:M:303:BCL:HHC	5:M:303:BCL:OBB	2.19	0.42
4:M:705:LDA:HM13	4:M:705:LDA:H21	1.73	0.42
1:H:212:LEU:HD23	1:H:212:LEU:HA	1.87	0.42
2:L:100:TRP:CH2	7:M:501:U10:H261	2.54	0.42
3:M:135:LEU:HD23	3:M:135:LEU:HA	1.92	0.42
2:L:52:SER:O	2:L:56:GLN:HB2	2.20	0.42
5:M:303:BCL:H102	5:M:303:BCL:H61	1.93	0.41
3:M:24:VAL:HG11	3:M:29:ARG:NH1	2.36	0.41
3:M:157:TRP:CE2	10:M:600:SPN:HM73	2.55	0.41
4:H:702:LDA:H121	4:M:701:LDA:H91	2.02	0.41
2:L:67:TYR:HA	2:L:68:PRO:HD3	1.93	0.41
6:M:401:BPH:HBA2	6:M:401:BPH:H3A	1.82	0.41
3:M:140:LEU:HA	3:M:140:LEU:HD23	1.95	0.41
2:L:272:TRP:CG	3:M:87:ARG:HB2	2.56	0.41
1:H:208:LEU:HA	1:H:208:LEU:HD23	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:702:LDA:HM22	3:M:253:ARG:NH2	2.31	0.41
2:L:2:LEU:HB3	2:L:6:GLU:HB3	2.02	0.41
5:L:302:BCL:HBB3	5:L:302:BCL:HMB1	2.03	0.41
3:M:152:SER:O	3:M:155:TRP:HB3	2.21	0.41
2:L:207:ARG:HG3	2:L:211:HIS:CD2	2.57	0.40
2:L:168:HIS:HE1	3:M:186:THR:HB	1.87	0.40
2:L:173:HIS:O	2:L:177:ILE:HG13	2.21	0.40
3:M:162:PHE:C	3:M:165:PRO:HD2	2.42	0.40
3:M:88:ASP:HB2	3:M:92:PHE:CZ	2.56	0.40
2:L:21:LEU:HA	2:L:21:LEU:HD13	1.86	0.40
2:L:241:VAL:HG21	6:L:402:BPH:H2C	2.04	0.40
6:L:402:BPH:H112	6:L:402:BPH:H7C2	1.65	0.40
3:M:132:ARG:O	3:M:136:ARG:HG2	2.20	0.40
1:H:160:ILE:HD13	1:H:160:ILE:HA	1.88	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	H	239/241 (99%)	232 (97%)	7 (3%)	0	100	100
2	L	279/281 (99%)	271 (97%)	8 (3%)	0	100	100
3	M	300/302 (99%)	282 (94%)	18 (6%)	0	100	100
All	All	818/824 (99%)	785 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	H	196/196 (100%)	188 (96%)	8 (4%)	33	67
2	L	220/220 (100%)	206 (94%)	14 (6%)	19	48
3	M	236/236 (100%)	228 (97%)	8 (3%)	40	74
All	All	652/652 (100%)	622 (95%)	30 (5%)	29	63

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	10	PHE
1	H	15	LEU
1	H	45	GLU
1	H	46	ASP
1	H	79	GLU
1	H	221	SER
1	H	223	THR
1	H	231	ASP
2	L	21	LEU
2	L	46	ILE
2	L	52	SER
2	L	56	GLN
2	L	63	LEU
2	L	72	GLU
2	L	85	LEU
2	L	126	LEU
2	L	154	LEU
2	L	158	SER
2	L	210	ASP
2	L	226	THR
2	L	247	CYS
2	L	254	ILE
3	M	12	VAL
3	M	60	LEU
3	M	114	LEU
3	M	144	LYS

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Mol	Chain	Res	Type
3	M	148	TRP
3	M	216	PHE
3	M	247	ARG
