



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:38 am GMT

PDB ID : 1QOV
Title : PHOTOSYNTHETIC REACTION CENTER MUTANT WITH ALA M260
REPLACED WITH TRP (CHAIN M, A260W)
Authors : Mcauley, K.E.; Fyfe, P.K.; Ridge, J.P.; Isaacs, N.W.; Cogdell, R.J.; Jones,
M.R.
Deposited on : 1999-11-17
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

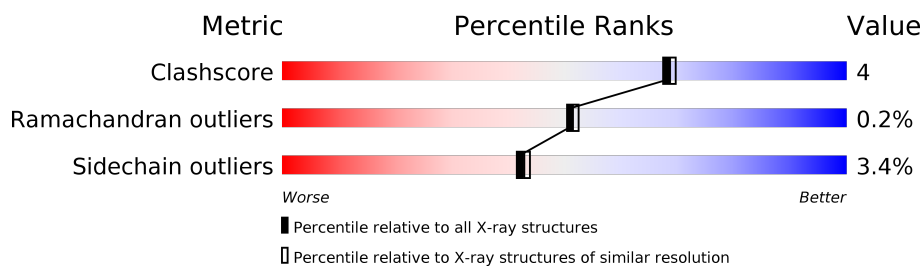
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BCL	M	1301	X	-	-	-
6	BPH	M	1401	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7312 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	1	0
			2235	1509	355	363	8			

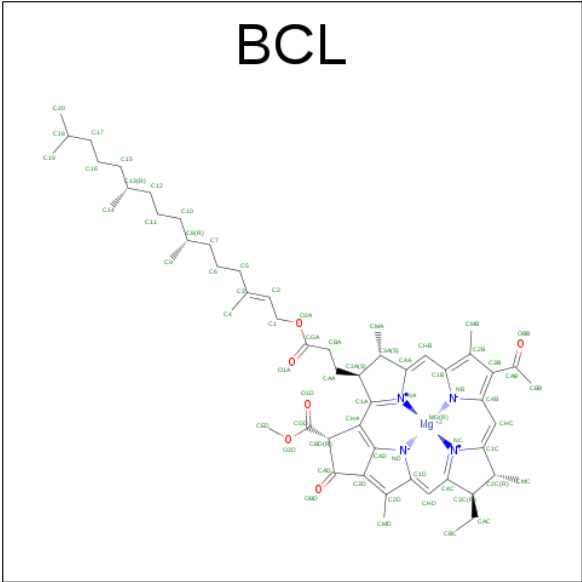
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	2	0
			2430	1622	401	397	10			

There is a discrepancy between the modelled and reference sequences:

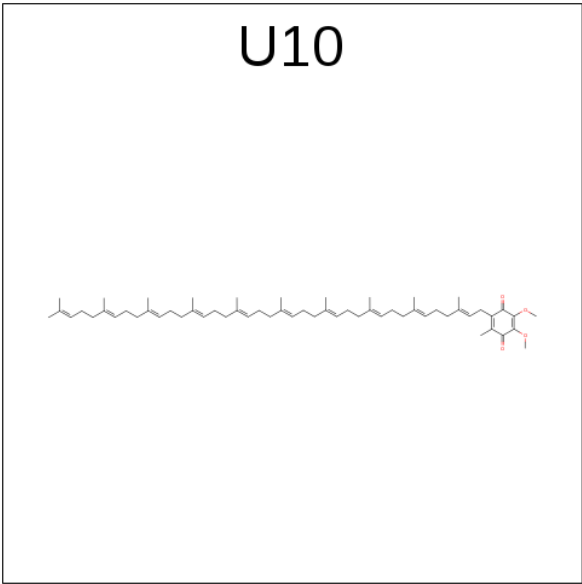
Chain	Residue	Modelled	Actual	Comment	Reference
M	260	TRP	ALA	ENGINEERED MUTATION	UNP P02953

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



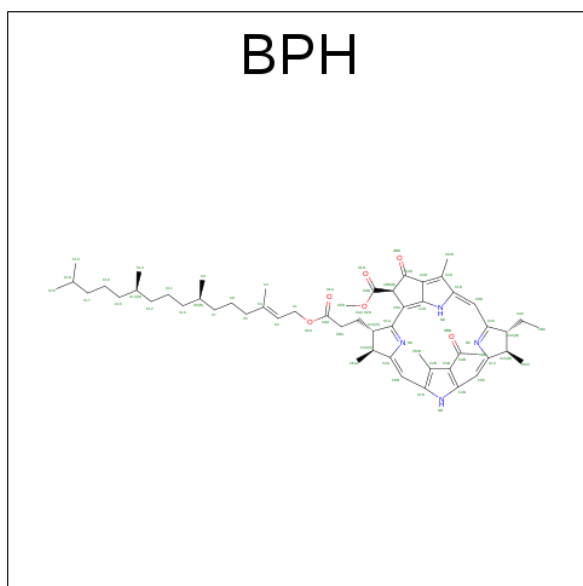
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 5 is UBIQUINONE-10 (three-letter code: U10) (formula: C₅₉H₉₀O₄).



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

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).

