



Full wwPDB X-ray Structure Validation Report i

Mar 1, 2014 – 01:26 AM GMT

PDB ID : 2GNU
Title : The crystallization of reaction center from Rhodobacter sphaeroides occurs via a new route
Authors : Wadsten, P.; Woehri, A.B.; Snijder, A.; Katona, G.; Gardiner, A.T.; Cogdell, R.J.; Neutze, R.; Engstroem, S.
Deposited on : 2006-04-11
Resolution : 2.20 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>

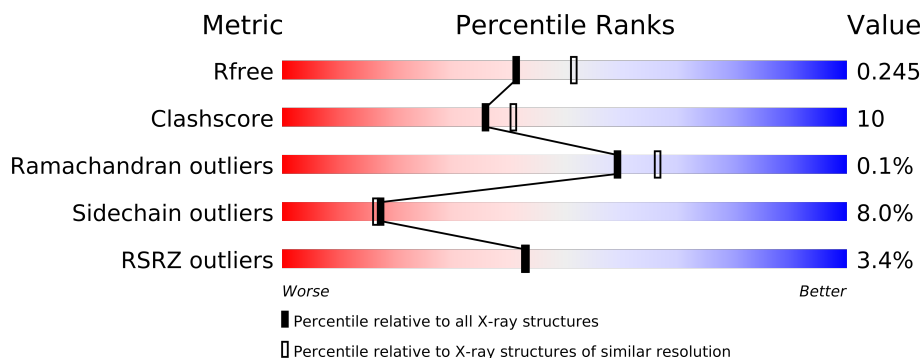
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.20 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	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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	H	235	
2	L	281	
3	M	300	

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

Mol	Type	Chain	Res	Geometry	Electron density
8	U10	L	1306	-	X
9	CDL	M	1309	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7045 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 H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	235	Total	C	N	O	S	0	0	0
			1787	1143	304	331	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
			2232	1507	355	362	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	300	Total	C	N	O	S	0	0	0
			2400	1602	392	396	10			

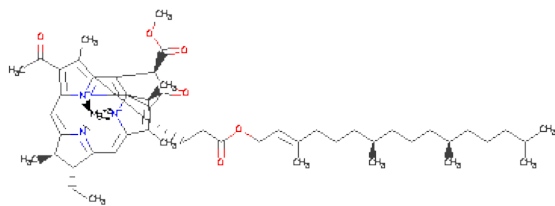
- Molecule 4 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

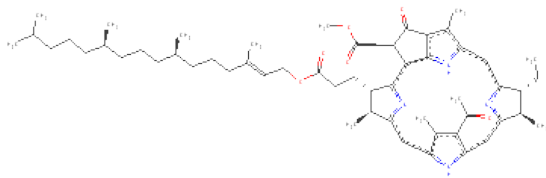
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	1	Total	Cl	0	0
			1	1		

- Molecule 6 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



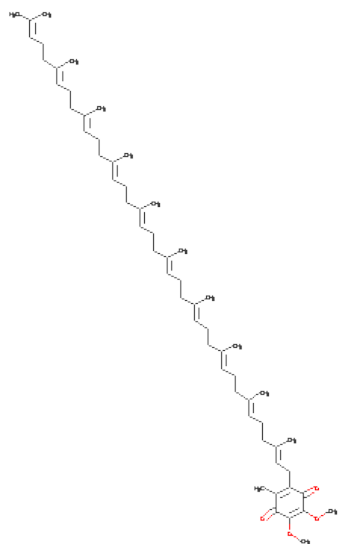
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆).



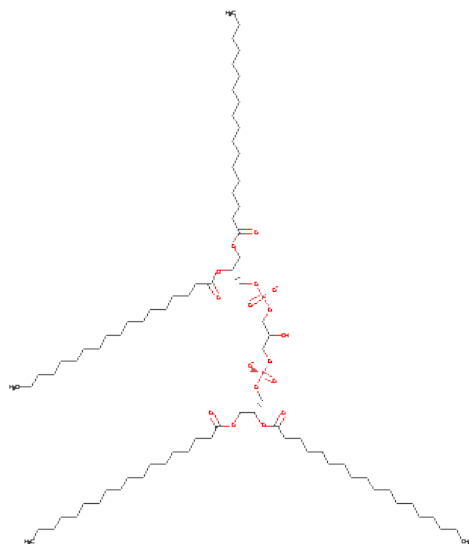
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 8 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



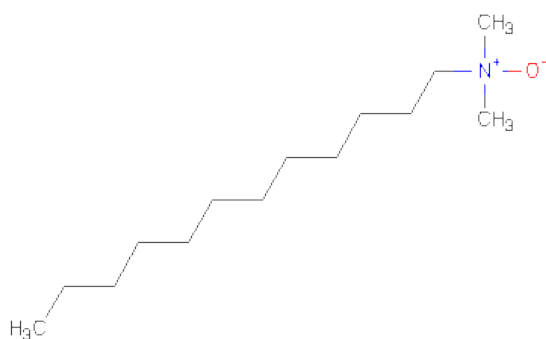
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			45	41	4		
8	L	1	Total	C	O	0	0
			24	20	4		

- Molecule 9 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	O	P	0	0
			10	8	2		

- Molecule 10 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	H	1	Total	C	N	O	0	0
			14	12	1	1		

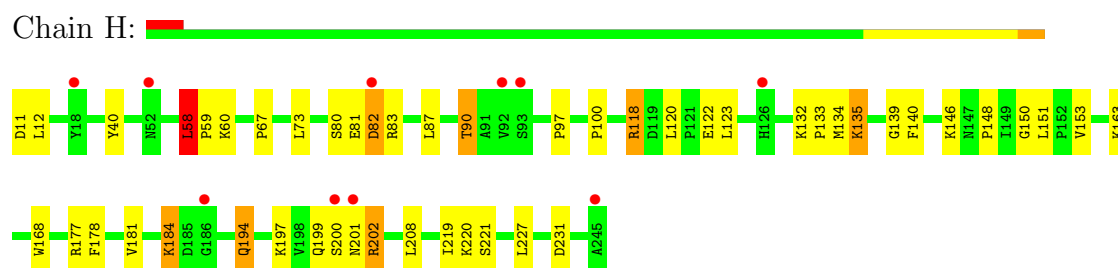
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	64	Total 64	O 64	0	0
11	L	43	Total 43	O 43	0	0
11	M	48	Total 48	O 48	0	0

