



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:45 AM GMT

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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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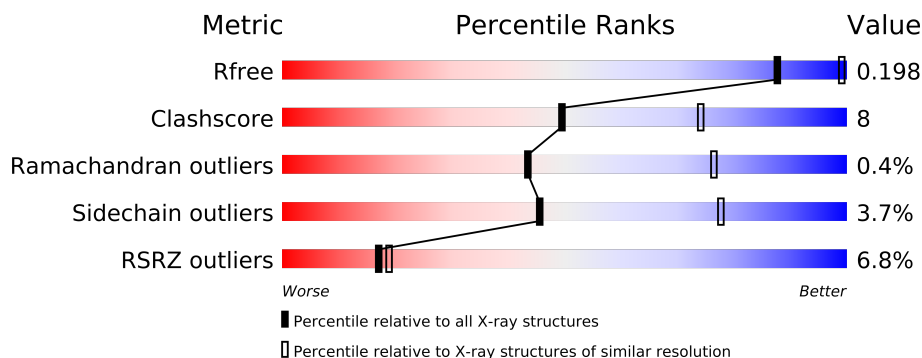
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.70 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))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	L	281	
2	M	307	
3	H	260	

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

Mol	Type	Chain	Res	Geometry	Electron density
10	HTO	L	705	-	X
11	CDL	M	800	-	X
12	PC9	M	801	-	X
12	PC9	M	802	-	X
13	LDA	H	901	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
13	LDA	H	902	-	X
13	LDA	H	903	-	X
13	LDA	L	905	-	X
13	LDA	L	906	-	X
13	LDA	L	909	-	X
13	LDA	M	907	-	X
13	LDA	M	920	-	X
14	GOL	H	706	-	X
14	GOL	H	709	-	X
14	GOL	L	708	-	X
6	PO4	L	701	-	X
6	PO4	M	703	-	X
9	U10	L	502	-	X

## 2 Entry composition

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	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 FE (III) ION (three-letter code: FE) (formula: Fe).

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

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

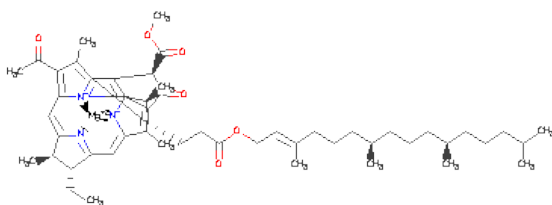
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	K	0	0
			1	1		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



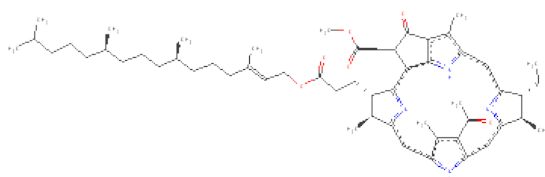
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	O	P	0	0
			5	4	1		
6	L	1	Total	O	P	0	0
			5	4	1		
6	M	1	Total	O	P	0	0
			5	4	1		
6	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula:  $C_{55}H_{74}MgN_4O_6$ ).



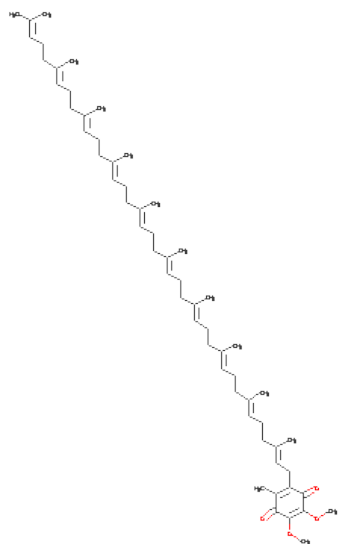
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 8 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).



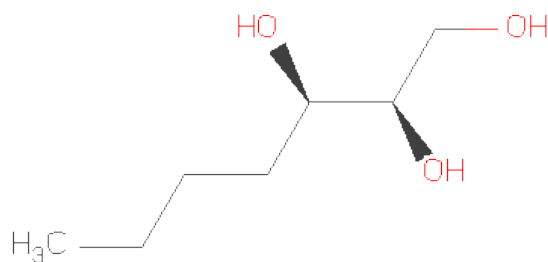
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	M	1	Total	C	N	O	0	0
			65	55	4	6		
8	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 9 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).



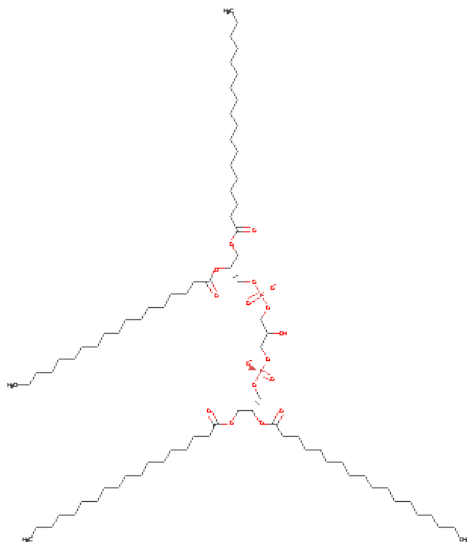
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			48	44	4		
9	L	1	Total	C	O	0	0
			48	44	4		

- Molecule 10 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula:  $C_7H_{16}O_3$ ).



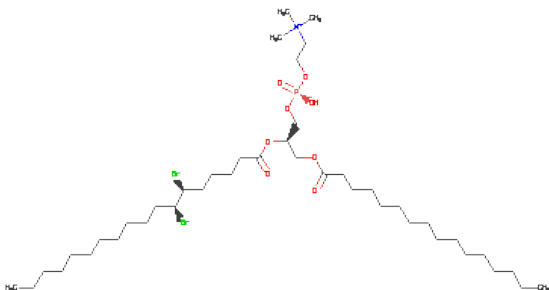
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 11 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



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

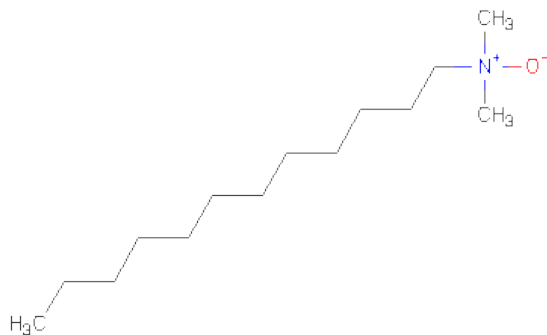
- Molecule 12 is (7R,14S)-14,15-DIBROMO-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM4-OXIDE (three-letter code: PC9) (formula: C<sub>42</sub>H<sub>83</sub>Br<sub>2</sub>NO<sub>8</sub>P).