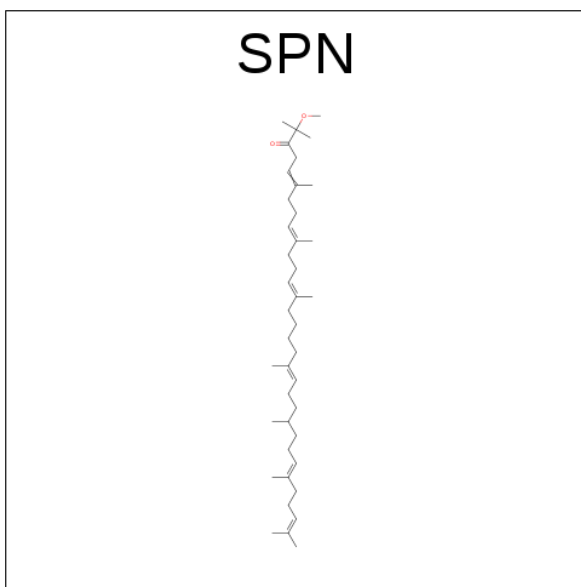


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	M	1	Total	C	N	O	10	0
			65	55	4	6		
6	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 7 is FE (II) ION (three-letter code: FE2) (formula: Fe).

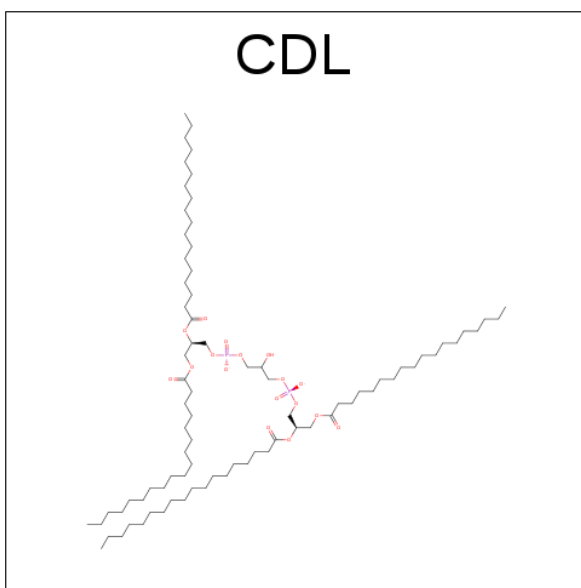
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Fe	0	0
			1	1		

- Molecule 8 is SPEROIDENONE (three-letter code: SPN) (formula: $C_{41}H_{70}O_2$).



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

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



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

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 11 is water.

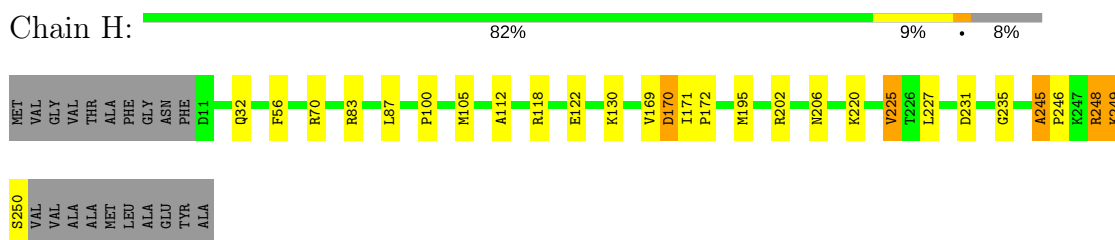
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	118	Total 118	O 118	0	0
11	L	59	Total 59	O 59	0	0
11	M	73	Total 73	O 73	0	0

3 Residue-property plots [i](#)

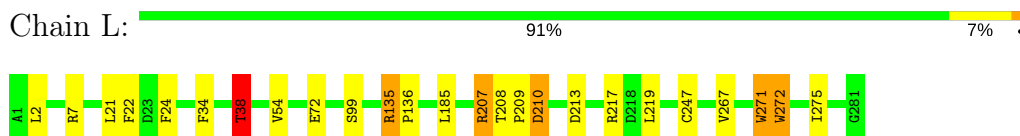
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

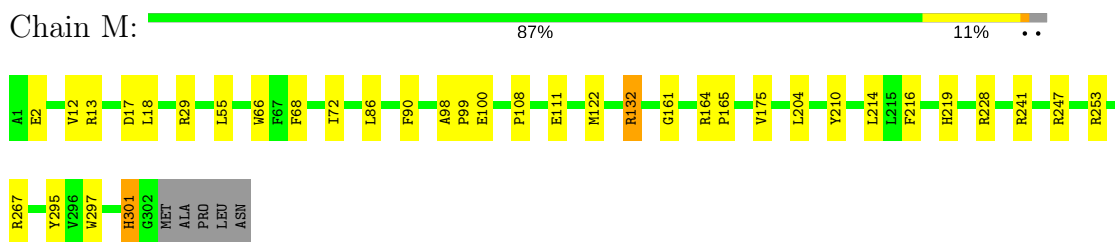
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER



• Molecule 2: PHOTOSYNTHETIC REACTION CENTER



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.05Å 142.05Å 186.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.10	Depositor
% Data completeness (in resolution range)	97.6 (30.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.169 , 0.186	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7312	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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, CL, CDL, BPH, FE2, 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	0.60	0/1877	1.28	14/2553 (0.5%)
2	L	0.61	0/2326	1.08	11/3183 (0.3%)
3	M	0.57	0/2533	1.19	20/3457 (0.6%)
All	All	0.59	0/6736	1.18	45/9193 (0.5%)

