



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:42 AM GMT

PDB ID : 1UMX
Title : PHOTOSYNTHETIC REACTION CENTER MUTANT WITH ARG M267
REPLACED WITH LEU (CHAIN M, R267L)
Authors : Fyfe, P.K.; Isaacs, N.W.; Cogdell, R.J.; Jones, M.R.
Deposited on : 2003-09-02
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

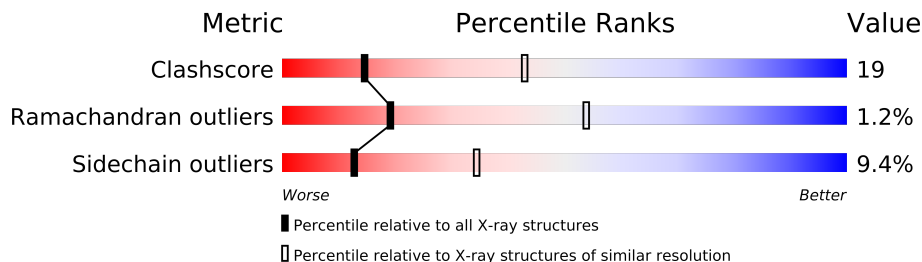
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
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 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

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

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7007 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	14	0	1
			1830	1169	315	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	10	0	0
			2232	1507	355	362	8			

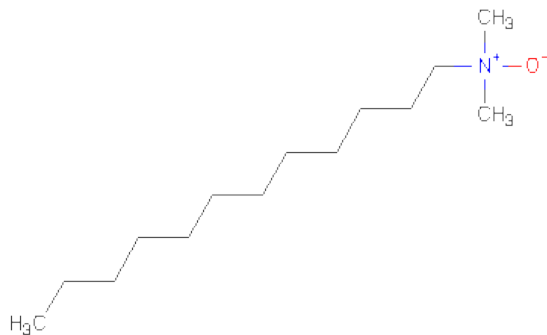
- Molecule 3 is a protein called REACTION CENTER PROTEIN M CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2406	1607	392	397	10			

There is a discrepancy between the modelled and reference sequences:

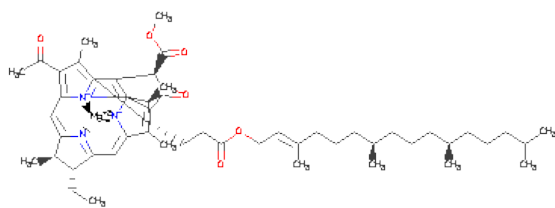
Chain	Residue	Modelled	Actual	Comment	Reference
M	267	LEU	ARG	ENGINEERED MUTATION	UNP P02953

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



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

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



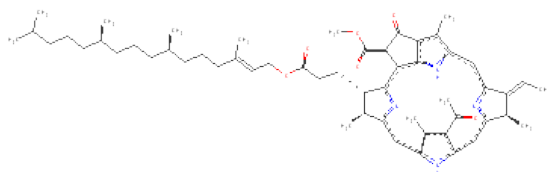
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: C₅₅H₇₄N₄O₆).

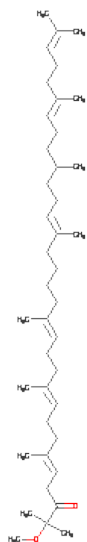


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			65	55	4	6		
6	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 7 is FE (III) ION (three-letter code: FE) (formula: Fe).

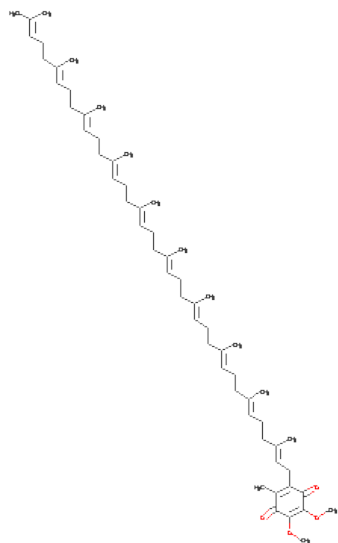
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Fe	0	0
			1	1		

- Molecule 8 is SPEROIDENONE (three-letter code: SPN) (formula: C₄₁H₇₀O₂).



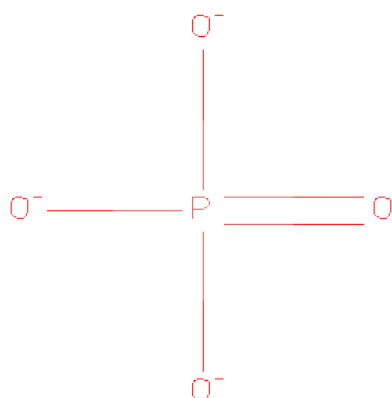
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			43	41	2		

- 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		

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	6	Total	O	0	0
			6	6		
11	L	6	Total	O	0	0
			6	6		
11	M	4	Total	O	0	0
			4	4		

3 Residue-property plots

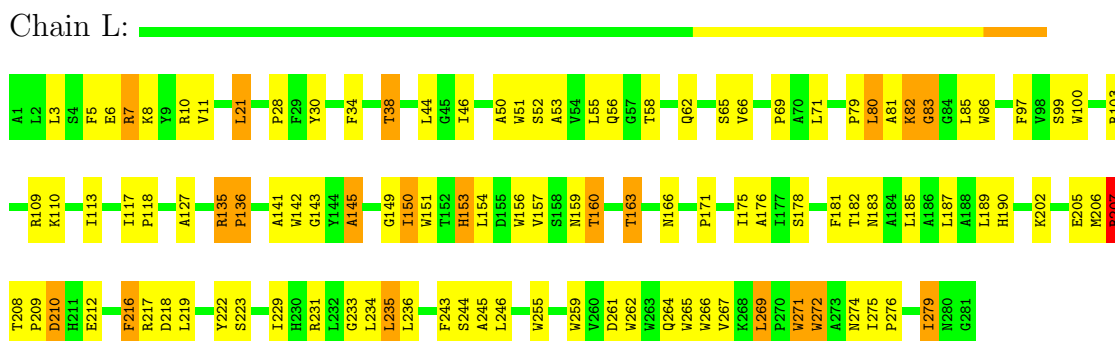
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

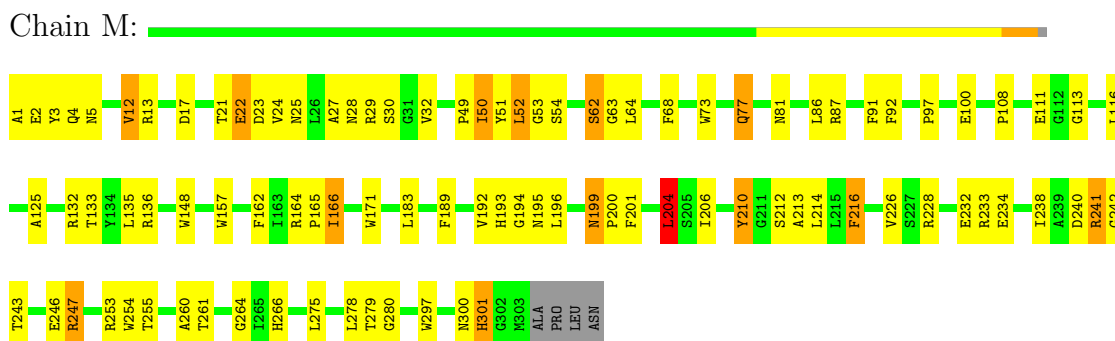
• Molecule 1: REACTION CENTER PROTEIN H CHAIN



• Molecule 2: REACTION CENTER PROTEIN L CHAIN



• Molecule 3: REACTION CENTER PROTEIN M CHAIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.64Å 141.64Å 187.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.00 – 2.80	Depositor
% Data completeness (in resolution range)	97.5 (29.00-2.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.224 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7007	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	H	1.09	0/1878	1.34	18/2555 (0.7%)
2	L	1.29	3/2320 (0.1%)	1.15	13/3175 (0.4%)
3	M	0.98	0/2498	1.09	8/3412 (0.2%)
All	All	1.13	3/6696 (0.0%)	1.18	39/9142 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	1	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	202	LYS	CD-CE	30.62	2.27	1.51
2	L	202	LYS	CG-CD	-24.89	0.67	1.52
2	L	5	PHE	CD2-CE2	5.88	1.51	1.39