3	M	292	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules 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 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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	$\# Z > 2$
4	LDA	H	702	-	12,15,15	1.88	1 (8%)	14,17,17	0.72	0
4	LDA	H	704	-	12,15,15	1.87	1 (8%)	14,17,17	0.51	0
4	LDA	H	709	-	12,15,15	1.89	1 (8%)	14,17,17	0.71	0
5	BCL	L	302	-	58,74,74	0.84	3 (5%)	66,115,115	1.66	18 (27%)
6	BPH	L	402	-	65,70,70	1.32	7 (10%)	75,101,101	1.73	14 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	U10	L	502	-	48,48,63	2.70	12 (25%)	56,61,79	1.64	17 (30%)
8	DIO	L	900	-	6,6,6	0.81	0	6,6,6	0.82	0
8	DIO	L	901	-	6,6,6	0.75	0	6,6,6	0.99	0
5	BCL	M	303	-	58,74,74	0.88	3 (5%)	66,115,115	1.81	23 (34%)
5	BCL	M	304	-	58,74,74	0.83	4 (6%)	66,115,115	1.75	16 (24%)
5	BCL	M	305	-	58,74,74	0.80	4 (6%)	66,115,115	1.90	16 (24%)
6	BPH	M	401	-	65,70,70	1.44	8 (12%)	75,101,101	1.44	8 (10%)
7	U10	M	501	-	48,48,63	2.61	13 (27%)	56,61,79	1.64	15 (26%)
10	SPN	M	600	-	40,42,42	1.08	4 (10%)	51,52,52	1.69	12 (23%)
4	LDA	M	701	-	12,15,15	1.94	1 (8%)	14,17,17	0.46	0
4	LDA	M	703	-	12,15,15	1.86	1 (8%)	14,17,17	0.64	0
4	LDA	M	705	-	12,15,15	1.94	1 (8%)	14,17,17	0.52	0
4	LDA	M	707	-	12,15,15	1.88	1 (8%)	14,17,17	0.71	1 (7%)
4	LDA	M	708	-	12,15,15	1.97	1 (8%)	14,17,17	0.64	0
11	PO4	M	800	-	4,4,4	0.93	0	6,6,6	0.46	0
11	PO4	M	801	-	4,4,4	0.52	0	6,6,6	0.68	0
11	PO4	M	803	-	4,4,4	0.67	0	6,6,6	0.51	0
8	DIO	M	902	-	6,6,6	0.74	0	6,6,6	0.93	0

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
4	LDA	H	702	-	-	0/13/13/13	0/0/0/0
4	LDA	H	704	-	-	0/13/13/13	0/0/0/0
4	LDA	H	709	-	-	0/13/13/13	0/0/0/0
5	BCL	L	302	-	-	0/37/137/137	0/0/9/9
6	BPH	L	402	-	2/2/18/22	0/52/105/105	0/5/6/6
7	U10	L	502	-	-	0/45/69/87	0/1/1/1
8	DIO	L	900	-	-	0/0/6/6	0/1/1/1
8	DIO	L	901	-	-	0/0/6/6	0/1/1/1
5	BCL	M	303	-	-	0/37/137/137	0/0/9/9
5	BCL	M	304	-	-	0/37/137/137	0/0/9/9
5	BCL	M	305	-	-	0/37/137/137	0/0/9/9
6	BPH	M	401	-	2/2/18/22	0/52/105/105	0/5/6/6
7	U10	M	501	-	-	0/45/69/87	0/1/1/1
10	SPN	M	600	-	-	0/50/51/51	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LDA	M	701	-	-	0/13/13/13	0/0/0/0
4	LDA	M	703	-	-	0/13/13/13	0/0/0/0
4	LDA	M	705	-	-	0/13/13/13	0/0/0/0
4	LDA	M	707	-	-	0/13/13/13	0/0/0/0
