



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 12:37 PM GMT

PDB ID : 2UX5  
Title : X-RAY HIGH RESOLUTION STRUCTURE OF THE PHOTOSYNTHETIC  
REACTION CENTER FROM RB. SPHAEROIDES AT PH 9 IN THE  
CHARGE-SEPARATED STATE  
Authors : Koepke, J.; Diehm, R.; Fritzsche, G.  
Deposited on : 2007-03-26  
Resolution : 2.21 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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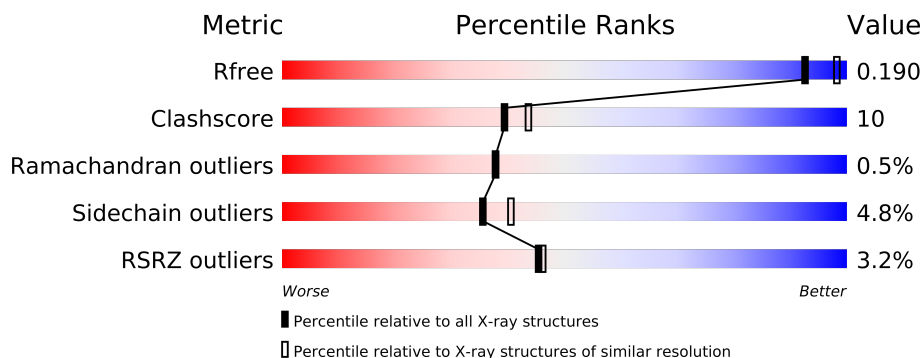
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.21 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	3340 (2.24-2.20)
Clashscore	79885	4208 (2.24-2.20)
Ramachandran outliers	78287	4135 (2.24-2.20)
Sidechain outliers	78261	4136 (2.24-2.20)
RSRZ outliers	66119	3341 (2.24-2.20)

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  $\geq 3$ , 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	H	260	
2	L	281	
3	M	307	

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	1289	-	X
14	CDL	M	1317	-	X
4	GOL	H	1252	-	X
4	GOL	H	1253	-	X
4	GOL	H	1254	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	GOL	L	1291	-	X
6	LDA	L	1283	-	X
6	LDA	L	1284	-	X
6	LDA	M	1306	-	X
6	LDA	M	1307	-	X
6	LDA	M	1308	-	X
6	LDA	M	1309	-	X
6	LDA	M	1310	-	X
6	LDA	M	1311	-	X
6	LDA	M	1312	-	X
8	UQ2	L	1286[A]	-	X
8	UQ2	L	1286[B]	-	X

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 7706 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	241	Total	C	N	O	S	0	3	1
			1846	1181	319	337	9			

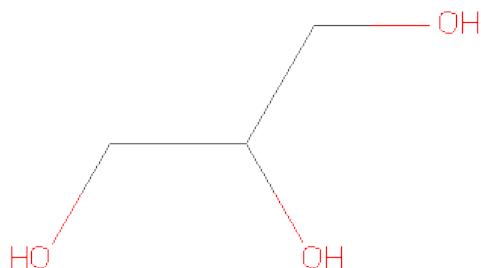
- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

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.

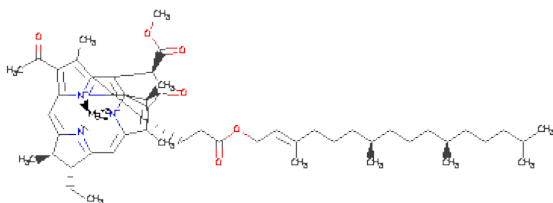
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2409	1607	395	397	10			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

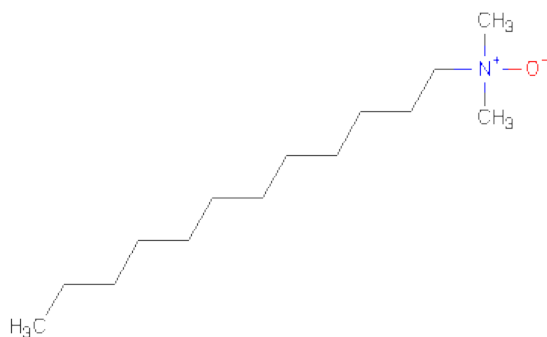
- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula:  $C_{55}H_{74}MgN_4O_6$ ).



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

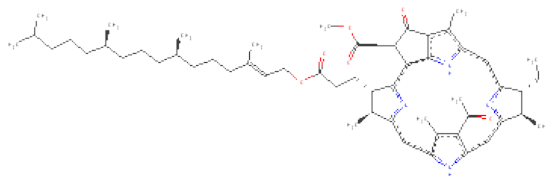
- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:

C<sub>14</sub>H<sub>31</sub>NO).



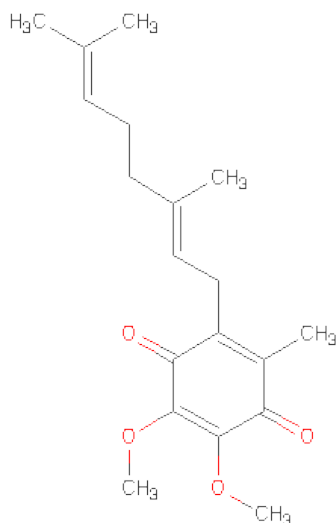
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1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

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C<sub>55</sub>H<sub>76</sub>N<sub>4</sub>O<sub>6</sub>).



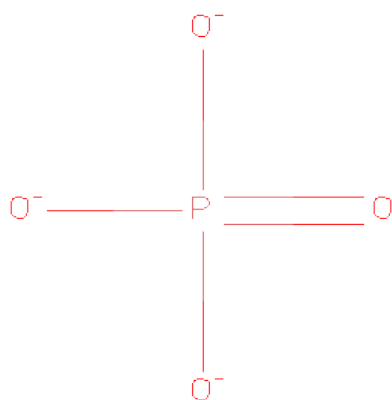
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 8 is UBIQUINONE-2 (three-letter code: UQ2) (formula:  $C_{19}H_{26}O_4$ ).



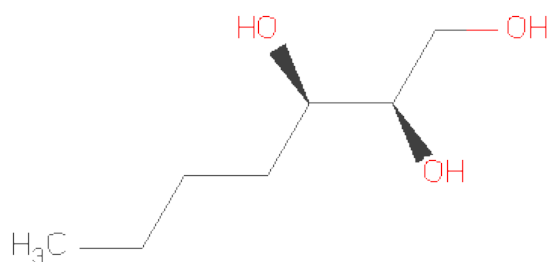
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	1
			46	38	8		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



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

- Molecule 10 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C<sub>7</sub>H<sub>16</sub>O<sub>3</sub>).

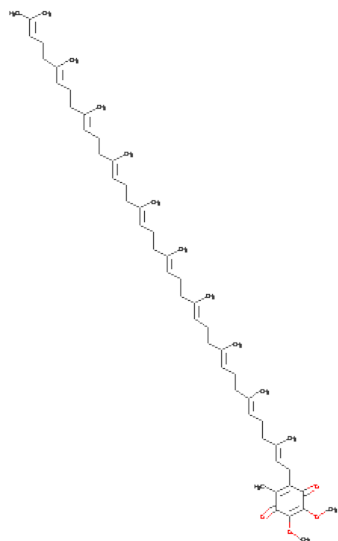


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			10	7	3		

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

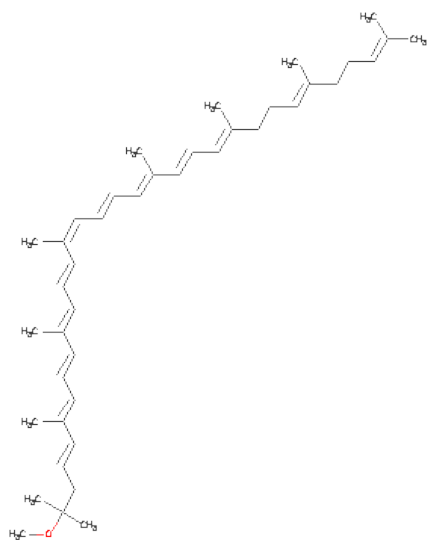
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

- Molecule 12 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).