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	202	LYS	CB-CG-CD	-17.59	65.86	111.60
1	H	31	LEU	N-CA-C	-15.57	68.97	111.00
2	L	202	LYS	CD-CE-NZ	11.23	137.54	111.70
3	M	17	ASP	CB-CG-OD2	10.95	128.16	118.30
1	H	65	ILE	C-N-CA	9.02	144.24	121.70
2	L	231	ARG	NE-CZ-NH2	-8.97	115.81	120.30
2	L	82	LYS	N-CA-CB	8.83	126.49	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	30	TYR	O-C-N	-8.71	108.75	122.70
1	H	66	LEU	CB-CA-C	8.18	125.75	110.20
2	L	261	ASP	CB-CG-OD2	7.99	125.49	118.30
1	H	82	ASP	CB-CG-OD2	7.70	125.23	118.30
1	H	31	LEU	N-CA-CB	7.50	125.41	110.40
1	H	83	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	H	30	TYR	CA-C-N	7.14	132.92	117.20
1	H	30	TYR	CB-CA-C	6.84	124.08	110.40
1	H	66	LEU	N-CA-CB	6.78	123.96	110.40
1	H	65	ILE	CA-C-N	6.68	131.89	117.20
2	L	207	ARG	NE-CZ-NH1	-6.50	117.05	120.30
3	M	241	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	H	30	TYR	C-N-CA	6.41	137.74	121.70
1	H	166	ASP	CB-CG-OD2	6.41	124.06	118.30
1	H	65	ILE	O-C-N	-6.36	112.52	122.70
3	M	29	ARG	NE-CZ-NH2	-6.27	117.17	120.30
3	M	240	ASP	CB-CG-OD2	6.19	123.87	118.30
2	L	10	ARG	NE-CZ-NH1	-6.11	117.24	120.30
2	L	231	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	H	119	ASP	CB-CG-OD2	5.95	123.66	118.30
1	H	65	ILE	N-CA-C	-5.82	95.28	111.00
3	M	23	ASP	CB-CG-OD2	5.67	123.40	118.30
2	L	83	GLY	N-CA-C	5.65	127.23	113.10
2	L	109	ARG	NE-CZ-NH1	-5.65	117.48	120.30
3	M	204	LEU	CB-CG-CD1	5.51	120.37	111.00
2	L	135	ARG	NE-CZ-NH1	5.48	123.04	120.30
3	M	210	TYR	CB-CG-CD2	-5.47	117.72	121.00
3	M	241	ARG	CG-CD-NE	-5.36	100.55	111.80
2	L	210	ASP	CB-CG-OD1	5.24	123.02	118.30
1	H	118	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	H	74	THR	OG1-CB-CG2	-5.12	98.24	110.00
2	L	10	ARG	NE-CZ-NH2	5.01	122.80	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	H	66	LEU	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	30	TYR	Mainchain,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	1830	0	1836	64	0
2	L	2232	0	2187	92	0
3	M	2406	0	2319	98	0
4	H	16	0	31	4	0
4	M	16	0	31	5	0
5	L	132	0	148	11	0
5	M	132	0	148	28	0
6	L	65	0	74	5	0
6	M	65	0	74	11	0
7	M	1	0	0	0	0
8	M	43	0	69	8	0
9	M	48	0	63	2	0
10	M	5	0	0	0	0
11	H	6	0	0	1	0
11	L	6	0	0	1	0
11	M	4	0	0	0	0
All	All	7007	0	6980	268	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 19.

All (268) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:M:1303:BCL:H51	6:M:1307:BPB:HMBB	1.25	1.12
3:M:50:ILE:HD13	3:M:51:TYR:N	1.67	1.09
3:M:50:ILE:HD13	3:M:51:TYR:H	1.16	1.07
4:H:1251:LDA:H121	4:M:1305:LDA:H91	1.14	1.07
2:L:272:TRP:HA	2:L:275:ILE:HD12	1.36	1.05
4:H:1251:LDA:H121	4:M:1305:LDA:C9	1.94	0.98
3:M:108:PRO:HG2	3:M:111:GLU:HG3	1.51	0.93
1:H:98:HIS:CD2	2:L:7:ARG:HH21	1.88	0.90
3:M:25:ASN:ND2	3:M:27:ALA:H	1.69	0.89
4:H:1251:LDA:C12	4:M:1305:LDA:H91	2.02	0.88
5:L:1282:BCL:HBB3	5:L:1282:BCL:HMB1	1.53	0.88

