



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:09 PM GMT

PDB ID : 2HH1  
Title : Reaction centre from Rhodobacter sphaeroides strain R-26.1 complexed with dibrominated phosphatidylcholine  
Authors : Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.  
Deposited on : 2006-06-27  
Resolution : 2.55 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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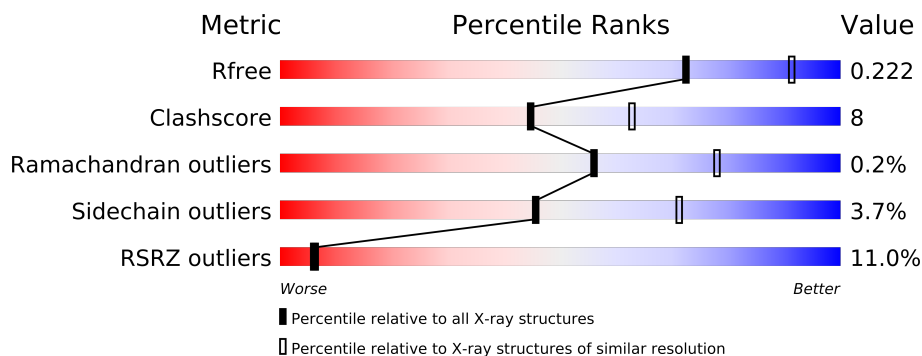
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.55 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	3413 (2.58-2.50)
Clashscore	79885	4284 (2.58-2.50)
Ramachandran outliers	78287	4193 (2.58-2.50)
Sidechain outliers	78261	4195 (2.58-2.50)
RSRZ outliers	66119	3414 (2.58-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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
11	CDL	M	800	-	X
12	PC7	H	801	-	X
13	PC9	L	802	-	X
14	LDA	H	901	-	X
14	LDA	H	903	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
14	LDA	H	904	-	X
14	LDA	H	905	-	X
14	LDA	L	902	-	X
14	LDA	L	906	-	X
14	LDA	M	907	-	X
14	LDA	M	920	-	X
15	GOL	H	705	-	X
15	GOL	H	706	-	X
15	GOL	H	708	-	X
6	PO4	M	704	-	X
9	U10	L	502	-	X

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 7923 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	2	0
			2234	1508	355	363	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	9	0
			2466	1643	403	409	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	244	Total	C	N	O	S	0	9	0
			1891	1207	328	346	10			

- 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).

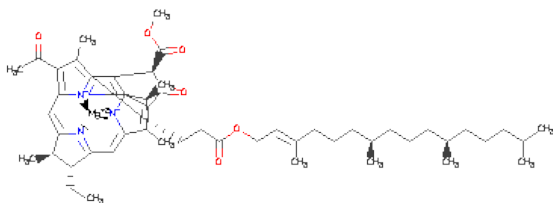
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	K	0	0
			1	1		

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



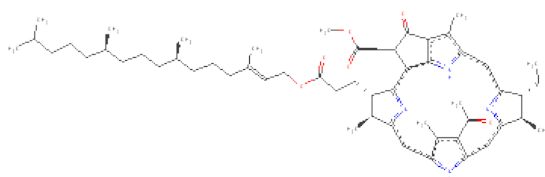
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	M	1	Total	O	P	0	0
			5	4	1		
6	M	1	Total	O	P	0	0
			5	4	1		
6	L	1	Total	O	P	0	0
			5	4	1		
6	M	1	Total	O	P	0	0
			5	4	1		

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



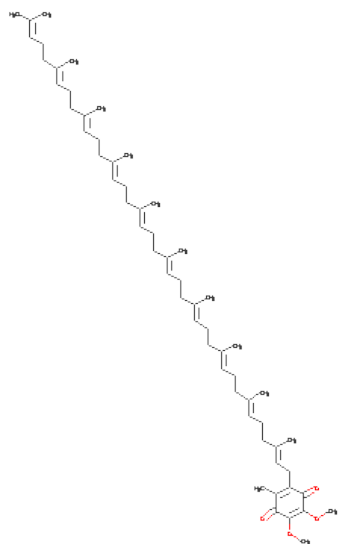
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



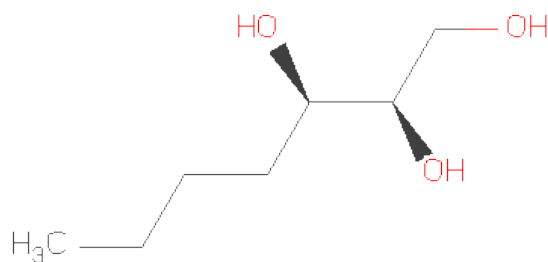
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	M	1	Total	C	N	O	0	0
			65	55	4	6		
8	L	1	Total	C	N	O	0	0
			65	55	4	6		

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



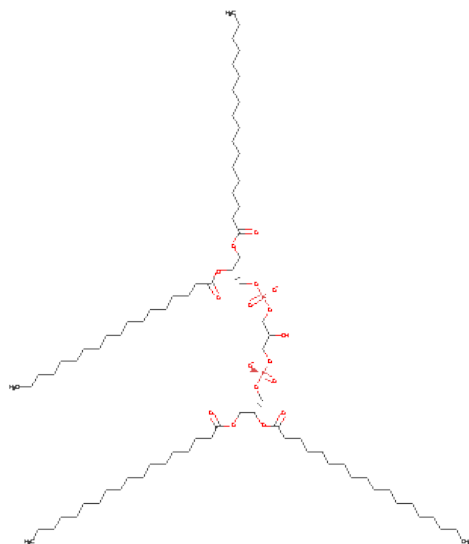
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			48	44	4		
9	L	1	Total	C	O	0	0
			48	44	4		

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



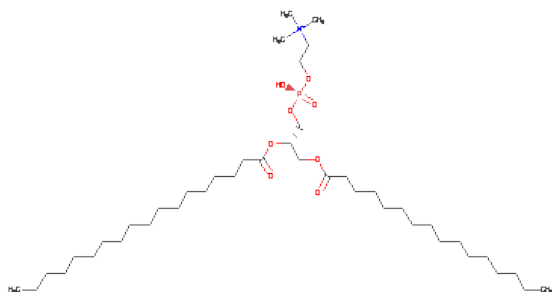
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	H	1	Total	C	O	0	0
			10	7	3		

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



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

- Molecule 12 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM4-OXIDE (three-letter code: PC7) (formula: C<sub>42</sub>H<sub>85</sub>NO<sub>8</sub>P).