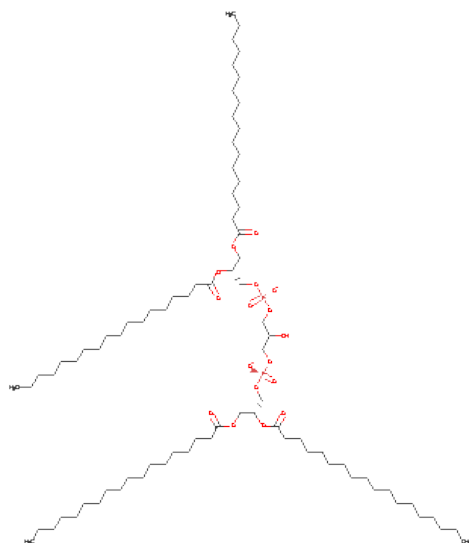
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 13 is SPHEROIDENE (three-letter code: SPO) (formula:  $C_{41}H_{60}O$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



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

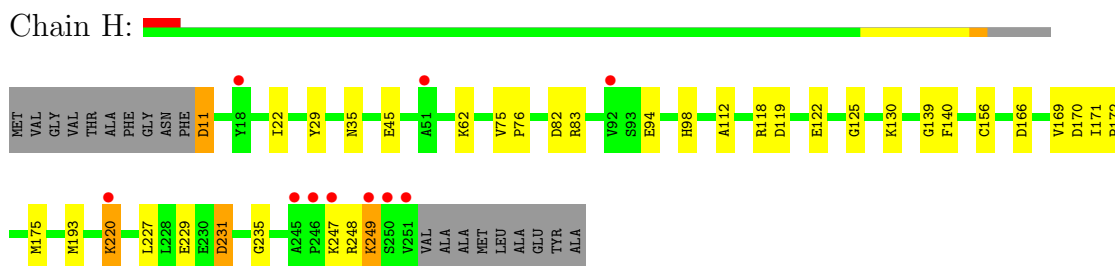
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	167	Total	O	0	0
			167	167		
15	L	115	Total	O	0	0
			115	115		
15	M	124	Total	O	0	0
			124	124		

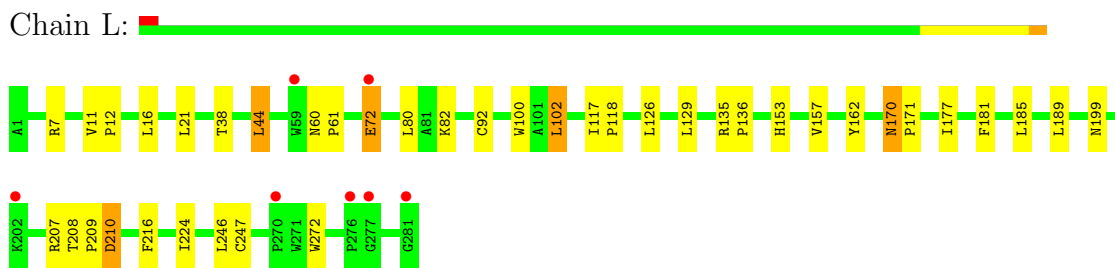
### 3 Residue-property plots

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.

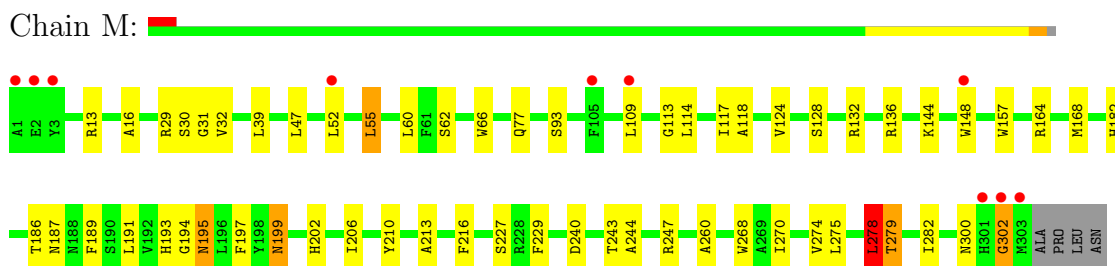
- Molecule 1: REACTION CENTER PROTEIN H CHAIN



- 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 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.46Å 139.46Å 184.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.21 19.86 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.21) 96.4 (19.86-2.21)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.37 (at 2.21Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.202 , 0.236 0.197 , 0.190	Depositor DCC
$R_{free}$ test set	3021 reflections (3.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.2	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.6	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 103484 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7706	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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, CDL, BPH, PO4, HTO, FE, SPO, U10, UQ2

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	0.88	0/1906	0.92	6/2591 (0.2%)
2	L	0.91	0/2320	0.78	1/3175 (0.0%)
3	M	0.88	3/2501 (0.1%)	0.80	2/3415 (0.1%)
All	All	0.89	3/6727 (0.0%)	0.83	9/9181 (0.1%)