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:M:1303:BCL:C5	6:M:1307:BPB:HMBB	2.04	0.87
2:L:156:TRP:O	2:L:160:THR:HG23	1.75	0.86
6:L:1284:BPB:HBBA	3:M:210:TYR:HB3	1.57	0.86
2:L:205:GLU:O	2:L:207:ARG:NH2	2.10	0.84
2:L:56:GLN:HE22	2:L:65:SER:H	1.23	0.84
2:L:266:TRP:O	2:L:269:LEU:HD22	1.78	0.82
3:M:25:ASN:HD21	3:M:27:ALA:CB	1.92	0.82
3:M:199:ASN:HD22	3:M:199:ASN:C	1.80	0.81
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.61	0.81
2:L:156:TRP:O	2:L:160:THR:CG2	2.29	0.80
2:L:264:GLN:HA	2:L:267:VAL:HG12	1.62	0.80
2:L:11:VAL:O	2:L:110:LYS:HE3	1.82	0.80
1:H:42:LEU:H	1:H:53:GLN:HE22	1.31	0.79
1:H:197:LYS:HE2	3:M:1:ALA:O	1.82	0.78
2:L:30:TYR:O	2:L:103:ARG:NH1	2.17	0.77
2:L:159:ASN:O	2:L:163:THR:HG22	1.85	0.76
2:L:272:TRP:HA	2:L:275:ILE:CD1	2.15	0.74
5:M:1303:BCL:H102	5:M:1304:BCL:H171	1.69	0.74
1:H:98:HIS:CD2	2:L:7:ARG:NH2	2.56	0.74
5:M:1303:BCL:H51	6:M:1307:BPB:CMB	2.12	0.73
5:L:1282:BCL:HMB1	5:L:1282:BCL:CBB	2.18	0.73
2:L:272:TRP:CA	2:L:275:ILE:HD12	2.17	0.73
6:M:1307:BPB:HBBB	6:M:1307:BPB:HHC	1.69	0.73
1:H:132:LYS:HG3	1:H:171:ILE:CD1	2.18	0.72
5:M:1303:BCL:HMB1	5:M:1303:BCL:HBB2	1.72	0.72
2:L:271:TRP:CD1	2:L:271:TRP:N	2.56	0.72
2:L:38:THR:HG22	2:L:99:SER:HB3	1.70	0.72
2:L:181:PHE:HB3	6:M:1307:BPB:HBBA	1.70	0.71
5:M:1303:BCL:CBB	5:M:1303:BCL:HMB1	2.22	0.70
2:L:71:LEU:HD23	2:L:143:GLY:HA3	1.75	0.68
1:H:35:ASN:HD22	3:M:261:THR:H	1.41	0.67
2:L:182:THR:HG22	2:L:236:LEU:HD13	1.75	0.67
5:M:1303:BCL:H102	5:M:1304:BCL:C17	2.25	0.66
5:M:1304:BCL:OBB	5:M:1304:BCL:HHC	1.95	0.66
3:M:157:TRP:NE1	8:M:1308:SPN:H202	2.10	0.66
1:H:148:PRO:HA	1:H:151:LEU:CD1	2.27	0.65
5:M:1303:BCL:C3B	8:M:1308:SPN:H152	2.27	0.65
1:H:197:LYS:CE	3:M:1:ALA:O	2.44	0.65
1:H:35:ASN:ND2	3:M:264:GLY:HA3	2.12	0.64
3:M:108:PRO:HD2	3:M:111:GLU:HB2	1.80	0.64
1:H:70:ARG:NH1	1:H:121:PRO:O	2.31	0.64
2:L:181:PHE:HB3	6:M:1307:BPB:CBB	2.28	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:199:ASN:HD22	3:M:200:PRO:N	1.95	0.64
2:L:208:THR:HB	2:L:209:PRO:HD2	1.81	0.63
2:L:269:LEU:HB2	2:L:272:TRP:NE1	2.13	0.63
1:H:202:ARG:HG2	1:H:203:VAL:N	2.11	0.63
2:L:34:PHE:O	2:L:38:THR:HG23	1.99	0.62
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.80	0.61
3:M:21:THR:O	3:M:24:VAL:HG23	2.01	0.61
3:M:113:GLY:HA2	3:M:116:LEU:HD12	1.81	0.61
3:M:97:PRO:HG2	3:M:171:TRP:HB2	1.82	0.61
2:L:103:ARG:NH2	3:M:255:THR:O	2.33	0.60
1:H:156:CYS:HB3	1:H:206:ASN:O	2.02	0.60
5:M:1303:BCL:CAB	8:M:1308:SPN:H162	2.31	0.60
1:H:117:ARG:HD2	3:M:242:GLY:HA2	1.83	0.60
2:L:100:TRP:CZ2	9:M:1309:U10:H251	2.36	0.60
3:M:108:PRO:CG	3:M:111:GLU:HG3	2.29	0.59
3:M:189:PHE:O	3:M:193:HIS:HD2	1.85	0.59
1:H:35:ASN:ND2	3:M:260:ALA:HB1	2.18	0.59
3:M:192:VAL:CG1	3:M:192:VAL:O	2.50	0.59
3:M:157:TRP:HB2	5:M:1304:BCL:H71	1.83	0.59
3:M:25:ASN:HD21	3:M:27:ALA:HB3	1.66	0.58
2:L:269:LEU:HD23	2:L:272:TRP:CZ2	2.38	0.58
2:L:274:ASN:O	2:L:275:ILE:C	2.40	0.58
3:M:199:ASN:C	3:M:199:ASN:ND2	2.55	0.58
3:M:25:ASN:HD21	3:M:27:ALA:HB2	1.69	0.58
1:H:42:LEU:N	1:H:53:GLN:HE22	2.00	0.58
3:M:243:THR:OG1	3:M:247:ARG:HD3	2.04	0.57
2:L:150:ILE:N	2:L:150:ILE:HD13	2.20	0.57
1:H:27:LEU:O	1:H:31:LEU:HB2	2.04	0.57
3:M:28:ASN:HB3	3:M:52:LEU:O	2.04	0.57
3:M:192:VAL:O	3:M:192:VAL:HG12	2.04	0.56
5:M:1303:BCL:C14	8:M:1308:SPN:H112	2.36	0.56
3:M:162:PHE:O	3:M:166:ILE:HD13	2.04	0.56
3:M:195:ASN:OD1	3:M:195:ASN:C	2.44	0.56
6:L:1284:BPB:HBBB	6:L:1284:BPB:HHC	1.88	0.56
1:H:148:PRO:HD2	1:H:167:ILE:HD11	1.86	0.56
3:M:206:ILE:HG13	5:M:1304:BCL:HMB3	1.88	0.55
3:M:97:PRO:HA	3:M:111:GLU:O	2.05	0.55
2:L:150:ILE:HD13	2:L:150:ILE:H	1.72	0.55
3:M:148:TRP:HA	3:M:148:TRP:CE3	2.41	0.55
1:H:96:PHE:HB3	1:H:97:PRO:CD	2.37	0.55
1:H:87:LEU:HD11	2:L:8:LYS:HA	1.87	0.55
2:L:38:THR:HG22	2:L:99:SER:CB	2.37	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:122:GLU:OE1	3:M:233:ARG:NH2	2.35	0.55
1:H:81:GLU:HG3	1:H:85:ILE:HD11	1.88	0.55
2:L:66:VAL:HG12	2:L:86:TRP:HB2	1.88	0.55
5:L:1283:BCL:H192	6:L:1284:BPB:H11A	1.88	0.54
2:L:181:PHE:CD2	6:M:1307:BPB:HBB	2.42	0.54
1:H:194:GLN:H	1:H:194:GLN:NE2	2.05	0.54
3:M:194:GLY:O	3:M:195:ASN:HB3	2.07	0.54
2:L:269:LEU:HD23	2:L:272:TRP:HZ2	1.72	0.54
5:L:1282:BCL:H2C	5:M:1304:BCL:HBC2	1.90	0.54
1:H:197:LYS:NZ	3:M:1:ALA:O	2.41	0.54
1:H:175:MET:HE1	3:M:232:GLU:OE2	2.08	0.54
1:H:201:ASN:O	1:H:202:ARG:HB3	2.07	0.53
3:M:157:TRP:CD1	8:M:1308:SPN:H202	2.44	0.53
1:H:89:ARG:HD3	1:H:91:ALA:O	2.09	0.53
2:L:52:SER:HB2	2:L:85:LEU:HD12	1.90	0.53
5:L:1283:BCL:HMB1	5:L:1283:BCL:HBB2	1.88	0.53
4:H:1251:LDA:H121	4:M:1305:LDA:C10	2.39	0.52
2:L:272:TRP:CD1	3:M:87:ARG:HG3	2.44	0.52
2:L:175:ILE:O	2:L:178:SER:HB2	2.09	0.52
6:M:1307:BPB:HBBB	6:M:1307:BPB:CHC	2.37	0.52
2:L:156:TRP:O	2:L:160:THR:HG22	2.07	0.52
5:M:1303:BCL:H8	5:M:1304:BCL:C20	2.39	0.52
2:L:145:ALA:O	2:L:156:TRP:NE1	2.43	0.52
1:H:96:PHE:CD1	1:H:96:PHE:N	2.77	0.52
3:M:21:THR:O	3:M:22:GLU:O	2.28	0.51
3:M:204:LEU:HD13	4:M:1305:LDA:HM13	1.91	0.51
2:L:209:PRO:O	2:L:212:GLU:HB2	2.11	0.51
1:H:96:PHE:HB3	1:H:97:PRO:HD2	1.92	0.51
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.91	0.51
2:L:217:ARG:O	2:L:218:ASP:C	2.48	0.51
2:L:279:ILE:HG21	3:M:91:PHE:HB3	1.92	0.51
3:M:21:THR:O	3:M:22:GLU:C	2.47	0.51
1:H:117:ARG:HD2	3:M:242:GLY:CA	2.41	0.51
2:L:6:GLU:OE1	3:M:253:ARG:NH1	2.44	0.51
1:H:121:PRO:HB3	1:H:225:VAL:O	2.10	0.51
1:H:206:ASN:O	1:H:248:ARG:NH1	2.44	0.50
3:M:234:GLU:O	3:M:238:ILE:HG13	2.12	0.50
2:L:113:ILE:CG2	3:M:226:VAL:HG12	2.41	0.50
3:M:50:ILE:CD1	3:M:51:TYR:N	2.57	0.50
1:H:219:ILE:HG21	1:H:225:VAL:HG13	1.93	0.50
3:M:148:TRP:HA	3:M:148:TRP:HE3	1.75	0.50
2:L:79:PRO:O	2:L:80:LEU:C	2.49	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:241:ARG:HD2	3:M:246:GLU:OE2	2.12	0.50
2:L:149:GLY:O	2:L:153:HIS:HB3	2.12	0.50
2:L:271:TRP:HD1	2:L:271:TRP:H	1.51	0.49
2:L:156:TRP:CE2	2:L:160:THR:HG21	2.46	0.49