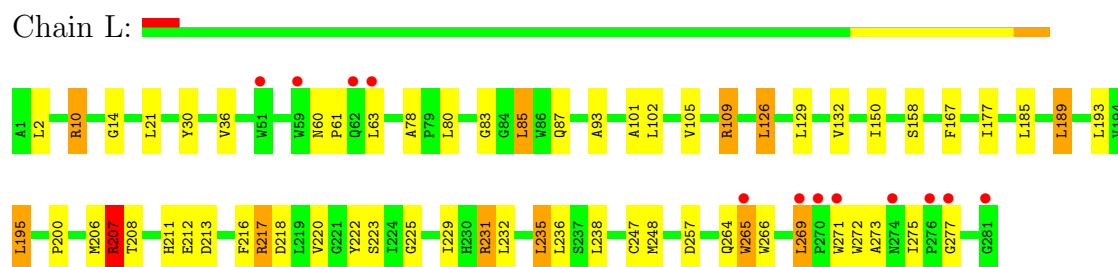
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

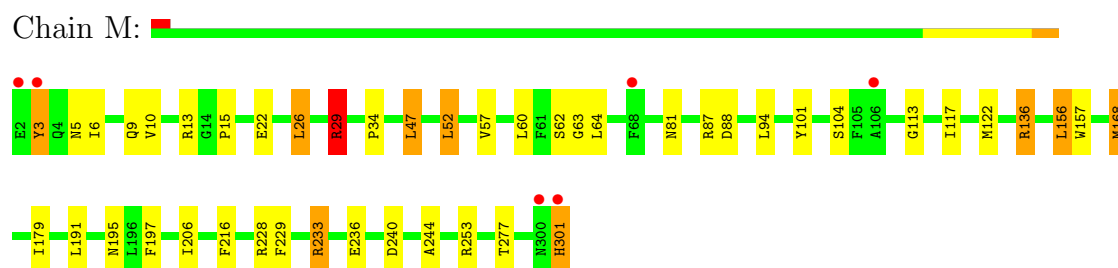
- Molecule 1: Reaction center protein H chain



- 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 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.42 Å 100.42 Å 235.41 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.80 – 2.20 19.80 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.80-2.20) 99.6 (19.80-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.19 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.200 , 0.246 0.202 , 0.245	Depositor DCC
R_{free} test set	3129 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 48.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 61641 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7045	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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, LDA, CL, CDL, BPH, FE2, 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	0.92	2/1834 (0.1%)	0.89	5/2497 (0.2%)
2	L	0.92	1/2320 (0.0%)	0.98	13/3175 (0.4%)
3	M	0.91	0/2492	0.92	10/3401 (0.3%)
All	All	0.91	3/6646 (0.0%)	0.94	28/9073 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	30	TYR	CD1-CE1	-5.93	1.30	1.39
1	H	132	LYS	CE-NZ	5.41	1.62	1.49
1	H	132	LYS	CD-CE	5.15	1.64	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	207	ARG	NE-CZ-NH2	-14.31	113.14	120.30
3	M	136	ARG	NE-CZ-NH2	-12.97	113.81	120.30
3	M	136	ARG	NE-CZ-NH1	11.77	126.19	120.30
2	L	217	ARG	NE-CZ-NH1	10.68	125.64	120.30
3	M	253	ARG	NE-CZ-NH2	-10.07	115.26	120.30
2	L	207	ARG	NE-CZ-NH1	9.75	125.17	120.30
3	M	233	ARG	NE-CZ-NH1	-9.60	115.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	29	ARG	NE-CZ-NH2	-8.28	116.16	120.30
2	L	195	LEU	CB-CG-CD1	7.97	124.56	111.00
3	M	29	ARG	NE-CZ-NH1	7.84	124.22	120.30
2	L	217	ARG	NE-CZ-NH2	-7.77	116.42	120.30
2	L	10	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	H	132	LYS	CD-CE-NZ	6.90	127.58	111.70
2	L	10	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	H	58	LEU	CA-CB-CG	6.56	130.38	115.30
3	M	240	ASP	CB-CG-OD1	6.43	124.09	118.30
1	H	118	ARG	NE-CZ-NH2	6.40	123.50	120.30
2	L	235	LEU	CA-CB-CG	6.36	129.92	115.30
2	L	231	ARG	NE-CZ-NH2	-6.23	117.18	120.30
2	L	126	LEU	CB-CG-CD1	6.23	121.59	111.00
1	H	118	ARG	NE-CZ-NH1	-5.69	117.46	120.30
1	H	83	ARG	NE-CZ-NH2	-5.61	117.50	120.30
2	L	109	ARG	NE-CZ-NH2	-5.61	117.50	120.30
2	L	231	ARG	NE-CZ-NH1	5.59	123.10	120.30
3	M	26	LEU	CA-CB-CG	5.52	127.99	115.30
3	M	233	ARG	NE-CZ-NH2	5.39	122.99	120.30
2	L	217	ARG	CB-CG-CD	5.30	125.39	111.60
3	M	240	ASP	CB-CG-OD2	-5.00	113.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	80	SER	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	H	1787	0	1785	42	0
2	L	2232	0	2187	47	0
3	M	2400	0	2310	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	1	0	0	0	0
5	M	1	0	0	0	0
6	L	132	0	147	12	0
6	M	114	0	111	13	0
7	M	130	0	152	17	0
8	L	24	0	25	14	0
8	M	45	0	59	3	0
9	M	10	0	0	0	0
10	H	14	0	24	3	0
11	H	64	0	0	3	0
11	L	43	0	0	3	0
11	M	48	0	0	1	0
All	All	7045	0	6800	142	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 10.