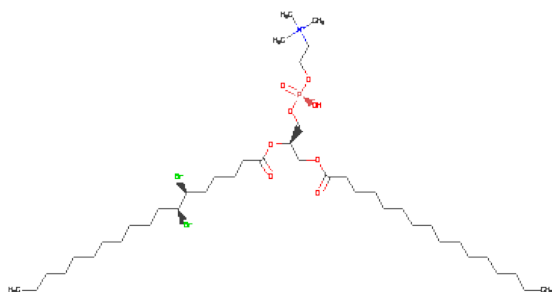


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	H	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 13 is (7R,14S)-14,15-DIBROMO-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-

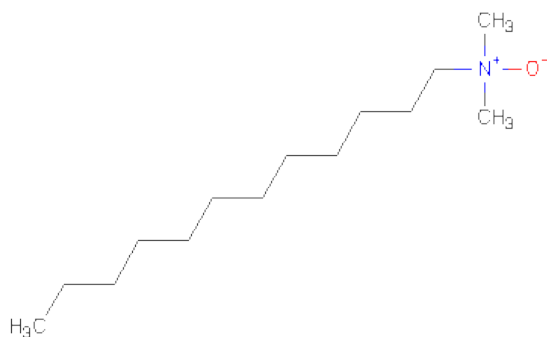


-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM  
M4-OXIDE (three-letter code: PC9) (formula:  $C_{42}H_{83}Br_2NO_8P$ ).



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

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



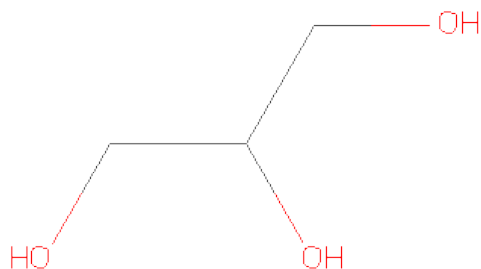
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
14	H	1	16	14	1	1	0	0

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

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



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

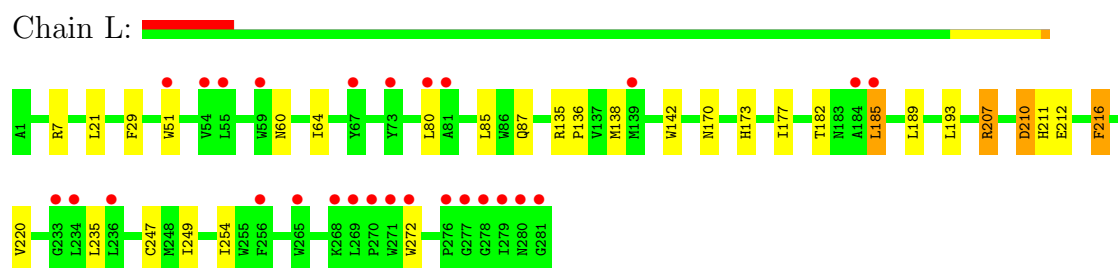
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	H	225	Total 225	O 225	0	0
16	L	113	Total 113	O 113	0	0
16	M	139	Total 139	O 139	0	0

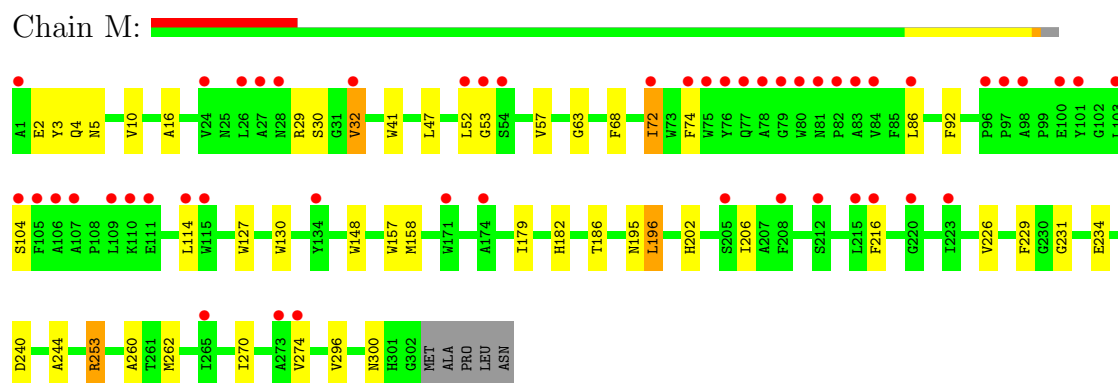
### 3 Residue-property plots

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.

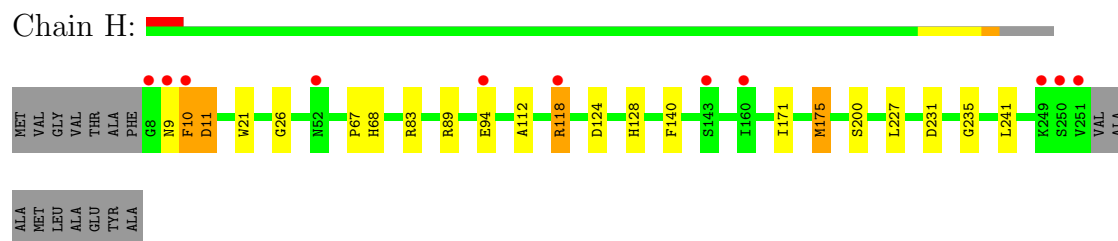
- Molecule 1: Reaction center protein L chain



- 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, $\alpha$ , $\beta$ , $\gamma$	139.54Å 139.54Å 183.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.03 – 2.55 45.68 – 2.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.03-2.55) 100.0 (45.68-2.55)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.69 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.178 , 0.210 0.197 , 0.222	Depositor DCC
$R_{free}$ test set	3362 reflections (5.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.3	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 78.0	EDS
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 67963 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7923	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, GOL, LDA, PC9, HTO, BPH, K, PC7, CDL, 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	0.89	0/2334	0.75	2/3194 (0.1%)
2	M	0.88	1/2590 (0.0%)	0.80	5/3532 (0.1%)
3	H	0.93	0/1986	0.86	3/2697 (0.1%)
All	All	0.90	1/6910 (0.0%)	0.80	10/9423 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	260	ALA	CA-CB	5.14	1.63	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	253[A]	ARG	NE-CZ-NH2	-7.34	116.63	120.30
2	M	253[B]	ARG	NE-CZ-NH2	-7.34	116.63	120.30
3	H	83	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	L	210	ASP	CB-CG-OD1	5.57	123.32	118.30
1	L	7	ARG	NE-CZ-NH2	5.51	123.05	120.30
3	H	124	ASP	CB-CG-OD1	5.42	123.18	118.30
2	M	240	ASP	CB-CG-OD1	5.33	123.09	118.30
3	H	83	ARG	NE-CZ-NH1	5.29	122.94	120.30
2	M	29	ARG	NE-CZ-NH1	5.11	122.86	120.30
2	M	29	ARG	NE-CZ-NH2	-5.10	117.75	120.30