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	253[A]	ARG	NE-CZ-NH2	-14.39	113.10	120.30
3	M	253[B]	ARG	NE-CZ-NH2	-14.39	113.10	120.30
1	H	83	ARG	CD-NE-CZ	14.06	143.28	123.60
1	H	248	ARG	NE-CZ-NH1	13.96	127.28	120.30
1	H	248	ARG	CD-NE-CZ	12.23	140.72	123.60
3	M	253[A]	ARG	NE-CZ-NH1	11.63	126.11	120.30
3	M	253[B]	ARG	NE-CZ-NH1	11.63	126.11	120.30
3	M	132[A]	ARG	NE-CZ-NH2	-10.89	114.86	120.30
3	M	132[B]	ARG	NE-CZ-NH2	-10.89	114.86	120.30
2	L	217	ARG	NE-CZ-NH1	-10.43	115.09	120.30
1	H	248	ARG	NE-CZ-NH2	-10.28	115.16	120.30
1	H	70	ARG	NE-CZ-NH2	-9.83	115.39	120.30
3	M	132[A]	ARG	CD-NE-CZ	9.76	137.26	123.60
3	M	132[B]	ARG	CD-NE-CZ	9.76	137.26	123.60
2	L	207	ARG	CD-NE-CZ	8.88	136.03	123.60
2	L	210	ASP	CB-CG-OD1	8.63	126.06	118.30
1	H	83	ARG	NE-CZ-NH2	-8.16	116.22	120.30
3	M	267	ARG	NE-CZ-NH2	-7.67	116.46	120.30
1	H	225	VAL	CB-CA-C	-7.14	97.83	111.40
2	L	217	ARG	NE-CZ-NH2	6.84	123.72	120.30
2	L	207	ARG	NE-CZ-NH2	-6.73	116.93	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	70	ARG	NH1-CZ-NH2	6.63	126.69	119.40
3	M	29	ARG	CD-NE-CZ	6.46	132.65	123.60
3	M	241	ARG	NE-CZ-NH1	6.38	123.49	120.30
3	M	247	ARG	NE-CZ-NH1	6.36	123.48	120.30
2	L	207	ARG	NE-CZ-NH1	6.35	123.47	120.30
3	M	17	ASP	CB-CG-OD1	6.31	123.98	118.30
3	M	210	TYR	CB-CG-CD1	6.15	124.69	121.00
2	L	7	ARG	NE-CZ-NH1	6.12	123.36	120.30
2	L	38	THR	N-CA-CB	5.98	121.67	110.30
1	H	83	ARG	NE-CZ-NH1	5.94	123.27	120.30
2	L	213	ASP	CB-CG-OD1	5.88	123.59	118.30
2	L	135	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	H	118	ARG	CD-NE-CZ	5.81	131.73	123.60
3	M	247	ARG	NE-CZ-NH2	-5.80	117.40	120.30
3	M	253[A]	ARG	CD-NE-CZ	5.74	131.63	123.60
3	M	253[B]	ARG	CD-NE-CZ	5.74	131.63	123.60
1	H	118	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	H	225	VAL	CG1-CB-CG2	5.46	119.64	110.90
3	M	295	TYR	CB-CG-CD2	-5.40	117.76	121.00
3	M	13	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	H	170	ASP	CB-CG-OD1	5.37	123.13	118.30
1	H	202	ARG	NE-CZ-NH2	-5.18	117.71	120.30
2	L	2	LEU	CA-CB-CG	5.11	127.05	115.30
3	M	210	TYR	CB-CG-CD2	-5.00	118.00	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1829	0	1836	17	0
2	L	2235	0	2192	9	0
3	M	2430	0	2344	17	0
4	L	198	0	222	8	0
4	M	66	0	71	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	48	0	62	11	0
6	M	130	0	145	2	0
7	M	1	0	0	0	0
8	M	43	0	69	2	0
9	M	81	0	106	0	0
10	M	1	0	0	1	0
11	H	118	0	0	2	0
11	L	59	0	0	0	0
11	M	73	0	0	1	0
All	All	7312	0	7047	62	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (62) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:1502:U10:H301	5:L:1502:U10:H38	1.29	1.07
5:L:1502:U10:C30	5:L:1502:U10:H38	1.80	0.94
5:L:1502:U10:H301	5:L:1502:U10:C38	2.03	0.87
5:L:1502:U10:H371	4:M:1301:BCL:HED2	1.63	0.80
5:L:1502:U10:H351	3:M:90:PHE:HE2	1.54	0.71
5:L:1502:U10:C38	5:L:1502:U10:C30	2.66	0.69