All (142) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:L:1306:U10:H4M3	8:L:1306:U10:O3	1.42	1.14
1:H:118:ARG:HD3	1:H:120:LEU:HD12	1.28	1.13
2:L:206:MET:O	11:L:1348:HOH:O	1.69	1.08
8:L:1306:U10:O3	8:L:1306:U10:C4M	2.14	0.95
1:H:90:THR:HB	1:H:97:PRO:O	1.65	0.95
3:M:122:MET:HE3	3:M:157:TRP:HE1	1.32	0.95
3:M:168:MET:HA	3:M:168:MET:CE	2.05	0.86
6:M:1303:BCL:CBB	6:M:1303:BCL:HHC	2.09	0.82
2:L:269:LEU:O	2:L:273:ALA:HB2	1.80	0.80
7:M:1304:BPH:H111	7:M:1304:BPH:H162	1.61	0.80
3:M:168:MET:HA	3:M:168:MET:HE3	1.65	0.77
1:H:118:ARG:CD	1:H:120:LEU:HD12	2.11	0.77
2:L:223:SER:OG	8:L:1306:U10:H4M1	1.85	0.77
3:M:197:PHE:CZ	6:M:1303:BCL:HBB2	2.20	0.76
1:H:194:GLN:CG	3:M:228:ARG:HA	2.16	0.76
6:M:1303:BCL:HBB2	6:M:1303:BCL:HHC	1.68	0.75
1:H:67:PRO:HG3	11:L:1348:HOH:O	1.88	0.74
1:H:81:GLU:HA	11:H:1339:HOH:O	1.87	0.73
1:H:40:TYR:OH	10:H:1310:LDA:CM1	2.36	0.72
1:H:194:GLN:HG3	3:M:228:ARG:HA	1.71	0.72
3:M:197:PHE:HZ	6:M:1303:BCL:HBB2	1.55	0.70
2:L:223:SER:OG	8:L:1306:U10:C4M	2.40	0.70
2:L:275:ILE:HG21	3:M:81:ASN:HD21	1.57	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:177:ILE:HG12	6:L:1282:BCL:HMB3	1.73	0.69
6:M:1302:BCL:HBB3	6:M:1302:BCL:HMB1	1.74	0.69
2:L:269:LEU:HG	2:L:271:TRP:CZ2	2.27	0.69
3:M:63:GLY:HA3	7:M:1304:BPH:H5C2	1.75	0.69
1:H:150:GLY:HA2	1:H:163:LYS:HE2	1.75	0.69
1:H:40:TYR:OH	10:H:1310:LDA:HM13	1.93	0.68
3:M:122:MET:CE	3:M:157:TRP:HE1	2.06	0.68
3:M:64:LEU:CD2	7:M:1304:BPH:H121	2.24	0.67
2:L:189:LEU:HD13	7:M:1304:BPH:HMD2	1.76	0.67
3:M:64:LEU:HD23	7:M:1304:BPH:H102	1.78	0.66
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.77	0.65
2:L:275:ILE:HG21	3:M:81:ASN:ND2	2.12	0.65
1:H:146:LYS:NZ	1:H:200:SER:O	2.29	0.65
7:M:1304:BPH:C11	7:M:1304:BPH:H162	2.26	0.64
3:M:122:MET:HE3	3:M:157:TRP:NE1	2.09	0.63
1:H:184:LYS:HE3	1:H:184:LYS:HA	1.79	0.63
1:H:82:ASP:N	11:H:1339:HOH:O	2.33	0.62
2:L:211:HIS:HE1	3:M:22:GLU:OE1	1.82	0.61
1:H:122:GLU:HB2	1:H:227:LEU:HD21	1.82	0.60
1:H:140:PHE:HA	3:M:13:ARG:O	2.01	0.59
1:H:81:GLU:CA	11:H:1339:HOH:O	2.47	0.59
3:M:3:TYR:H	3:M:3:TYR:HD2	1.51	0.58
8:L:1306:U10:H3M2	11:L:1327:HOH:O	2.05	0.57
7:M:1304:BPH:HHD	7:M:1304:BPH:HBC2	1.87	0.56
3:M:64:LEU:HD23	7:M:1304:BPH:H121	1.86	0.56
3:M:52:LEU:HD13	3:M:57:VAL:HG23	1.85	0.56
1:H:197:LYS:HA	3:M:9:GLN:HE22	1.69	0.56
8:L:1306:U10:H4M3	8:L:1306:U10:C3M	2.32	0.56
1:H:184:LYS:CE	1:H:184:LYS:HA	2.36	0.56
2:L:264:GLN:C	2:L:266:TRP:H	2.08	0.56
1:H:11:ASP:HB3	3:M:301:HIS:HD2	1.71	0.55
6:M:1303:BCL:HBB3	6:M:1303:BCL:HHC	1.87	0.55
2:L:277:GLY:O	3:M:87:ARG:NH2	2.39	0.55
1:H:194:GLN:HG3	3:M:228:ARG:CA	2.35	0.54
3:M:168:MET:HA	3:M:168:MET:HE2	1.87	0.54
1:H:40:TYR:OH	10:H:1310:LDA:HM11	2.06	0.54
2:L:217:ARG:HD2	11:M:1318:HOH:O	2.07	0.54
6:M:1302:BCL:HHC	6:M:1302:BCL:OBB	2.08	0.54
1:H:122:GLU:HG3	3:M:236:GLU:HG3	1.90	0.54
1:H:194:GLN:HG2	3:M:228:ARG:HA	1.87	0.53
2:L:101:ALA:O	2:L:105:VAL:HG23	2.08	0.53
1:H:148:PRO:O	1:H:151:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:14:GLY:O	2:L:109:ARG:HD3	2.08	0.52
2:L:208:THR:H	2:L:211:HIS:CD2	2.27	0.52
3:M:101:TYR:O	3:M:104:SER:HB3	2.10	0.52
1:H:184:LYS:CA	1:H:184:LYS:HE3	2.39	0.52
6:L:1283:BCL:C4A	6:L:1283:BCL:HBA1	2.39	0.51
2:L:264:GLN:C	2:L:266:TRP:N	2.64	0.51
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.93	0.51
2:L:193:LEU:HD21	2:L:212:GLU:HB3	1.93	0.51
6:L:1282:BCL:NC	6:M:1303:BCL:HBB3	2.25	0.51
6:L:1282:BCL:H142	6:L:1283:BCL:HMB1	1.93	0.51
8:M:1305:U10:O3	8:M:1305:U10:H4M2	2.11	0.51
2:L:231:ARG:HD3	3:M:5:ASN:O	2.10	0.51
2:L:213:ASP:OD2	8:L:1306:U10:H4M1	2.11	0.50
2:L:225:GLY:C	8:L:1306:U10:H3M3	2.32	0.50
2:L:248:MET:HE2	6:L:1282:BCL:OBD	2.12	0.50
2:L:265:TRP:O	2:L:269:LEU:HD13	2.12	0.50
1:H:87:LEU:HD23	1:H:100:PRO:HA	1.93	0.50
8:L:1306:U10:C8	8:L:1306:U10:H1M1	2.41	0.50
1:H:201:ASN:N	1:H:201:ASN:OD1	2.44	0.50
2:L:150:ILE:HG23	6:L:1283:BCL:HED1	1.93	0.49
1:H:11:ASP:HB3	3:M:301:HIS:CD2	2.47	0.49
2:L:208:THR:H	2:L:211:HIS:HD2	1.60	0.49
2:L:105:VAL:O	2:L:109:ARG:HG3	2.13	0.49
2:L:269:LEU:O	2:L:273:ALA:CB	2.57	0.49
3:M:87:ARG:HG2	3:M:88:ASP:OD1	2.13	0.48
1:H:194:GLN:HG3	3:M:228:ARG:N	2.28	0.48
2:L:264:GLN:O	2:L:266:TRP:N	2.47	0.48
2:L:80:LEU:HD22	2:L:85:LEU:HD13	1.95	0.47
2:L:222:TYR:HD2	8:L:1306:U10:H13	1.80	0.47
1:H:90:THR:CB	1:H:97:PRO:O	2.52	0.46
2:L:60:ASN:ND2	2:L:63:LEU:HD23	2.30	0.46
1:H:139:GLY:HA3	3:M:15:PRO:HD3	1.96	0.46
2:L:93:ALA:HA	7:M:1284:BPH:H9C2	1.98	0.46
2:L:229:ILE:HD13	8:L:1306:U10:H8	1.97	0.45
7:M:1284:BPH:HBB3	7:M:1284:BPH:CMB	2.46	0.45
7:M:1284:BPH:ND	7:M:1284:BPH:NC	2.64	0.45
3:M:206:ILE:HG12	6:M:1303:BCL:HMB3	1.99	0.45
2:L:61:PRO:O	2:L:150:ILE:HD12	2.17	0.45
2:L:185:LEU:HD13	7:M:1304:BPH:ND	2.31	0.45
1:H:11:ASP:CB	3:M:301:HIS:HD2	2.29	0.45
2:L:225:GLY:O	8:L:1306:U10:H3M3	2.16	0.45
6:L:1282:BCL:HHC	6:L:1282:BCL:OBB	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:156:LEU:HD13	6:M:1303:BCL:H43	1.99	0.45
2:L:218:ASP:OD1	3:M:29:ARG:HD2	2.17	0.45
2:L:223:SER:HG	8:L:1306:U10:H4M1	1.81	0.44
6:L:1283:BCL:HBB3	7:M:1284:BPH:H141	1.98	0.44
2:L:231:ARG:HD2	3:M:6:ILE:O	2.18	0.44
1:H:153:VAL:HG21	1:H:181:VAL:HG22	1.99	0.44
2:L:207:ARG:HD2	2:L:207:ARG:N	2.31	0.44
7:M:1304:BPH:CHD	7:M:1304:BPH:CBC	2.96	0.44
2:L:207:ARG:HA	2:L:207:ARG:HD2	1.86	0.44
2:L:200:PRO:HB3	2:L:207:ARG:HD3	1.98	0.43
1:H:194:GLN:H	1:H:194:GLN:CD	2.20	0.43
2:L:189:LEU:CD1	7:M:1304:BPH:HMD2	2.44	0.43
1:H:168:TRP:HB2	1:H:178:PHE:HB2	2.00	0.43
6:L:1282:BCL:HBB3	6:L:1282:BCL:HMB1	2.00	0.43
3:M:34:PRO:O	3:M:47:LEU:HB2	2.18	0.43
2:L:78:ALA:H	2:L:87:GLN:HE22	1.67	0.43
7:M:1304:BPH:HHD	7:M:1304:BPH:CBC	2.49	0.42
8:M:1305:U10:C4M	8:M:1305:U10:O3	2.68	0.42
6:L:1282:BCL:H193	8:M:1305:U10:H252	2.01	0.42
1:H:177:ARG:CZ	3:M:233:ARG:HD2	2.49	0.42
6:L:1282:BCL:H2C	6:M:1303:BCL:H2C	2.02	0.42
2:L:223:SER:OG	8:L:1306:U10:O4	2.38	0.42
3:M:156:LEU:HD12	3:M:277:THR:HG22	2.02	0.42
1:H:58:LEU:HD22	1:H:59:PRO:HD2	2.02	0.42
6:M:1303:BCL:CBB	6:M:1303:BCL:CHC	2.82	0.42
1:H:219:ILE:HD12	1:H:221:SER:O	2.20	0.41
7:M:1284:BPH:H7C1	7:M:1284:BPH:H112	1.80	0.41
2:L:83:GLY:O	2:L:87:GLN:HG3	2.20	0.41
1:H:133:PRO:HB2	1:H:135:LYS:HE3	2.02	0.41
3:M:179:ILE:HG23	6:M:1302:BCL:HED1	2.02	0.41
6:L:1283:BCL:HHC	6:L:1283:BCL:OBB	2.21	0.40
3:M:113:GLY:O	3:M:117:ILE:HG13	2.20	0.40
2:L:232:LEU:O	2:L:236:LEU:HG	2.21	0.40
1:H:199:GLN:OE1	1:H:202:ARG:HD3	2.20	0.40
1:H:60:LYS:CD	1:H:60:LYS:N	2.85	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	H	233/235 (99%)	225 (97%)	8 (3%)	0	100	100
2	L	279/281 (99%)	265 (95%)	13 (5%)	1 (0%)	43	45
3	M	298/300 (99%)	288 (97%)	10 (3%)	0	100	100
All	All	810/816 (99%)	778 (96%)	31 (4%)	1 (0%)	59	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	265	TRP