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
3	M	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	278	LEU	CG-CD2	7.91	1.81	1.51
3	M	213	ALA	CA-CB	6.24	1.65	1.52
3	M	227	SER	CA-CB	5.32	1.60	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	278	LEU	CA-CB-CG	-13.19	84.97	115.30
1	H	11	ASP	CB-CG-OD2	8.98	126.38	118.30
1	H	166	ASP	CB-CG-OD2	8.16	125.64	118.30
1	H	83	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	H	231	ASP	CB-CG-OD2	7.12	124.71	118.30
1	H	82	ASP	CB-CG-OD2	6.78	124.40	118.30
1	H	139	GLY	N-CA-C	-6.73	96.27	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	240	ASP	CB-CG-OD2	6.22	123.90	118.30
2	L	102	LEU	CB-CG-CD1	5.06	119.60	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	M	300	ASN	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	1846	0	1861	24	0
2	L	2232	0	2187	28	0
3	M	2409	0	2321	53	0
4	H	24	0	32	4	0
4	L	12	0	16	1	0
4	M	6	0	8	1	0
5	L	132	0	148	6	0
5	M	132	0	148	20	0
6	L	32	0	62	2	0
6	M	112	0	217	8	0
7	L	65	0	76	6	0
7	M	65	0	76	14	0
8	L	46	0	52	6	0
9	L	5	0	0	0	0
10	L	10	0	16	0	0
11	M	1	0	0	0	0
12	M	48	0	63	3	0
13	M	42	0	60	2	0
14	M	81	0	86	4	0
15	H	167	0	0	3	0
15	L	115	0	0	2	0
15	M	124	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7706	0	7429	141	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 (141) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:278:LEU:CG	3:M:278:LEU:CD2	1.81	1.56
3:M:278:LEU:CD2	3:M:279:THR:H	1.18	1.55
3:M:278:LEU:CD2	3:M:279:THR:N	1.74	1.38
3:M:278:LEU:HA	3:M:278:LEU:CD2	1.61	1.28
3:M:278:LEU:CA	3:M:278:LEU:CD2	2.11	1.27
3:M:278:LEU:HD22	3:M:278:LEU:C	1.56	1.26
3:M:278:LEU:HD22	3:M:279:THR:N	0.79	1.10
3:M:278:LEU:HA	3:M:278:LEU:HD23	1.20	1.08
7:L:1285:BPH:HHC	7:L:1285:BPH:HBB3	1.42	0.99
3:M:275:LEU:O	3:M:278:LEU:O	1.83	0.97
3:M:278:LEU:CD2	3:M:278:LEU:C	2.20	0.94
1:H:220[A]:LYS:HD2	1:H:229:GLU:OE2	1.71	0.90
3:M:197:PHE:CZ	5:M:1305:BCL:HBB2	2.10	0.86
3:M:197:PHE:HZ	5:M:1305:BCL:HBB2	1.39	0.85
3:M:278:LEU:HD22	3:M:279:THR:CA	2.08	0.83
4:H:1252:GOL:H31	15:H:2003:HOH:O	1.78	0.83
6:M:1306:LDA:H101	6:M:1308:LDA:H121	1.62	0.80
5:M:1305:BCL:HBB3	5:M:1305:BCL:HHC	1.67	0.77
1:H:248:ARG:HA	1:H:249:LYS:HB3	1.67	0.77
3:M:189:PHE:O	3:M:193:HIS:HD2	1.70	0.75
5:M:1305:BCL:HHC	5:M:1305:BCL:CBB	2.18	0.74
7:M:1314:BPH:HBB3	7:M:1314:BPH:HHC	1.68	0.74
6:M:1306:LDA:H101	6:M:1308:LDA:C12	2.19	0.73
7:L:1285:BPH:HHC	7:L:1285:BPH:CBB	2.19	0.72
2:L:181:PHE:CD2	7:M:1314:BPH:HBB1	2.24	0.71
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.71	0.71
2:L:199:ASN:HA	4:L:1290:GOL:H31	1.76	0.68
5:M:1304:BCL:CBB	5:M:1304:BCL:HHC	2.24	0.68
5:M:1304:BCL:HBB2	5:M:1304:BCL:HHC	1.77	0.67
2:L:170:ASN:C	2:L:170:ASN:HD22	1.99	0.66
7:M:1314:BPH:HBC3	7:M:1314:BPH:HHD	1.76	0.66
5:M:1304:BCL:HBB3	5:M:1305:BCL:H41	1.76	0.66
6:M:1308:LDA:H112	12:M:1315:U10:H202	1.79	0.65
1:H:35:ASN:OD1	3:M:260:ALA:HB1	1.97	0.65
7:M:1314:BPH:CBB	7:M:1314:BPH:HHC	2.28	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:175:MET:HE1	15:M:2097:HOH:O	1.97	0.63
3:M:157:TRP:HB2	5:M:1305:BCL:H71	1.81	0.63
2:L:72:GLU:HG2	15:L:2042:HOH:O	1.97	0.63
2:L:224:ILE:HG22	8:L:1286[B]:UQ2:H8	1.81	0.63
3:M:77:GLN:HE22	3:M:93:SER:H	1.44	0.62
4:H:1252:GOL:C3	15:H:2003:HOH:O	2.45	0.61
1:H:119:ASP:OD1	1:H:220[A]:LYS:NZ	2.34	0.60
3:M:197:PHE:HZ	5:M:1305:BCL:CBB	2.13	0.60
2:L:181:PHE:HB3	7:M:1314:BPH:HBB2	1.84	0.60
1:H:118[A]:ARG:HD3	15:M:2102:HOH:O	2.01	0.59
7:L:1285:BPH:HBB2	3:M:210:TYR:HB3	1.84	0.59
2:L:72:GLU:CG	15:L:2042:HOH:O	2.50	0.58
1:H:169:VAL:HG23	1:H:171:ILE:HD13	1.85	0.58
3:M:55:LEU:HD22	3:M:128:SER:HB2	1.86	0.58
5:L:1282:BCL:HBB3	5:L:1287:BCL:H52	1.85	0.58
3:M:194:GLY:O	3:M:195:ASN:HB3	2.04	0.57
2:L:208:THR:HB	2:L:209:PRO:HD2	1.86	0.57
3:M:62:SER:OG	3:M:124:VAL:HG22	2.05	0.56
1:H:11:ASP:OD1	3:M:302:GLY:HA2	2.06	0.56
1:H:248:ARG:HA	1:H:249:LYS:CB	2.36	0.56
6:L:1284:LDA:H121	8:L:1286[B]:UQ2:C16	2.36	0.55
1:H:62:LYS:HE3	4:H:1252:GOL:H11	1.88	0.55
6:M:1308:LDA:HM22	6:M:1309:LDA:H11	1.89	0.55
5:L:1287:BCL:CBB	5:L:1287:BCL:HMB1	2.37	0.54
5:M:1305:BCL:HBD	5:M:1305:BCL:HAA2	1.90	0.54
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.90	0.54
1:H:171:ILE:HB	1:H:172:PRO:HD3	1.88	0.53
6:L:1284:LDA:H121	8:L:1286[B]:UQ2:H162	1.90	0.52
2:L:162:TYR:OH	3:M:187:ASN:ND2	2.43	0.52
7:M:1314:BPH:HBB3	7:M:1314:BPH:CHC	2.38	0.52
2:L:199:ASN:O	14:M:1317:CDL:HB22	2.09	0.51
3:M:202:HIS:CE1	3:M:206:ILE:HD11	2.45	0.51
5:L:1287:BCL:HBB3	5:L:1287:BCL:HMB1	1.93	0.51
3:M:189:PHE:O	3:M:193:HIS:CD2	2.58	0.51
7:M:1314:BPH:HHD	7:M:1314:BPH:CBC	2.39	0.50
5:L:1282:BCL:HHC	5:L:1282:BCL:HBB2	1.94	0.50
3:M:278:LEU:CA	3:M:278:LEU:HD23	1.99	0.49
1:H:122:GLU:HB2	1:H:227:LEU:HD21	1.94	0.49
1:H:140:PHE:HA	3:M:13:ARG:O	2.13	0.49
8:L:1286[A]:UQ2:H152	6:M:1310:LDA:H91	1.95	0.49
3:M:194:GLY:O	3:M:195:ASN:CB	2.61	0.48
7:L:1285:BPH:CHC	7:L:1285:BPH:HBB3	2.29	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:M:1314:BPH:HBC3	7:M:1314:BPH:CHD	2.44	0.48
3:M:199:ASN:C	3:M:199:ASN:HD22	2.15	0.48
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.95	0.48
7:L:1285:BPH:CHC	7:L:1285:BPH:CBB	2.89	0.48
5:M:1304:BCL:H13	5:M:1304:BCL:H102	1.64	0.48
1:H:45:GLU:HG3	1:H:94:GLU:OE1	2.14	0.47
5:M:1304:BCL:HBB2	13:M:1316:SPO:H243	1.96	0.47
3:M:197:PHE:CE1	5:M:1305:BCL:HBB2	2.50	0.47
2:L:181:PHE:HB3	7:M:1314:BPH:CBB	2.44	0.47
15:H:2003:HOH:O	14:M:1317:CDL:HA32	2.14	0.47
1:H:130:LYS:HE3	1:H:170:ASP:OD2	2.14	0.47
6:M:1309:LDA:H91	12:M:1315:U10:H23	1.97	0.47
3:M:144:LYS:N	14:M:1317:CDL:OB3	2.39	0.47
3:M:278:LEU:O	3:M:279:THR:OG1	2.30	0.46
3:M:278:LEU:CG	3:M:279:THR:N	2.75	0.46
2:L:11:VAL:HB	2:L:12:PRO:HD2	1.96	0.46
2:L:210:ASP:OD1	2:L:210:ASP:N	2.48	0.46
3:M:278:LEU:HG	3:M:278:LEU:CD2	2.22	0.46
3:M:47:LEU:HD12	6:M:1310:LDA:H62	1.97	0.45
5:M:1305:BCL:CHC	5:M:1305:BCL:CBB	2.88	0.45
3:M:109:LEU:O	3:M:114:LEU:HB2	2.16	0.45
7:L:1285:BPH:HBB1	3:M:210:TYR:CD2	2.52	0.45
2:L:72:GLU:H	2:L:72:GLU:HG3	1.50	0.45
2:L:44:LEU:HD13	2:L:92:CYS:SG	2.57	0.45
1:H:156:CYS:SG	1:H:248:ARG:HB2	2.57	0.44
8:L:1286[B]:UQ2:H71	8:L:1286[B]:UQ2:H5M1	1.61	0.44
3:M:66:TRP:HD1	3:M:118:ALA:O	2.01	0.44
3:M:186:THR:HG23	5:M:1305:BCL:HMD2	2.00	0.44
6:M:1306:LDA:H32	4:M:1318:GOL:H32	2.00	0.44
2:L:38:THR:HG21	2:L:100:TRP:HE3	1.82	0.44
1:H:22:ILE:HG23	14:M:1317:CDL:H231	1.99	0.43
1:H:125:GLY:HA2	2:L:208:THR:HG21	2.00	0.43
1:H:112:ALA:HA	1:H:235:GLY:O	2.18	0.43
2:L:189:LEU:HB3	8:L:1286[A]:UQ2:H3M3	2.00	0.43
2:L:157:VAL:HG11	5:M:1305:BCL:HBB1	2.00	0.43
2:L:177:ILE:HG12	5:L:1287:BCL:HMB3	2.00	0.43
3:M:113:GLY:O	3:M:117:ILE:HG13	2.18	0.43
7:M:1314:BPH:H13	7:M:1314:BPH:H102	1.88	0.43
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.36	0.43
3:M:268:TRP:CD1	12:M:1315:U10:H111	2.54	0.42
3:M:132:ARG:O	3:M:136:ARG:HG2	2.20	0.42
1:H:75:VAL:HA	1:H:76:PRO:C	2.40	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:170:ASN:HD22	2:L:171:PRO:N	2.18	0.42
5:M:1305:BCL:H61	7:M:1314:BPH:C4B	2.49	0.42
2:L:117:ILE:N	2:L:118:PRO:HD2	2.35	0.42
1:H:29:TYR:HB2	4:H:1253:GOL:H12	2.01	0.41
2:L:189:LEU:HD23	7:M:1314:BPH:HMD2	2.02	0.41
2:L:153:HIS:CD2	5:L:1282:BCL:NC	2.88	0.41
3:M:270:ILE:O	3:M:274:VAL:HG13	2.20	0.41
5:M:1304:BCL:CBB	13:M:1316:SPO:H243	2.51	0.41
1:H:171:ILE:HB	1:H:172:PRO:CD	2.51	0.41
1:H:171:ILE:N	1:H:172:PRO:HD2	2.36	0.41
3:M:30:SER:OG	3:M:31:GLY:O	2.35	0.41
7:M:1314:BPH:CBB	7:M:1314:BPH:CHC	2.97	0.41
3:M:278:LEU:HD21	3:M:282:ILE:HG13	2.03	0.41
3:M:278:LEU:CD2	3:M:278:LEU:CD1	2.86	0.41
5:M:1304:BCL:H71	5:M:1305:BCL:H202	2.03	0.41
5:M:1304:BCL:HHB	5:M:1304:BCL:H112	2.02	0.41
3:M:164:ARG:O	3:M:168:MET:HG2	2.21	0.41
3:M:243:THR:O	3:M:247:ARG:HG3	2.20	0.40
3:M:278:LEU:HD22	3:M:279:THR:H	0.59	0.40
3:M:77:GLN:NE2	3:M:93:SER:H	2.15	0.40
2:L:60:ASN:HA	2:L:61:PRO:HD3	1.94	0.40
2:L:185:LEU:HD13	7:M:1314:BPH:ND	2.37	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	242/260 (93%)	235 (97%)	6 (2%)	1 (0%)	43	45
2	L	279/281 (99%)	272 (98%)	7 (2%)	0	100	100
3	M	301/307 (98%)	289 (96%)	9 (3%)	3 (1%)	22	18
All	All	822/848 (97%)	796 (97%)	22 (3%)	4 (0%)	38	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249	LYS
3	M	195	ASN
3	M	279	THR
3	M	302	GLY