2:L:117:ILE:N	2:L:118:PRO:HD2	2.28	0.49
1:H:132:LYS:HG3	1:H:171:ILE:HD11	1.93	0.49
1:H:140:PHE:HA	3:M:13:ARG:O	2.12	0.49
3:M:25:ASN:OD1	3:M:27:ALA:HB3	2.13	0.49
3:M:64:LEU:HB3	3:M:68:PHE:CE2	2.47	0.49
5:M:1303:BCL:H3A	5:M:1303:BCL:HBA1	1.48	0.49
2:L:160:THR:O	2:L:163:THR:HG23	2.12	0.48
3:M:25:ASN:ND2	3:M:27:ALA:HB3	2.27	0.48
2:L:69:PRO:HD3	2:L:83:GLY:O	2.13	0.48
1:H:142:VAL:HG21	1:H:147:ASN:ND2	2.29	0.48
1:H:14:SER:HA	1:H:17:ILE:HG22	1.94	0.48
5:M:1303:BCL:H141	8:M:1308:SPN:CM4	2.44	0.48
1:H:201:ASN:O	1:H:202:ARG:CB	2.62	0.48
3:M:21:THR:C	3:M:22:GLU:O	2.51	0.48
2:L:208:THR:O	2:L:209:PRO:C	2.52	0.47
1:H:35:ASN:HD21	3:M:264:GLY:HA3	1.78	0.47
2:L:153:HIS:CE1	2:L:154:LEU:CD1	2.97	0.47
3:M:275:LEU:HD23	3:M:278:LEU:HD23	1.95	0.47
3:M:300:ASN:O	3:M:301:HIS:HB2	2.14	0.47
2:L:246:LEU:HA	2:L:246:LEU:HD12	1.64	0.47
3:M:297:TRP:O	3:M:301:HIS:N	2.47	0.47
2:L:187:LEU:HD13	3:M:216:PHE:CG	2.49	0.47
5:M:1304:BCL:H161	5:M:1304:BCL:H192	1.55	0.47
3:M:199:ASN:ND2	3:M:201:PHE:H	2.12	0.47
1:H:248:ARG:CZ	1:H:248:ARG:HB2	2.45	0.47
5:M:1303:BCL:H8	5:M:1304:BCL:H203	1.96	0.47
1:H:154:ARG:NH1	1:H:202:ARG:NH2	2.63	0.47
3:M:243:THR:OG1	3:M:247:ARG:CD	2.62	0.47
2:L:190:HIS:CD2	3:M:266:HIS:CD2	3.03	0.47
1:H:199:GLN:OE1	1:H:202:ARG:HD3	2.15	0.46
1:H:156:CYS:SG	1:H:248:ARG:HA	2.55	0.46
3:M:73:TRP:HE1	3:M:77:GLN:NE2	2.13	0.46
2:L:166:ASN:OD1	2:L:166:ASN:C	2.51	0.46
1:H:135:LYS:HB3	1:H:135:LYS:HE3	1.73	0.46
1:H:83:ARG:HD2	1:H:114:TRP:CH2	2.50	0.46
5:M:1304:BCL:HBC2	5:M:1304:BCL:H2C	1.53	0.46
2:L:141:ALA:HB1	11:L:2003:HOH:O	2.16	0.46
3:M:62:SER:O	3:M:63:GLY:C	2.54	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:M:1309:U10:H322	9:M:1309:U10:H28	1.46	0.46
3:M:232:GLU:OE1	3:M:232:GLU:N	2.41	0.46
3:M:135:LEU:HD23	3:M:135:LEU:HA	1.78	0.46
1:H:35:ASN:ND2	3:M:261:THR:H	2.11	0.46
1:H:229:GLU:O	1:H:233:ILE:HD12	2.15	0.46
2:L:50:ALA:O	2:L:53:ALA:HB3	2.15	0.45
2:L:113:ILE:HG21	3:M:226:VAL:HG12	1.98	0.45
3:M:62:SER:HB2	3:M:125:ALA:HB2	1.98	0.45
1:H:245:ALA:N	1:H:246:PRO:CD	2.79	0.45
5:M:1304:BCL:HMB1	5:M:1304:BCL:CBB	2.46	0.45
6:M:1307:BPB:H44	6:M:1307:BPB:HBAA	1.42	0.45
3:M:2:GLU:HG3	3:M:4:GLN:NE2	2.30	0.45
2:L:235:LEU:HD12	2:L:235:LEU:HA	1.72	0.45
2:L:244:SER:O	2:L:245:ALA:C	2.55	0.45
3:M:3:TYR:CZ	3:M:5:ASN:HA	2.51	0.45
3:M:25:ASN:HD21	3:M:27:ALA:H	1.57	0.45
3:M:25:ASN:ND2	3:M:27:ALA:N	2.51	0.45
2:L:55:LEU:HD13	2:L:81:ALA:HB2	1.99	0.45
2:L:182:THR:HG22	2:L:236:LEU:CD1	2.45	0.44
2:L:171:PRO:HD2	2:L:259:TRP:CZ3	2.52	0.44
3:M:73:TRP:NE1	3:M:77:GLN:NE2	2.65	0.44
1:H:63:THR:HA	1:H:73:LEU:O	2.18	0.44
2:L:28:PRO:O	3:M:254:TRP:HA	2.17	0.44
5:M:1304:BCL:HAA2	5:M:1304:BCL:HBD	2.00	0.44
1:H:15:LEU:HD22	1:H:15:LEU:HA	1.71	0.44
1:H:181:VAL:O	1:H:188:THR:HA	2.17	0.44
1:H:119:ASP:OD1	1:H:226:THR:HG21	2.18	0.44
2:L:127:ALA:CB	5:L:1282:BCL:H43	2.48	0.44
2:L:176:ALA:HB2	2:L:243:PHE:HB3	2.00	0.44
1:H:173:GLU:OE1	1:H:177:ARG:NH1	2.51	0.44
6:M:1307:BPB:H14A	6:M:1307:BPB:H10	2.00	0.43
2:L:183:ASN:OD1	3:M:213:ALA:HA	2.17	0.43
2:L:265:TRP:CG	2:L:266:TRP:N	2.86	0.43
2:L:219:LEU:O	3:M:132:ARG:NH1	2.40	0.43
2:L:229:ILE:HG13	2:L:229:ILE:O	2.17	0.43
2:L:69:PRO:HG2	2:L:142:TRP:HB2	2.01	0.43
2:L:80:LEU:HD13	2:L:85:LEU:HD21	1.99	0.43
3:M:77:GLN:HB3	3:M:92:PHE:CD1	2.53	0.43
3:M:243:THR:O	3:M:247:ARG:HG2	2.18	0.43
2:L:3:LEU:HD23	2:L:3:LEU:HA	1.85	0.42
1:H:245:ALA:HB3	1:H:246:PRO:HD3	2.01	0.42
5:M:1303:BCL:H102	5:M:1304:BCL:C20	2.49	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:M:1308:SPN:C3	8:M:1308:SPN:HMA3	2.50	0.42
5:M:1303:BCL:H141	8:M:1308:SPN:HM43	2.02	0.42
5:L:1283:BCL:HMB1	5:L:1283:BCL:CBB	2.50	0.42
1:H:147:ASN:OD1	1:H:149:ILE:N	2.52	0.42
2:L:62:GLN:OE1	2:L:151:TRP:NE1	2.51	0.42
5:L:1283:BCL:H3A	5:L:1283:BCL:HBA1	1.72	0.42
2:L:51:TRP:O	2:L:52:SER:C	2.58	0.42
2:L:219:LEU:HA	3:M:132:ARG:HH12	1.85	0.42
5:L:1282:BCL:OB	5:L:1282:BCL:HHC	2.20	0.42
5:M:1303:BCL:H162	5:M:1303:BCL:H141	1.85	0.42
6:L:1284:BPB:HBB	3:M:210:TYR:CD2	2.55	0.42
1:H:20:PHE:CE1	3:M:279:THR:HG22	2.55	0.42
3:M:280:GLY:O	5:M:1304:BCL:HED3	2.20	0.42
2:L:189:LEU:HD13	2:L:216:PHE:HZ	1.85	0.42
2:L:222:TYR:CG	2:L:223:SER:N	2.87	0.41
3:M:228:ARG:HG2	3:M:228:ARG:H	1.72	0.41
1:H:143:SER:OG	3:M:13:ARG:HB2	2.20	0.41
1:H:124:ASP:OD2	1:H:128:HIS:HB2	2.20	0.41
1:H:117:ARG:O	1:H:228:LEU:HB2	2.20	0.41
6:L:1284:BPB:ND	6:L:1284:BPB:NC	2.68	0.41
6:M:1307:BPB:H6	6:M:1307:BPB:H9A	1.63	0.41
3:M:183:LEU:HA	3:M:183:LEU:HD23	1.84	0.41
2:L:233:GLY:O	2:L:234:LEU:C	2.57	0.41
5:L:1282:BCL:H2C	5:L:1282:BCL:HBC2	1.91	0.41
3:M:206:ILE:CG2	3:M:210:TYR:CE2	3.04	0.41
3:M:73:TRP:HE1	3:M:77:GLN:HE22	1.69	0.41
1:H:60:LYS:HA	1:H:61:PRO:HD3	1.89	0.41
3:M:12:VAL:HG12	3:M:12:VAL:O	2.21	0.41
3:M:32:VAL:HG22	3:M:49:PRO:HD3	2.02	0.41
1:H:48:THR:HA	1:H:49:PRO:HD3	1.91	0.41
5:M:1303:BCL:H111	5:M:1303:BCL:H91	1.34	0.41
2:L:97:PHE:CE1	5:L:1282:BCL:H121	2.56	0.41
2:L:275:ILE:HA	2:L:276:PRO:HD3	1.87	0.41
2:L:156:TRP:O	2:L:157:VAL:C	2.58	0.41
2:L:150:ILE:N	2:L:150:ILE:CD1	2.83	0.41
1:H:111:PRO:O	3:M:247:ARG:NH1	2.53	0.41
2:L:255:TRP:CZ2	2:L:262:TRP:HB2	2.56	0.41
5:M:1304:BCL:H162	5:M:1304:BCL:H121	1.91	0.40
2:L:265:TRP:CD2	2:L:266:TRP:N	2.90	0.40
2:L:160:THR:HA	2:L:163:THR:CG2	2.51	0.40
2:L:30:TYR:HB2	3:M:254:TRP:HB3	2.03	0.40
2:L:135:ARG:HB3	2:L:136:PRO:CD	2.48	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:227:LEU:HA	1:H:227:LEU:HD23	1.76	0.40
3:M:53:GLY:O	3:M:54:SER:C	2.59	0.40
1:H:89:ARG:HG2	11:H:2002:HOH:O	2.22	0.40
3:M:212:SER:O	3:M:213:ALA:C	2.57	0.40
2:L:21:LEU:HD13	2:L:21:LEU:HA	1.86	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	239/260 (92%)	221 (92%)	14 (6%)	4 (2%)	14	42
2	L	279/281 (99%)	251 (90%)	26 (9%)	2 (1%)	30	69
3	M	301/307 (98%)	267 (89%)	30 (10%)	4 (1%)	18	51
All	All	819/848 (97%)	739 (90%)	70 (8%)	10 (1%)	19	54