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	190/190 (100%)	176 (93%)	14 (7%)	20	19
2	L	220/220 (100%)	198 (90%)	22 (10%)	11	10
3	M	236/236 (100%)	220 (93%)	16 (7%)	22	23
All	All	646/646 (100%)	594 (92%)	52 (8%)	17	16

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	12	LEU
1	H	58	LEU
1	H	73	LEU
1	H	82	ASP
1	H	90	THR

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Mol	Chain	Res	Type
1	H	123	LEU
1	H	134	MET
1	H	135	LYS
1	H	184	LYS
1	H	194	GLN
1	H	202	ARG
1	H	208	LEU
1	H	220	LYS
1	H	231	ASP
2	L	2	LEU
2	L	10	ARG
2	L	21	LEU
2	L	36	VAL
2	L	85	LEU
2	L	102	LEU
2	L	126	LEU
2	L	129	LEU
2	L	132	VAL
2	L	158	SER
2	L	167	PHE
2	L	189	LEU
2	L	195	LEU
2	L	207	ARG
2	L	216	PHE
2	L	220	VAL
2	L	235	LEU
2	L	238	LEU
2	L	247	CYS
2	L	257	ASP
2	L	269	LEU
2	L	272	TRP
3	M	3	TYR
3	M	10	VAL
3	M	26	LEU
3	M	29	ARG
3	M	47	LEU
3	M	52	LEU
3	M	60	LEU
3	M	62	SER
3	M	94	LEU
3	M	136	ARG
3	M	156	LEU