4	LDA	M	708	-	-	0/13/13/13	0/0/0/0
11	PO4	M	800	-	-	0/0/0/0	0/0/0/0
11	PO4	M	801	-	-	0/0/0/0	0/0/0/0
11	PO4	M	803	-	-	0/0/0/0	0/0/0/0
8	DIO	M	902	-	-	0/0/6/6	0/1/1/1

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	708	LDA	O1-N1	-6.70	1.25	1.42
4	M	705	LDA	O1-N1	-6.64	1.25	1.42
4	M	701	LDA	O1-N1	-6.55	1.26	1.42
4	H	709	LDA	O1-N1	-6.44	1.26	1.42
4	H	702	LDA	O1-N1	-6.43	1.26	1.42
4	M	707	LDA	O1-N1	-6.41	1.26	1.42
4	H	704	LDA	O1-N1	-6.38	1.26	1.42
4	M	703	LDA	O1-N1	-6.31	1.26	1.42
7	M	501	U10	O3-C3	-4.94	1.24	1.36
7	L	502	U10	O3-C3	-4.75	1.25	1.36
7	M	501	U10	O4-C4	-4.46	1.25	1.36
6	M	401	BPH	C4C-NC	-4.16	1.28	1.37
7	L	502	U10	O4-C4	-4.13	1.26	1.36
6	M	401	BPH	C1B-C2B	-3.74	1.37	1.45
6	M	401	BPH	C1A-NA	-3.47	1.30	1.37
6	L	402	BPH	C1A-NA	-3.28	1.30	1.37
6	L	402	BPH	C4C-NC	-3.17	1.30	1.37
6	L	402	BPH	C1B-C2B	-3.08	1.39	1.45
5	M	303	BCL	C1C-NC	-3.02	1.33	1.38
7	L	502	U10	C3-C2	-2.89	1.40	1.48
7	M	501	U10	C4-C5	-2.82	1.40	1.48
7	M	501	U10	C3-C2	-2.73	1.41	1.48
7	L	502	U10	C4-C5	-2.67	1.41	1.48
5	M	305	BCL	C1C-NC	-2.56	1.34	1.38
6	M	401	BPH	CHB-C4A	-2.38	1.34	1.40
5	M	304	BCL	C1C-NC	-2.34	1.34	1.38
5	L	302	BCL	C1C-NC	-2.33	1.34	1.38
6	L	402	BPH	C3D-C2D	-2.32	1.35	1.39
5	L	302	BCL	CHD-C4C	-2.29	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	305	BCL	CHD-C4C	-2.25	1.34	1.41
7	M	501	U10	C1-C2	-2.23	1.38	1.47
7	M	501	U10	C6-C5	-2.21	1.40	1.46
5	M	304	BCL	CHD-C4C	-2.10	1.35	1.41
6	M	401	BPH	C3D-C2D	-2.06	1.35	1.39
5	M	303	BCL	CHD-C4C	-2.04	1.35	1.41
5	M	304	BCL	C4A-NA	-2.03	1.35	1.38
5	M	305	BCL	C4A-NA	-2.00	1.35	1.38
5	M	305	BCL	CHC-C1C	2.08	1.36	1.33
10	M	600	SPN	C12-C13	2.13	1.38	1.33
7	L	502	U10	C6-C1	2.21	1.40	1.35
5	M	303	BCL	CHC-C1C	2.43	1.36	1.33
6	M	401	BPH	C3D-C4D	2.53	1.44	1.41
10	M	600	SPN	C19-C18	2.55	1.39	1.33
6	L	402	BPH	CHB-C1B	2.55	1.43	1.38
5	M	304	BCL	CHC-C1C	2.64	1.36	1.33
5	L	302	BCL	CHC-C1C	2.66	1.36	1.33
10	M	600	SPN	C8-C9	2.70	1.39	1.33
10	M	600	SPN	C25-C26	2.90	1.40	1.33
6	M	401	BPH	CHD-C4C	4.14	1.48	1.37
6	L	402	BPH	CHA-C1A	4.27	1.47	1.38
6	L	402	BPH	CHD-C4C	4.30	1.49	1.37
6	M	401	BPH	CHA-C1A	4.77	1.48	1.38
7	M	501	U10	C23-C24	5.38	1.46	1.33
7	M	501	U10	C38-C39	5.50	1.48	1.32
7	L	502	U10	C38-C39	5.55	1.48	1.32