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

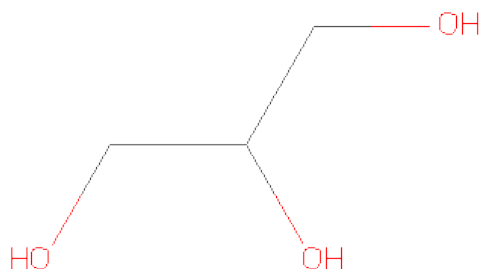


- Molecule 13 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



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

- Molecule 14 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 15 is water.

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

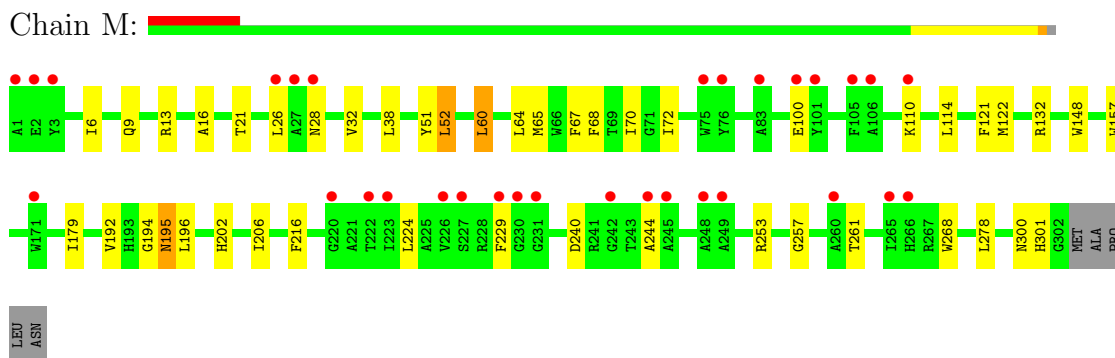
### 3 Residue-property plots

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

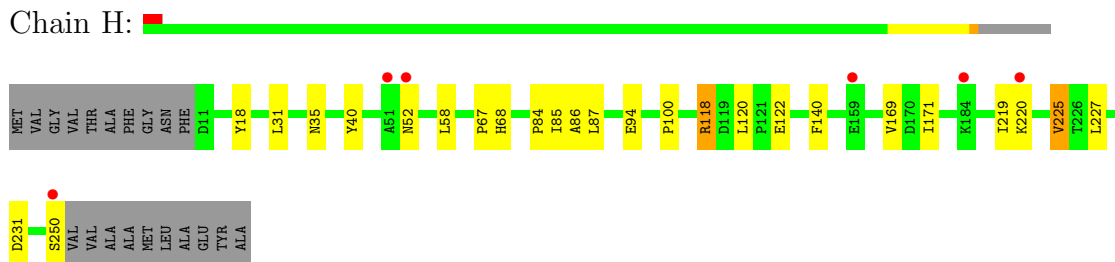
- Molecule 1: Reaction center protein L chain



- Molecule 2: Reaction center protein M chain



- Molecule 3: Reaction center protein H chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.164 , 0.199 0.169 , 0.198	Depositor DCC
$R_{free}$ test set	2853 reflections (4.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.8	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.9	EDS
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 57529 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7921	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, 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 Close contacts ⓘ