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	2234	0	2193	21	0
2	M	2466	0	2371	35	0
3	H	1891	0	1902	14	0
4	M	1	0	0	0	0
5	H	1	0	0	0	0
6	L	5	0	0	1	0
6	M	15	0	0	0	0
7	L	132	0	148	6	0
7	M	132	0	148	19	0
8	L	65	0	75	0	0
8	M	65	0	76	11	0
9	L	48	0	63	12	0
9	M	48	0	63	1	0
10	H	10	0	16	1	0
11	M	81	0	106	2	0
12	H	52	0	84	8	0
13	L	54	0	80	36	0
14	H	64	0	124	7	0
14	L	32	0	62	1	0
14	M	32	0	62	1	0
15	H	18	0	24	2	0
16	H	225	0	0	2	0
16	L	113	0	0	1	0
16	M	139	0	0	3	0
All	All	7923	0	7597	128	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 (128) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:L:802:PC9:H442	13:L:802:PC9:C48	1.58	1.26
13:L:802:PC9:C44	13:L:802:PC9:H482	1.67	1.19
9:L:502:U10:H351	9:L:502:U10:H38	1.28	1.15

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:L:802:PC9:H483	8:M:401:BPH:HED1	1.40	1.03
9:L:502:U10:H153	13:L:802:PC9:H471	1.38	1.02
1:L:189:LEU:CD1	13:L:802:PC9:H472	1.96	0.95
13:L:802:PC9:C48	13:L:802:PC9:C44	2.29	0.94
12:H:801:PC7:H73	14:H:905:LDA:H112	1.50	0.92
12:H:801:PC7:H451	14:H:901:LDA:H122	1.53	0.89
9:L:502:U10:H351	9:L:502:U10:C38	2.04	0.87
9:L:502:U10:H153	13:L:802:PC9:C47	2.03	0.87
2:M:253[B]:ARG:NH1	16:M:1468:HOH:O	2.07	0.85
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.59	0.84
7:M:311:BCL:H41	7:M:311:BCL:H71	1.61	0.81
13:L:802:PC9:C26	8:M:401:BPH:HED2	2.12	0.79
12:H:801:PC7:H431	14:H:901:LDA:H121	1.69	0.75
13:L:802:PC9:H483	8:M:401:BPH:CED	2.17	0.73
12:H:801:PC7:O31	12:H:801:PC7:H32	1.87	0.72
9:L:502:U10:C15	13:L:802:PC9:H471	2.18	0.69
1:L:189:LEU:HD12	13:L:802:PC9:H472	1.72	0.69
13:L:802:PC9:H231	7:M:313:BCL:C20	2.23	0.69
2:M:2[B]:GLU:O	2:M:4:GLN:NE2	2.26	0.68
7:L:314:BCL:HBB2	7:L:314:BCL:HMB1	1.77	0.67
13:L:802:PC9:C23	7:M:313:BCL:C20	2.73	0.66
3:H:128[B]:HIS:HD1	15:H:708:GOL:C2	2.09	0.65
7:M:311:BCL:C7	7:M:311:BCL:H41	2.19	0.65
7:M:311:BCL:H102	7:M:313:BCL:H191	1.79	0.65
13:L:802:PC9:H52	2:M:30:SER:HA	1.79	0.64
13:L:802:PC9:H442	13:L:802:PC9:H482	0.75	0.64
13:L:802:PC9:C23	7:M:313:BCL:H201	2.28	0.64
2:M:63:GLY:HA3	8:M:401:BPH:H5C2	1.79	0.63
2:M:270:ILE:HD13	11:M:800:CDL:H711	1.81	0.62
7:M:311:BCL:HBB2	7:M:311:BCL:HMB1	1.81	0.62
12:H:801:PC7:C7	14:H:905:LDA:H112	2.28	0.62
9:L:502:U10:C12	13:L:802:PC9:H471	2.30	0.61
7:M:311:BCL:CBB	7:M:311:BCL:HMB1	2.31	0.61
2:M:179:ILE:HG23	7:M:311:BCL:HED1	1.83	0.60
2:M:72:ILE:HD13	2:M:72:ILE:N	2.17	0.59
2:M:262:MET:HE3	2:M:262:MET:CA	2.31	0.59
13:L:802:PC9:BR2	2:M:47:LEU:HD22	2.58	0.59
2:M:68[A]:PHE:CD1	2:M:72:ILE:HD11	2.38	0.58
2:M:253[A]:ARG:NH2	16:M:1461:HOH:O	2.36	0.58
13:L:802:PC9:H231	7:M:313:BCL:H203	1.86	0.58
13:L:802:PC9:H202	13:L:802:PC9:H251	1.85	0.57
1:L:185:LEU:HD13	13:L:802:PC9:H461	1.86	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:200:SER:H	10:H:709:HTO:H73	1.69	0.57
9:L:502:U10:H153	13:L:802:PC9:C46	2.35	0.57
7:M:311:BCL:C4	7:M:311:BCL:H71	2.34	0.56
9:L:502:U10:H122	13:L:802:PC9:C48	2.36	0.56
2:M:68[A]:PHE:CE1	2:M:72:ILE:HD11	2.41	0.56
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.88	0.56
7:L:314:BCL:CBB	7:L:314:BCL:HMB1	2.37	0.55
1:L:51:TRP:CZ3	1:L:80:LEU:HD13	2.42	0.54
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.43	0.53
2:M:179:ILE:CG2	7:M:311:BCL:HED1	2.39	0.53
1:L:189:LEU:HD11	13:L:802:PC9:H472	1.89	0.53
14:H:904:LDA:HM13	14:H:904:LDA:C3	2.39	0.53
3:H:9:ASN:C	3:H:11:ASP:H	2.13	0.52
13:L:802:PC9:H31	13:L:802:PC9:O1P	2.09	0.52