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Mol	Chain	Res	Type
3	M	168	MET
3	M	191	LEU
3	M	195	ASN
3	M	216	PHE
3	M	301	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	194	GLN
2	L	87	GLN
2	L	211	HIS
2	L	258	GLN
3	M	9	GLN
3	M	195	ASN
3	M	301	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	LDA	H	1310	-	13,13,15	3.82	2 (15%)	15,15,17	1.62	3 (20%)
6	BCL	L	1282	2	74,74,74	1.73	13 (17%)	97,115,115	2.05	28 (28%)
6	BCL	L	1283	2	74,74,74	1.96	14 (18%)	97,115,115	1.92	25 (25%)
8	U10	L	1306	-	24,24,63	2.79	7 (29%)	31,32,79	2.40	15 (48%)
7	BPH	M	1284	-	70,70,70	1.89	8 (11%)	94,101,101	1.78	20 (21%)
6	BCL	M	1302	3	55,56,74	1.99	11 (20%)	74,93,115	2.55	22 (29%)
6	BCL	M	1303	3	74,74,74	2.03	12 (16%)	97,115,115	1.96	25 (25%)
7	BPH	M	1304	-	70,70,70	2.04	10 (14%)	94,101,101	1.99	21 (22%)
8	U10	M	1305	-	44,45,63	2.93	10 (22%)	56,57,79	2.01	17 (30%)
9	CDL	M	1309	-	8,8,99	1.09	0	12,12,111	1.29	3 (25%)

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	LDA	H	1310	-	-	0/11/11/13	0/0/0/0
6	BCL	L	1282	2	2/2/21/25	0/41/137/137	0/0/9/9
6	BCL	L	1283	2	2/2/21/25	0/41/137/137	0/0/9/9
8	U10	L	1306	-	-	0/17/41/87	0/1/1/1
7	BPH	M	1284	-	1/1/18/22	0/49/105/105	0/0/6/6
6	BCL	M	1302	3	-	0/20/116/137	0/0/9/9
6	BCL	M	1303	3	2/2/21/25	0/41/137/137	0/0/9/9
7	BPH	M	1304	-	1/1/18/22	0/49/105/105	0/0/6/6
8	U10	M	1305	-	-	0/42/66/87	0/1/1/1
9	CDL	M	1309	-	-	0/0/0/110	0/0/0/0

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	H	1310	LDA	O1-N1	-13.37	1.26	1.39
7	M	1304	BPH	C1D-CHD	11.31	1.48	1.35
7	M	1284	BPH	C1D-CHD	10.77	1.47	1.35
8	M	1305	U10	C28-C29	8.18	1.49	1.32
6	M	1303	BCL	MG-NB	8.09	2.23	2.05
8	M	1305	U10	C33-C34	7.76	1.48	1.32
8	L	1306	U10	C13-C14	7.34	1.47	1.32
8	M	1305	U10	C18-C19	7.03	1.47	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	1305	U10	C8-C9	6.94	1.47	1.32
8	L	1306	U10	C8-C9	6.78	1.46	1.32
8	M	1305	U10	C23-C24	6.61	1.46	1.32
8	M	1305	U10	C13-C14	6.56	1.46	1.32
6	L	1282	BCL	C4D-C3D	-6.34	1.33	1.41
6	M	1302	BCL	C4D-C3D	-6.30	1.33	1.41
6	M	1303	BCL	C4D-C3D	-5.71	1.34	1.41
6	L	1282	BCL	C4C-NC	5.65	1.44	1.32
6	L	1283	BCL	C4D-C3D	-5.60	1.34	1.41
7	M	1304	BPH	C4D-C3D	-5.45	1.34	1.41
6	L	1283	BCL	C1A-NA	5.41	1.44	1.32
6	M	1303	BCL	C4C-NC	5.35	1.44	1.32
8	L	1306	U10	O4-C4	-5.32	1.23	1.36
6	L	1283	BCL	MG-NC	-5.30	1.91	2.07
6	L	1282	BCL	C1A-NA	5.19	1.43	1.32
6	M	1303	BCL	MG-NA	5.18	2.22	2.07
7	M	1304	BPH	C1C-NC	-5.13	1.27	1.38
6	L	1283	BCL	OBD-CAD	5.11	1.29	1.22
6	M	1303	BCL	MG-ND	-5.03	1.93	2.05
6	M	1302	BCL	O2A-CGA	4.96	1.48	1.33
6	M	1303	BCL	C1A-NA	4.95	1.43	1.32
6	M	1302	BCL	C1A-NA	4.89	1.43	1.32
7	M	1284	BPH	C1C-NC	-4.69	1.28	1.38
7	M	1304	BPH	O2D-CGD	4.59	1.45	1.33
6	M	1303	BCL	O2D-CGD	4.52	1.45	1.33
7	M	1284	BPH	O2D-CGD	4.51	1.45	1.33
7	M	1284	BPH	OBD-CAD	4.37	1.28	1.22
6	M	1302	BCL	C4C-NC	4.37	1.41	1.32
6	L	1283	BCL	C4C-NC	4.35	1.41	1.32
8	M	1305	U10	O4-C4	-4.35	1.25	1.36
6	L	1283	BCL	O2A-CGA	4.34	1.46	1.33
6	M	1302	BCL	O2D-CGD	4.33	1.44	1.33
6	L	1282	BCL	O2D-CGD	4.28	1.44	1.33
7	M	1284	BPH	C4D-C3D	-4.06	1.36	1.41
6	M	1302	BCL	OBD-CAD	4.05	1.28	1.22
7	M	1304	BPH	OBD-CAD	4.03	1.28	1.22
6	L	1283	BCL	MG-NA	3.97	2.19	2.07
8	L	1306	U10	O3-C3	-3.88	1.26	1.36
6	L	1283	BCL	MG-NB	3.87	2.13	2.05
6	L	1283	BCL	O2D-CGD	3.87	1.43	1.33
6	M	1303	BCL	O2A-CGA	3.79	1.45	1.33
6	L	1282	BCL	MG-NA	3.77	2.18	2.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1284	BPH	O2A-CGA	3.59	1.44	1.33
8	M	1305	U10	O3-C3	-3.53	1.27	1.36
7	M	1304	BPH	C1A-NA	-3.27	1.26	1.35
6	L	1282	BCL	MG-NB	3.23	2.12	2.05
6	L	1283	BCL	C1C-NC	3.15	1.45	1.39
8	L	1306	U10	C17-C16	-3.14	1.53	1.55
7	M	1304	BPH	O2A-CGA	3.07	1.42	1.33
6	L	1283	BCL	CAA-C2A	3.05	1.59	1.54
6	M	1303	BCL	OBD-CAD	2.95	1.26	1.22
6	L	1282	BCL	C1C-NC	2.91	1.45	1.39
7	M	1284	BPH	C1A-NA	-2.88	1.27	1.35
6	L	1282	BCL	O2A-CGA	2.88	1.42	1.33
6	L	1283	BCL	C2A-C1A	-2.87	1.47	1.52
7	M	1304	BPH	C1B-NB	2.84	1.39	1.36
6	L	1282	BCL	C2A-C1A	-2.73	1.47	1.52
6	L	1283	BCL	C3C-C4C	-2.72	1.48	1.51
6	L	1282	BCL	C3C-C4C	-2.70	1.48	1.51
6	L	1283	BCL	C4B-NB	2.65	1.37	1.34
6	M	1303	BCL	C1B-NB	2.59	1.37	1.34
6	M	1302	BCL	C2A-C1A	-2.57	1.47	1.52
7	M	1304	BPH	C4D-CHA	2.57	1.49	1.39
6	L	1282	BCL	CHC-C1C	2.55	1.42	1.36
8	M	1305	U10	C3-C2	-2.50	1.41	1.48
6	L	1282	BCL	C4D-CHA	2.43	1.49	1.39
10	H	1310	LDA	CM1-N1	-2.42	1.45	1.49
8	M	1305	U10	C6-C1	2.36	1.40	1.35
8	L	1306	U10	C6-C1	2.35	1.40	1.35
6	L	1282	BCL	C1B-NB	2.35	1.37	1.34
6	M	1303	BCL	C4D-CHA	2.34	1.48	1.39
6	M	1302	BCL	C3C-C4C	-2.31	1.48	1.51
7	M	1284	BPH	CHD-C4C	-2.24	1.36	1.41
6	M	1303	BCL	C1C-NC	2.17	1.43	1.39
6	M	1302	BCL	C1C-NC	2.16	1.43	1.39
6	M	1302	BCL	C1B-NB	2.15	1.37	1.34
6	M	1302	BCL	MG-ND	-2.07	2.00	2.05
8	L	1306	U10	C4-C5	-2.06	1.42	1.48
7	M	1304	BPH	CHD-C4C	-2.00	1.36	1.41