### 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	198/208 (95%)	193 (98%)	5 (2%)	60	71
2	L	220/220 (100%)	204 (93%)	16 (7%)	20	19
3	M	236/240 (98%)	225 (95%)	11 (5%)	36	42
All	All	654/668 (98%)	622 (95%)	32 (5%)	35	39

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	193	MET
1	H	220[A]	LYS
1	H	220[B]	LYS
1	H	231	ASP
1	H	247	LYS
2	L	16	LEU
2	L	21	LEU
2	L	44	LEU
2	L	72	GLU
2	L	80	LEU
2	L	82	LYS
2	L	102	LEU
2	L	126	LEU
2	L	129	LEU
2	L	170	ASN
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	246	LEU

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Mol	Chain	Res	Type
2	L	247	CYS
2	L	272	TRP
3	M	29	ARG
3	M	39	LEU
3	M	52	LEU
3	M	55	LEU
3	M	60	LEU
3	M	148	TRP
3	M	182	HIS
3	M	191	LEU
3	M	199	ASN
3	M	216	PHE
3	M	278	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
2	L	159	ASN
2	L	170	ASN
2	L	264	GLN
3	M	77	GLN
3	M	187	ASN
3	M	193	HIS
3	M	199	ASN

### 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 30 ligands modelled in this entry, 1 is monoatomic - leaving 29 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	H	1252	-	5,5,5	0.52	0	5,5,5	1.17	0
4	GOL	H	1253	-	5,5,5	0.46	0	5,5,5	0.64	0
4	GOL	H	1254	-	5,5,5	0.30	0	5,5,5	0.42	0
4	GOL	H	1255	-	5,5,5	0.33	0	5,5,5	0.38	0
5	BCL	L	1282	2	74,74,74	2.08	9 (12%)	97,115,115	1.81	28 (28%)
6	LDA	L	1283	-	15,15,15	3.64	1 (6%)	17,17,17	0.52	0
6	LDA	L	1284	-	15,15,15	3.86	2 (13%)	17,17,17	0.90	1 (5%)
7	BPH	L	1285	-	70,70,70	2.79	16 (22%)	94,101,101	1.91	19 (20%)
8	UQ2	L	1286[A]	-	23,23,23	2.71	7 (30%)	31,31,31	1.25	3 (9%)
8	UQ2	L	1286[B]	-	23,23,23	2.60	8 (34%)	31,31,31	1.64	5 (16%)
5	BCL	L	1287	2	74,74,74	2.18	10 (13%)	97,115,115	1.98	25 (25%)
9	PO4	L	1288	-	4,4,4	0.15	0	6,6,6	0.31	0
10	HTO	L	1289	-	9,9,9	0.51	0	10,10,10	0.57	0
4	GOL	L	1290	-	5,5,5	0.36	0	5,5,5	0.96	0
4	GOL	L	1291	-	5,5,5	0.29	0	5,5,5	0.35	0
5	BCL	M	1304	3	74,74,74	2.14	13 (17%)	97,115,115	1.86	21 (21%)
5	BCL	M	1305	3	74,74,74	2.20	12 (16%)	97,115,115	1.90	25 (25%)
6	LDA	M	1306	-	15,15,15	3.87	1 (6%)	17,17,17	1.24	3 (17%)
6	LDA	M	1307	-	15,15,15	3.77	1 (6%)	17,17,17	0.59	0
6	LDA	M	1308	-	15,15,15	3.56	2 (13%)	17,17,17	0.81	1 (5%)
6	LDA	M	1309	-	15,15,15	3.71	2 (13%)	17,17,17	0.47	0
6	LDA	M	1310	-	15,15,15	3.77	2 (13%)	17,17,17	0.60	0
6	LDA	M	1311	-	15,15,15	3.76	2 (13%)	17,17,17	0.68	0
6	LDA	M	1312	-	15,15,15	3.65	1 (6%)	17,17,17	0.80	1 (5%)
7	BPH	M	1314	-	70,70,70	2.93	16 (22%)	94,101,101	1.97	18 (19%)
12	U10	M	1315	-	48,48,63	3.04	14 (29%)	59,61,79	1.93	13 (22%)
13	SPO	M	1316	-	41,41,41	3.92	13 (31%)	50,50,50	2.29	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CDL	M	1317	-	80,80,99	2.61	21 (26%)	92,92,111	3.16	16 (17%)
4	GOL	M	1318	-	5,5,5	0.29	0	5,5,5	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	H	1252	-	-	0/4/4/4	0/0/0/0
4	GOL	H	1253	-	-	0/4/4/4	0/0/0/0
4	GOL	H	1254	-	-	0/4/4/4	0/0/0/0
4	GOL	H	1255	-	-	0/4/4/4	0/0/0/0
5	BCL	L	1282	2	2/2/21/25	0/41/137/137	0/0/9/9
6	LDA	L	1283	-	-	0/13/13/13	0/0/0/0
6	LDA	L	1284	-	-	0/13/13/13	0/0/0/0
7	BPH	L	1285	-	2/2/18/22	0/49/105/105	0/0/6/6
8	UQ2	L	1286[A]	-	-	0/15/39/39	0/1/1/1
8	UQ2	L	1286[B]	-	-	0/15/39/39	0/1/1/1
5	BCL	L	1287	2	2/2/21/25	0/41/137/137	0/0/9/9
9	PO4	L	1288	-	-	0/0/0/0	0/0/0/0
10	HTO	L	1289	-	-	0/10/10/10	0/0/0/0
4	GOL	L	1290	-	-	0/4/4/4	0/0/0/0
4	GOL	L	1291	-	-	0/4/4/4	0/0/0/0
5	BCL	M	1304	3	2/2/21/25	0/41/137/137	0/0/9/9
5	BCL	M	1305	3	2/2/21/25	0/41/137/137	0/0/9/9
6	LDA	M	1306	-	-	0/13/13/13	0/0/0/0
6	LDA	M	1307	-	-	0/13/13/13	0/0/0/0
6	LDA	M	1308	-	-	0/13/13/13	0/0/0/0
6	LDA	M	1309	-	-	0/13/13/13	0/0/0/0
6	LDA	M	1310	-	-	0/13/13/13	0/0/0/0
6	LDA	M	1311	-	-	0/13/13/13	0/0/0/0
6	LDA	M	1312	-	-	0/13/13/13	0/0/0/0
7	BPH	M	1314	-	2/2/18/22	0/49/105/105	0/0/6/6
12	U10	M	1315	-	-	0/45/69/87	0/1/1/1
13	SPO	M	1316	-	-	0/47/47/47	0/0/0/0
14	CDL	M	1317	-	1/1/9/9	0/91/91/110	0/0/0/0
4	GOL	M	1318	-	-	0/4/4/4	0/0/0/0