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	250	SER
2	L	145	ALA
3	M	22	GLU
3	M	301	HIS
2	L	80	LEU
3	M	100	GLU
1	H	66	LEU
3	M	30	SER
1	H	202	ARG
1	H	211	ASP

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	195/208 (94%)	172 (88%)	23 (12%)	8	22
2	L	220/220 (100%)	198 (90%)	22 (10%)	11	30
3	M	236/240 (98%)	220 (93%)	16 (7%)	22	54
All	All	651/668 (98%)	590 (91%)	61 (9%)	13	34

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	11	ASP
1	H	15	LEU
1	H	62	LYS
1	H	70	ARG
1	H	72	THR
1	H	73	LEU
1	H	80	SER
1	H	94	GLU
1	H	117	ARG
1	H	134	MET
1	H	143	SER
1	H	146	LYS
1	H	190	LEU
1	H	193	MET
1	H	194	GLN
1	H	200	SER
1	H	202	ARG
1	H	208	LEU
1	H	217	PRO
1	H	221	SER
1	H	225	VAL
1	H	231	ASP
1	H	249	LYS
2	L	7	ARG
2	L	21	LEU
2	L	38	THR
2	L	44	LEU

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Mol	Chain	Res	Type
2	L	46	ILE
2	L	58	THR
2	L	82	LYS
2	L	136	PRO
2	L	150	ILE
2	L	153	HIS
2	L	160	THR
2	L	163	THR
2	L	185	LEU
2	L	206	MET
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	235	LEU
2	L	269	LEU
2	L	271	TRP
2	L	272	TRP
2	L	279	ILE
3	M	12	VAL
3	M	50	ILE
3	M	52	LEU
3	M	62	SER
3	M	77	GLN
3	M	81	ASN
3	M	86	LEU
3	M	133	THR
3	M	136	ARG
3	M	166	ILE
3	M	196	LEU
3	M	199	ASN
3	M	204	LEU
3	M	214	LEU
3	M	216	PHE
3	M	247	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	35	ASN
1	H	53	GLN
1	H	98	HIS
1	H	194	GLN

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Mol	Chain	Res	Type
2	L	56	GLN
2	L	280	ASN
3	M	4	GLN
3	M	11	GLN
3	M	25	ASN
3	M	28	ASN
3	M	44	ASN
3	M	77	GLN
3	M	193	HIS
3	M	199	ASN
3	M	299	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	LDA	H	1251	-	15,15,15	4.55	2 (13%)	17,17,17	4.82	7 (41%)
5	BCL	L	1282	2	74,74,74	1.49	14 (18%)	97,115,115	1.79	28 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BCL	L	1283	2	74,74,74	1.60	13 (17%)	97,115,115	2.14	34 (35%)
6	BPB	L	1284	-	70,70,70	2.39	13 (18%)	93,101,101	2.07	23 (24%)
5	BCL	M	1303	3	74,74,74	1.36	11 (14%)	97,115,115	2.08	29 (29%)
5	BCL	M	1304	3	74,74,74	1.50	14 (18%)	97,115,115	1.78	23 (23%)
4	LDA	M	1305	-	15,15,15	5.57	3 (20%)	17,17,17	3.48	6 (35%)
6	BPB	M	1307	-	70,70,70	2.05	6 (8%)	93,101,101	2.41	23 (24%)
8	SPN	M	1308	-	42,42,42	3.65	14 (33%)	52,52,52	2.27	20 (38%)
9	U10	M	1309	-	48,48,63	1.48	4 (8%)	59,61,79	2.05	17 (28%)
10	PO4	M	1310	-	4,4,4	0.16	0	6,6,6	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LDA	H	1251	-	-	0/13/13/13	0/0/0/0
5	BCL	L	1282	2	-	0/41/137/137	0/0/9/9
5	BCL	L	1283	2	-	0/41/137/137	0/0/9/9
6	BPB	L	1284	-	-	1/52/105/105	0/0/6/6
5	BCL	M	1303	3	-	0/41/137/137	0/0/9/9
5	BCL	M	1304	3	-	0/41/137/137	0/0/9/9
4	LDA	M	1305	-	-	0/13/13/13	0/0/0/0
6	BPB	M	1307	-	-	1/52/105/105	0/0/6/6
8	SPN	M	1308	-	-	0/51/51/51	0/0/0/0
9	U10	M	1309	-	-	0/45/69/87	0/1/1/1
10	PO4	M	1310	-	-	0/0/0/0	0/0/0/0