2:M:68[A]:PHE:O	2:M:72:ILE:HD13	2.10	0.52
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.45	0.51
2:M:41:TRP:CZ3	14:M:907:LDA:HM22	2.45	0.51
13:L:802:PC9:H483	13:L:802:PC9:C44	2.32	0.51
9:L:502:U10:H153	13:L:802:PC9:H461	1.92	0.51
2:M:72:ILE:N	2:M:72:ILE:CD1	2.74	0.51
2:M:68[B]:PHE:O	2:M:72:ILE:HD13	2.11	0.50
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.47	0.50
8:M:401:BPH:H192	8:M:401:BPH:C15	2.42	0.49
8:M:401:BPH:CBC	8:M:401:BPH:HHD	2.43	0.49
1:L:29:PHE:CE1	9:M:501:U10:H311	2.48	0.49
1:L:182:THR:OG1	7:M:311:BCL:H2	2.13	0.49
9:L:502:U10:H122	13:L:802:PC9:H471	1.95	0.49
6:L:703:PO4:O1	16:L:1467:HOH:O	2.20	0.49
3:H:21:TRP:CZ3	12:H:801:PC7:H72	2.48	0.48
13:L:802:PC9:BR1	7:M:311:BCL:H193	2.68	0.48
13:L:802:PC9:C48	8:M:401:BPH:HED1	2.27	0.47
2:M:10:VAL:HG22	16:H:1457:HOH:O	2.14	0.47
3:H:112:ALA:HA	3:H:235:GLY:O	2.14	0.47
2:M:234:GLU:CG	2:M:262:MET:HE1	2.45	0.47
13:L:802:PC9:H232	7:M:313:BCL:C20	2.44	0.47
1:L:207:ARG:HG2	1:L:211:HIS:CG	2.50	0.47
3:H:128[B]:HIS:HD1	15:H:708:GOL:H2	1.80	0.47
16:M:1078:HOH:O	3:H:175:MET:HE1	2.14	0.47
13:L:802:PC9:H261	8:M:401:BPH:HED2	1.95	0.47
7:L:312:BCL:CBB	7:L:312:BCL:HMB1	2.45	0.46
13:L:802:PC9:H232	7:M:313:BCL:H201	1.97	0.46
8:M:401:BPH:H152	8:M:401:BPH:H192	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:207:ARG:CG	1:L:211:HIS:CG	2.99	0.46
7:L:312:BCL:OBB	7:L:312:BCL:HHC	2.15	0.46
11:M:800:CDL:H172	3:H:26:GLY:HA3	1.97	0.46
1:L:138:MET:SD	1:L:249:ILE:HD11	2.56	0.46
3:H:118[A]:ARG:NH2	16:H:1237:HOH:O	2.48	0.46
2:M:53:GLY:O	2:M:57:VAL:HG23	2.16	0.45
7:M:311:BCL:H102	7:M:313:BCL:C19	2.45	0.45
2:M:186:THR:HG23	7:M:313:BCL:HMD2	1.98	0.45
12:H:801:PC7:C43	14:H:901:LDA:H121	2.43	0.45
7:L:314:BCL:C4A	7:L:314:BCL:HBA1	2.47	0.45
2:M:262:MET:HA	2:M:262:MET:HE3	1.99	0.45
2:M:157:TRP:CE3	2:M:158:MET:HG2	2.52	0.44
1:L:51:TRP:HZ3	1:L:80:LEU:HD13	1.83	0.44
3:H:89:ARG:NH2	3:H:94[A]:GLU:HG2	2.31	0.44
1:L:135:ARG:HB3	1:L:136:PRO:HD3	2.00	0.43
3:H:67:PRO:HB2	3:H:68:HIS:CD2	2.52	0.43
2:M:226:VAL:HG23	2:M:231:GLY:HA3	2.00	0.43
1:L:216:PHE:CD2	9:L:502:U10:H102	2.54	0.43
13:L:802:PC9:H241	8:M:401:BPH:HMA1	2.00	0.43
7:L:312:BCL:NA	7:M:313:BCL:HBB2	2.34	0.43
14:H:904:LDA:H31	14:H:904:LDA:HM13	2.00	0.43
1:L:170:ASN:HB3	1:L:173:HIS:HB3	2.01	0.43
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.53	0.42
2:M:74:PHE:CD1	2:M:92:PHE:HB3	2.54	0.42
14:L:906:LDA:H32	14:L:906:LDA:HM13	2.01	0.42
2:M:196:LEU:HA	2:M:196:LEU:HD12	1.82	0.42
2:M:296:VAL:O	2:M:300:ASN:ND2	2.49	0.42
1:L:220:VAL:HG11	13:L:802:PC9:H263	2.02	0.42
13:L:802:PC9:H263	8:M:401:BPH:HED2	1.98	0.42
1:L:51:TRP:CE3	1:L:85:LEU:HD21	2.55	0.42
1:L:60:ASN:O	1:L:64:ILE:HG13	2.20	0.42
9:L:502:U10:H301	9:L:502:U10:H322	1.81	0.42
1:L:87:GLN:NE2	1:L:142:TRP:CD1	2.88	0.41
12:H:801:PC7:H11	12:H:801:PC7:H41	2.02	0.41
2:M:2[B]:GLU:OE2	3:H:241:LEU:HD21	2.20	0.41
1:L:80:LEU:O	1:L:85:LEU:HD12	2.21	0.41
3:H:140:PHE:CE1	3:H:171:ILE:HG23	2.56	0.41
2:M:127:TRP:O	2:M:130:TRP:HB3	2.21	0.41
2:M:148:TRP:HA	2:M:148:TRP:HE3	1.85	0.40
1:L:193:LEU:HD21	1:L:212:GLU:HB3	2.03	0.40
3:H:227:LEU:HA	3:H:227:LEU:HD23	1.89	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	281/281 (100%)	275 (98%)	6 (2%)	0	100	100
2	M	310/307 (101%)	299 (96%)	10 (3%)	1 (0%)	50	71
3	H	251/260 (96%)	245 (98%)	5 (2%)	1 (0%)	43	66
All	All	842/848 (99%)	819 (97%)	21 (2%)	2 (0%)	56	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	10	PHE
2	M	195	ASN