All (153) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1306	LDA	O1-N1	-14.70	1.25	1.39
6	L	1284	LDA	O1-N1	-14.70	1.25	1.39
6	M	1307	LDA	O1-N1	-14.38	1.25	1.39
6	M	1310	LDA	O1-N1	-14.34	1.25	1.39
6	M	1311	LDA	O1-N1	-14.31	1.25	1.39
6	M	1309	LDA	O1-N1	-14.10	1.26	1.39
7	M	1314	BPH	C1D-CHD	14.06	1.51	1.35
6	M	1312	LDA	O1-N1	-13.93	1.26	1.39
6	L	1283	LDA	O1-N1	-13.89	1.26	1.39
5	M	1305	BCL	OBD-CAD	13.57	1.42	1.22
6	M	1308	LDA	O1-N1	-13.51	1.26	1.39
5	L	1287	BCL	OBD-CAD	12.79	1.40	1.22
5	L	1282	BCL	OBD-CAD	12.47	1.40	1.22
5	M	1304	BCL	OBD-CAD	12.45	1.40	1.22
13	M	1316	SPO	C27-C28	12.30	1.47	1.34
7	L	1285	BPH	OBD-CAD	12.24	1.40	1.22
7	M	1314	BPH	OBD-CAD	11.65	1.39	1.22
7	L	1285	BPH	C1D-CHD	10.87	1.47	1.35
13	M	1316	SPO	C9-C7	9.09	1.47	1.35
13	M	1316	SPO	C19-C17	9.08	1.47	1.35
12	M	1315	U10	C33-C34	8.27	1.49	1.32
13	M	1316	SPO	C14-C12	8.21	1.46	1.35
8	L	1286[A]	UQ2	C8-C9	8.06	1.49	1.32
12	M	1315	U10	C13-C14	7.95	1.49	1.32
14	M	1317	CDL	C84-C83	-7.92	1.52	1.55
14	M	1317	CDL	C58-C57	-7.85	1.52	1.55
13	M	1316	SPO	C22-C23	7.83	1.46	1.35
14	M	1317	CDL	C43-C42	-7.80	1.52	1.55
13	M	1316	SPO	C32-C33	7.79	1.48	1.32
7	M	1314	BPH	C2-C3	7.62	1.48	1.32
8	L	1286[B]	UQ2	C8-C9	7.18	1.47	1.32
7	L	1285	BPH	C2-C3	7.15	1.47	1.32
12	M	1315	U10	C28-C29	7.10	1.47	1.32
12	M	1315	U10	C8-C9	6.97	1.47	1.32
12	M	1315	U10	C38-C39	6.89	1.48	1.34
7	L	1285	BPH	O1D-CGD	6.78	1.38	1.21
12	M	1315	U10	C23-C24	6.75	1.46	1.32
12	M	1315	U10	C18-C19	6.70	1.46	1.32
7	M	1314	BPH	O1D-CGD	6.60	1.37	1.21
14	M	1317	CDL	C24-C23	-6.46	1.52	1.55
7	L	1285	BPH	OBG-CAB	6.40	1.44	1.22
7	L	1285	BPH	O1A-CGA	6.37	1.41	1.22
14	M	1317	CDL	C32-C31	-6.34	1.27	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1314	BPH	O1A-CGA	5.91	1.40	1.22
5	M	1304	BCL	O1A-CGA	5.88	1.40	1.22
5	L	1287	BCL	O1A-CGA	5.82	1.40	1.22
5	L	1282	BCL	O1A-CGA	5.73	1.39	1.22
14	M	1317	CDL	C11-CA5	-5.53	1.33	1.50
13	M	1316	SPO	C37-C38	5.22	1.49	1.32
5	M	1305	BCL	O1A-CGA	5.18	1.38	1.22
7	M	1314	BPH	OB6-CAB	5.12	1.40	1.22
8	L	1286[B]	UQ2	C13-C14	4.99	1.48	1.32
8	L	1286[B]	UQ2	O2-C2	-4.99	1.24	1.36
5	M	1305	BCL	C4D-C3D	-4.93	1.35	1.41
8	L	1286[A]	UQ2	O2-C2	-4.93	1.24	1.36
14	M	1317	CDL	C33-C32	-4.81	1.22	1.51
14	M	1317	CDL	OB6-CB5	4.78	1.48	1.34
5	L	1287	BCL	C2-C3	4.70	1.42	1.32
5	L	1287	BCL	C1B-NB	4.67	1.40	1.34
8	L	1286[A]	UQ2	C13-C14	4.60	1.47	1.32
14	M	1317	CDL	OA6-CA5	4.57	1.48	1.34
14	M	1317	CDL	OA8-CA7	4.57	1.47	1.33
13	M	1316	SPO	C10-C11	4.47	1.46	1.34
13	M	1316	SPO	C6-C5	4.44	1.44	1.31
8	L	1286[A]	UQ2	O3-C3	-4.43	1.25	1.36
5	L	1287	BCL	C4B-NB	4.39	1.40	1.34
13	M	1316	SPO	C15-C16	4.36	1.46	1.34
8	L	1286[B]	UQ2	O3-C3	-4.34	1.25	1.36
14	M	1317	CDL	OB8-CB7	4.31	1.46	1.33
5	L	1282	BCL	C1B-NB	4.31	1.39	1.34
7	M	1314	BPH	C3D-CAD	-4.31	1.38	1.47
14	M	1317	CDL	C34-C33	-4.13	1.26	1.51
5	M	1304	BCL	C4D-C3D	-4.09	1.36	1.41
5	L	1282	BCL	C2-C3	4.09	1.41	1.32
5	M	1305	BCL	C1B-NB	4.03	1.39	1.34
13	M	1316	SPO	C26-C25	3.89	1.45	1.34
14	M	1317	CDL	C17-C16	-3.89	1.27	1.51
5	L	1282	BCL	C4B-NB	3.84	1.39	1.34
14	M	1317	CDL	C16-C15	-3.76	1.28	1.51
14	M	1317	CDL	C13-C12	-3.75	1.28	1.51
12	M	1315	U10	O3-C3	-3.70	1.27	1.36
5	L	1287	BCL	C3D-CAD	-3.69	1.39	1.47
5	L	1287	BCL	O2D-CGD	-3.67	1.23	1.33
5	M	1304	BCL	C2-C3	3.67	1.40	1.32
5	M	1304	BCL	C1B-NB	3.65	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	1285	BPH	C4D-C3D	-3.64	1.37	1.41
14	M	1317	CDL	C20-C19	-3.61	1.29	1.51
7	L	1285	BPH	C3D-CAD	-3.56	1.40	1.47
5	M	1305	BCL	C3D-CAD	-3.56	1.40	1.47
13	M	1316	SPO	C21-C20	3.48	1.45	1.35
14	M	1317	CDL	C19-C18	-3.44	1.30	1.51
5	M	1304	BCL	C1C-NC	-3.39	1.31	1.39
5	L	1282	BCL	C3D-CAD	-3.38	1.40	1.47
8	L	1286[B]	UQ2	C3-C4	-3.35	1.39	1.48
5	M	1305	BCL	C2-C3	3.31	1.39	1.32
12	M	1315	U10	O4-C4	-3.31	1.28	1.36
5	M	1304	BCL	MG-ND	-3.19	1.97	2.05
5	M	1304	BCL	C3D-CAD	-3.19	1.40	1.47
7	M	1314	BPH	CHD-C4C	3.15	1.48	1.41
5	L	1287	BCL	C1A-NA	3.13	1.39	1.32
12	M	1315	U10	C4-C5	-3.10	1.39	1.48
5	M	1304	BCL	O2D-CGD	-3.10	1.24	1.33
7	L	1285	BPH	O2A-CGA	-3.07	1.23	1.33
8	L	1286[A]	UQ2	C3-C4	-3.06	1.40	1.48
7	M	1314	BPH	C4D-ND	-3.04	1.34	1.38
7	M	1314	BPH	C4D-C3D	-2.97	1.38	1.41
5	L	1282	BCL	C4D-C3D	-2.91	1.38	1.41
7	L	1285	BPH	C1C-NC	-2.88	1.32	1.38
7	M	1314	BPH	C3D-C2D	2.85	1.49	1.40
7	M	1314	BPH	O2D-CGD	-2.85	1.25	1.33
5	L	1282	BCL	C1A-NA	2.79	1.38	1.32
14	M	1317	CDL	C79-C78	-2.77	1.34	1.51
7	L	1285	BPH	O2D-CGD	-2.75	1.25	1.33
14	M	1317	CDL	C37-C36	-2.74	1.34	1.51
5	M	1305	BCL	C4B-NB	2.72	1.38	1.34
14	M	1317	CDL	C80-C79	-2.72	1.34	1.51
12	M	1315	U10	C6-C1	2.68	1.41	1.35
14	M	1317	CDL	C22-C21	-2.68	1.35	1.51
5	M	1305	BCL	C1C-NC	-2.60	1.33	1.39
5	L	1282	BCL	O2A-CGA	-2.53	1.25	1.33
8	L	1286[A]	UQ2	C6-C5	2.52	1.41	1.35
5	M	1305	BCL	C1A-NA	2.48	1.37	1.32
7	M	1314	BPH	CHC-C1C	2.47	1.47	1.38
5	M	1305	BCL	O2D-CGD	-2.45	1.26	1.33
12	M	1315	U10	O3-C3M	-2.45	1.39	1.45
8	L	1286[B]	UQ2	C6-C1	-2.44	1.39	1.46
7	L	1285	BPH	C3D-C2D	2.43	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	1285	BPH	CHD-C4C	2.41	1.46	1.41
5	M	1304	BCL	C1A-NA	2.40	1.37	1.32
7	M	1314	BPH	O2A-CGA	-2.39	1.25	1.33
6	M	1308	LDA	C1-N1	-2.33	1.46	1.51
5	L	1287	BCL	C4D-C3D	-2.33	1.38	1.41
7	M	1314	BPH	C1C-NC	-2.32	1.33	1.38
7	L	1285	BPH	CHC-C1C	2.30	1.47	1.38
5	M	1304	BCL	C4B-NB	2.28	1.37	1.34
8	L	1286[B]	UQ2	C2-C1	-2.27	1.42	1.48
5	M	1304	BCL	C2A-C1A	-2.25	1.48	1.52
5	M	1304	BCL	O2A-CGA	-2.24	1.26	1.33
7	L	1285	BPH	CHB-C4A	2.23	1.46	1.38
7	M	1314	BPH	CHB-C4A	2.21	1.46	1.38
8	L	1286[A]	UQ2	C2-C1	-2.20	1.42	1.48
6	L	1284	LDA	C1-N1	-2.20	1.47	1.51
6	M	1310	LDA	C1-N1	-2.14	1.47	1.51
5	M	1305	BCL	O2D-CED	-2.13	1.40	1.45
12	M	1315	U10	C41-C39	2.12	1.52	1.40
5	L	1287	BCL	C1C-NC	-2.08	1.34	1.39
6	M	1311	LDA	C1-N1	-2.06	1.47	1.51
8	L	1286[B]	UQ2	C6-C5	2.05	1.40	1.35
7	L	1285	BPH	C4A-NA	-2.05	1.34	1.38
13	M	1316	SPO	C4-C1	-2.04	1.52	1.54
5	M	1305	BCL	C3C-C4C	2.02	1.54	1.51
12	M	1315	U10	C4-C3	2.01	1.44	1.35
6	M	1309	LDA	C1-N1	-2.00	1.47	1.51