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	1305	LDA	O1-N1	-20.89	1.19	1.39
4	H	1251	LDA	O1-N1	-17.24	1.23	1.39
6	L	1284	BPB	CAC-C3C	14.95	1.52	1.33
6	M	1307	BPB	CAC-C3C	14.17	1.51	1.33
8	M	1308	SPN	C3-C4	-8.52	1.37	1.50
8	M	1308	SPN	C4-C5	7.35	1.47	1.32
8	M	1308	SPN	C10-C9	-7.21	1.34	1.51
8	M	1308	SPN	C8-C9	7.18	1.47	1.32
8	M	1308	SPN	C19-C18	7.01	1.47	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	1308	SPN	C17-C18	-6.79	1.35	1.51
8	M	1308	SPN	C6-C5	-6.36	1.36	1.51
8	M	1308	SPN	C14-C13	-6.29	1.36	1.51
5	L	1283	BCL	C1B-C2B	6.28	1.48	1.40
9	M	1309	U10	C36-C34	-5.90	1.37	1.51
8	M	1308	SPN	C12-C13	5.82	1.44	1.32
6	L	1284	BPB	CHD-C4C	5.61	1.38	1.35
5	M	1304	BCL	MG-NA	5.48	2.23	2.07
8	M	1308	SPN	C20-C19	-5.31	1.35	1.50
8	M	1308	SPN	C11-C12	-5.26	1.35	1.50
6	M	1307	BPB	CHD-C4C	5.25	1.38	1.35
5	L	1282	BCL	MG-NA	4.91	2.21	2.07
9	M	1309	U10	C6-C1	4.78	1.47	1.35
8	M	1308	SPN	C7-C8	-4.72	1.36	1.50
6	L	1284	BPB	C1D-ND	4.67	1.41	1.36
6	L	1284	BPB	C4D-CHA	-4.54	1.39	1.45
5	L	1283	BCL	MG-NC	-4.52	1.93	2.07
5	M	1304	BCL	C1B-C2B	4.37	1.45	1.40
6	M	1307	BPB	C4D-CHA	-4.35	1.39	1.45
5	M	1304	BCL	C1B-NB	4.34	1.39	1.34
5	M	1303	BCL	C1B-NB	4.22	1.39	1.34
5	L	1282	BCL	C1A-NA	4.18	1.41	1.32
5	L	1282	BCL	C1B-C2B	4.18	1.45	1.40
4	M	1305	LDA	CM1-N1	-3.97	1.43	1.49
6	L	1284	BPB	C4D-ND	3.70	1.40	1.36
5	L	1282	BCL	C4C-NC	3.68	1.40	1.32
5	L	1283	BCL	C1B-NB	3.59	1.39	1.34
5	L	1283	BCL	C3B-C4B	3.45	1.45	1.40
5	M	1303	BCL	C1B-C2B	3.37	1.44	1.40
6	L	1284	BPB	OBD-CAD	3.32	1.27	1.22
6	L	1284	BPB	C2C-C3C	3.31	1.58	1.52
4	M	1305	LDA	CM2-N1	-3.21	1.44	1.49
5	M	1303	BCL	MG-NA	3.20	2.16	2.07
5	M	1304	BCL	C1A-NA	3.15	1.39	1.32
5	M	1304	BCL	C3B-C4B	3.14	1.45	1.40
5	L	1283	BCL	C1C-NC	-3.13	1.32	1.39
5	M	1303	BCL	C4D-C3D	-3.12	1.37	1.41
5	M	1303	BCL	C4B-NB	3.10	1.38	1.34
8	M	1308	SPN	C21-C22	-3.07	1.36	1.52
5	M	1304	BCL	C4C-NC	3.05	1.39	1.32
5	L	1283	BCL	C1A-NA	3.02	1.38	1.32
5	L	1282	BCL	C4B-NB	2.95	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1283	BCL	CHC-C1C	2.95	1.43	1.36
5	M	1304	BCL	CHC-C1C	2.94	1.43	1.36
5	L	1282	BCL	C3D-CAD	-2.88	1.41	1.47
5	L	1283	BCL	MG-NB	2.88	2.11	2.05
6	L	1284	BPB	C1-C2	2.86	1.58	1.49
5	M	1303	BCL	C4C-NC	2.81	1.38	1.32
5	L	1282	BCL	MG-ND	2.80	2.11	2.05
4	H	1251	LDA	CM1-N1	-2.74	1.45	1.49
5	M	1303	BCL	C3B-C4B	2.74	1.44	1.40
5	L	1282	BCL	CHC-C1C	2.69	1.42	1.36
9	M	1309	U10	C4-C3	2.67	1.47	1.35
6	L	1284	BPB	C4B-CHC	2.65	1.38	1.35
6	M	1307	BPB	C1D-ND	2.61	1.39	1.36
5	L	1283	BCL	C4B-NB	2.58	1.37	1.34
5	M	1304	BCL	C4A-NA	-2.56	1.33	1.39
5	L	1282	BCL	C1B-NB	2.56	1.37	1.34
6	L	1284	BPB	C4C-C3C	2.50	1.53	1.44
5	M	1303	BCL	C1C-NC	-2.41	1.34	1.39
5	L	1283	BCL	C3C-C4C	-2.39	1.48	1.51
5	M	1304	BCL	C3D-CAD	-2.38	1.42	1.47
5	L	1282	BCL	C4A-NA	-2.35	1.34	1.39
5	M	1303	BCL	C1A-NA	2.35	1.37	1.32
5	L	1283	BCL	CMB-C2B	-2.34	1.46	1.51
5	L	1283	BCL	CHB-C4A	2.31	1.41	1.36
8	M	1308	SPN	C16-C15	-2.26	1.37	1.51
5	L	1282	BCL	MG-NC	2.24	2.13	2.07
5	M	1304	BCL	CBA-CGA	-2.17	1.43	1.50
5	M	1304	BCL	C2A-C1A	-2.16	1.48	1.52
6	M	1307	BPB	C4D-ND	-2.15	1.34	1.36
5	M	1304	BCL	C1C-NC	-2.14	1.34	1.39
9	M	1309	U10	C41-C39	2.14	1.52	1.40
5	L	1282	BCL	C3B-C4B	2.12	1.43	1.40
5	L	1282	BCL	O2D-CGD	2.11	1.38	1.33
5	M	1304	BCL	C4B-NB	2.11	1.37	1.34
6	M	1307	BPB	C4B-NB	-2.10	1.35	1.38
5	M	1303	BCL	CHC-C1C	2.09	1.41	1.36
5	L	1283	BCL	C4D-C3D	2.09	1.44	1.41
6	L	1284	BPB	CHC-C1C	-2.08	1.36	1.41
6	L	1284	BPB	C1B-NB	-2.06	1.35	1.38
6	L	1284	BPB	C3D-CAD	-2.06	1.43	1.47
5	M	1304	BCL	C3C-C4C	-2.03	1.49	1.51
5	M	1303	BCL	C4A-NA	-2.02	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1282	BCL	C1C-NC	-2.00	1.34	1.39