7	M	501	U10	C28-C29	5.69	1.47	1.33
7	M	501	U10	C8-C9	5.71	1.47	1.33
7	M	501	U10	C18-C19	6.03	1.47	1.33
7	L	502	U10	C33-C34	6.11	1.48	1.33
7	L	502	U10	C23-C24	6.13	1.48	1.33
7	L	502	U10	C28-C29	6.21	1.48	1.33
7	M	501	U10	C33-C34	6.23	1.48	1.33
7	L	502	U10	C18-C19	6.26	1.48	1.33
7	M	501	U10	C13-C14	6.50	1.49	1.33
7	L	502	U10	C8-C9	6.57	1.49	1.33
7	L	502	U10	C13-C14	6.66	1.49	1.33

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	600	SPN	C3-C4-C5	-5.19	118.00	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	402	BPH	C1C-NC-C4C	-4.77	106.25	110.54
6	L	402	BPH	C4D-CHA-C1A	-4.44	119.57	130.51
6	M	401	BPH	C4D-C3D-CAD	-4.27	105.34	107.78
7	M	501	U10	C32-C33-C34	-3.96	117.86	127.66
5	L	302	BCL	CMB-C2B-C1B	-3.96	122.38	128.46
6	M	401	BPH	C4D-CHA-C1A	-3.75	121.26	130.51
7	M	501	U10	C22-C23-C24	-3.71	118.48	127.66
7	L	502	U10	O5-C5-C4	-3.68	113.10	120.93
5	M	303	BCL	C3A-C2A-C1A	-3.65	95.87	101.34
5	M	305	BCL	O2D-CGD-O1D	-3.65	116.58	123.82
5	M	304	BCL	CMB-C2B-C1B	-3.64	122.87	128.46
5	M	303	BCL	CMB-C2B-C1B	-3.53	123.05	128.46
5	M	303	BCL	O1D-CGD-CBD	-3.42	118.24	124.58
5	M	303	BCL	C1B-CHB-C4A	-3.37	123.44	130.12
5	M	303	BCL	C1D-CHD-C4C	-3.37	120.91	125.92
5	M	304	BCL	O2D-CGD-O1D	-3.25	117.37	123.82
5	M	305	BCL	O1D-CGD-CBD	-3.16	118.72	124.58
6	L	402	BPH	C3A-C2A-C1A	-3.15	97.97	101.68
10	M	600	SPN	C7-C8-C9	-3.12	119.94	127.66
5	M	305	BCL	CMB-C2B-C1B	-3.02	123.82	128.46
5	M	305	BCL	C1D-CHD-C4C	-3.01	121.44	125.92
7	M	501	U10	C17-C18-C19	-2.96	120.34	127.66
6	L	402	BPH	C4D-C3D-CAD	-2.84	106.15	107.78
5	M	304	BCL	C1D-CHD-C4C	-2.83	121.70	125.92
10	M	600	SPN	C24-C25-C26	-2.81	120.70	127.66
5	M	304	BCL	CAA-C2A-C3A	-2.79	105.15	112.81
7	L	502	U10	C22-C23-C24	-2.78	120.77	127.66
5	M	304	BCL	C1-C2-C3	-2.78	120.84	125.96
5	M	305	BCL	C3C-C4C-CHD	-2.73	117.62	123.31
7	M	501	U10	C12-C13-C14	-2.72	120.93	127.66
5	L	302	BCL	C1D-CHD-C4C	-2.67	121.94	125.92
5	M	304	BCL	CAC-C3C-C2C	-2.67	107.54	114.24
5	M	304	BCL	CGD-CBD-CAD	-2.66	102.11	110.73
6	L	402	BPH	C1-O2A-CGA	-2.66	110.65	116.77
7	L	502	U10	C17-C18-C19	-2.65	121.10	127.66
7	L	502	U10	C32-C33-C34	-2.65	121.11	127.66
10	M	600	SPN	C20-C19-C18	-2.59	121.25	127.66
5	M	303	BCL	C6-C5-C3	-2.56	106.62	112.82