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1302	BCL	C1-O2A-CGA	13.04	130.37	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1282	BCL	CMB-C2B-C3B	7.15	136.23	124.97
6	M	1302	BCL	CMB-C2B-C3B	7.05	136.08	124.97
7	M	1304	BPH	C3B-C2B-C1B	-6.99	102.83	107.01
6	L	1282	BCL	CMB-C2B-C1B	-6.92	117.98	128.62
6	L	1283	BCL	CMB-C2B-C1B	-6.67	118.36	128.62
6	M	1302	BCL	CMB-C2B-C1B	-6.44	118.71	128.62
6	L	1282	BCL	CAC-C3C-C4C	-6.14	98.97	112.58
6	L	1283	BCL	CMB-C2B-C3B	6.00	134.41	124.97
7	M	1304	BPH	CMD-C2D-C1D	5.98	135.50	125.81
7	M	1284	BPH	C1D-C2D-C3D	-5.97	101.77	106.89
7	M	1304	BPH	C1D-C2D-C3D	-5.86	101.86	106.89
7	M	1284	BPH	C3B-C2B-C1B	-5.82	103.53	107.01
7	M	1304	BPH	C4-C3-C5	5.68	124.02	115.39
7	M	1284	BPH	CMD-C2D-C1D	5.63	134.93	125.81
8	L	1306	U10	C7-C8-C9	-5.53	117.42	126.76
8	M	1305	U10	C25-C24-C26	5.38	123.57	115.39
6	M	1303	BCL	CAC-C3C-C2C	-5.30	101.72	113.89
6	L	1283	BCL	C2C-C3C-C4C	5.25	108.32	101.05
6	M	1303	BCL	CMB-C2B-C3B	5.13	133.05	124.97
6	M	1303	BCL	CMB-C2B-C1B	-5.09	120.79	128.62
6	L	1283	BCL	O2D-CGD-CBD	4.98	121.47	111.33
7	M	1304	BPH	C3B-C4B-NB	4.95	112.69	107.10
6	M	1303	BCL	O2D-CGD-O1D	-4.85	113.93	123.79
6	M	1303	BCL	CED-O2D-CGD	4.77	127.38	116.02
6	L	1283	BCL	CAC-C3C-C2C	-4.71	103.07	113.89
7	M	1284	BPH	C3B-C4B-NB	4.57	112.26	107.10
8	M	1305	U10	C15-C14-C16	4.48	122.20	115.39
8	M	1305	U10	C17-C18-C19	-4.47	118.15	127.80
6	L	1283	BCL	CAA-C2A-C3A	-4.42	102.58	113.04
6	M	1303	BCL	O2D-CGD-CBD	4.37	120.22	111.33
7	M	1304	BPH	C5-C3-C2	-4.34	112.73	121.08
6	L	1282	BCL	C2A-C3A-C4A	4.32	108.05	101.40
7	M	1304	BPH	O2D-CGD-CBD	4.32	120.12	111.33
8	M	1305	U10	C35-C34-C33	-4.15	115.30	123.52
7	M	1284	BPH	C4D-ND-C1D	-4.09	99.35	108.72
8	L	1306	U10	C10-C9-C11	4.04	121.53	115.39
7	M	1304	BPH	CED-O2D-CGD	4.01	125.55	116.02
6	M	1302	BCL	O2A-CGA-CBA	4.00	124.53	111.94
6	M	1302	BCL	CAA-C2A-C3A	-3.97	103.66	113.04
6	M	1302	BCL	C3A-C2A-C1A	3.96	106.68	101.08
7	M	1284	BPH	O2D-CGD-CBD	3.90	119.28	111.33
10	H	1310	LDA	CM2-N1-CM1	-3.86	104.44	108.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1302	BCL	O2D-CGD-CBD	3.79	119.05	111.33
6	L	1282	BCL	C2C-C3C-C4C	3.77	106.28	101.05
6	M	1303	BCL	CAC-C3C-C4C	-3.73	104.31	112.58
6	M	1303	BCL	CMC-C2C-C1C	-3.71	101.00	111.76
8	M	1305	U10	C36-C34-C33	3.68	128.16	121.08
8	L	1306	U10	O3-C3-C2	3.63	127.93	116.54
6	L	1282	BCL	C3B-C4B-NB	-3.62	105.12	108.64
10	H	1310	LDA	O1-N1-CM1	-3.60	104.17	109.01
8	L	1306	U10	C15-C14-C16	3.57	122.92	114.77
6	L	1282	BCL	C4B-NB-C1B	3.57	111.46	106.76
7	M	1304	BPH	C4D-ND-C1D	-3.54	100.60	108.72
6	L	1282	BCL	CGD-CBD-CHA	3.49	122.82	110.96
8	L	1306	U10	C1M-C1-C6	-3.47	117.31	124.20
6	M	1303	BCL	CMC-C2C-C3C	-3.47	99.24	114.14
8	L	1306	U10	C3M-O3-C3	3.45	128.20	116.48
6	M	1303	BCL	C3C-C2C-C1C	3.44	106.69	101.40
6	M	1303	BCL	C2A-C3A-C4A	3.33	106.53	101.40
6	M	1303	BCL	O2A-CGA-CBA	3.31	122.34	111.94
6	M	1302	BCL	C3B-C4B-NB	-3.31	105.43	108.64
8	L	1306	U10	C7-C6-C5	3.26	122.29	118.75
7	M	1284	BPH	CAA-C2A-C3A	-3.26	105.33	113.04
6	L	1282	BCL	C2D-C1D-ND	-3.26	106.95	109.41
7	M	1304	BPH	CMB-C2B-C3B	3.26	130.10	124.97
6	L	1283	BCL	O2A-CGA-CBA	3.22	122.07	111.94
8	L	1306	U10	C15-C14-C13	-3.21	117.15	123.52
7	M	1304	BPH	C2B-C1B-NB	3.19	114.36	108.16
6	L	1282	BCL	CAC-C3C-C2C	-3.18	106.59	113.89
8	M	1305	U10	C4M-O4-C4	3.12	127.09	116.48
6	M	1302	BCL	C3C-C2C-C1C	3.10	106.17	101.40
6	M	1303	BCL	CHA-C1A-NA	-3.04	119.98	126.22
6	M	1302	BCL	CMA-C3A-C2A	-3.04	101.09	114.14
6	L	1283	BCL	CMC-C2C-C3C	-3.03	101.10	114.14
6	L	1282	BCL	C1-O2A-CGA	3.02	125.43	116.98
7	M	1284	BPH	C2D-C1D-ND	3.00	116.52	106.38
6	M	1302	BCL	C4B-C3B-C2B	3.00	110.60	106.97
6	L	1283	BCL	C4-C3-C5	2.99	119.93	115.39
7	M	1284	BPH	C2B-C1B-NB	2.98	113.96	108.16
6	L	1283	BCL	C1-O2A-CGA	2.98	125.31	116.98
6	L	1282	BCL	CMA-C3A-C2A	-2.97	101.38	114.14
6	L	1282	BCL	CHA-C1A-NA	-2.96	120.14	126.22
8	L	1306	U10	O3-C3-C4	-2.95	112.09	123.80
8	L	1306	U10	C12-C13-C14	-2.94	121.46	127.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	1304	BPH	C1B-NB-C4B	-2.93	101.99	108.72
6	M	1303	BCL	C2B-C1B-NB	-2.90	107.22	109.41
6	M	1303	BCL	OBD-CAD-CBD	-2.89	121.57	125.94