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

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (116) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:M:801:PC9:H261	13:H:903:LDA:H121	1.33	1.05
2:M:257:GLY:O	12:M:801:PC9:H32	1.64	0.98
7:M:311:BCL:H41	12: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
11:M:800:CDL:HB4	11:M:800:CDL:HA61	1.66	0.74
7:L:312:BCL:CBB	7:L:312:BCL:HMB1	2.18	0.74
2:M:122:MET:SD	13:M:920:LDA:H123	2.28	0.74
2:M:253[B]:ARG:NH2	12:M:801:PC9:O2	2.24	0.71
7:M:311:BCL:H41	12:M:802:PC9:C44	2.19	0.70
12:M:801:PC9:H141	12:M:801:PC9:H31	1.72	0.70
12:M:801:PC9:H261	13:H:903:LDA:C12	2.16	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:M:311:BCL:CBB	7:M:311:BCL:HMB1	2.22	0.69
9:L:502:U10:H303	7:M:311:BCL:C14	2.25	0.66
7:L:312:BCL:HMB1	7: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:70:ILE:HD13	13:M:920:LDA:HM22	1.78	0.65
2:M:52:LEU:HD21	2:M:60[A]:LEU:HD21	1.78	0.65
12:M:801:PC9:C4	3:H:52:ASN:HD21	2.10	0.64
12:M:801:PC9:C26	13:H:903:LDA:H121	2.20	0.63
7:M:311:BCL:C4	12: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	13:M:920:LDA:HM23	1.80	0.62
2:M:157:TRP:HE1	13:M:920:LDA:H122	1.65	0.61
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.84	0.59
12:M:802:PC9:H121	12:M:802:PC9:H162	1.84	0.59
3:H:118[B]:ARG:CD	3:H:120:LEU:HD12	2.31	0.59
7:M:313:BCL:H191	12:M:802:PC9:C26	2.33	0.58
1:L:178:SER:OG	9:L:502:U10:H302	2.03	0.58
7:M:311:BCL:HBB2	7:M:311:BCL:HMB1	1.86	0.58
11:M:800:CDL:HB4	11:M:800:CDL:CA6	2.33	0.58
2:M:21:THR:HG23	2:M:26:LEU:HD21	1.85	0.57
8:M:401:BPH:CB	8:M:401:BPH:HH	2.35	0.57
7:L:314:BCL:HBB2	7:L:314:BCL:HMB1	1.86	0.56
13:L:906:LDA:HM22	13:L:908:LDA:H52	1.88	0.56
3:H:18:TYR:CD1	13:H:903:LDA:O1	2.59	0.55
9:L:502:U10:H303	7:M:311:BCL:H143	1.88	0.55
13:H:903:LDA:H62	13: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
2:M:67[B]:PHE:HZ	7:M:313:BCL:H203	1.73	0.54
8:L:402:BPH:HBB3	8:L:402:BPH:CMB	2.38	0.54
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.42	0.54
2:M:60[A]:LEU:HD12	8:M:401:BPH:H4C1	1.89	0.53
1:L:119:PHE:CD2	13: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
7:M:313:BCL:H191	12:M:802:PC9:H263	1.90	0.52
13:L:906:LDA:H32	13:L:906:LDA:HM11	1.91	0.51
12:M:801:PC9:H41	3:H:52:ASN:HD21	1.74	0.51
12:M:802:PC9:H51	12:M:802:PC9:O11	2.11	0.51
12:M:802:PC9:H412	12:M:802:PC9:H451	1.93	0.51
9:L:502:U10:H351	9:L:502:U10:H38	1.92	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:76:GLY:HA3	13:L:909:LDA:HM13	1.94	0.50
9:M:501:U10:H23	12:M:801:PC9:H191	1.94	0.50
13:H:903:LDA:H62	13:H:904:LDA:HM21	1.93	0.50
9:L:502:U10:H351	9:L:502:U10:C38	2.42	0.49
8:M:401:BPH:HBC2	8:M:401:BPH:HHD	1.94	0.49
2:M:157:TRP:NE1	13:M:920:LDA:H122	2.26	0.49
13:L:906:LDA:CM2	13:L:908:LDA:H52	2.42	0.49
2:M:65[A]:MET:CE	2:M:121:PHE:CE2	2.95	0.49
2:M:70:ILE:HD13	13:M:920:LDA:CM2	2.42	0.48
1:L:241:VAL:HG21	8:L:402:BPH:HAC1	1.95	0.48
3:H:40:TYR:HB3	3:H:58:LEU:HD21	1.96	0.48
6:M:703:PO4:O3	15:M:1448:HOH:O	2.20	0.48
13:M:920:LDA:HM11	13:M:920:LDA:H22	1.56	0.48
7:M:313:BCL:HMB1	7: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	9:L:502:U10:H352	1.80	0.46
12:M:801:PC9:H2	12:M:801:PC9:O1P	2.16	0.46
2:M:52:LEU:HD21	2:M:60[A]:LEU:CD2	2.46	0.46
12:M:801:PC9:H141	12:M:801:PC9:C3	2.42	0.46
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.98	0.46
12:M:802:PC9:C12	12: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
7:M:311:BCL:HMB1	7:M:311:BCL:HBB3	1.98	0.45
2:M:28:ASN:HB2	2:M:51:TYR:CE2	2.52	0.45
7:L:312:BCL:CGA	7:L:314:BCL:HBC1	2.47	0.45
12:M:801:PC9:BR1	13:H:902:LDA:H102	2.72	0.44
13:L:908:LDA:C3	13:L:908:LDA:HM11	2.46	0.44
1:L:263:TRP:CH2	9:L:502:U10:H352	2.52	0.44
13:L:906:LDA:HM21	13:L:906:LDA:H22	1.71	0.44
2:M:68[A]:PHE:CE1	2:M:72:ILE:HD11	2.52	0.44
12:M:801:PC9:H222	12:M:801:PC9:H252	1.31	0.44
2:M:194:GLY:O	2:M:195:ASN:HB3	2.17	0.44
8:L:402:BPH:CMB	8:L:402:BPH:CBB	2.95	0.43
3:H:122:GLU:HB2	3:H:227:LEU:HD21	1.99	0.43
1:L:53:ALA:HB1	1:L:58:THR:O	2.18	0.43
7:L:314:BCL:CBB	7:L:314:BCL:HMB1	2.49	0.43
8:M:401:BPH:CBC	8: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:M:703:PO4:P	15:M:1448:HOH:O	2.77	0.42
2:M:261:THR:HG23	3:H:35:ASN:O	2.19	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:253[B]:ARG:HH21	12:M:801:PC9:H12	1.85	0.42
2:M:68[A]:PHE:O	2:M:72:ILE:HD13	2.18	0.42
1:L:216:PHE:CD2	9:L:502:U10:H102	2.55	0.42
2:M:301[A]:HIS:HE1	15:M:1031:HOH:O	1.99	0.42
13:L:908:LDA:C3	13:L:908:LDA:CM1	2.97	0.42
2:M:179:ILE:HG23	7:M:311:BCL:HED1	2.02	0.42
1:L:119:PHE:CE2	13:L:908:LDA:H111	2.55	0.42
2:M:6:ILE:HD13	2:M:224:LEU:HD13	2.02	0.41
1:L:76:GLY:CA	13:L:909:LDA:HM13	2.51	0.41
7:M:311:BCL:H61	7: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	11:M:800:CDL:OB6	2.74	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	283/281 (101%)	272 (96%)	10 (4%)	1 (0%)	43	76
2	M	314/307 (102%)	298 (95%)	15 (5%)	1 (0%)	50	82
3	H	246/260 (95%)	240 (98%)	5 (2%)	1 (0%)	43	76
All	All	843/848 (99%)	810 (96%)	30 (4%)	3 (0%)	43	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	195	ASN
3	H	86	ALA

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Mol	Chain	Res	Type
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%)	42	75
2	M	250/240 (104%)	239 (96%)	11 (4%)	39	71
3	H	203/208 (98%)	197 (97%)	6 (3%)	53	84
All	All	677/668 (101%)	651 (96%)	26 (4%)	45	76

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
2	M	216	PHE
2	M	278	LEU
3	H	118[A]	ARG
3	H	118[B]	ARG

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Mol	Chain	Res	Type
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 ⓘ