3:M:108:PRO:HG2	3:M:111:GLU:HG3	1.77	0.66
1:H:195:MET:HE3	3:M:228:ARG:NE	2.10	0.65
4:L:1303:BCL:HMB1	4:L:1303:BCL:CBB	2.27	0.65
1:H:220:LYS:HE3	11:H:2107:HOH:O	1.99	0.62
1:H:32:GLN:HG2	1:H:56:PHE:CE2	2.37	0.60
1:H:195:MET:HE3	3:M:228:ARG:CZ	2.32	0.60
2:L:208:THR:HB	2:L:209:PRO:HD2	1.84	0.59
4:M:1301:BCL:CBB	4:M:1301:BCL:HMB1	2.32	0.59
5:L:1502:U10:H351	3:M:90:PHE:CE2	2.38	0.58
4:M:1301:BCL:HBB2	4:M:1301:BCL:HMB1	1.85	0.58
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.86	0.58
1:H:171:ILE:HB	1:H:172:PRO:HD3	1.85	0.57
4:L:1302:BCL:CBB	4:L:1302:BCL:HMB1	2.35	0.57
4:L:1303:BCL:HBB3	4:L:1303:BCL:HMB1	1.88	0.56
4:L:1302:BCL:HMB1	4:L:1302:BCL:HBB3	1.88	0.56
4:L:1304:BCL:HBB2	4:L:1304:BCL:HMB1	1.87	0.56
3:M:164:ARG:N	3:M:165:PRO:CD	2.68	0.55
5:L:1502:U10:C29	5:L:1502:U10:C41	2.67	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:175:VAL:HG11	8:M:1600:SPN:H161	1.91	0.52
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.93	0.51
1:H:195:MET:HE1	11:M:2006:HOH:O	2.10	0.51
1:H:206:ASN:HD21	1:H:248:ARG:HD2	1.76	0.49
1:H:249:LYS:O	1:H:250:SER:C	2.50	0.49
1:H:245:ALA:HB3	1:H:246:PRO:HD3	1.95	0.49
5:L:1502:U10:C33	5:L:1502:U10:C38	2.66	0.49
3:M:219:HIS:HA	10:M:1900:CL:CL	2.50	0.49
5:L:1502:U10:H371	4:M:1301:BCL:CED	2.39	0.48
3:M:214:LEU:HD13	6:M:1402:BPH:ND	2.29	0.48
3:M:98:ALA:HB1	3:M:99:PRO:HD2	1.96	0.48
2:L:34:PHE:O	2:L:38:THR:HG23	2.13	0.47
5:L:1502:U10:H403	4:M:1301:BCL:HMA2	1.95	0.47
3:M:161:GLY:HA3	8:M:1600:SPN:H201	1.97	0.47
1:H:32:GLN:HG2	1:H:56:PHE:CZ	2.50	0.46
2:L:219:LEU:HD12	3:M:132[B]:ARG:NH1	2.31	0.46
2:L:22:PHE:HA	2:L:24:PHE:CE2	2.50	0.46
1:H:112:ALA:HA	1:H:235:GLY:O	2.17	0.45
3:M:66:TRP:CD1	3:M:122:MET:HB2	2.52	0.45
4:M:1301:BCL:H112	4:M:1301:BCL:H151	1.67	0.45
4:L:1303:BCL:OBB	4:L:1303:BCL:HHC	2.17	0.44
1:H:171:ILE:HB	1:H:172:PRO:CD	2.48	0.44
1:H:32:GLN:NE2	11:H:2004:HOH:O	2.50	0.43
2:L:271:TRP:N	2:L:271:TRP:CD1	2.85	0.43
3:M:68:PHE:O	3:M:72:ILE:HG12	2.18	0.43
2:L:38:THR:HG22	2:L:99:SER:HB3	1.98	0.43
4:L:1304:BCL:C4A	4:L:1304:BCL:HBA1	2.49	0.42
1:H:130:LYS:HE3	1:H:170:ASP:OD2	2.20	0.42
1:H:122:GLU:HB2	1:H:227:LEU:HD21	2.01	0.42
2:L:272:TRP:HA	2:L:275:ILE:HG13	2.02	0.41
3:M:297:TRP:O	3:M:301:HIS:N	2.45	0.41
4:M:1301:BCL:OBB	4:M:1301:BCL:HHC	2.21	0.41
4:L:1302:BCL:OBB	4:L:1302:BCL:HHC	2.21	0.41
1:H:87:LEU:HD23	1:H:100:PRO:HA	2.03	0.41
2:L:38:THR:HG22	2:L:99:SER:CB	2.51	0.41
6:M:1402:BPH:HBA2	6:M:1402:BPH:H3A	1.92	0.41
1:H:169:VAL:HG23	1:H:171:ILE:HD13	2.03	0.41
3:M:100:GLU:HG3	3:M:100:GLU:H	1.70	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	238/260 (92%)	235 (99%)	2 (1%)	1 (0%)	38	35
2	L	280/281 (100%)	275 (98%)	5 (2%)	0	100	100
3	M	302/307 (98%)	292 (97%)	9 (3%)	1 (0%)	44	44
All	All	820/848 (97%)	802 (98%)	16 (2%)	2 (0%)	51	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	301	HIS
1	H	245	ALA