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1251	LDA	CM2-N1-CM1	14.19	125.07	108.85
6	M	1307	BPB	CAC-C3C-C4C	-8.99	109.29	127.18
4	H	1251	LDA	O1-N1-C1	-8.79	97.93	110.19
6	M	1307	BPB	CBC-CAC-C3C	-8.70	107.21	126.93
4	M	1305	LDA	CM2-N1-CM1	-8.63	98.99	108.85
6	M	1307	BPB	C1-C2-C3	-8.19	111.62	126.19
6	L	1284	BPB	C2C-C3C-CAC	-7.24	112.74	129.36
4	M	1305	LDA	O1-N1-CM1	7.00	118.43	109.01
5	L	1283	BCL	C2B-C1B-NB	-6.53	104.48	109.41
4	H	1251	LDA	O1-N1-CM1	6.44	117.68	109.01
6	L	1284	BPB	CHD-C4C-NC	-6.22	117.11	128.59
5	M	1303	BCL	C11-C12-C13	-6.08	97.62	115.14
5	L	1282	BCL	CAA-C2A-C3A	-6.05	98.73	113.04
5	M	1303	BCL	CMB-C2B-C1B	-5.93	119.49	128.62
5	L	1283	BCL	CMB-C2B-C1B	-5.92	119.52	128.62
4	M	1305	LDA	O1-N1-CM2	5.89	116.94	109.01
9	M	1309	U10	C30-C29-C31	5.77	124.17	115.39
5	L	1282	BCL	C2B-C1B-NB	-5.77	105.06	109.41
5	M	1303	BCL	O2A-C1-C2	5.76	121.03	108.55
4	M	1305	LDA	O1-N1-C1	-5.75	102.16	110.19
6	M	1307	BPB	C3D-C4D-CHA	5.52	115.29	109.18
8	M	1308	SPN	CM5-C13-C14	5.42	123.63	115.39
6	L	1284	BPB	C2C-C3C-C4C	-5.36	100.81	108.73
9	M	1309	U10	C26-C27-C28	-5.34	96.37	111.62
8	M	1308	SPN	C7-C6-C5	5.13	129.74	112.74
6	L	1284	BPB	CAC-C3C-C4C	-5.10	117.02	127.18
6	M	1307	BPB	O2A-C1-C2	-5.07	97.57	108.55
4	H	1251	LDA	CM2-N1-C1	-5.00	93.50	109.86
8	M	1308	SPN	C15-C14-C13	4.84	124.29	112.78
4	H	1251	LDA	CM1-N1-C1	-4.76	94.28	109.86
6	M	1307	BPB	C2C-C3C-CAC	-4.76	118.44	129.36
5	M	1304	BCL	O2D-CGD-CBD	4.71	120.93	111.33
5	M	1304	BCL	O2D-CGD-O1D	-4.60	114.45	123.79
5	M	1303	BCL	CMB-C2B-C3B	4.57	132.17	124.97
5	M	1303	BCL	C2B-C1B-NB	-4.56	105.97	109.41
6	L	1284	BPB	CBC-CAC-C3C	-4.42	116.92	126.93
5	L	1282	BCL	C4B-NB-C1B	4.39	112.54	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	1308	SPN	CM6-C18-C17	4.38	122.05	115.39
4	H	1251	LDA	O1-N1-CM2	4.33	114.84	109.01
9	M	1309	U10	C37-C36-C34	4.33	127.06	112.74
8	M	1308	SPN	CM3-C5-C6	4.28	121.90	115.39
5	L	1283	BCL	CHD-C4C-NC	4.28	132.04	125.86
6	L	1284	BPB	O2D-CGD-CBD	4.26	120.01	111.33
9	M	1309	U10	C17-C18-C19	-4.25	118.64	127.80
5	M	1303	BCL	C2C-C1C-NC	4.21	116.07	110.95
5	M	1303	BCL	CAA-C2A-C3A	-4.15	103.22	113.04
5	L	1283	BCL	CAA-C2A-C3A	-4.14	103.25	113.04
5	L	1283	BCL	CHC-C1C-NC	4.10	129.44	124.58
5	M	1304	BCL	C2A-C1A-NA	4.07	115.75	111.24
5	L	1283	BCL	C1B-CHB-C4A	-4.03	121.68	130.06
6	M	1307	BPB	O2D-CGD-CBD	4.02	119.52	111.33
5	M	1304	BCL	C11-C10-C8	-3.99	103.64	115.14
6	M	1307	BPB	C6-C5-C3	-3.99	103.30	112.78
6	M	1307	BPB	CMB-C2B-C3B	3.95	131.19	124.97
5	L	1283	BCL	CMB-C2B-C3B	3.94	131.18	124.97
5	L	1283	BCL	CAC-C3C-C4C	-3.92	103.89	112.58
6	M	1307	BPB	C4B-C3B-C2B	3.91	109.65	106.92
5	M	1303	BCL	CAC-C3C-C2C	-3.88	104.98	113.89
6	L	1284	BPB	CAA-C2A-C3A	-3.86	103.90	113.04
6	M	1307	BPB	C5-C3-C2	3.84	128.48	121.08
5	M	1303	BCL	C16-C15-C13	-3.83	104.10	115.14
8	M	1308	SPN	CM7-C22-C21	3.82	125.03	111.02
5	M	1304	BCL	CHA-C1A-NA	-3.80	118.43	126.22
9	M	1309	U10	C35-C34-C36	3.80	121.16	115.39
5	L	1283	BCL	CAC-C3C-C2C	-3.76	105.27	113.89
5	L	1283	BCL	C4B-NB-C1B	3.74	111.68	106.76
5	M	1304	BCL	OBB-CAB-C3B	-3.61	114.66	120.07
5	M	1304	BCL	C7-C6-C5	-3.60	102.40	113.01
6	M	1307	BPB	CAA-C2A-C3A	-3.57	104.61	113.04
9	M	1309	U10	C32-C33-C34	-3.56	120.11	127.80
6	M	1307	BPB	C4-C3-C2	-3.55	116.48	123.52
5	L	1282	BCL	C11-C12-C13	-3.53	104.97	115.14
6	M	1307	BPB	C1-O2A-CGA	3.52	126.84	116.98
5	L	1282	BCL	C3B-C4B-NB	-3.51	105.23	108.64
6	L	1284	BPB	C3D-C2D-C1D	3.43	109.06	107.01
5	L	1283	BCL	C1D-CHD-C4C	-3.43	119.63	125.55
8	M	1308	SPN	C20-C21-C22	3.37	127.29	116.60
9	M	1309	U10	C22-C23-C24	-3.36	120.55	127.80
5	M	1304	BCL	C2B-C1B-NB	-3.35	106.88	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1282	BCL	CED-O2D-CGD	3.34	123.96	116.02
5	L	1283	BCL	O2A-C1-C2	-3.31	101.38	108.55
6	L	1284	BPB	C4D-C3D-CAD	3.31	111.37	108.14
5	M	1304	BCL	C4B-NB-C1B	3.30	111.11	106.76
6	M	1307	BPB	CMA-C3A-C4A	-3.29	102.46	112.94
5	L	1282	BCL	OBb-CAB-C3B	3.29	125.01	120.07
5	L	1283	BCL	CBD-CHA-C1A	-3.29	124.47	128.77
5	M	1303	BCL	C1B-CHB-C4A	-3.29	123.22	130.06
9	M	1309	U10	C35-C34-C33	-3.28	117.03	123.52
5	L	1283	BCL	C2C-C1C-CHC	-3.27	117.54	124.33
5	M	1303	BCL	OBb-CAB-C3B	3.26	124.96	120.07
5	L	1282	BCL	CMA-C3A-C2A	-3.20	100.39	114.14
5	M	1304	BCL	CAA-C2A-C3A	-3.18	105.51	113.04
8	M	1308	SPN	C16-C17-C18	3.18	120.33	112.78
6	L	1284	BPB	C7-C6-C5	-3.16	103.69	113.01
6	L	1284	BPB	C4B-C3B-C2B	3.15	109.12	106.92
9	M	1309	U10	C4M-O4-C4	3.14	127.16	116.48
5	M	1304	BCL	C3B-C4B-NB	-3.14	105.59	108.64
5	M	1304	BCL	CGD-CBD-CAD	-3.14	100.30	110.96
5	M	1303	BCL	C4B-NB-C1B	3.12	110.88	106.76
6	M	1307	BPB	C2C-C3C-C4C	-3.08	104.17	108.73
5	L	1283	BCL	C3C-C4C-CHD	-3.06	116.64	123.35
6	M	1307	BPB	CHD-C4C-NC	-3.06	122.94	128.59
5	L	1283	BCL	C4D-CHA-C1A	3.06	129.18	120.32
8	M	1308	SPN	C16-C15-C14	3.04	124.75	113.28
5	L	1283	BCL	O2D-CGD-CBD	3.04	117.52	111.33
6	L	1284	BPB	CBB-CAB-C3B	3.04	129.17	120.21
6	L	1284	BPB	OBb-CAB-CBB	-3.03	112.60	120.13