7	L	502	U10	O5-C5-C6	-2.54	117.33	121.88
5	M	305	BCL	C11-C12-C13	-2.53	107.42	115.73
6	L	402	BPH	OBB-CAB-CBB	-2.51	114.09	119.72
6	L	402	BPH	C2B-C1B-NB	-2.50	106.00	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	302	BCL	OBB-CAB-CBB	-2.43	114.67	120.15
5	M	305	BCL	O2A-CGA-O1A	-2.43	117.65	123.58
5	L	302	BCL	C7-C6-C5	-2.42	106.58	113.17
5	M	303	BCL	OBB-CAB-CBB	-2.41	114.73	120.15
5	M	303	BCL	C3C-C4C-CHD	-2.38	118.34	123.31
5	L	302	BCL	C1B-CHB-C4A	-2.37	125.42	130.12
7	L	502	U10	C27-C28-C29	-2.36	121.82	127.66
7	M	501	U10	C27-C28-C29	-2.31	121.95	127.66
10	M	600	SPN	C11-C12-C13	-2.27	122.03	127.66
5	L	302	BCL	C1-C2-C3	-2.27	121.78	125.96
7	L	502	U10	O2-C2-C3	-2.26	116.12	120.93
5	M	303	BCL	O2A-CGA-O1A	-2.26	118.08	123.58
5	L	302	BCL	C11-C10-C8	-2.25	108.35	115.73
5	M	303	BCL	CBC-CAC-C3C	-2.24	108.36	113.45
5	M	305	BCL	C16-C15-C13	-2.22	108.46	115.73
7	M	501	U10	C22-C21-C19	-2.22	105.53	112.85
10	M	600	SPN	O1-C1-C2	-2.22	104.54	108.93
6	M	401	BPH	OBB-CAB-CBB	-2.21	114.77	119.72
6	L	402	BPH	C4-C3-C5	-2.20	111.48	115.29
5	L	302	BCL	C11-C12-C13	-2.19	108.55	115.73
4	M	707	LDA	CM2-N1-CM1	-2.19	107.42	110.91
5	M	305	BCL	C6-C5-C3	-2.18	107.53	112.82
5	L	302	BCL	C3C-C4C-CHD	-2.17	118.78	123.31
5	M	304	BCL	CBC-CAC-C3C	-2.17	108.52	113.45
5	M	303	BCL	CAC-C3C-C2C	-2.16	108.80	114.24
7	M	501	U10	C25-C24-C23	-2.14	118.07	123.70
5	L	302	BCL	O2A-CGA-O1A	-2.13	118.39	123.58
10	M	600	SPN	C28-C29-C30	-2.10	120.53	127.84
5	M	304	BCL	OBB-CAB-CBB	-2.09	115.45	120.15
5	M	303	BCL	C5-C3-C2	-2.08	116.86	121.10
5	M	303	BCL	C3D-CAD-CBD	-2.08	104.81	107.61
5	M	303	BCL	C11-C12-C13	-2.07	108.92	115.73
7	L	502	U10	C7-C8-C9	-2.06	123.30	126.79
5	M	304	BCL	C11-C10-C8	-2.05	109.00	115.73
7	M	501	U10	O5-C5-C6	-2.05	118.21	121.88
7	L	502	U10	C37-C38-C39	-2.04	120.76	127.84
5	M	303	BCL	CMA-C3A-C4A	-2.01	106.36	111.77
5	M	303	BCL	C1-C2-C3	-2.01	122.25	125.96
5	M	303	BCL	CBB-CAB-C3B	2.02	126.26	120.35
7	M	501	U10	C10-C9-C11	2.04	118.81	115.29
7	M	501	U10	C41-C39-C40	2.07	119.27	114.59
5	M	305	BCL	CMB-C2B-C3B	2.09	128.68	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	600	SPN	CM5-C13-C14	2.14	118.97	115.29
7	L	502	U10	C41-C39-C40	2.17	119.48	114.59
5	L	302	BCL	CHB-C4A-NA	2.18	127.52	124.51