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%)	191 (98%)	4 (2%)	59	64
2	L	221/220 (100%)	210 (95%)	11 (5%)	28	26
3	M	239/241 (99%)	232 (97%)	7 (3%)	48	51
All	All	655/669 (98%)	633 (97%)	22 (3%)	42	43

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	105	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	225	VAL
1	H	231	ASP
1	H	249	LYS
2	L	21	LEU
2	L	38	THR
2	L	54	VAL
2	L	72	GLU
2	L	185	LEU
2	L	207	ARG
2	L	210	ASP
2	L	247	CYS
2	L	267	VAL
2	L	271	TRP
2	L	272	TRP
3	M	2	GLU
3	M	12	VAL
3	M	18	LEU
3	M	55	LEU
3	M	86	LEU
3	M	204	LEU
3	M	216	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	32	GLN
1	H	206	ASN
3	M	188	ASN
3	M	299	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	BCL	L	1302	2	55,74,74	1.59	8 (14%)	65,115,115	1.92	17 (26%)
4	BCL	L	1303	3	55,74,74	1.57	7 (12%)	65,115,115	1.87	17 (26%)
4	BCL	L	1304	2	55,74,74	1.75	12 (21%)	65,115,115	1.99	20 (30%)
5	U10	L	1502	-	48,48,63	1.73	11 (22%)	58,61,79	2.67	13 (22%)
4	BCL	M	1301	3,6	55,74,74	1.72	9 (16%)	65,115,115	2.38	23 (35%)
6	BPH	M	1401	3,4	65,70,70	1.39	7 (10%)	75,101,101	2.19	23 (30%)
6	BPH	M	1402	-	65,70,70	1.29	9 (13%)	75,101,101	1.93	20 (26%)
8	SPN	M	1600	-	40,42,42	3.60	18 (45%)	48,52,52	2.59	16 (33%)
9	CDL	M	1800	-	80,80,99	0.47	0	82,92,111	0.96	5 (6%)

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	BCL	L	1302	2	-	0/37/137/137	0/0/9/9
4	BCL	L	1303	3	-	0/37/137/137	0/0/9/9
4	BCL	L	1304	2	-	0/37/137/137	0/0/9/9
5	U10	L	1502	-	-	0/45/69/87	0/1/1/1
4	BCL	M	1301	3,6	2/2/21/25	1/37/137/137	0/0/9/9
6	BPH	M	1401	3,4	2/2/18/22	0/54/105/105	0/1/6/6
6	BPH	M	1402	-	-	0/54/105/105	0/1/6/6
8	SPN	M	1600	-	-	0/50/51/51	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CDL	M	1800	-	-	0/91/91/110	0/0/0/0

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	1600	SPN	C3-C4	-6.13	1.41	1.50
8	M	1600	SPN	C17-C18	-5.61	1.39	1.51
8	M	1600	SPN	C10-C9	-5.53	1.39	1.51
6	M	1401	BPH	C11-C10	-5.30	1.28	1.52
8	M	1600	SPN	C14-C13	-5.04	1.40	1.51
8	M	1600	SPN	C6-C5	-4.92	1.40	1.51
5	L	1502	U10	C7-C8	-3.60	1.45	1.50
8	M	1600	SPN	C20-C19	-3.34	1.39	1.50
8	M	1600	SPN	C7-C8	-2.96	1.40	1.50
5	L	1502	U10	O3-C3M	-2.93	1.38	1.45
8	M	1600	SPN	C11-C12	-2.93	1.40	1.50
4	L	1304	BCL	C2C-C3C	-2.87	1.46	1.54
6	M	1401	BPH	O2D-CED	-2.80	1.38	1.45
5	L	1502	U10	C32-C33	-2.58	1.41	1.50
8	M	1600	SPN	C21-C22	-2.48	1.39	1.52
6	M	1402	BPH	O2D-CED	-2.42	1.39	1.45
6	M	1401	BPH	C2C-C3C	-2.32	1.47	1.54