All (197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	1317	CDL	C33-C32-C31	17.25	178.30	113.28
14	M	1317	CDL	C17-C16-C15	10.65	172.22	114.61
14	M	1317	CDL	C12-C11-CA5	10.02	152.78	113.51
14	M	1317	CDL	C20-C19-C18	9.45	165.72	114.61
5	L	1287	BCL	CMB-C2B-C1B	-8.47	115.59	128.62
7	M	1314	BPH	C3B-C2B-C1B	-7.94	102.26	107.01
14	M	1317	CDL	C35-C34-C33	7.86	157.13	114.61
5	M	1304	BCL	CMB-C2B-C1B	-7.71	116.76	128.62
5	M	1305	BCL	CMB-C2B-C1B	-7.64	116.86	128.62
7	L	1285	BPH	C3B-C2B-C1B	-7.32	102.63	107.01
14	M	1317	CDL	C34-C33-C32	7.25	153.85	114.61
14	M	1317	CDL	C13-C12-C11	7.07	139.94	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1282	BCL	CMB-C2B-C1B	-6.70	118.32	128.62
7	M	1314	BPH	O2D-CGD-CBD	6.04	123.62	111.33
5	M	1304	BCL	CMB-C2B-C3B	5.95	134.34	124.97
7	M	1314	BPH	OBD-CAD-C3D	-5.95	116.85	127.91
5	L	1287	BCL	CMB-C2B-C3B	5.89	134.25	124.97
7	L	1285	BPH	O2D-CGD-CBD	5.75	123.04	111.33
13	M	1316	SPO	C15-C14-C12	-5.53	119.32	127.29
12	M	1315	U10	C30-C29-C31	5.50	123.75	115.39
13	M	1316	SPO	C20-C19-C17	-5.48	119.39	127.29
14	M	1317	CDL	OA6-CA5-C11	5.44	123.48	111.56
5	M	1305	BCL	CMB-C2B-C3B	5.42	133.50	124.97
5	L	1282	BCL	O2D-CGD-CBD	5.31	122.15	111.33
7	L	1285	BPH	OBD-CAD-CBD	-5.09	118.25	125.94
7	M	1314	BPH	C1D-C2D-C3D	-5.01	102.59	106.89
7	L	1285	BPH	C3B-C4B-NB	4.77	112.48	107.10
13	M	1316	SPO	C26-C27-C28	-4.71	123.40	127.91
5	L	1282	BCL	CMB-C2B-C3B	4.63	132.26	124.97
12	M	1315	U10	C15-C14-C16	4.61	122.40	115.39
12	M	1315	U10	C25-C24-C26	4.48	122.19	115.39
7	M	1314	BPH	OBD-CAD-CBD	-4.41	119.28	125.94
13	M	1316	SPO	C4-C5-C6	-4.39	117.70	124.95
5	L	1287	BCL	C2B-C1B-NB	-4.36	106.12	109.41
12	M	1315	U10	C10-C9-C11	4.33	121.98	115.39
13	M	1316	SPO	C10-C9-C7	-4.32	121.08	127.29
13	M	1316	SPO	C21-C22-C23	-4.31	121.09	127.29
5	M	1304	BCL	C3A-C4A-CHB	-4.30	115.40	124.33
7	M	1314	BPH	CMD-C2D-C1D	4.21	132.64	125.81
7	L	1285	BPH	CMD-C2D-C1D	4.17	132.56	125.81
7	M	1314	BPH	O2D-CGD-O1D	-4.14	115.38	123.79
7	L	1285	BPH	OBD-CAD-C3D	-4.04	120.39	127.91
7	L	1285	BPH	CED-O2D-CGD	3.96	125.45	116.02
13	M	1316	SPO	C29-C28-C30	3.85	121.24	115.39
5	M	1305	BCL	CED-O2D-CGD	3.82	125.10	116.02
7	L	1285	BPH	O1D-CGD-CBD	-3.80	116.64	124.42
5	M	1304	BCL	O2D-CGD-CBD	3.80	119.07	111.33
5	M	1304	BCL	C2C-C1C-CHC	-3.76	116.51	124.33
5	L	1282	BCL	C4B-CHC-C1C	-3.74	122.27	130.06
5	M	1305	BCL	C2D-C1D-ND	-3.73	106.59	109.41
5	L	1287	BCL	O2A-CGA-CBA	3.69	123.55	111.94
5	M	1305	BCL	O2A-CGA-CBA	3.69	123.54	111.94
5	M	1305	BCL	O2D-CGD-CBD	3.68	118.83	111.33
5	M	1305	BCL	OBB-CAB-C3B	3.66	125.57	120.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	1315	U10	C17-C18-C19	-3.66	119.90	127.80
5	M	1305	BCL	C1C-NC-C4C	-3.64	103.37	107.79
7	L	1285	BPH	C1D-C2D-C3D	-3.58	103.82	106.89
5	L	1287	BCL	OBD-CAD-CBD	-3.58	120.54	125.94
12	M	1315	U10	C30-C29-C28	-3.57	116.45	123.52
7	M	1314	BPH	CMD-C2D-C3D	-3.57	119.35	124.97
5	L	1282	BCL	C4-C3-C5	3.56	120.81	115.39
5	M	1305	BCL	C2C-C1C-CHC	-3.56	116.94	124.33
14	M	1317	CDL	OB6-CB5-C51	3.54	119.31	111.56
7	L	1285	BPH	C2B-C1B-NB	3.53	115.03	108.16
8	L	1286[B]	UQ2	C10-C9-C11	3.48	120.68	115.39
5	L	1287	BCL	CMD-C2D-C1D	3.48	133.04	126.16
5	M	1304	BCL	CAA-C2A-C3A	-3.46	104.86	113.04
7	M	1314	BPH	C2B-C1B-NB	3.45	114.87	108.16
5	M	1305	BCL	CMD-C2D-C1D	3.44	132.96	126.16
8	L	1286[B]	UQ2	CM5-C5-C6	-3.38	117.49	124.20
5	L	1287	BCL	CGD-CBD-CHA	3.37	122.43	110.96
5	L	1287	BCL	C2A-C3A-C4A	3.33	106.52	101.40
5	L	1282	BCL	C2D-C1D-ND	-3.32	106.90	109.41
5	M	1304	BCL	C1-O2A-CGA	3.30	126.23	116.98
5	L	1287	BCL	C4B-CHC-C1C	-3.30	123.19	130.06
5	M	1305	BCL	OBD-CAD-CBD	-3.30	120.96	125.94
12	M	1315	U10	C27-C28-C29	-3.29	120.70	127.80
5	M	1304	BCL	C2D-C1D-ND	-3.26	106.95	109.41
7	M	1314	BPH	CAC-C3C-C2C	-3.25	106.44	113.89
7	M	1314	BPH	C4B-C3B-C2B	3.24	109.95	107.60
5	L	1287	BCL	C11-C12-C13	3.23	124.44	115.14
5	L	1287	BCL	C1-O2A-CGA	3.21	125.97	116.98
5	L	1287	BCL	O2D-CGD-O1D	-3.20	117.30	123.79
8	L	1286[B]	UQ2	CM3-O3-C3	3.19	127.32	116.48
5	M	1304	BCL	C1B-CHB-C4A	-3.18	123.44	130.06
5	M	1304	BCL	O2A-CGA-CBA	3.16	121.87	111.94
12	M	1315	U10	C22-C23-C24	-3.12	121.06	127.80
5	M	1304	BCL	CMA-C3A-C4A	-3.08	102.82	111.76
7	L	1285	BPH	C1B-NB-C4B	-3.07	101.69	108.72
5	L	1282	BCL	O2A-CGA-CBA	3.06	121.56	111.94
14	M	1317	CDL	OB8-CB7-C71	2.97	121.27	111.94
7	M	1314	BPH	O2A-CGA-CBA	2.95	121.21	111.94
6	M	1306	LDA	O1-N1-C1	2.94	114.29	110.19
13	M	1316	SPO	C24-C23-C25	2.93	122.83	118.09
7	L	1285	BPH	O2A-CGA-O1A	-2.91	115.48	123.43
5	L	1282	BCL	C2A-C3A-C4A	2.90	105.87	101.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1282	BCL	C2B-C1B-NB	-2.90	107.22	109.41