6	L	402	BPH	C3B-C2B-C1B	2.21	109.16	105.85
5	M	303	BCL	CMB-C2B-C3B	2.21	128.91	124.88
5	L	302	BCL	C1-O2A-CGA	2.26	121.98	116.77
5	M	305	BCL	OBD-CAD-CBD	2.27	129.25	125.91
5	M	305	BCL	C4-C3-C5	2.29	119.24	115.29
6	L	402	BPH	C1B-NB-C4B	2.32	111.02	106.51
7	M	501	U10	C4M-O4-C4	2.34	124.79	116.45
7	L	502	U10	C30-C29-C31	2.36	119.35	115.29
6	M	401	BPH	CAC-C3C-C4C	2.38	118.78	112.67
10	M	600	SPN	C7-C6-C5	2.38	120.71	112.85
7	L	502	U10	C3M-O3-C3	2.38	124.94	116.45
6	L	402	BPH	CMD-C2D-C3D	2.41	129.27	124.88
7	L	502	U10	C25-C24-C26	2.44	119.49	115.29
7	L	502	U10	C4M-O4-C4	2.45	125.16	116.45
7	L	502	U10	C35-C34-C36	2.47	119.54	115.29
7	M	501	U10	C15-C14-C16	2.47	119.55	115.29
5	M	304	BCL	C4-C3-C5	2.53	119.66	115.29
10	M	600	SPN	CMA-O1-C1	2.55	126.25	112.32
7	L	502	U10	C20-C19-C21	2.58	119.73	115.29
5	L	302	BCL	CMB-C2B-C3B	2.60	129.61	124.88
10	M	600	SPN	CM6-C18-C17	2.69	119.93	115.29
5	M	303	BCL	O2A-CGA-CBA	2.71	119.76	111.92
5	L	302	BCL	O2D-CGD-CBD	2.72	116.11	111.28
6	M	401	BPH	OBB-CAB-C3B	2.74	125.29	120.38
5	L	302	BCL	O2A-CGA-CBA	2.89	120.28	111.92
5	M	303	BCL	CHB-C4A-NA	2.92	128.55	124.51
5	M	304	BCL	O2A-CGA-CBA	2.92	120.36	111.92
5	M	305	BCL	CHB-C4A-NA	2.93	128.56	124.51
5	M	304	BCL	CMB-C2B-C3B	2.96	130.27	124.88
7	M	501	U10	C25-C24-C26	2.99	120.45	115.29
6	M	401	BPH	CMD-C2D-C3D	3.11	130.54	124.88
5	L	302	BCL	C4-C3-C5	3.13	120.69	115.29
10	M	600	SPN	CM3-C5-C6	3.14	120.70	115.29
6	L	402	BPH	C6-C5-C3	3.18	120.52	112.82
7	L	502	U10	C7-C6-C5	3.18	122.45	118.48
5	L	302	BCL	CED-O2D-CGD	3.21	123.36	115.97
6	L	402	BPH	OBB-CAB-C3B	3.24	126.18	120.38
5	M	305	BCL	O2A-CGA-CBA	3.35	121.61	111.92
7	M	501	U10	C35-C34-C36	3.43	121.21	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	501	U10	C30-C29-C31	3.47	121.27	115.29
5	M	304	BCL	CHB-C4A-NA	3.47	129.31	124.51
6	M	401	BPH	C6-C5-C3	3.73	121.86	112.82
5	M	303	BCL	O2D-CGD-CBD	3.81	118.03	111.28
5	L	302	BCL	CHD-C4C-NC	3.83	129.33	125.08
5	M	303	BCL	C4-C3-C5	3.83	121.90	115.29
5	M	303	BCL	CHD-C4C-NC	4.09	129.62	125.08
5	M	304	BCL	CHD-C4C-NC	4.20	129.74	125.08
5	M	305	BCL	CHD-C4C-NC	4.93	130.55	125.08
5	M	304	BCL	O2D-CGD-CBD	5.02	120.18	111.28
6	M	401	BPH	C3C-C4C-NC	5.39	113.33	108.11