### 5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	222/220 (101%)	213 (96%)	9 (4%)	41	66
2	M	246/240 (102%)	236 (96%)	10 (4%)	41	66
3	H	207/208 (100%)	201 (97%)	6 (3%)	55	80
All	All	675/668 (101%)	650 (96%)	25 (4%)	45	71

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	21	LEU
1	L	185	LEU
1	L	207	ARG
1	L	210	ASP

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Mol	Chain	Res	Type
1	L	216	PHE
1	L	235	LEU
1	L	247	CYS
1	L	254	ILE
1	L	272	TRP
2	M	32	VAL
2	M	52	LEU
2	M	72	ILE
2	M	86	LEU
2	M	104	SER
2	M	114	LEU
2	M	182	HIS
2	M	196	LEU
2	M	216	PHE
2	M	274	VAL
3	H	10	PHE
3	H	11	ASP
3	H	118[A]	ARG
3	H	118[B]	ARG
3	H	175	MET
3	H	231	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
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 29 ligands modelled in this entry, 2 are monoatomic - leaving 27 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	$\# Z  > 2$
15	GOL	H	705	-	5,5,5	0.42	0	5,5,5	0.58	0
15	GOL	H	706	-	5,5,5	0.41	0	5,5,5	0.96	0
15	GOL	H	708	-	5,5,5	0.37	0	5,5,5	0.52	0
10	HTO	H	709	-	9,9,9	0.49	0	10,10,10	0.43	0
12	PC7	H	801	-	51,51,51	0.89	1 (1%)	59,59,59	0.99	3 (5%)
14	LDA	H	901	-	15,15,15	3.18	1 (6%)	17,17,17	0.96	1 (5%)
14	LDA	H	903	-	15,15,15	3.69	2 (13%)	17,17,17	0.85	0
14	LDA	H	904	-	15,15,15	3.55	1 (6%)	17,17,17	0.99	1 (5%)
14	LDA	H	905	-	15,15,15	3.69	1 (6%)	17,17,17	0.71	1 (5%)
7	BCL	L	312	1	74,74,74	1.35	10 (13%)	97,115,115	1.50	19 (19%)
7	BCL	L	314	1	74,74,74	1.51	9 (12%)	97,115,115	1.58	17 (17%)
8	BPH	L	402	-	70,70,70	1.41	7 (10%)	94,101,101	1.26	11 (11%)
9	U10	L	502	-	48,48,63	1.06	4 (8%)	59,61,79	1.92	16 (27%)
6	PO4	L	703	-	4,4,4	0.14	0	6,6,6	0.32	0
13	PC9	L	802	-	53,53,53	0.79	2 (3%)	63,63,63	1.21	5 (7%)
14	LDA	L	902	-	15,15,15	3.42	2 (13%)	17,17,17	1.80	3 (17%)
14	LDA	L	906	-	15,15,15	3.72	2 (13%)	17,17,17	0.82	0
7	BCL	M	311	2	74,74,74	1.32	9 (12%)	97,115,115	1.67	19 (19%)
7	BCL	M	313	2	74,74,74	1.44	11 (14%)	97,115,115	1.77	24 (24%)
8	BPH	M	401	-	70,70,70	1.26	6 (8%)	94,101,101	1.49	16 (17%)
9	U10	M	501	-	48,48,63	1.23	7 (14%)	59,61,79	1.80	15 (25%)
6	PO4	M	701	-	4,4,4	0.11	0	6,6,6	0.31	0
6	PO4	M	702	-	4,4,4	0.16	0	6,6,6	0.32	0
6	PO4	M	704	-	4,4,4	0.23	0	6,6,6	0.33	0
11	CDL	M	800	-	80,80,99	1.60	8 (10%)	92,92,111	1.31	10 (10%)
14	LDA	M	907	-	15,15,15	3.47	1 (6%)	17,17,17	0.74	0
14	LDA	M	920	-	15,15,15	3.16	1 (6%)	17,17,17	1.20	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	GOL	H	705	-	-	0/4/4/4	0/0/0/0
15	GOL	H	706	-	-	0/4/4/4	0/0/0/0
15	GOL	H	708	-	-	0/4/4/4	0/0/0/0
10	HTO	H	709	-	-	0/10/10/10	0/0/0/0
12	PC7	H	801	-	-	0/55/55/55	0/0/0/0
14	LDA	H	901	-	-	0/13/13/13	0/0/0/0
14	LDA	H	903	-	-	0/13/13/13	0/0/0/0
14	LDA	H	904	-	-	0/13/13/13	0/0/0/0
14	LDA	H	905	-	-	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	703	-	-	0/0/0/0	0/0/0/0
13	PC9	L	802	-	-	0/60/60/60	0/0/0/0
14	LDA	L	902	-	-	0/13/13/13	0/0/0/0
14	LDA	L	906	-	-	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	701	-	-	0/0/0/0	0/0/0/0
6	PO4	M	702	-	-	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
14	LDA	M	907	-	-	0/13/13/13	0/0/0/0
14	LDA	M	920	-	-	0/13/13/13	0/0/0/0

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	L	906	LDA	O1-N1	-14.13	1.26	1.39
14	H	905	LDA	O1-N1	-14.10	1.26	1.39
14	H	903	LDA	O1-N1	-14.04	1.26	1.39
14	H	904	LDA	O1-N1	-13.51	1.26	1.39
14	M	907	LDA	O1-N1	-13.17	1.27	1.39
14	L	902	LDA	O1-N1	-12.98	1.27	1.39
14	H	901	LDA	O1-N1	-12.08	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	920	LDA	O1-N1	-12.03	1.28	1.39
11	M	800	CDL	C84-C83	-7.02	1.52	1.55
8	M	401	BPH	C1D-CHD	6.59	1.42	1.35
7	L	314	BCL	C1B-C2B	6.48	1.48	1.40
8	L	402	BPH	C1D-CHD	6.12	1.42	1.35
11	M	800	CDL	C43-C42	-5.69	1.52	1.55
8	L	402	BPH	C3B-C4B	4.92	1.47	1.40
11	M	800	CDL	OA8-CA7	4.55	1.47	1.33
7	L	312	BCL	C3B-C4B	4.54	1.47	1.40
11	M	800	CDL	OB6-CB5	4.50	1.48	1.34
7	L	314	BCL	C3B-C4B	4.40	1.47	1.40
11	M	800	CDL	OA6-CA5	4.35	1.47	1.34
7	M	311	BCL	C3B-C4B	4.29	1.46	1.40
7	M	313	BCL	C4B-NB	4.15	1.39	1.34
9	M	501	U10	O3-C3	4.07	1.47	1.36
9	L	502	U10	O3-C3	4.04	1.47	1.36
7	L	314	BCL	C1A-NA	4.03	1.41	1.32
7	M	311	BCL	MG-NA	4.02	2.19	2.07
7	L	312	BCL	MG-NA	3.83	2.18	2.07
11	M	800	CDL	C58-C57	-3.78	1.53	1.55
11	M	800	CDL	OB8-CB7	3.75	1.45	1.33
7	M	311	BCL	C1A-NA	3.72	1.40	1.32
7	M	313	BCL	C3B-C4B	3.62	1.45	1.40
7	L	312	BCL	C1B-C2B	3.56	1.44	1.40
7	L	314	BCL	C4C-NC	3.56	1.40	1.32
7	M	313	BCL	C3C-C4C	-3.51	1.47	1.51
7	M	311	BCL	C1B-C2B	3.41	1.44	1.40
7	M	313	BCL	C1B-C2B	3.39	1.44	1.40
7	M	313	BCL	MG-NA	3.39	2.17	2.07
7	M	313	BCL	C1A-NA	3.36	1.39	1.32
7	L	312	BCL	C1A-NA	3.27	1.39	1.32
7	L	314	BCL	MG-NA	3.20	2.16	2.07
8	M	401	BPH	C3B-C4B	3.11	1.45	1.40
7	M	313	BCL	MG-ND	3.11	2.11	2.05
9	M	501	U10	C13-C14	2.95	1.38	1.32
9	L	502	U10	C13-C14	2.95	1.38	1.32
7	L	312	BCL	C1B-NB	2.93	1.38	1.34
7	M	313	BCL	C4C-NC	2.84	1.38	1.32
7	M	311	BCL	MG-NB	2.84	2.11	2.05
7	M	311	BCL	C1B-NB	2.82	1.38	1.34
9	M	501	U10	C33-C34	2.71	1.38	1.32
7	L	314	BCL	C4B-NB	2.70	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	401	BPH	CHA-C1A	-2.68	1.35	1.45
13	L	802	PC9	P-O1P	2.64	1.61	1.51
9	M	501	U10	O2-C2	2.60	1.29	1.23
7	L	312	BCL	C1C-NC	-2.60	1.33	1.39
7	L	312	BCL	C4C-NC	2.59	1.37	1.32
8	L	402	BPH	CHA-C1A	-2.53	1.36	1.45
7	M	313	BCL	CHC-C1C	2.50	1.42	1.36
7	L	312	BCL	C4-C3	2.48	1.57	1.50
7	M	311	BCL	CHC-C1C	2.46	1.42	1.36
8	L	402	BPH	C4C-NC	2.45	1.41	1.34
7	M	313	BCL	C4A-NA	-2.44	1.33	1.39
7	M	311	BCL	C4A-NA	-2.40	1.34	1.39
12	H	801	PC7	C1-C2	2.39	1.57	1.50
7	L	312	BCL	MG-NB	2.39	2.10	2.05
8	L	402	BPH	C1C-NC	-2.39	1.33	1.38
7	L	312	BCL	C4A-NA	-2.35	1.34	1.39
9	L	502	U10	O4-C4	2.35	1.42	1.36
7	L	314	BCL	C1B-NB	2.30	1.37	1.34
8	M	401	BPH	C1B-NB	2.30	1.39	1.36
8	L	402	BPH	C1B-NB	2.28	1.39	1.36
7	M	313	BCL	C1C-NC	-2.27	1.34	1.39
7	M	311	BCL	C1C-NC	-2.21	1.34	1.39
9	M	501	U10	C41-C39	2.20	1.52	1.40
8	M	401	BPH	C4B-CHC	-2.18	1.37	1.46
14	L	902	LDA	C1-N1	-2.18	1.47	1.51
8	M	401	BPH	C4C-NC	2.15	1.40	1.34
9	L	502	U10	C41-C39	2.15	1.52	1.40
13	L	802	PC9	O3-C3	2.15	1.50	1.45
14	L	906	LDA	C1-N1	-2.14	1.47	1.51
11	M	800	CDL	PA1-OA3	-2.14	1.43	1.48
7	L	314	BCL	C4A-NA	-2.13	1.34	1.39
7	L	314	BCL	C1C-NC	-2.10	1.34	1.39
9	M	501	U10	O3-C3M	-2.10	1.40	1.45
9	M	501	U10	O4-C4	2.07	1.42	1.36
8	L	402	BPH	C4D-ND	-2.05	1.35	1.38
14	H	903	LDA	C1-N1	-2.03	1.47	1.51