4	M	1301	BCL	C2C-C3C	-2.31	1.47	1.54
4	L	1303	BCL	O2D-CED	-2.28	1.39	1.45
4	L	1304	BCL	C3B-C2B	-2.19	1.35	1.39
4	L	1302	BCL	C2C-C3C	-2.19	1.48	1.54
8	M	1600	SPN	C16-C15	-2.15	1.39	1.51
4	M	1301	BCL	C3B-C2B	-2.06	1.35	1.39
4	L	1304	BCL	O2D-CED	-2.01	1.40	1.45
5	L	1502	U10	C28-C29	2.03	1.38	1.33
6	M	1402	BPH	C4C-NC	2.03	1.41	1.37
4	L	1303	BCL	C4-C3	2.03	1.55	1.50
8	M	1600	SPN	O1-C1	2.08	1.52	1.41
4	L	1302	BCL	CMA-C3A	2.09	1.57	1.53
6	M	1402	BPH	C4A-NA	2.13	1.40	1.35
6	M	1401	BPH	CAA-C2A	2.16	1.58	1.54
4	L	1304	BCL	CMB-C2B	2.20	1.56	1.51
4	M	1301	BCL	C2-C3	2.26	1.38	1.33
6	M	1402	BPH	C3D-C4D	2.31	1.44	1.41
4	M	1301	BCL	CMA-C3A	2.32	1.58	1.53
6	M	1402	BPH	O1D-CGD	2.35	1.27	1.21
4	L	1304	BCL	O1D-CGD	2.36	1.27	1.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1401	BPH	C2-C3	2.38	1.38	1.33
4	L	1304	BCL	C2-C3	2.41	1.39	1.33
6	M	1402	BPH	CAA-C2A	2.41	1.58	1.54
6	M	1402	BPH	C2-C3	2.42	1.39	1.33
4	L	1304	BCL	CMC-C2C	2.47	1.58	1.53
4	L	1304	BCL	CAA-C2A	2.47	1.58	1.54
5	L	1502	U10	C18-C19	2.53	1.39	1.33
5	L	1502	U10	C38-C39	2.59	1.39	1.32
4	M	1301	BCL	CAA-C2A	2.59	1.59	1.54
5	L	1502	U10	C8-C9	2.63	1.39	1.33
4	L	1304	BCL	O2A-CGA	2.70	1.41	1.33
4	L	1302	BCL	C4-C3	2.79	1.57	1.50
4	L	1302	BCL	C2-C3	2.92	1.40	1.33
5	L	1502	U10	C23-C24	2.94	1.40	1.33
8	M	1600	SPN	O1-CMA	2.95	1.52	1.43
8	M	1600	SPN	C29-C30	3.04	1.41	1.32
4	L	1303	BCL	C2-C3	3.11	1.40	1.33
4	L	1302	BCL	O2A-CGA	3.12	1.42	1.33
5	L	1502	U10	O3-C3	3.15	1.44	1.36
8	M	1600	SPN	C25-C26	3.17	1.40	1.33
4	L	1303	BCL	O2A-CGA	3.28	1.43	1.33
5	L	1502	U10	C13-C14	3.29	1.41	1.33
4	L	1302	BCL	CHB-C4A	3.31	1.37	1.33
6	M	1402	BPH	O2A-CGA	3.43	1.43	1.33
6	M	1401	BPH	O2D-CGD	3.68	1.42	1.33
4	M	1301	BCL	O2A-CGA	3.69	1.44	1.33
6	M	1402	BPH	O2D-CGD	3.70	1.42	1.33
6	M	1401	BPH	O2A-CGA	3.85	1.44	1.33
4	L	1302	BCL	O2D-CGD	3.99	1.43	1.33
4	L	1303	BCL	CHB-C4A	4.24	1.38	1.33
5	L	1502	U10	O4-C4	4.33	1.47	1.36
4	M	1301	BCL	O2D-CGD	4.60	1.44	1.33
4	L	1303	BCL	O2D-CGD	4.69	1.45	1.33
4	L	1304	BCL	O2D-CGD	5.04	1.46	1.33
4	M	1301	BCL	CHB-C4A	5.28	1.40	1.33
4	L	1304	BCL	CHC-C1C	5.40	1.40	1.33
4	L	1303	BCL	CHC-C1C	5.43	1.40	1.33
4	L	1304	BCL	CHB-C4A	5.63	1.40	1.33
4	L	1302	BCL	CHC-C1C	6.68	1.42	1.33
4	M	1301	BCL	CHC-C1C	6.82	1.42	1.33
8	M	1600	SPN	C12-C13	7.83	1.52	1.33
8	M	1600	SPN	C8-C9	8.13	1.53	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	1600	SPN	C19-C18	8.41	1.54	1.33
8	M	1600	SPN	C4-C5	8.52	1.54	1.33