9	M	1309	U10	C27-C28-C29	-3.03	121.27	127.80
5	L	1283	BCL	CMD-C2D-C3D	3.01	129.72	124.97
5	M	1303	BCL	C11-C10-C8	-3.00	106.50	115.14
5	M	1303	BCL	C2A-C1A-NA	2.98	114.54	111.24
5	M	1303	BCL	CHA-C1A-NA	-2.97	120.13	126.22
6	L	1284	BPB	C3D-C4D-CHA	2.89	112.38	109.18
6	L	1284	BPB	O2A-CGA-O1A	-2.87	115.60	123.43
9	M	1309	U10	C20-C19-C18	-2.86	117.85	123.52
5	L	1283	BCL	CGD-CBD-CHA	2.83	120.58	110.96
6	L	1284	BPB	CMA-C3A-C2A	-2.81	102.08	114.14
5	M	1303	BCL	CHB-C1B-NB	2.79	129.25	124.58
5	M	1304	BCL	CAC-C3C-C2C	-2.79	107.48	113.89
5	M	1304	BCL	C1-C2-C3	-2.79	121.23	126.19
8	M	1308	SPN	CM7-C22-C23	2.77	121.18	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1284	BPB	C3D-CAD-CBD	-2.76	103.69	107.60
5	M	1304	BCL	C11-C12-C13	-2.75	107.21	115.14
5	L	1283	BCL	C4-C3-C5	2.75	119.57	115.39
5	L	1282	BCL	CBA-CAA-C2A	2.72	122.09	114.01
5	L	1283	BCL	CAA-CBA-CGA	2.69	121.94	113.27
5	L	1282	BCL	CHA-C1A-NA	-2.68	120.71	126.22
8	M	1308	SPN	CM5-C13-C12	-2.68	118.22	123.52
5	M	1303	BCL	C3B-C4B-NB	-2.67	106.04	108.64
5	L	1283	BCL	C2C-C3C-C4C	2.67	104.75	101.05
5	L	1282	BCL	O2A-CGA-O1A	-2.66	116.16	123.43
5	M	1304	BCL	C2C-C3C-C4C	2.66	104.74	101.05
5	M	1303	BCL	C16-C17-C18	-2.64	102.29	115.69
5	M	1303	BCL	C2C-C3C-C4C	2.64	104.71	101.05
8	M	1308	SPN	CM2-C1-C2	-2.63	104.75	110.87
5	L	1283	BCL	C4D-C3D-C2D	-2.62	104.22	107.42
5	M	1303	BCL	C3A-C4A-NA	2.61	114.13	110.95
5	M	1303	BCL	CMA-C3A-C2A	-2.59	103.03	114.14
5	M	1304	BCL	C4B-C3B-C2B	2.58	110.09	106.97
5	L	1282	BCL	C4-C3-C5	2.57	119.30	115.39
6	M	1307	BPB	O2D-CGD-O1D	-2.55	118.62	123.79
8	M	1308	SPN	O2-C2-C1	-2.54	115.78	119.39
5	L	1283	BCL	CHB-C1B-NB	2.53	128.81	124.58
8	M	1308	SPN	CM8-C26-C27	2.52	119.23	115.39
5	M	1304	BCL	C3A-C4A-NA	2.52	114.01	110.95
5	L	1283	BCL	C5-C3-C2	-2.52	116.24	121.08
6	L	1284	BPB	CMA-C3A-C4A	-2.51	104.95	112.94
5	M	1303	BCL	O2D-CGD-CBD	2.49	116.41	111.33
9	M	1309	U10	C30-C29-C28	-2.49	118.60	123.52
8	M	1308	SPN	C15-C16-C17	2.47	122.60	113.28
4	M	1305	LDA	CM2-N1-C1	2.47	117.92	109.86
5	L	1282	BCL	C2A-C3A-C4A	2.45	105.18	101.40
5	L	1283	BCL	O1D-CGD-CBD	-2.45	119.40	124.42
9	M	1309	U10	O5-C5-C6	-2.44	117.18	121.67
9	M	1309	U10	C40-C39-C38	-2.44	117.76	123.62
6	L	1284	BPB	C16-C15-C13	-2.44	108.12	115.14
5	L	1282	BCL	C2C-C1C-NC	2.43	113.91	110.95
5	L	1283	BCL	C2A-C1A-NA	2.39	113.88	111.24
5	M	1304	BCL	C1D-C2D-C3D	-2.38	104.84	106.78
5	L	1283	BCL	C3A-C4A-CHB	-2.37	119.41	124.33
4	H	1251	LDA	C2-C1-N1	2.36	117.87	113.80
6	M	1307	BPB	C2D-C1D-CHD	2.36	132.42	125.72
5	L	1282	BCL	CHC-C4B-NB	2.35	128.51	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1283	BCL	C6-C5-C3	-2.35	107.20	112.78
6	L	1284	BPB	O2D-CGD-O1D	-2.34	119.04	123.79
5	M	1303	BCL	CBA-CAA-C2A	-2.34	107.08	114.01
5	L	1282	BCL	CAC-C3C-C2C	-2.33	108.54	113.89
5	M	1303	BCL	C2D-C1D-ND	-2.32	107.66	109.41
4	M	1305	LDA	CM1-N1-C1	-2.31	102.30	109.86
9	M	1309	U10	C21-C19-C18	2.31	125.53	121.08
6	L	1284	BPB	C11-C10-C8	-2.31	108.50	115.14
5	M	1303	BCL	O2D-CGD-O1D	-2.30	119.11	123.79
8	M	1308	SPN	O1-C1-C2	2.28	113.87	109.32
5	M	1304	BCL	C4D-CHA-C1A	2.28	126.91	120.32
6	L	1284	BPB	C1D-CHD-C4C	-2.27	125.49	129.92
5	L	1282	BCL	C2A-C1A-NA	2.27	113.75	111.24
6	L	1284	BPB	OBD-CAD-C3D	2.26	132.27	127.96
6	M	1307	BPB	C6-C7-C8	-2.25	108.67	115.14
5	L	1283	BCL	CHB-C4A-NA	2.25	127.24	124.58
6	M	1307	BPB	CMB-C2B-C1B	-2.25	122.18	125.81
6	M	1307	BPB	CMA-C3A-C2A	-2.22	104.58	114.14
8	M	1308	SPN	C6-C5-C4	-2.22	116.82	121.08
5	M	1304	BCL	CHB-C1B-NB	2.21	128.27	124.58
5	M	1304	BCL	CBB-CAB-C3B	2.15	126.58	120.30
5	L	1283	BCL	C2A-C3A-C4A	2.14	104.69	101.40
9	M	1309	U10	C7-C8-C9	-2.14	123.14	126.76
8	M	1308	SPN	C23-C24-C25	-2.13	106.47	112.46
5	M	1303	BCL	CHD-C4C-NC	-2.13	122.78	125.86
5	L	1283	BCL	CHA-C1A-NA	-2.12	121.87	126.22
5	L	1282	BCL	C4B-CHC-C1C	-2.12	125.65	130.06
5	M	1303	BCL	CMA-C3A-C4A	-2.11	105.65	111.76
5	L	1282	BCL	C1-C2-C3	-2.10	122.44	126.19
5	L	1283	BCL	CMD-C2D-C1D	-2.10	122.01	126.16
5	M	1303	BCL	CMD-C2D-C1D	2.09	130.30	126.16
5	L	1282	BCL	O1D-CGD-CBD	-2.09	120.14	124.42
5	L	1282	BCL	CMB-C2B-C1B	-2.08	125.42	128.62
5	L	1282	BCL	C1-O2A-CGA	2.08	122.80	116.98
5	L	1282	BCL	CMD-C2D-C3D	2.06	128.21	124.97
6	M	1307	BPB	CMD-C2D-C3D	2.06	128.21	124.97
5	L	1282	BCL	C2D-C1D-ND	-2.04	107.87	109.41
8	M	1308	SPN	CM6-C18-C19	-2.03	119.50	123.52
5	L	1283	BCL	CMC-C2C-C3C	-2.03	105.43	114.14
5	M	1303	BCL	CHC-C1C-NC	-2.03	122.17	124.58
8	M	1308	SPN	C6-C7-C8	2.02	117.39	111.62
5	L	1282	BCL	O2A-CGA-CBA	2.02	118.31	111.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1282	BCL	C4D-CHA-CBD	-2.01	104.64	109.37
5	L	1282	BCL	C2C-C3C-C4C	2.01	103.83	101.05
5	M	1304	BCL	C4D-C3D-C2D	2.00	109.87	107.42
5	L	1282	BCL	C17-C16-C15	-2.00	102.75	113.02
9	M	1309	U10	C31-C29-C28	-2.00	117.23	121.08

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	M	1307	BPB	CBC-CAC-C3C-C2C
6	L	1284	BPB	CBC-CAC-C3C-C2C

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.