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	313	BCL	CMB-C2B-C1B	-6.55	118.55	128.62
14	L	902	LDA	CM2-N1-CM1	-5.93	102.07	108.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	800	CDL	OA6-CA5-C11	5.72	124.10	111.56
7	M	311	BCL	C4-C3-C2	-5.05	113.52	123.52
9	M	501	U10	C30-C29-C31	5.00	122.99	115.39
9	L	502	U10	C30-C29-C31	4.84	122.76	115.39
9	M	501	U10	C32-C33-C34	-4.74	117.57	127.80
8	M	401	BPH	OBD-CAD-CBD	-4.70	118.85	125.94
9	M	501	U10	C17-C18-C19	-4.66	117.74	127.80
9	L	502	U10	C35-C34-C33	-4.55	114.51	123.52
11	M	800	CDL	OB6-CB5-C51	4.54	121.50	111.56
7	L	314	BCL	CAA-C2A-C3A	-4.52	102.34	113.04
9	L	502	U10	C25-C24-C26	4.44	122.14	115.39
9	M	501	U10	C7-C6-C5	-4.38	114.00	118.75
7	M	311	BCL	CMB-C2B-C1B	-4.36	121.91	128.62
7	M	313	BCL	CMB-C2B-C3B	4.31	131.76	124.97
7	L	312	BCL	CAA-C2A-C3A	-4.26	102.97	113.04
7	L	312	BCL	CMB-C2B-C3B	4.18	131.55	124.97
7	L	312	BCL	CMB-C2B-C1B	-4.12	122.29	128.62
12	H	801	PC7	O2-C31-C32	4.06	120.45	111.56
9	M	501	U10	C26-C27-C28	-3.98	100.23	111.62
13	L	802	PC9	C2-O2-C31	-3.96	108.15	117.92
9	L	502	U10	C31-C29-C28	-3.92	113.55	121.08
7	M	313	BCL	CAC-C3C-C2C	-3.91	104.91	113.89
7	M	311	BCL	C2C-C1C-NC	3.88	115.68	110.95
7	L	314	BCL	CMB-C2B-C1B	-3.85	122.71	128.62
7	L	314	BCL	CAC-C3C-C2C	-3.85	105.06	113.89
7	M	311	BCL	C4B-NB-C1B	3.82	111.80	106.76
7	M	311	BCL	C2B-C1B-NB	-3.77	106.57	109.41
13	L	802	PC9	O2-C31-C32	3.76	119.79	111.56
14	M	920	LDA	O1-N1-C1	3.74	115.41	110.19
7	M	313	BCL	C2B-C1B-NB	-3.72	106.60	109.41
8	M	401	BPH	CAC-C3C-C4C	3.70	122.87	112.68
8	M	401	BPH	C1-C2-C3	-3.69	119.62	126.19
8	M	401	BPH	C4B-C3B-C2B	3.69	110.27	107.60
8	M	401	BPH	CMB-C2B-C3B	3.68	130.77	124.97
8	M	401	BPH	CMB-C2B-C1B	-3.62	123.14	128.65
7	L	314	BCL	CAC-C3C-C4C	-3.59	104.61	112.58
9	L	502	U10	C35-C34-C36	3.57	120.81	115.39
8	M	401	BPH	CAA-C2A-C3A	-3.54	104.68	113.04
8	L	402	BPH	C1-C2-C3	-3.51	119.94	126.19
7	L	314	BCL	OBB-CAB-C3B	3.48	125.30	120.07
7	L	314	BCL	O2D-CGD-CBD	3.43	118.32	111.33
7	M	313	BCL	O2A-C1-C2	3.42	115.95	108.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	402	BPH	CMB-C2B-C1B	-3.39	123.49	128.65
8	L	402	BPH	O2D-CGD-O1D	-3.38	116.92	123.79
8	L	402	BPH	O2D-CGD-CBD	3.37	118.19	111.33
14	H	904	LDA	CM2-N1-CM1	-3.34	105.04	108.85
9	L	502	U10	O2-C2-C3	-3.29	113.66	120.96
11	M	800	CDL	CB6-CB4-CB3	-3.28	104.38	111.86
8	M	401	BPH	O2D-CGD-CBD	3.28	118.02	111.33
7	L	312	BCL	C2C-C1C-NC	3.24	114.90	110.95
9	M	501	U10	C31-C29-C28	-3.23	114.86	121.08
7	M	311	BCL	CMB-C2B-C3B	3.22	130.04	124.97
7	L	312	BCL	CHA-C1A-NA	-3.19	119.68	126.22
7	M	311	BCL	CED-O2D-CGD	-3.17	108.47	116.02
7	M	313	BCL	C3A-C4A-NA	3.17	114.80	110.95
7	M	313	BCL	CHA-C1A-NA	-3.16	119.73	126.22
7	M	311	BCL	OB8-CAB-C3B	3.14	124.79	120.07
7	L	314	BCL	CAA-CBA-CGA	3.13	123.36	113.27
7	L	314	BCL	C5-C3-C2	-3.13	115.07	121.08
7	M	313	BCL	C4B-NB-C1B	3.10	110.85	106.76
9	L	502	U10	C12-C13-C14	-3.09	121.14	127.80
7	L	312	BCL	C3A-C4A-NA	3.06	114.67	110.95
7	M	311	BCL	CHA-C1A-NA	-3.05	119.95	126.22
7	M	313	BCL	CHC-C1C-NC	3.04	128.18	124.58
9	M	501	U10	C22-C23-C24	-3.03	121.26	127.80
7	M	311	BCL	C5-C3-C2	2.99	126.85	121.08
8	L	402	BPH	CMB-C2B-C3B	2.98	129.66	124.97
12	H	801	PC7	C3-C2-C1	2.95	118.59	111.86
7	L	314	BCL	O1D-CGD-CBD	-2.93	118.41	124.42
7	L	314	BCL	C2B-C1B-NB	-2.86	107.25	109.41
7	M	313	BCL	CMD-C2D-C3D	2.85	129.46	124.97
7	L	312	BCL	CGD-CBD-CHA	2.84	120.61	110.96
8	L	402	BPH	CMD-C2D-C3D	2.82	129.42	124.97
11	M	800	CDL	OB8-CB7-C71	2.82	120.80	111.94
7	L	312	BCL	C2A-C1A-NA	2.81	114.36	111.24
7	L	312	BCL	C4B-NB-C1B	2.81	110.47	106.76
7	M	311	BCL	CMA-C3A-C4A	-2.80	103.63	111.76
7	M	311	BCL	C4-C3-C5	2.79	119.63	115.39
8	L	402	BPH	CAC-C3C-C4C	2.78	120.35	112.68
7	L	314	BCL	C2C-C1C-NC	2.77	114.32	110.95