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 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	$\# Z  > 2$
14	GOL	H	706	-	5,5,5	0.31	0	5,5,5	0.87	0
14	GOL	H	709	-	5,5,5	0.50	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	LDA	H	901	-	15,15,15	3.65	1 (6%)	17,17,17	0.82	1 (5%)
13	LDA	H	902	-	15,15,15	3.59	1 (6%)	17,17,17	0.72	1 (5%)
13	LDA	H	903	-	15,15,15	3.71	1 (6%)	17,17,17	0.95	1 (5%)
13	LDA	H	904	-	15,15,15	3.82	2 (13%)	17,17,17	0.80	1 (5%)
7	BCL	L	312	1	74,74,74	1.43	10 (13%)	97,115,115	1.35	12 (12%)
7	BCL	L	314	1	74,74,74	1.40	7 (9%)	97,115,115	1.64	23 (23%)
8	BPH	L	402	-	70,70,70	1.42	6 (8%)	94,101,101	1.29	12 (12%)
9	U10	L	502	-	48,48,63	1.38	7 (14%)	59,61,79	2.00	17 (28%)
6	PO4	L	701	-	4,4,4	0.29	0	6,6,6	0.31	0
6	PO4	L	702	-	4,4,4	2.07	2 (50%)	6,6,6	0.34	0
10	HTO	L	705	-	9,9,9	0.64	0	10,10,10	0.68	0
14	GOL	L	707	-	5,5,5	0.62	0	5,5,5	1.02	0
14	GOL	L	708	-	5,5,5	0.50	0	5,5,5	0.33	0
13	LDA	L	905	-	15,15,15	3.60	1 (6%)	17,17,17	0.82	0
13	LDA	L	906	-	15,15,15	3.00	1 (6%)	17,17,17	0.50	0
13	LDA	L	908	-	15,15,15	3.51	1 (6%)	17,17,17	0.92	1 (5%)
13	LDA	L	909	-	15,15,15	3.60	1 (6%)	17,17,17	1.12	2 (11%)
7	BCL	M	311	2	74,74,74	1.44	9 (12%)	97,115,115	1.80	25 (25%)
7	BCL	M	313	2	74,74,74	1.50	11 (14%)	97,115,115	1.63	22 (22%)
8	BPH	M	401	-	70,70,70	1.48	11 (15%)	94,101,101	1.62	21 (22%)
9	U10	M	501	-	48,48,63	1.11	4 (8%)	59,61,79	1.95	14 (23%)
6	PO4	M	703	-	4,4,4	0.22	0	6,6,6	0.31	0
6	PO4	M	704	-	4,4,4	0.83	0	6,6,6	0.34	0
11	CDL	M	800	-	80,80,99	1.53	6 (7%)	92,92,111	1.38	10 (10%)
12	PC9	M	801	-	53,53,53	1.09	6 (11%)	63,63,63	1.46	9 (14%)
12	PC9	M	802	-	53,53,53	0.98	4 (7%)	63,63,63	1.43	7 (11%)
13	LDA	M	907	-	15,15,15	3.32	1 (6%)	17,17,17	1.18	2 (11%)
13	LDA	M	920	-	15,15,15	3.16	1 (6%)	17,17,17	1.45	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	GOL	H	706	-	-	0/4/4/4	0/0/0/0
14	GOL	H	709	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	LDA	H	901	-	-	0/13/13/13	0/0/0/0
13	LDA	H	902	-	-	0/13/13/13	0/0/0/0
13	LDA	H	903	-	-	0/13/13/13	0/0/0/0
13	LDA	H	904	-	-	0/13/13/13	0/0/0/0
7	BCL	L	312	1	-	0/41/137/137	0/0/9/9
7	BCL	L	314	1	-	0/41/137/137	0/0/9/9
8	BPH	L	402	-	2/2/18/22	0/49/105/105	0/0/6/6
9	U10	L	502	-	-	0/45/69/87	0/1/1/1
6	PO4	L	701	-	-	0/0/0/0	0/0/0/0
6	PO4	L	702	-	-	0/0/0/0	0/0/0/0
10	HTO	L	705	-	-	0/10/10/10	0/0/0/0
14	GOL	L	707	-	-	0/4/4/4	0/0/0/0
14	GOL	L	708	-	-	0/4/4/4	0/0/0/0
13	LDA	L	905	-	-	0/13/13/13	0/0/0/0
13	LDA	L	906	-	-	0/13/13/13	0/0/0/0
13	LDA	L	908	-	-	0/13/13/13	0/0/0/0
13	LDA	L	909	-	-	0/13/13/13	0/0/0/0
7	BCL	M	311	2	-	0/41/137/137	0/0/9/9
7	BCL	M	313	2	-	0/41/137/137	0/0/9/9
8	BPH	M	401	-	2/2/18/22	0/49/105/105	0/0/6/6
9	U10	M	501	-	-	0/45/69/87	0/1/1/1
6	PO4	M	703	-	-	0/0/0/0	0/0/0/0
6	PO4	M	704	-	-	0/0/0/0	0/0/0/0
11	CDL	M	800	-	1/1/9/9	0/91/91/110	0/0/0/0
12	PC9	M	801	-	-	0/60/60/60	0/0/0/0
12	PC9	M	802	-	-	0/60/60/60	0/0/0/0
13	LDA	M	907	-	-	0/13/13/13	0/0/0/0
13	LDA	M	920	-	-	0/13/13/13	0/0/0/0