5	L	1287	BCL	CAA-C2A-C1A	-2.89	104.41	111.62
12	M	1315	U10	C11-C9-C8	-2.89	115.53	121.08
14	M	1317	CDL	OA8-CA7-C31	2.88	121.01	111.94
8	L	1286[B]	UQ2	O1-C1-C6	-2.85	116.42	121.67
5	L	1287	BCL	C1B-CHB-C4A	-2.85	124.13	130.06
5	L	1287	BCL	C14-C13-C12	2.83	121.42	111.02
6	L	1284	LDA	O1-N1-C1	-2.81	106.27	110.19
5	M	1304	BCL	O2A-C1-C2	2.80	114.62	108.55
5	L	1282	BCL	OBD-CAD-CBD	-2.80	121.72	125.94
14	M	1317	CDL	C21-C22-C23	2.78	124.32	113.78
5	L	1282	BCL	O2D-CGD-O1D	-2.77	118.17	123.79
5	L	1282	BCL	C4D-ND-C1D	2.68	109.81	106.57
7	M	1314	BPH	CBA-CAA-C2A	-2.67	106.08	114.01
5	M	1305	BCL	O2D-CGD-O1D	-2.66	118.39	123.79
6	M	1306	LDA	CM2-N1-CM1	-2.65	105.82	108.85
7	L	1285	BPH	C1-C2-C3	-2.63	121.50	126.19
13	M	1316	SPO	C15-C16-C17	-2.63	118.87	126.38
5	M	1304	BCL	C4D-ND-C1D	2.63	109.74	106.57
5	L	1287	BCL	CHB-C4A-NA	-2.62	121.47	124.58
5	M	1305	BCL	C3C-C4C-CHD	-2.59	117.67	123.35
13	M	1316	SPO	C8-C7-C6	2.59	122.28	118.09
5	M	1304	BCL	O2D-CGD-O1D	-2.59	118.54	123.79
5	L	1287	BCL	C3A-C4A-CHB	-2.58	118.96	124.33
5	L	1282	BCL	C1C-NC-C4C	-2.58	104.66	107.79
8	L	1286[A]	UQ2	C10-C9-C11	2.57	119.30	115.39
13	M	1316	SPO	C25-C23-C22	-2.57	115.03	118.97
7	L	1285	BPH	C11-C10-C8	-2.56	107.77	115.14
13	M	1316	SPO	C34-C33-C35	2.56	119.28	115.39
5	L	1287	BCL	C11-C10-C8	2.54	122.46	115.14
6	M	1308	LDA	C2-C1-N1	-2.54	109.43	113.80
5	L	1287	BCL	C2D-C1D-ND	-2.53	107.50	109.41
5	M	1304	BCL	CED-O2D-CGD	2.53	122.03	116.02
8	L	1286[A]	UQ2	O2-C2-C3	-2.52	113.80	123.80
5	L	1287	BCL	C2A-C1A-NA	2.52	114.03	111.24
5	M	1305	BCL	C1-C2-C3	-2.52	121.71	126.19
5	M	1304	BCL	C4B-CHC-C1C	-2.51	124.83	130.06
5	M	1304	BCL	OBD-CAD-CBD	-2.50	122.16	125.94
5	L	1282	BCL	CAC-C3C-C2C	-2.47	108.22	113.89
5	M	1304	BCL	CBD-CHA-C1A	2.46	131.99	128.77
5	L	1287	BCL	C2C-C1C-CHC	-2.45	119.23	124.33
12	M	1315	U10	C16-C14-C13	-2.44	116.38	121.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1287	BCL	CMD-C2D-C3D	-2.42	121.15	124.97
12	M	1315	U10	C7-C8-C9	2.42	130.85	126.76
13	M	1316	SPO	C31-C32-C33	-2.39	122.63	127.80
7	L	1285	BPH	O2A-CGA-CBA	2.39	119.46	111.94
12	M	1315	U10	C12-C13-C14	-2.39	122.64	127.80
5	L	1282	BCL	O2A-CGA-O1A	-2.38	116.94	123.43
13	M	1316	SPO	C13-C12-C11	2.37	121.93	118.09
5	L	1282	BCL	O1D-CGD-CBD	-2.37	119.57	124.42
7	M	1314	BPH	CMB-C2B-C1B	-2.34	125.08	128.65
13	M	1316	SPO	C20-C21-C22	-2.32	118.23	123.36
14	M	1317	CDL	OA6-CA5-OA7	-2.30	117.49	123.65
5	L	1282	BCL	C5-C3-C2	-2.30	116.66	121.08
5	L	1287	BCL	C3C-C4C-CHD	-2.29	118.33	123.35
5	L	1282	BCL	C2C-C1C-CHC	-2.29	119.56	124.33
5	M	1305	BCL	CMD-C2D-C3D	-2.29	121.36	124.97
13	M	1316	SPO	C27-C26-C25	-2.29	115.52	123.24
5	L	1282	BCL	C1B-CHB-C4A	-2.29	125.30	130.06
5	M	1305	BCL	CGD-CBD-CHA	-2.29	103.19	110.96
5	M	1305	BCL	C4D-ND-C1D	2.28	109.33	106.57
5	L	1287	BCL	O2D-CGD-CBD	2.27	115.96	111.33
7	L	1285	BPH	C4D-ND-C1D	-2.27	103.51	108.72
5	M	1305	BCL	CAC-C3C-C2C	-2.27	108.68	113.89
5	L	1282	BCL	C3C-C4C-NC	2.26	114.50	111.60
6	M	1306	LDA	O1-N1-CM2	-2.25	105.98	109.01
5	L	1282	BCL	CAA-C2A-C3A	-2.25	107.72	113.04
5	M	1304	BCL	C3B-C4B-NB	2.25	110.83	108.64
7	M	1314	BPH	CMB-C2B-C3B	2.23	128.47	124.97
6	M	1312	LDA	O1-N1-CM2	-2.22	106.02	109.01
5	M	1304	BCL	C3C-C4C-CHD	-2.21	118.51	123.35
5	L	1282	BCL	CBD-CHA-C1A	2.21	131.66	128.77
13	M	1316	SPO	C3-C1-C4	-2.19	107.35	110.97
13	M	1316	SPO	C14-C15-C16	-2.19	115.86	123.24
7	L	1285	BPH	C4D-C3D-C2D	-2.18	104.73	107.37
12	M	1315	U10	C21-C22-C23	-2.18	105.38	111.62
5	M	1305	BCL	C2B-C1B-NB	-2.18	107.77	109.41
5	M	1305	BCL	CHC-C1C-NC	-2.18	121.99	124.58
5	L	1282	BCL	CHA-C1A-NA	-2.15	121.80	126.22
5	M	1305	BCL	C3A-C4A-NA	2.14	113.55	110.95
5	L	1282	BCL	CHC-C4B-NB	-2.12	121.03	124.58
14	M	1317	CDL	C32-C31-CA7	2.12	121.81	113.51
7	M	1314	BPH	CED-O2D-CGD	2.11	121.03	116.02
5	L	1282	BCL	C2A-C1A-NA	2.11	113.58	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1282	BCL	CAA-C2A-C1A	-2.11	106.37	111.62
7	M	1314	BPH	C3B-C4B-CHC	-2.09	119.46	126.11
5	M	1305	BCL	C1D-CHD-C4C	-2.09	121.94	125.55
5	L	1287	BCL	C4D-ND-C1D	2.07	109.07	106.57
5	M	1305	BCL	C7-C6-C5	-2.07	106.91	113.01
14	M	1317	CDL	C80-C79-C78	2.06	125.73	114.61
5	M	1305	BCL	C16-C15-C13	-2.05	109.23	115.14
8	L	1286[B]	UQ2	O4-C4-C3	-2.04	116.43	120.96
7	L	1285	BPH	C2D-C1D-ND	2.04	113.28	106.38
7	L	1285	BPH	CMB-C2B-C3B	2.04	128.19	124.97
5	L	1282	BCL	C3A-C4A-CHB	-2.04	120.08	124.33
5	L	1282	BCL	CMD-C2D-C1D	2.04	130.18	126.16
14	M	1317	CDL	OB2-CB2-C1	2.02	114.96	108.62
7	M	1314	BPH	C3C-C4C-CHD	2.01	126.01	121.83
5	M	1305	BCL	C2C-C1C-NC	2.01	113.39	110.95
5	M	1304	BCL	C3D-CAD-CBD	2.01	110.43	107.60
8	L	1286[A]	UQ2	CM2-O2-C2	2.01	123.29	116.48