7	M	1284	BPH	O2D-CGD-O1D	-2.89	117.91	123.79
6	M	1303	BCL	C4B-NB-C1B	2.89	110.57	106.76
6	M	1303	BCL	C2C-C3C-C4C	2.89	105.06	101.05
6	L	1282	BCL	CMA-C3A-C4A	-2.88	103.41	111.76
6	L	1282	BCL	C4-C3-C5	2.87	119.75	115.39
6	L	1283	BCL	CMA-C3A-C2A	-2.86	101.85	114.14
6	L	1283	BCL	CAA-CBA-CGA	2.84	122.43	113.27
8	M	1305	U10	C3M-O3-C3	2.84	126.13	116.48
8	M	1305	U10	C16-C14-C13	-2.83	115.64	121.08
8	L	1306	U10	C6-C1-C2	2.83	123.05	120.18
7	M	1304	BPH	CAC-C3C-C4C	2.79	120.36	112.68
6	L	1282	BCL	C3D-CAD-CBD	2.78	111.53	107.60
8	L	1306	U10	O4-C4-C3	-2.78	112.77	123.80
6	L	1282	BCL	O2A-CGA-CBA	2.78	120.67	111.94
8	M	1305	U10	C27-C28-C29	-2.77	121.82	127.80
6	M	1302	BCL	O1D-CGD-CBD	-2.73	118.82	124.42
6	M	1302	BCL	C2A-C1A-CHA	2.70	128.51	123.83
6	M	1303	BCL	C2A-C1A-CHA	2.69	128.50	123.83
6	M	1302	BCL	CBB-CAB-C3B	-2.68	112.45	120.30
8	M	1305	U10	C30-C29-C31	2.66	119.44	115.39
7	M	1284	BPH	C1-O2A-CGA	2.66	124.42	116.98
6	L	1282	BCL	C16-C15-C13	2.66	122.79	115.14
6	L	1283	BCL	CAC-C3C-C4C	-2.65	106.69	112.58
8	M	1305	U10	C32-C33-C34	-2.64	122.10	127.80
6	M	1302	BCL	CHC-C4B-NB	2.64	128.98	124.58
7	M	1284	BPH	C1B-NB-C4B	-2.63	102.69	108.72
6	M	1302	BCL	OBB-CAB-C3B	2.62	124.01	120.07
6	L	1282	BCL	C11-C12-C13	2.62	122.69	115.14
6	L	1283	BCL	CAA-C2A-C1A	-2.62	105.09	111.62
6	M	1302	BCL	C2D-C1D-ND	-2.60	107.45	109.41
6	L	1283	BCL	O1D-CGD-CBD	-2.57	119.15	124.42
6	L	1283	BCL	C2A-C3A-C4A	2.55	105.33	101.40
7	M	1284	BPH	CMB-C2B-C3B	2.55	128.98	124.97
7	M	1304	BPH	CMA-C3A-C4A	-2.53	104.90	112.94
7	M	1304	BPH	C1-O2A-CGA	2.53	124.06	116.98
6	M	1303	BCL	C2D-C1D-ND	-2.53	107.50	109.41
7	M	1284	BPH	C6-C7-C8	-2.52	107.87	115.14
6	M	1303	BCL	C1D-CHD-C4C	-2.51	121.21	125.55
7	M	1304	BPH	OBD-CAD-CBD	-2.50	122.16	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1283	BCL	O2A-CGA-O1A	-2.47	116.69	123.43
7	M	1284	BPH	C4-C3-C5	2.46	119.12	115.39
10	H	1310	LDA	O1-N1-CM2	2.45	112.31	109.01
7	M	1284	BPH	O2A-CGA-CBA	2.44	119.62	111.94
6	M	1302	BCL	C4B-NB-C1B	2.44	109.97	106.76
6	L	1283	BCL	C3A-C2A-C1A	2.43	104.51	101.08
8	L	1306	U10	C7-C6-C1	-2.41	117.43	123.35
6	M	1303	BCL	CHC-C1C-NC	2.40	127.42	124.58
7	M	1304	BPH	O2A-CGA-O1A	-2.39	116.91	123.43
7	M	1284	BPH	CED-O2D-CGD	2.37	121.66	116.02
6	M	1303	BCL	CGD-CBD-CAD	-2.37	102.91	110.96
6	L	1282	BCL	C4B-C3B-C2B	2.36	109.82	106.97
6	L	1283	BCL	C5-C3-C2	-2.35	116.56	121.08
7	M	1304	BPH	C4D-C3D-C2D	2.34	110.20	107.37
7	M	1304	BPH	C2D-C1D-ND	2.34	114.28	106.38
6	L	1282	BCL	CAA-C2A-C3A	-2.33	107.53	113.04
8	M	1305	U10	C22-C23-C24	-2.31	122.81	127.80
6	M	1303	BCL	CMD-C2D-C3D	2.31	128.61	124.97
6	L	1282	BCL	C3C-C2C-C1C	2.29	104.92	101.40
8	L	1306	U10	O4-C4-C5	2.27	123.66	116.54
8	M	1305	U10	C30-C29-C28	-2.27	119.03	123.52
6	L	1282	BCL	C14-C13-C12	2.25	119.27	111.02
7	M	1284	BPH	CBA-CAA-C2A	-2.23	107.41	114.01
6	L	1282	BCL	CHB-C1B-NB	2.22	128.28	124.58
6	M	1302	BCL	CHA-C1A-NA	-2.21	121.68	126.22
8	M	1305	U10	C37-C36-C34	2.21	119.49	114.02
8	M	1305	U10	C26-C24-C23	-2.20	116.84	121.08
6	L	1282	BCL	C2B-C1B-NB	-2.20	107.75	109.41
6	L	1282	BCL	CAA-C2A-C1A	-2.20	106.14	111.62
6	L	1282	BCL	O2D-CGD-CBD	2.19	115.79	111.33
6	L	1283	BCL	O2D-CGD-O1D	-2.19	119.35	123.79
9	M	1309	CDL	OB5-PB2-OB2	-2.18	99.56	106.45
9	M	1309	CDL	OA5-PA1-OA3	-2.16	102.41	109.00
6	M	1302	BCL	CAA-C2A-C1A	-2.16	106.22	111.62
7	M	1304	BPH	O1D-CGD-CBD	-2.16	120.00	124.42
7	M	1284	BPH	C5-C3-C2	-2.13	116.98	121.08
6	L	1283	BCL	C2D-C1D-ND	-2.13	107.80	109.41
6	M	1302	BCL	C2C-C3C-C4C	2.12	103.99	101.05
8	M	1305	U10	C7-C8-C9	-2.10	123.21	126.76
6	M	1303	BCL	C3B-C4B-NB	-2.08	106.61	108.64
6	L	1282	BCL	O2A-CGA-O1A	-2.09	117.73	123.43
6	L	1283	BCL	C1B-CHB-C4A	-2.08	125.73	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1283	BCL	C16-C17-C18	-2.07	105.19	115.69
9	M	1309	CDL	OA2-PA1-OA4	2.06	115.20	109.10
6	M	1302	BCL	O2A-CGA-O1A	-2.06	117.81	123.43
7	M	1284	BPH	OBD-CAD-CBD	-2.06	122.83	125.94
8	M	1305	U10	C20-C19-C21	2.05	118.51	115.39
6	M	1303	BCL	C4A-NA-C1A	2.03	109.32	106.52
6	L	1283	BCL	C3C-C4C-NC	-2.02	109.00	111.60
8	L	1306	U10	C8-C7-C6	2.01	118.04	111.61
7	M	1304	BPH	C3D-CAD-CBD	2.01	110.44	107.60
6	L	1283	BCL	C1D-CHD-C4C	-2.01	122.08	125.55