6	L	402	BPH	C3C-C4C-NC	7.55	115.42	108.11
5	M	305	BCL	O2D-CGD-CBD	7.56	124.68	111.28

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	M	401	BPH	C8
6	M	401	BPH	C13
6	L	402	BPH	C8
6	L	402	BPH	C13

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	702	LDA	3	0
4	H	704	LDA	2	0
5	L	302	BCL	4	0
6	L	402	BPH	6	0
7	L	502	U10	5	0
8	L	900	DIO	2	0
5	M	303	BCL	7	0
5	M	304	BCL	5	0
5	M	305	BCL	2	0
6	M	401	BPH	5	0
7	M	501	U10	1	0
10	M	600	SPN	6	0
4	M	701	LDA	1	0
4	M	703	LDA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	705	LDA	1	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	H	241/241 (100%)	-0.45	4 (1%) 70 63	19, 35, 54, 102	0
2	L	281/281 (100%)	-0.46	2 (0%) 87 83	20, 36, 70, 94	0
3	M	302/302 (100%)	-0.64	0 100 100	21, 39, 65, 82	0
All	All	824/824 (100%)	-0.52	6 (0%) 87 83	19, 36, 65, 102	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	250	SER	4.3
1	H	10	PHE	3.8
2	L	59	TRP	3.1
1	H	245	ALA	2.6
1	H	246	PRO	2.3
2	L	281	GLY	2.3

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. 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	B-factors(\AA^2)	Q<0.9
4	LDA	M	707	16/16	0.73	0.29	42,59,91,96	0
11	PO4	M	801	5/5	0.73	0.28	54,68,85,101	0
7	U10	L	502	48/63	0.74	0.48	31,64,107,115	0
4	LDA	M	708	16/16	0.76	0.32	35,64,90,93	0
4	LDA	H	704	16/16	0.83	0.36	40,50,73,75	0
4	LDA	M	705	16/16	0.85	0.41	36,50,81,81	0
8	DIO	M	902	6/6	0.85	0.56	45,53,62,68	0
4	LDA	H	709	16/16	0.87	0.37	32,57,87,89	0
4	LDA	M	703	16/16	0.87	0.29	38,49,69,73	0
4	LDA	M	701	16/16	0.88	0.21	21,41,51,55	0
10	SPN	M	600	43/43	0.90	0.21	29,49,77,87	0
4	LDA	H	702	16/16	0.90	0.22	46,59,70,73	0
8	DIO	L	901	6/6	0.90	0.26	46,48,53,58	0
8	DIO	L	900	6/6	0.91	0.33	51,55,63,70	0
6	BPH	M	401	65/65	0.92	0.17	23,32,93,104	0
11	PO4	M	803	5/5	0.94	0.14	66,72,79,87	0
5	BCL	M	303	66/66	0.94	0.17	20,29,53,63	0
7	U10	M	501	48/63	0.94	0.17	19,30,50,61	0
5	BCL	L	302	66/66	0.94	0.16	21,29,38,55	0
5	BCL	M	305	66/66	0.95	0.13	21,26,38,52	0
12	CL	M	306	1/1	0.95	0.09	50,50,50,50	0
5	BCL	M	304	66/66	0.96	0.14	22,30,43,60	0
6	BPH	L	402	65/65	0.96	0.15	14,28,39,42	0
11	PO4	M	800	5/5	0.98	0.07	24,33,44,47	0
9	FE	M	500	1/1	0.99	0.11	24,24,24,24	0

6.5 Other polymers

There are no such residues in this entry.