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	L	1285	BPH	C8
7	L	1285	BPH	C13
5	L	1287	BCL	C8
5	L	1287	BCL	C13
5	L	1282	BCL	C8
5	L	1282	BCL	C13
5	M	1304	BCL	C8
5	M	1304	BCL	C13
7	M	1314	BPH	C8
7	M	1314	BPH	C13
5	M	1305	BCL	C8
5	M	1305	BCL	C13
14	M	1317	CDL	CA4

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	H	241/260 (92%)	-0.26	10 (4%) 35 36	29, 39, 51, 96	0
2	L	281/281 (100%)	-0.38	7 (2%) 54 55	27, 37, 61, 67	0
3	M	303/307 (98%)	-0.39	10 (3%) 44 45	24, 41, 63, 75	0
All	All	825/848 (97%)	-0.35	27 (3%) 45 45	24, 39, 61, 96	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	251	VAL	20.4
3	M	303	MET	9.5
3	M	1	ALA	8.5
1	H	250	SER	8.4
1	H	249	LYS	6.2
3	M	302	GLY	4.4
2	L	281	GLY	3.7
2	L	59	TRP	3.7
3	M	148	TRP	3.6
1	H	245	ALA	3.5
1	H	247	LYS	3.4
3	M	2	GLU	3.2
1	H	246	PRO	3.1
2	L	270	PRO	2.9
3	M	301	HIS	2.8
3	M	52	LEU	2.7
2	L	202	LYS	2.7
3	M	3	TYR	2.7
1	H	51	ALA	2.5
1	H	220[A]	LYS	2.4
2	L	276	PRO	2.3
3	M	109	LEU	2.2
1	H	18	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	72	GLU	2.1
2	L	277	GLY	2.1
3	M	105	PHE	2.1
1	H	92	VAL	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
6	LDA	M	1312	16/16	0.29	20.43	78,90,101,101	0
4	GOL	H	1254	6/6	0.35	13.41	103,104,105,105	0
6	LDA	L	1284	16/16	0.34	13.16	109,110,114,114	0
6	LDA	L	1283	16/16	0.46	11.50	61,91,105,105	0
4	GOL	H	1253	6/6	0.28	9.89	74,77,77,80	0
4	GOL	H	1252	6/6	0.31	8.47	46,60,63,65	0
6	LDA	M	1306	16/16	0.26	8.10	54,70,75,76	0
6	LDA	M	1310	16/16	0.33	8.09	110,113,119,120	0
6	LDA	M	1309	16/16	0.37	7.48	98,102,109,110	0
14	CDL	M	1317	81/100	0.41	5.94	78,104,124,124	0
8	UQ2	L	1286[B]	23/23	0.18	4.82	32,41,50,51	23
4	GOL	L	1291	6/6	0.25	4.67	94,95,96,96	0
8	UQ2	L	1286[A]	23/23	0.18	4.50	36,41,50,52	23
10	HTO	L	1289	10/10	0.26	4.44	85,87,88,89	0
6	LDA	M	1308	16/16	0.17	4.16	61,67,75,75	0
6	LDA	M	1311	16/16	0.45	3.87	95,104,112,113	0
6	LDA	M	1307	16/16	0.21	3.52	66,69,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
12	U10	M	1315	48/63	0.13	1.43	26,45,73,75	0
13	SPO	M	1316	42/42	0.16	1.23	36,49,68,72	0
4	GOL	L	1290	6/6	0.20	1.09	49,57,57,61	0
7	BPH	M	1314	65/65	0.12	0.58	26,41,98,101	0
9	PO4	L	1288	5/5	0.21	0.56	89,89,90,90	0
5	BCL	L	1287	66/66	0.12	0.44	19,30,50,57	0
5	BCL	M	1305	66/66	0.10	0.36	22,29,59,67	0
5	BCL	L	1282	66/66	0.08	-0.13	24,32,59,63	0
7	BPH	L	1285	65/65	0.09	-0.26	23,31,44,48	0
5	BCL	M	1304	66/66	0.09	-0.28	21,32,75,76	0
4	GOL	M	1318	6/6	0.09	-0.78	83,84,84,85	0
11	FE	M	1313	1/1	0.01	-4.35	26,26,26,26	0
4	GOL	H	1255	6/6	0.34	-	101,101,102,102	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.