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	904	LDA	O1-N1	-14.39	1.25	1.39
13	H	903	LDA	O1-N1	-14.27	1.26	1.39
13	H	901	LDA	O1-N1	-13.94	1.26	1.39
13	L	909	LDA	O1-N1	-13.77	1.26	1.39
13	L	905	LDA	O1-N1	-13.72	1.26	1.39
13	H	902	LDA	O1-N1	-13.70	1.26	1.39
13	L	908	LDA	O1-N1	-13.41	1.26	1.39
13	M	907	LDA	O1-N1	-12.64	1.27	1.39
13	M	920	LDA	O1-N1	-11.88	1.28	1.39
13	L	906	LDA	O1-N1	-11.38	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	402	BPH	C1D-CHD	7.56	1.43	1.35
11	M	800	CDL	C43-C42	-7.31	1.52	1.55
8	M	401	BPH	C1D-CHD	6.32	1.42	1.35
7	M	313	BCL	MG-NA	6.10	2.25	2.07
7	L	312	BCL	C1B-C2B	5.51	1.47	1.40
7	L	314	BCL	C1B-C2B	5.16	1.46	1.40
11	M	800	CDL	OA8-CA7	5.15	1.49	1.33
11	M	800	CDL	OB6-CB5	5.10	1.49	1.34
7	M	311	BCL	C1B-NB	5.08	1.40	1.34
7	M	311	BCL	C3B-C4B	4.97	1.48	1.40
7	M	313	BCL	C1B-C2B	4.52	1.45	1.40
8	M	401	BPH	C3B-C4B	4.42	1.47	1.40
11	M	800	CDL	OA6-CA5	4.39	1.47	1.34
9	L	502	U10	O3-C3	4.32	1.47	1.36
7	L	314	BCL	C3B-C4B	4.17	1.46	1.40
8	L	402	BPH	C3B-C4B	4.16	1.46	1.40
11	M	800	CDL	OB8-CB7	3.98	1.45	1.33
7	L	314	BCL	MG-NB	3.92	2.13	2.05
9	L	502	U10	O4-C4	3.78	1.46	1.36
7	L	314	BCL	C1A-NA	3.64	1.40	1.32
7	M	311	BCL	C1B-C2B	3.55	1.44	1.40
7	L	312	BCL	C3B-C4B	3.54	1.45	1.40
7	L	312	BCL	MG-NA	3.45	2.17	2.07
7	M	311	BCL	MG-NA	3.42	2.17	2.07
9	M	501	U10	O3-C3	3.38	1.45	1.36
7	L	312	BCL	C4B-NB	3.35	1.38	1.34
7	M	313	BCL	C3B-C4B	3.31	1.45	1.40
7	M	313	BCL	C3C-C4C	-3.27	1.47	1.51
7	M	313	BCL	C1C-NC	-3.21	1.32	1.39
7	M	311	BCL	C4C-NC	3.21	1.39	1.32
8	M	401	BPH	C1B-NB	3.17	1.39	1.36
9	L	502	U10	C28-C29	3.14	1.39	1.32
12	M	801	PC9	C1-C2	3.12	1.59	1.50
7	M	311	BCL	C1A-NA	3.07	1.39	1.32
8	M	401	BPH	OBD-CAD	-2.98	1.18	1.22
9	M	501	U10	O4-C4	2.97	1.44	1.36
12	M	801	PC9	P-O1P	2.96	1.62	1.51
7	L	314	BCL	C4C-NC	2.96	1.38	1.32
7	L	314	BCL	C1C-NC	-2.93	1.32	1.39
7	M	313	BCL	C4C-NC	2.91	1.38	1.32
7	L	312	BCL	C1B-NB	2.91	1.38	1.34
7	L	312	BCL	MG-NB	2.88	2.11	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	802	PC9	O2-C2	-2.83	1.39	1.46
6	L	702	PO4	P-O2	2.82	1.64	1.52
7	L	312	BCL	C1A-NA	2.81	1.38	1.32
6	L	702	PO4	P-O1	2.80	1.67	1.52
7	M	313	BCL	C1A-NA	2.77	1.38	1.32
7	M	313	BCL	C4B-NB	2.74	1.38	1.34
13	H	904	LDA	C1-N1	-2.72	1.46	1.51
8	L	402	BPH	C4C-NC	2.68	1.41	1.34
12	M	802	PC9	O3-C3	2.66	1.51	1.45
12	M	802	PC9	P-O1P	2.63	1.61	1.51
7	L	312	BCL	C4C-NC	2.61	1.38	1.32
7	L	312	BCL	MG-NC	2.59	2.14	2.07
8	M	401	BPH	C4D-ND	-2.58	1.34	1.38
9	L	502	U10	C13-C14	2.57	1.38	1.32
11	M	800	CDL	C58-C57	-2.54	1.54	1.55
7	M	313	BCL	MG-NB	2.49	2.10	2.05
8	M	401	BPH	CHA-C1A	-2.47	1.36	1.45
12	M	801	PC9	O3-C3	2.42	1.50	1.45
12	M	801	PC9	BR1-C36	-2.39	1.91	1.97
8	M	401	BPH	C3D-CAD	-2.39	1.42	1.47
7	L	312	BCL	C1C-NC	-2.38	1.34	1.39
8	L	402	BPH	CHA-C1A	-2.38	1.36	1.45
8	M	401	BPH	C1C-NC	-2.33	1.33	1.38
9	L	502	U10	C41-C39	2.30	1.53	1.40
7	M	311	BCL	OBD-CAD	2.25	1.25	1.22
8	L	402	BPH	C1B-NB	2.23	1.38	1.36
12	M	801	PC9	O2-C2	2.22	1.52	1.46
8	L	402	BPH	C4-C3	2.22	1.56	1.50
7	L	314	BCL	C4B-NB	2.20	1.37	1.34
8	M	401	BPH	C1B-CHB	-2.19	1.37	1.46
12	M	802	PC9	O3-C11	2.18	1.40	1.33
9	L	502	U10	C3-C2	-2.14	1.42	1.48
9	M	501	U10	C41-C39	2.12	1.52	1.40
7	M	311	BCL	CHC-C1C	2.12	1.41	1.36
7	M	311	BCL	C4A-NA	-2.12	1.34	1.39
7	M	313	BCL	CHB-C4A	2.11	1.41	1.36
9	M	501	U10	C13-C14	2.08	1.37	1.32
9	L	502	U10	C26-C24	2.07	1.56	1.51
7	M	313	BCL	CBA-CGA	-2.07	1.44	1.50
8	M	401	BPH	C4A-NA	-2.06	1.34	1.38
8	M	401	BPH	C5-C3	2.04	1.56	1.51
12	M	801	PC9	C32-C31	2.02	1.56	1.50