8	L	402	BPH	CAC-C3C-C2C	2.76	120.22	113.89
7	L	314	BCL	CMB-C2B-C3B	2.73	129.27	124.97
9	L	502	U10	C21-C22-C23	-2.72	103.84	111.62
7	M	313	BCL	C2C-C3C-C4C	2.71	104.81	101.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	311	BCL	C3B-C4B-NB	-2.71	106.01	108.64
14	M	920	LDA	CM2-N1-CM1	-2.69	105.78	108.85
7	M	313	BCL	O2D-CGD-O1D	-2.64	118.42	123.79
9	M	501	U10	C37-C38-C39	-2.64	122.23	128.63
9	L	502	U10	C3M-O3-C3	2.62	125.37	116.48
8	L	402	BPH	C4B-C3B-C2B	2.61	109.49	107.60
9	L	502	U10	C7-C6-C5	-2.60	115.93	118.75
11	M	800	CDL	OB8-CB7-OB9	-2.59	116.35	123.43
7	M	313	BCL	C4-C3-C5	2.59	119.33	115.39
7	L	314	BCL	C2C-C3C-C4C	2.55	104.59	101.05
7	L	312	BCL	C5-C3-C2	-2.54	116.19	121.08
9	M	501	U10	C4M-O4-C4	2.54	125.11	116.48
7	L	312	BCL	C3B-C4B-NB	-2.52	106.19	108.64
9	L	502	U10	C22-C23-C24	-2.49	122.42	127.80
11	M	800	CDL	OA8-CA7-C31	2.45	119.63	111.94
7	M	313	BCL	C4B-CHC-C1C	-2.44	124.97	130.06
8	M	401	BPH	OBD-CAD-C3D	2.44	132.45	127.91
9	L	502	U10	C37-C38-C39	-2.44	122.72	128.63
14	L	902	LDA	O1-N1-C1	-2.44	106.79	110.19
8	M	401	BPH	O2A-C1-C2	-2.43	103.28	108.55
7	M	311	BCL	CAA-C2A-C3A	-2.41	107.33	113.04
7	L	314	BCL	CMA-C3A-C2A	-2.41	103.78	114.14
9	L	502	U10	C16-C17-C18	-2.40	104.77	111.62
7	M	313	BCL	OBD-CAD-CBD	-2.39	122.32	125.94
7	M	313	BCL	C2C-C1C-CHC	-2.39	119.36	124.33
8	L	402	BPH	CAA-C2A-C3A	-2.38	107.41	113.04
9	M	501	U10	C15-C14-C16	2.36	118.97	115.39
13	L	802	PC9	C35-C36-C37	-2.35	109.55	115.69
13	L	802	PC9	O3-C11-C12	2.35	119.32	111.94
7	L	312	BCL	C4-C3-C5	2.35	118.96	115.39
7	M	311	BCL	C1-O2A-CGA	2.33	123.51	116.98
14	L	902	LDA	O1-N1-CM2	2.32	112.14	109.01
11	M	800	CDL	OB5-PB2-OB2	-2.31	98.20	104.53
9	L	502	U10	C1M-C1-C6	-2.31	119.62	124.20
7	M	313	BCL	CGD-CBD-CHA	-2.30	103.15	110.96
7	M	313	BCL	C1D-C2D-C3D	-2.30	104.91	106.78
9	L	502	U10	C25-C24-C23	-2.28	119.01	123.52
7	L	312	BCL	OBD-CAD-CBD	-2.26	122.52	125.94
7	M	311	BCL	CAA-CBA-CGA	2.25	120.53	113.27
8	M	401	BPH	C3C-C4C-NC	-2.25	109.57	113.49
14	H	905	LDA	O1-N1-CM2	-2.24	106.00	109.01
9	M	501	U10	C40-C39-C38	-2.24	118.26	123.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	401	BPH	CMA-C3A-C2A	-2.22	104.60	114.14
8	M	401	BPH	C3C-C4C-CHD	2.21	126.43	121.83
7	L	314	BCL	C4-C3-C5	2.20	118.73	115.39
7	M	313	BCL	C2A-C1A-NA	2.20	113.67	111.24
7	M	313	BCL	C3B-C4B-CHC	2.19	130.16	126.00
7	M	313	BCL	CAC-C3C-C4C	-2.19	107.72	112.58
7	L	312	BCL	C2C-C3C-C4C	2.19	104.08	101.05
7	L	314	BCL	C4B-NB-C1B	2.19	109.65	106.76
12	H	801	PC7	O3-C11-C12	2.18	118.81	111.94
11	M	800	CDL	CA6-OA8-CA7	2.18	123.52	117.13
7	M	313	BCL	C4D-CHA-C1A	2.17	126.61	120.32
13	L	802	PC9	O3-C3-C2	2.17	114.52	108.83
7	L	312	BCL	C2D-C1D-ND	-2.17	107.77	109.41
7	M	311	BCL	C2C-C3C-C4C	2.16	104.05	101.05
7	M	313	BCL	C1-C2-C3	-2.16	122.34	126.19
11	M	800	CDL	C43-C42-C41	-2.16	109.62	114.46
14	H	901	LDA	CM2-N1-CM1	-2.14	106.40	108.85
7	M	311	BCL	C1D-C2D-C3D	-2.14	105.04	106.78
9	M	501	U10	C22-C21-C19	-2.13	105.67	112.74
7	M	311	BCL	C3A-C4A-NA	2.13	113.54	110.95
8	M	401	BPH	C2C-C3C-C4C	2.12	104.95	102.06
8	M	401	BPH	CBB-CAB-C3B	-2.12	114.11	120.30
8	M	401	BPH	O2D-CGD-O1D	-2.11	119.50	123.79
7	L	312	BCL	C3A-C4A-CHB	-2.10	119.95	124.33
11	M	800	CDL	CA4-OA6-CA5	-2.09	112.75	117.92
7	L	312	BCL	C4D-ND-C1D	2.09	109.10	106.57
9	M	501	U10	C6-C1-C2	2.09	122.30	120.18
7	L	312	BCL	CED-O2D-CGD	2.08	120.98	116.02
7	L	312	BCL	C1-O2A-CGA	2.08	122.81	116.98
9	M	501	U10	C10-C9-C11	2.08	118.55	115.39
7	M	313	BCL	OBB-CAB-CBB	-2.06	115.00	120.13
7	L	314	BCL	C3A-C4A-NA	2.05	113.44	110.95
9	L	502	U10	C10-C9-C11	2.03	118.47	115.39
9	M	501	U10	C31-C32-C33	2.02	117.37	111.62
8	L	402	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	L	402	BPH	C8
8	L	402	BPH	C13