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	M	1284	BPH	C13
6	M	1303	BCL	C8
6	M	1303	BCL	C13
6	L	1282	BCL	C8
6	L	1282	BCL	C13
6	L	1283	BCL	C8
6	L	1283	BCL	C13
7	M	1304	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	H	235/235 (100%)	-0.11	10 (4%) 34 34	13, 28, 45, 50	0
2	L	281/281 (100%)	-0.22	12 (4%) 34 34	9, 24, 59, 65	0
3	M	300/300 (100%)	-0.40	6 (2%) 62 62	9, 23, 46, 68	0
All	All	816/816 (100%)	-0.25	28 (3%) 43 43	9, 25, 47, 68	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	59	TRP	6.4
2	L	281	GLY	6.2
3	M	301	HIS	5.7
2	L	270	PRO	4.9
1	H	245	ALA	4.5
3	M	300	ASN	4.2
2	L	265	TRP	4.2
2	L	276	PRO	4.1
1	H	92	VAL	4.1
3	M	68	PHE	3.1
1	H	186	GLY	3.0
2	L	274	ASN	3.0
2	L	277	GLY	3.0
2	L	51	TRP	2.9
2	L	62	GLN	2.9
1	H	52	ASN	2.7
1	H	126	HIS	2.7
2	L	63	LEU	2.7
1	H	200	SER	2.6
2	L	269	LEU	2.4
2	L	271	TRP	2.4
3	M	3	TYR	2.4
3	M	2	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	18	TYR	2.2
1	H	82	ASP	2.2
1	H	201	ASN	2.2
3	M	106	ALA	2.1
1	H	93	SER	2.1

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
8	U10	L	1306	24/63	0.21	8.81	46,49,55,56	0
9	CDL	M	1309	10/100	0.12	3.32	15,27,34,36	0
6	BCL	L	1282	66/66	0.13	1.70	15,22,28,37	0
6	BCL	M	1303	66/66	0.12	1.10	11,19,38,43	0
8	U10	M	1305	45/63	0.12	0.74	14,25,46,48	0
7	BPH	M	1304	65/65	0.14	0.62	11,19,73,74	0
10	LDA	H	1310	14/16	0.13	0.46	30,38,42,45	0
7	BPH	M	1284	65/65	0.10	0.04	9,15,31,33	0
6	BCL	M	1302	48/66	0.09	-0.21	14,19,27,29	0
6	BCL	L	1283	66/66	0.09	-0.60	17,19,32,41	0
5	CL	M	1308	1/1	0.05	-1.58	38,38,38,38	0
4	FE2	M	1307	1/1	0.04	-3.76	14,14,14,14	0

6.5 Other polymers ⓘ

There are no such residues in this entry.