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	502	U10	C25-C24-C26	6.62	125.46	115.39
12	M	802	PC9	O2-C31-C32	5.85	124.38	111.56
11	M	800	CDL	OB6-CB5-C51	5.81	124.28	111.56
9	M	501	U10	C30-C29-C31	5.42	123.63	115.39
12	M	801	PC9	O2-C31-C32	5.25	123.06	111.56
8	L	402	BPH	C1-C2-C3	-5.13	117.07	126.19
7	M	313	BCL	C2B-C1B-NB	-4.96	105.67	109.41
7	L	314	BCL	CAA-C2A-C3A	-4.92	101.40	113.04
9	M	501	U10	C17-C18-C19	-4.89	117.25	127.80
7	M	311	BCL	C5-C3-C2	4.87	130.46	121.08
7	M	311	BCL	C1-O2A-CGA	4.77	130.35	116.98
9	M	501	U10	C32-C33-C34	-4.62	117.82	127.80
8	M	401	BPH	OBD-CAD-CBD	-4.53	119.09	125.94
9	L	502	U10	C25-C24-C23	-4.48	114.65	123.52
7	M	311	BCL	CMB-C2B-C1B	-4.32	121.98	128.62
8	M	401	BPH	C1-C2-C3	-4.29	118.56	126.19
9	L	502	U10	C12-C13-C14	-4.28	118.56	127.80
7	M	313	BCL	CMD-C2D-C3D	4.21	131.60	124.97
7	L	314	BCL	CMB-C2B-C1B	-4.13	122.27	128.62
9	L	502	U10	C7-C8-C9	-4.11	119.81	126.76
8	M	401	BPH	O2D-CGD-CBD	4.07	119.62	111.33
7	M	313	BCL	CAC-C3C-C2C	-4.04	104.61	113.89
11	M	800	CDL	OB8-CB7-C71	4.01	124.57	111.94
11	M	800	CDL	OA6-CA5-C11	3.96	120.24	111.56
7	L	312	BCL	C2C-C1C-NC	3.95	115.75	110.95
12	M	801	PC9	O2-C2-C1	3.94	122.88	108.40
9	M	501	U10	C26-C27-C28	-3.93	100.39	111.62
9	M	501	U10	C7-C6-C5	-3.77	114.67	118.75
7	L	314	BCL	CAC-C3C-C2C	-3.73	105.33	113.89
12	M	802	PC9	C3-C2-C1	-3.71	103.39	111.86
8	M	401	BPH	CAC-C3C-C4C	3.69	122.85	112.68
7	M	311	BCL	O2A-C1-C2	3.67	116.51	108.55
7	M	313	BCL	CHA-C1A-NA	-3.64	118.74	126.22
11	M	800	CDL	OA8-CA7-C31	3.63	123.34	111.94
12	M	801	PC9	C2-O2-C31	-3.59	109.06	117.92
9	M	501	U10	C11-C9-C8	-3.58	114.19	121.08
7	M	311	BCL	C2C-C1C-NC	3.57	115.29	110.95
8	M	401	BPH	CAA-C2A-C3A	-3.56	104.62	113.04
13	M	920	LDA	O1-N1-C1	3.55	115.13	110.19
7	L	312	BCL	CAA-C2A-C3A	-3.54	104.67	113.04
9	M	501	U10	C15-C14-C16	3.47	120.67	115.39
8	M	401	BPH	C4-C3-C2	-3.44	116.71	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	312	BCL	C2B-C1B-NB	-3.38	106.86	109.41
12	M	801	PC9	O3-C3-C2	3.35	117.60	108.83
7	M	313	BCL	CMB-C2B-C1B	-3.34	123.48	128.62
11	M	800	CDL	CA4-OA6-CA5	-3.32	109.73	117.92
7	M	311	BCL	CMB-C2B-C3B	3.31	130.18	124.97
7	M	311	BCL	OBD-CAD-CBD	-3.31	120.95	125.94
9	L	502	U10	O2-C2-C3	-3.29	113.67	120.96
7	L	312	BCL	CAA-C2A-C1A	-3.28	103.45	111.62
7	M	311	BCL	OBB-CAB-C3B	3.26	124.96	120.07
7	M	313	BCL	OBD-CAD-CBD	-3.24	121.05	125.94
9	M	501	U10	C31-C29-C28	-3.21	114.90	121.08
9	L	502	U10	C3M-O3-C3	3.19	127.32	116.48
12	M	802	PC9	O3-C11-C12	3.18	121.95	111.94
13	M	907	LDA	O1-N1-C1	3.17	114.60	110.19
7	L	314	BCL	CMB-C2B-C3B	3.17	129.96	124.97
7	M	313	BCL	C4B-NB-C1B	3.14	110.90	106.76
8	M	401	BPH	C1-O2A-CGA	3.13	125.75	116.98
9	L	502	U10	C36-C34-C33	3.12	127.08	121.08
13	M	907	LDA	CM2-N1-CM1	-3.11	105.30	108.85
12	M	802	PC9	C34-C35-C36	-3.10	104.70	113.67
7	M	311	BCL	CAA-C2A-C3A	-3.09	105.73	113.04
7	M	313	BCL	C1-C2-C3	-3.08	120.71	126.19
13	M	920	LDA	C2-C1-N1	-3.04	108.56	113.80
7	M	313	BCL	C1D-C2D-C3D	-3.00	104.33	106.78
7	M	311	BCL	O2D-CGD-CBD	2.99	117.43	111.33
8	L	402	BPH	O2D-CGD-CBD	2.97	117.39	111.33
7	L	314	BCL	C4B-NB-C1B	2.97	110.68	106.76
7	M	311	BCL	C4-C3-C5	-2.95	110.90	115.39
7	L	314	BCL	C2C-C1C-NC	2.94	114.52	110.95
7	M	311	BCL	C6-C5-C3	-2.93	105.81	112.78
7	M	311	BCL	C2B-C1B-NB	-2.92	107.21	109.41
13	L	909	LDA	CM2-N1-CM1	-2.92	105.52	108.85
7	M	313	BCL	C3A-C4A-NA	2.92	114.50	110.95
7	L	314	BCL	C5-C3-C2	-2.91	115.48	121.08
7	M	311	BCL	OBD-CAD-C3D	2.90	133.31	127.91
12	M	802	PC9	O2-C2-C3	-2.90	97.75	108.40
8	L	402	BPH	C4B-C3B-C2B	2.88	109.69	107.60
9	M	501	U10	C26-C24-C23	-2.88	115.55	121.08
9	M	501	U10	C16-C14-C13	-2.87	115.56	121.08
7	L	314	BCL	C2B-C1B-NB	-2.85	107.26	109.41
11	M	800	CDL	OA6-CA5-OA7	-2.85	116.03	123.65
7	L	312	BCL	C4B-NB-C1B	2.84	110.50	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	402	BPH	CAA-C2A-C3A	-2.82	106.38	113.04
8	M	401	BPH	CMB-C2B-C3B	2.81	129.40	124.97
7	M	311	BCL	C4B-NB-C1B	2.81	110.46	106.76
8	M	401	BPH	C7-C6-C5	2.78	121.21	113.01
7	L	314	BCL	O2D-CGD-CBD	2.78	117.00	111.33
12	M	801	PC9	BR2-C37-C38	-2.77	103.99	108.90
8	M	401	BPH	CMC-C2C-C1C	2.76	121.70	112.94
7	M	311	BCL	CHA-C1A-NA	-2.74	120.59	126.22