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	1301	BCL	C4-C3-C5	-5.78	105.26	115.29
6	M	1402	BPH	O2A-CGA-O1A	-5.16	110.74	123.55
8	M	1600	SPN	C6-C5-C4	-5.06	110.74	121.10
8	M	1600	SPN	C17-C18-C19	-4.82	111.23	121.10
4	M	1301	BCL	O2A-CGA-O1A	-4.69	111.90	123.55
8	M	1600	SPN	C3-C4-C5	-4.53	119.14	126.71
4	M	1301	BCL	OBD-CAD-CBD	-4.46	119.21	125.94
6	M	1402	BPH	O2D-CGD-O1D	-4.40	114.98	123.82
5	L	1502	U10	O5-C5-C6	-4.39	113.73	121.82
4	L	1304	BCL	CMB-C2B-C1B	-4.06	122.23	128.46
4	L	1303	BCL	CAC-C3C-C2C	-4.01	104.16	114.24
4	L	1302	BCL	C4B-CHC-C1C	-3.98	122.23	130.12
6	M	1401	BPH	O2D-CGD-O1D	-3.93	115.91	123.82
4	M	1301	BCL	CAA-C2A-C3A	-3.92	102.07	112.81
8	M	1600	SPN	C20-C19-C18	-3.81	118.11	127.68
8	M	1600	SPN	C10-C9-C8	-3.81	113.31	121.10
4	L	1304	BCL	C1B-CHB-C4A	-3.79	122.61	130.12
4	L	1304	BCL	C4B-CHC-C1C	-3.78	122.63	130.12
6	M	1401	BPH	O1D-CGD-CBD	-3.74	117.88	124.60
4	L	1302	BCL	O2D-CGD-O1D	-3.71	116.35	123.82
4	L	1302	BCL	OB B-CAB-CBB	-3.69	111.74	120.16
4	L	1302	BCL	O2A-CGA-O1A	-3.69	114.38	123.55
8	M	1600	SPN	C14-C13-C12	-3.67	113.59	121.10
4	L	1304	BCL	CAC-C3C-C2C	-3.66	105.05	114.24
8	M	1600	SPN	C7-C8-C9	-3.64	118.53	127.68
4	L	1302	BCL	CAC-C3C-C4C	-3.64	104.51	112.58
4	M	1301	BCL	CMB-C2B-C1B	-3.61	122.92	128.46
8	M	1600	SPN	C11-C12-C13	-3.60	118.63	127.68
4	L	1302	BCL	OBD-CAD-CBD	-3.60	120.50	125.94
6	M	1402	BPH	OBD-CAD-CBD	-3.55	120.58	125.94
5	L	1502	U10	C30-C29-C31	-3.43	109.34	115.29
5	L	1502	U10	O2-C2-C3	-3.37	113.79	120.95
4	L	1303	BCL	C1-C2-C3	-3.25	119.97	125.96
6	M	1401	BPH	CAA-C2A-C3A	-3.25	103.91	112.81
4	M	1301	BCL	OB B-CAB-CBB	-3.17	112.93	120.16
4	L	1304	BCL	O2D-CGD-O1D	-3.17	117.45	123.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1302	BCL	CMA-C3A-C2A	-3.13	101.08	113.77
4	M	1301	BCL	O2D-CGD-O1D	-3.12	117.55	123.82
4	L	1303	BCL	CAC-C3C-C4C	-3.11	105.67	112.58
4	L	1303	BCL	O1D-CGD-CBD	-3.08	119.08	124.60
4	L	1303	BCL	C4B-CHC-C1C	-3.05	124.08	130.12
6	M	1402	BPH	CAA-C2A-C3A	-3.05	104.46	112.81
4	M	1301	BCL	C4B-CHC-C1C	-3.04	124.10	130.12
6	M	1401	BPH	O2A-CGA-O1A	-2.95	116.22	123.55
6	M	1401	BPH	CBB-CAB-C3B	-2.82	114.48	120.52
6	M	1402	BPH	CMA-C3A-C4A	-2.81	103.92	112.37
6	M	1401	BPH	C4D-CHA-C1A	-2.79	123.11	130.23
4	L	1304	BCL	OBD-CAD-CBD	-2.78	121.74	125.94
4	M	1301	BCL	CMA-C3A-C2A	-2.77	102.52	113.77
9	M	1800	CDL	CB6-CB4-CB3	-2.75	105.66	111.86
4	L	1302	BCL	CAC-C3C-C2C	-2.75	107.34	114.24
6	M	1401	BPH	C4B-C3B-CAB	-2.73	120.03	130.09
6	M	1402	BPH	O1D-CGD-CBD	-2.72	119.72	124.60
5	L	1502	U10	C20-C19-C21	-2.70	110.59	115.29
4	L	1302	BCL	CAA-C2A-C3A	-2.70	105.42	112.81
4	L	1303	BCL	O2D-CGD-O1D	-2.62	118.56	123.82
4	L	1304	BCL	OB B-CAB-CBB	-2.59	114.25	120.16
6	M	1402	BPH	C4D-CHA-C1A	-2.53	123.77	130.23
6	M	1402	BPH	C4B-C3B-CAB	-2.53	120.74	130.09
4	L	1304	BCL	O1D-CGD-CBD	-2.53	120.06	124.60
4	L	1304	BCL	CAA-C2A-C3A	-2.51	105.92	112.81
6	M	1401	BPH	C5-C3-C2	-2.47	116.06	121.10
4	M	1301	BCL	O1D-CGD-CBD	-2.45	120.20	124.60
6	M	1402	BPH	C4-C3-C5	-2.41	111.10	115.29
6	M	1402	BPH	CAA-C2A-C1A	-2.38	106.12	112.28
6	M	1402	BPH	C3A-C4A-NA	-2.36	108.99	113.06
6	M	1401	BPH	CAA-C2A-C1A	-2.34	106.22	112.28
4	M	1301	BCL	C1B-CHB-C4A	-2.26	125.65	130.12
9	M	1800	CDL	OA8-CA7-OA9	-2.23	118.02	123.55
4	L	1303	BCL	OBD-CAD-CBD	-2.23	122.58	125.94
6	M	1401	BPH	OBD-CAD-CBD	-2.21	122.60	125.94
4	L	1303	BCL	O2A-CGA-O1A	-2.17	118.15	123.55
9	M	1800	CDL	CA6-CA4-CA3	-2.16	106.98	111.86
6	M	1401	BPH	C2A-C1A-NA	-2.16	109.29	111.91
4	L	1302	BCL	CMA-C3A-C4A	-2.13	106.05	111.77
4	L	1303	BCL	C1B-CHB-C4A	-2.12	125.91	130.12
5	L	1502	U10	C4-C3-C2	-2.11	116.28	120.67
4	L	1303	BCL	CMB-C2B-C1B	-2.11	125.22	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	1301	BCL	CHA-C1A-NA	-2.10	121.30	126.18
6	M	1401	BPH	CMA-C3A-C4A	-2.09	106.08	112.37