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Mol	Chain	Res	Type	Atom
8	M	401	BPH	C8
8	M	401	BPH	C13

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.58	27 (9%) 8 8	38, 51, 61, 72	0
2	M	302/307 (98%)	0.83	50 (16%) 2 2	40, 50, 60, 76	0
3	H	244/260 (93%)	0.20	11 (4%) 32 34	42, 49, 60, 87	1 (0%)
All	All	827/848 (97%)	0.56	88 (10%) 6 6	38, 50, 61, 87	1 (0%)

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	8	GLY	7.5
3	H	251	VAL	7.1
3	H	10	PHE	6.8
3	H	9	ASN	6.8
1	L	277	GLY	6.5
1	L	279	ILE	6.3
1	L	281	GLY	6.1
2	M	109	LEU	5.3
1	L	59	TRP	5.2
1	L	280	ASN	4.9
2	M	80	TRP	4.9
2	M	174	ALA	4.8
2	M	171	TRP	4.8
2	M	83	ALA	4.7
2	M	76	TYR	4.7
1	L	55	LEU	4.6
2	M	82	PRO	4.5
3	H	250	SER	4.4
1	L	81	ALA	4.4
2	M	26	LEU	4.3
2	M	75	TRP	4.3
2	M	105	PHE	4.2
2	M	101	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	L	278	GLY	4.1
2	M	114	LEU	4.1
1	L	271	TRP	4.0
1	L	268	LYS	3.8
1	L	80	LEU	3.8
2	M	79	GLY	3.8
2	M	98	ALA	3.8
2	M	27	ALA	3.8
3	H	118[A]	ARG	3.7
1	L	276[A]	PRO	3.7
1	L	73	TYR	3.6
2	M	97	PRO	3.6
2	M	32	VAL	3.6
3	H	249	LYS	3.5
1	L	269	LEU	3.3
1	L	236	LEU	3.3
2	M	24	VAL	3.2
2	M	104	SER	3.1
2	M	77	GLN	3.1
2	M	54	SER	3.1
2	M	216	PHE	3.1
3	H	52	ASN	3.0
2	M	134	TYR	3.0
2	M	265	ILE	2.9
1	L	51	TRP	2.9
1	L	185	LEU	2.8
2	M	86	LEU	2.8
1	L	184	ALA	2.7
2	M	110	LYS	2.7
1	L	233	GLY	2.6
2	M	111	GLU	2.6
2	M	72	ILE	2.6
1	L	54	VAL	2.6
2	M	78	ALA	2.6
1	L	272	TRP	2.5
2	M	1	ALA	2.5
2	M	28	ASN	2.5
2	M	84	VAL	2.4
1	L	270	PRO	2.4
2	M	100	GLU	2.4
2	M	103	LEU	2.3
2	M	106	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	M	220	GLY	2.3
2	M	107	ALA	2.3
2	M	274	VAL	2.3
1	L	265	TRP	2.2
2	M	115	TRP	2.2
2	M	205[A]	SER	2.2
2	M	52	LEU	2.2
2	M	53	GLY	2.2
3	H	94[A]	GLU	2.2
2	M	212	SER	2.2
1	L	234	LEU	2.2
2	M	208	PHE	2.2
2	M	223	ILE	2.2
2	M	273	ALA	2.2
2	M	81	ASN	2.1
2	M	96	PRO	2.1
2	M	215	LEU	2.1
1	L	139	MET	2.1
2	M	74	PHE	2.1
3	H	143	SER	2.1
3	H	160	ILE	2.0
1	L	67	TYR	2.0
1	L	256	PHE	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( $\text{\AA}^2$ )	Q<0.9
15	GOL	H	708	6/6	0.70	27.01	46,46,47,49	6
14	LDA	H	905	16/16	0.78	17.82	61,69,78,78	16
14	LDA	M	907	16/16	0.45	12.65	56,61,66,67	16
14	LDA	H	904	16/16	0.52	11.40	65,68,72,72	16
14	LDA	L	902	16/16	0.48	10.37	68,73,77,80	16
12	PC7	H	801	52/52	0.77	10.15	26,68,76,78	52
9	U10	L	502	48/63	0.60	6.61	34,48,60,62	48
15	GOL	H	705	6/6	0.29	6.46	58,69,70,72	0
14	LDA	H	903	16/16	0.44	5.68	63,65,74,75	16
6	PO4	M	704	5/5	0.47	4.44	76,76,77,78	5
13	PC9	L	802	54/54	0.56	4.31	57,66,75,79	54
11	CDL	M	800	81/100	0.35	3.84	43,71,83,85	81
14	LDA	M	920	16/16	0.38	3.70	59,74,88,88	16
15	GOL	H	706	6/6	0.29	3.37	74,76,77,77	0
14	LDA	L	906	16/16	0.42	3.22	54,56,59,60	16
14	LDA	H	901	16/16	0.31	2.64	60,65,69,71	0
6	PO4	L	703	5/5	0.37	1.50	70,72,73,75	5
9	U10	M	501	48/63	0.24	0.76	43,54,77,80	0
7	BCL	L	314	66/66	0.21	0.61	38,47,62,66	0
6	PO4	M	702	5/5	0.27	0.07	66,67,68,68	5
8	BPH	L	402	65/65	0.17	0.05	35,47,52,53	0
10	HTO	H	709	10/10	0.21	-0.08	50,56,56,58	10
7	BCL	L	312	66/66	0.16	-0.12	41,46,58,61	0
8	BPH	M	401	65/65	0.17	-0.18	45,51,92,93	0
7	BCL	M	311	66/66	0.18	-0.24	42,51,96,97	0
7	BCL	M	313	66/66	0.14	-0.63	38,46,70,79	0
4	FE	M	500	1/1	0.20	-0.70	49,49,49,49	0
6	PO4	M	701	5/5	0.26	-0.91	57,59,62,63	0
5	K	H	700	1/1	0.06	-5.59	54,54,54,54	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.