7	L	314	BCL	C2C-C3C-C4C	2.73	104.84	101.05
9	L	502	U10	C6-C1-C2	-2.71	117.42	120.18
8	L	402	BPH	O2D-CGD-O1D	-2.71	118.29	123.79
7	M	313	BCL	C2A-C1A-CHA	2.70	128.50	123.83
9	L	502	U10	C35-C34-C33	-2.68	118.21	123.52
9	L	502	U10	C22-C23-C24	-2.67	122.05	127.80
13	M	920	LDA	O1-N1-CM1	-2.67	105.42	109.01
7	M	311	BCL	C2C-C3C-C4C	2.66	104.74	101.05
8	L	402	BPH	CAA-C2A-C1A	-2.66	105.74	112.72
7	L	314	BCL	CAA-CBA-CGA	2.65	121.82	113.27
12	M	802	PC9	O3-C3-C2	2.65	115.78	108.83
8	M	401	BPH	CMB-C2B-C1B	-2.64	124.63	128.65
9	L	502	U10	C37-C38-C39	-2.63	122.26	128.63
13	H	904	LDA	C2-C1-N1	-2.62	109.29	113.80
13	L	908	LDA	C2-C1-N1	-2.62	109.29	113.80
7	L	314	BCL	OBb-CAB-C3B	2.62	124.00	120.07
7	L	314	BCL	C1D-C2D-C3D	-2.62	104.64	106.78
8	M	401	BPH	C2C-C1C-NC	2.61	116.41	112.90
9	M	501	U10	C35-C34-C36	2.60	119.35	115.39
7	L	312	BCL	CHA-C1A-NA	-2.60	120.88	126.22
11	M	800	CDL	OB8-CB6-CB4	2.59	115.62	108.83
7	M	311	BCL	C4-C3-C2	-2.56	118.45	123.52
7	M	313	BCL	C4D-CHA-C1A	2.56	127.74	120.32
9	M	501	U10	C40-C39-C38	-2.55	117.51	123.62
7	M	311	BCL	C1-C2-C3	2.53	130.69	126.19
7	L	314	BCL	C4-C3-C5	2.51	119.21	115.39
9	L	502	U10	C36-C37-C38	2.51	118.80	111.62
7	M	313	BCL	C4D-C3D-CAD	-2.50	104.97	108.05
8	M	401	BPH	C5-C3-C2	2.50	125.89	121.08
7	M	311	BCL	C6-C7-C8	2.49	122.32	115.14
9	L	502	U10	C3-C2-C1	2.49	123.95	117.40
7	L	312	BCL	C2A-C1A-NA	2.49	114.00	111.24
9	M	501	U10	C10-C9-C11	2.48	119.17	115.39
7	L	312	BCL	C4-C3-C5	2.48	119.16	115.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	313	BCL	O2A-C1-C2	2.47	113.91	108.55
8	M	401	BPH	CMA-C3A-C4A	-2.46	105.10	112.94
8	M	401	BPH	C4B-C3B-C2B	2.46	109.38	107.60
8	L	402	BPH	CMB-C2B-C1B	-2.45	124.91	128.65
8	M	401	BPH	C2C-C3C-C4C	2.45	105.40	102.06
7	L	314	BCL	CAC-C3C-C4C	-2.44	107.18	112.58
9	M	501	U10	C22-C23-C24	-2.43	122.56	127.80
9	L	502	U10	O4-C4-C5	2.43	124.14	116.54
7	L	312	BCL	CGD-CBD-CHA	2.42	119.18	110.96
7	L	314	BCL	CHA-C1A-NA	-2.40	121.29	126.22
7	L	314	BCL	C2C-C1C-CHC	-2.39	119.37	124.33
8	M	401	BPH	CMD-C2D-C3D	2.39	128.73	124.97
7	L	314	BCL	CBC-CAC-C3C	2.38	119.47	113.61
13	L	909	LDA	O1-N1-CM1	-2.36	105.84	109.01
7	L	312	BCL	C3A-C4A-NA	2.35	113.81	110.95
7	L	314	BCL	C3A-C4A-NA	2.35	113.81	110.95
11	M	800	CDL	OA2-CA2-C1	2.35	115.99	108.62
12	M	801	PC9	O2-C31-O31	-2.33	117.42	123.65
8	M	401	BPH	O2D-CGD-O1D	-2.32	119.07	123.79
7	M	313	BCL	C2C-C1C-CHC	-2.31	119.53	124.33
11	M	800	CDL	OB6-CB4-CB6	2.29	116.82	108.40
9	L	502	U10	C12-C11-C9	-2.28	105.17	112.74
7	L	312	BCL	C1-O2A-CGA	2.27	123.34	116.98
7	L	312	BCL	OBD-CAD-CBD	-2.26	122.53	125.94
11	M	800	CDL	OB8-CB7-OB9	-2.26	117.27	123.43
12	M	802	PC9	BR2-C37-C36	-2.25	105.60	110.23
7	M	311	BCL	C3A-C4A-NA	2.23	113.66	110.95
8	L	402	BPH	CAC-C3C-C2C	2.23	119.00	113.89
13	H	902	LDA	CM2-N1-CM1	-2.22	106.31	108.85
8	L	402	BPH	OBD-CAD-CBD	-2.21	122.60	125.94
8	M	401	BPH	C4D-CHA-CBD	-2.21	104.69	110.15
7	M	313	BCL	CMC-C2C-C3C	-2.20	104.67	114.14
7	M	313	BCL	C2C-C1C-NC	2.18	113.60	110.95
7	M	313	BCL	C2C-C3C-C4C	2.18	104.07	101.05
8	L	402	BPH	CAC-C3C-C4C	2.16	118.63	112.68
12	M	801	PC9	C13-C12-C11	-2.14	105.13	113.51
12	M	801	PC9	BR2-C37-C36	2.12	114.61	110.23
7	M	313	BCL	CGD-CBD-CHA	-2.11	103.79	110.96
13	H	903	LDA	O1-N1-CM1	-2.11	106.17	109.01
13	H	901	LDA	O1-N1-CM2	-2.10	106.18	109.01
7	M	311	BCL	CGD-CBD-CHA	2.10	118.09	110.96
7	M	313	BCL	O2D-CGD-O1D	-2.09	119.53	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	313	BCL	C4-C3-C5	2.09	118.57	115.39
12	M	801	PC9	BR1-C36-C37	-2.09	105.93	110.23
7	M	311	BCL	C3B-C4B-NB	-2.08	106.62	108.64
7	L	314	BCL	C3A-C2A-C1A	2.06	103.99	101.08
7	L	314	BCL	CAA-C2A-C1A	-2.05	106.52	111.62
7	L	314	BCL	C3A-C4A-CHB	-2.04	120.08	124.33
9	L	502	U10	O5-C5-C6	-2.04	117.92	121.67
7	M	311	BCL	OBB-CAB-CBB	-2.03	115.08	120.13
9	L	502	U10	C21-C22-C23	-2.03	105.82	111.62
7	M	313	BCL	C4D-ND-C1D	2.03	109.02	106.57
8	M	401	BPH	CAA-CBA-CGA	2.03	119.80	113.27
7	L	314	BCL	O1D-CGD-CBD	-2.03	120.27	124.42
8	L	402	BPH	CMB-C2B-C3B	2.02	128.14	124.97
7	M	311	BCL	CMA-C3A-C2A	-2.01	105.49	114.14
8	L	402	BPH	C3A-C2A-C1A	2.01	104.47	101.91
8	M	401	BPH	CMA-C3A-C2A	-2.01	105.52	114.14