9	M	1800	CDL	OB6-CB5-OB7	-2.07	118.52	123.68
4	M	1301	BCL	CMA-C3A-C4A	-2.05	106.27	111.77
4	L	1304	BCL	O2A-CGA-O1A	-2.04	118.49	123.55
4	M	1301	BCL	C3C-C2C-C1C	2.02	105.13	101.87
4	L	1302	BCL	C3C-C2C-C1C	2.03	105.15	101.87
4	M	1301	BCL	CMB-C2B-C3B	2.04	128.68	124.89
6	M	1401	BPH	C4-C3-C5	2.05	118.85	115.29
5	L	1502	U10	C17-C18-C19	2.08	132.90	127.68
4	L	1304	BCL	C2A-C3A-C4A	2.09	105.25	101.87
4	M	1301	BCL	C6-C5-C3	2.09	117.40	112.66
5	L	1502	U10	O5-C5-C4	2.11	125.45	120.95
4	L	1303	BCL	C3A-C2A-C1A	2.13	104.53	101.34
4	L	1302	BCL	C2A-C3A-C4A	2.14	105.33	101.87
5	L	1502	U10	C21-C19-C18	2.14	125.49	121.10
8	M	1600	SPN	C7-C6-C5	2.16	120.23	112.93
8	M	1600	SPN	C15-C16-C17	2.19	121.26	113.24
6	M	1402	BPH	C2A-C3A-C4A	2.28	105.89	101.33
5	L	1502	U10	C31-C29-C28	2.28	125.78	121.10
6	M	1401	BPH	CMD-C2D-C3D	2.30	129.17	124.89
4	L	1303	BCL	C3C-C2C-C1C	2.37	105.69	101.87
6	M	1402	BPH	C3C-C2C-C1C	2.38	105.71	101.87
6	M	1402	BPH	C3A-C4A-CHB	2.39	125.80	121.75
8	M	1600	SPN	CM3-C5-C6	2.39	119.44	115.29
6	M	1402	BPH	C2C-C3C-C4C	2.40	104.94	101.34
4	L	1304	BCL	CHB-C4A-NA	2.41	127.85	124.51
4	M	1301	BCL	CMD-C2D-C3D	2.49	129.51	124.89
4	L	1304	BCL	C3C-C2C-C1C	2.50	105.91	101.87
6	M	1402	BPH	CED-O2D-CGD	2.58	122.01	115.97
4	L	1304	BCL	C4A-NA-C1A	2.58	109.66	106.45
6	M	1401	BPH	C3C-C2C-C1C	2.66	106.16	101.87
6	M	1402	BPH	CAC-C3C-C2C	2.68	120.98	114.24
4	L	1303	BCL	C5-C3-C2	2.68	126.59	121.10
4	L	1304	BCL	O2A-CGA-CBA	2.73	119.85	111.90
6	M	1401	BPH	C2C-C3C-C4C	2.86	105.62	101.34
6	M	1402	BPH	C4A-NA-C1A	2.86	110.48	108.16
4	L	1302	BCL	C2C-C3C-C4C	2.89	105.67	101.34
4	L	1304	BCL	CMB-C2B-C3B	2.93	130.34	124.89
4	M	1301	BCL	C2C-C3C-C4C	3.01	105.85	101.34
4	L	1302	BCL	OB6-CAB-C3B	3.04	125.75	119.95
5	L	1502	U10	C16-C14-C13	3.22	127.70	121.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	1800	CDL	OB8-CB6-CB4	3.25	116.83	108.66
4	L	1303	BCL	O2A-CGA-CBA	3.29	121.47	111.90
4	L	1303	BCL	CHC-C1C-NC	3.31	129.09	124.51
4	L	1304	BCL	C1-O2A-CGA	3.39	124.90	116.77
4	L	1304	BCL	OBB-CAB-C3B	3.39	126.41	119.95
4	L	1302	BCL	C4A-NA-C1A	3.47	110.76	106.45
4	L	1302	BCL	CHC-C1C-NC	3.50	129.35	124.51
4	L	1304	BCL	CHC-C1C-NC	3.60	129.50	124.51
6	M	1401	BPH	CBC-CAC-C3C	3.62	121.72	113.51
6	M	1401	BPH	CED-O2D-CGD	3.66	124.55	115.97
6	M	1401	BPH	C11-C10-C8	3.67	127.78	115.73
6	M	1402	BPH	O2A-CGA-CBA	3.71	122.70	111.90
8	M	1600	SPN	CM4-C9-C10	3.78	121.85	115.29
4	M	1301	BCL	C5-C3-C2	3.88	129.04	121.10
8	M	1600	SPN	C16-C17-C18	3.91	121.53	112.66
6	M	1401	BPH	C6-C5-C3	4.01	121.74	112.66
4	L	1303	BCL	C4A-NA-C1A	4.04	111.46	106.45
8	M	1600	SPN	CM7-C22-C21	4.20	126.68	111.36
4	L	1302	BCL	O2D-CGD-CBD	4.47	119.28	111.30
4	M	1301	BCL	O2D-CGD-CBD	4.56	119.44	111.30
6	M	1401	BPH	C4A-NA-C1A	4.64	111.91	108.16
4	M	1301	BCL	O2A-CGA-CBA	4.98	126.39	111.90
6	M	1401	BPH	C1-C2-C3	5.55	136.19	125.96
4	M	1301	BCL	OBB-CAB-C3B	5.56	130.55	119.95
4	L	1304	BCL	O2D-CGD-CBD	6.07	122.14	111.30
4	L	1303	BCL	O2D-CGD-CBD	6.07	122.15	111.30
5	L	1502	U10	C27-C28-C29	6.11	143.03	127.68
8	M	1600	SPN	CM5-C13-C14	6.20	126.06	115.29
5	L	1502	U10	C3M-O3-C3	6.31	139.02	116.44
8	M	1600	SPN	CM6-C18-C17	6.77	127.03	115.29
4	M	1301	BCL	C1-C2-C3	7.42	139.63	125.96
6	M	1402	BPH	O2D-CGD-CBD	7.81	125.25	111.30
6	M	1401	BPH	O2D-CGD-CBD	8.32	126.18	111.30
5	L	1502	U10	C32-C33-C34	14.01	162.88	127.68

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	M	1401	BPH	C8
6	M	1401	BPH	C13
4	M	1301	BCL	C8
4	M	1301	BCL	C13

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	1301	BCL	C1-C2-C3-C4

There are no ring outliers.

7 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1302	BCL	3	0
4	L	1303	BCL	3	0
4	L	1304	BCL	2	0
5	L	1502	U10	11	0
4	M	1301	BCL	7	0
6	M	1402	BPH	2	0
8	M	1600	SPN	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.