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	M	800	CDL	CA4
8	M	401	BPH	C8
8	M	401	BPH	C13
8	L	402	BPH	C8
8	L	402	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	L	281/281 (100%)	-0.00	16 (5%) 23 25	42, 51, 63, 72	0
2	M	302/307 (98%)	0.29	31 (10%) 7 7	40, 51, 61, 88	1 (0%)
3	H	240/260 (92%)	-0.15	6 (2%) 54 61	39, 51, 59, 83	0
All	All	823/848 (97%)	0.06	53 (6%) 17 21	39, 51, 62, 88	1 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	271	TRP	4.5
3	H	250	SER	4.0
2	M	1	ALA	3.9
1	L	281	GLY	3.8
2	M	244	ALA	3.7
2	M	76	TYR	3.3
1	L	277	GLY	3.2
2	M	265	ILE	3.2
2	M	27	ALA	3.0
3	H	51	ALA	3.0
2	M	231	GLY	3.0
1	L	269	LEU	3.0
1	L	59	TRP	2.9
1	L	270	PRO	2.8
1	L	73	TYR	2.8
2	M	248	ALA	2.7
1	L	274	ASN	2.7
2	M	227	SER	2.7
3	H	220	LYS	2.7
2	M	226	VAL	2.7
2	M	2[A]	GLU	2.7
2	M	223	ILE	2.7
1	L	278	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	276[A]	PRO	2.6
2	M	106	ALA	2.6
2	M	245	ALA	2.6
2	M	230	GLY	2.6
2	M	222	THR	2.6
3	H	159	GLU	2.6
2	M	249	ALA	2.6
2	M	266	HIS	2.6
2	M	171	TRP	2.3
2	M	83	ALA	2.3
2	M	100	GLU	2.3
1	L	279	ILE	2.3
2	M	105	PHE	2.3
3	H	52	ASN	2.3
1	L	22	PHE	2.3
2	M	3	TYR	2.2
2	M	220	GLY	2.2
2	M	28	ASN	2.2
2	M	110	LYS	2.2
2	M	75	TRP	2.1
1	L	265	TRP	2.1
1	L	280	ASN	2.1
2	M	242	GLY	2.1
3	H	184	LYS	2.1
1	L	26	VAL	2.1
2	M	101	TYR	2.1
2	M	229	PHE	2.1
2	M	260	ALA	2.0
1	L	272	TRP	2.0
2	M	26	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
13	LDA	H	902	16/16	0.72	31.58	64,66,72,72	16
13	LDA	L	905	16/16	0.96	20.85	61,66,70,71	16
13	LDA	L	906	16/16	0.43	16.69	51,55,69,70	16
13	LDA	M	920	16/16	0.62	13.23	49,53,65,66	16
6	PO4	M	703	5/5	0.47	6.88	64,65,66,67	5
13	LDA	H	901	16/16	0.55	6.64	52,55,66,66	16
13	LDA	H	903	16/16	0.59	6.50	49,55,63,63	16
13	LDA	L	909	16/16	0.46	6.35	50,54,71,73	16
12	PC9	M	802	54/54	0.45	4.78	42,54,70,73	54
10	HTO	L	705	10/10	0.23	4.46	56,60,62,65	10
9	U10	L	502	48/63	0.45	4.19	37,56,66,67	48
11	CDL	M	800	81/100	0.40	3.92	50,69,80,87	81
12	PC9	M	801	54/54	0.41	3.66	30,52,79,80	54
14	GOL	L	708	6/6	0.24	3.55	49,57,59,60	0
14	GOL	H	706	6/6	0.49	3.19	59,62,63,65	6
14	GOL	H	709	6/6	0.23	3.06	50,51,52,53	6
6	PO4	L	701	5/5	0.41	2.87	65,65,66,67	5
13	LDA	M	907	16/16	0.32	2.76	60,64,70,71	16
7	BCL	M	311	66/66	0.26	1.69	41,51,103,104	0
13	LDA	L	908	16/16	0.45	1.67	51,59,72,73	16
14	GOL	L	707	6/6	0.28	1.29	58,61,62,66	6
8	BPH	M	401	65/65	0.23	0.99	44,52,96,97	0
7	BCL	M	313	66/66	0.19	0.61	41,48,72,80	0
7	BCL	L	312	66/66	0.16	0.42	40,48,55,59	0
9	U10	M	501	48/63	0.26	0.31	46,54,80,83	0
7	BCL	L	314	66/66	0.15	0.21	38,46,66,73	0
8	BPH	L	402	65/65	0.15	-0.04	42,49,55,56	0
6	PO4	L	702	5/5	0.24	-0.10	64,65,66,68	5
6	PO4	M	704	5/5	0.22	-0.42	54,54,56,58	5
4	FE	M	500	1/1	0.19	-2.08	52,52,52,52	0
5	K	H	700	1/1	0.08	-2.58	52,52,52,52	0
13	LDA	H	904	16/16	0.35	-	60,62,66,66	16

## 6.5 Other polymers ⓘ

There are no such residues in this entry.