



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 06:08 am BST

PDB ID : 5N4A
Title : Crystal structure of Chlamydomonas IFT80
Authors : Taschner, M.; Mourao, A.
Deposited on : 2017-02-10
Resolution : 1.79 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

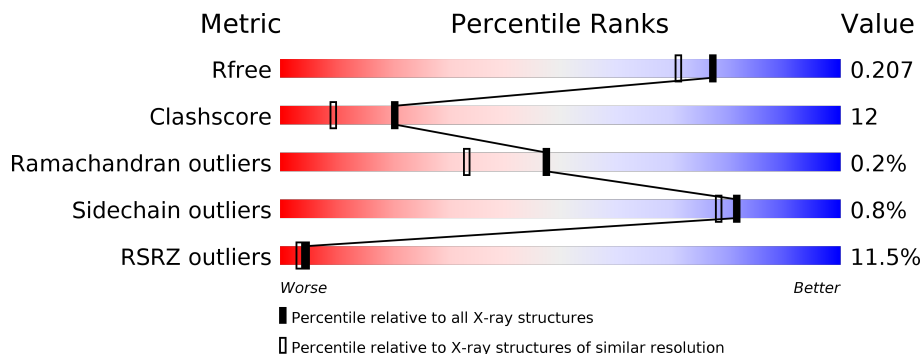
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 respectively. 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.

Mol	Chain	Length	Quality of chain
1	A	771	

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
2	GOL	A	802	-	-	X	-
2	GOL	A	805	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6130 atoms, of which 104 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.

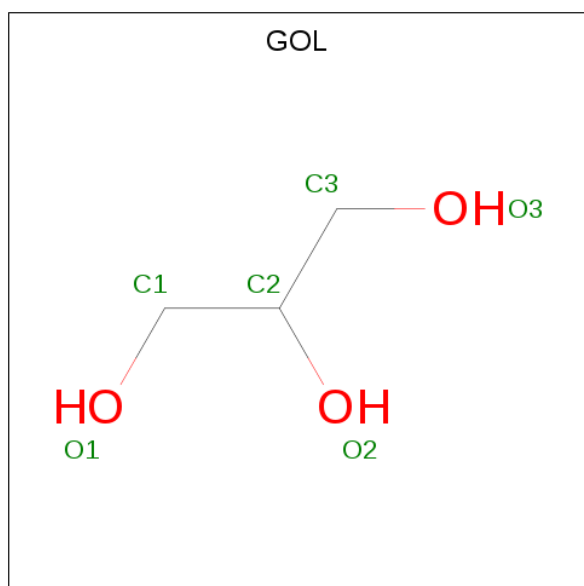
- Molecule 1 is a protein called Intraflagellar transport protein 80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	633	5208	3281	909	982	36	0	35	0

There are 6 discrepancies between the modelled and reference sequences:

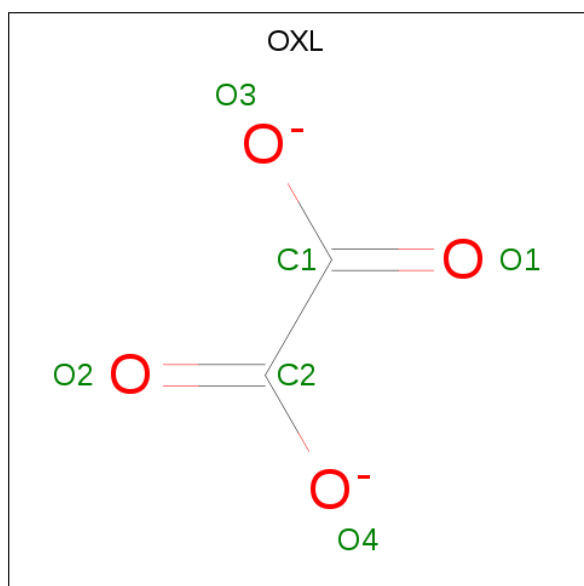
Chain	Residue	Modelled	Actual	Comment	Reference
A	766	HIS	-	expression tag	UNP A5Z0S9
A	767	HIS	-	expression tag	UNP A5Z0S9
A	768	HIS	-	expression tag	UNP A5Z0S9
A	769	HIS	-	expression tag	UNP A5Z0S9
A	770	HIS	-	expression tag	UNP A5Z0S9
A	771	HIS	-	expression tag	UNP A5Z0S9

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is OXALATE ION (three-letter code: OXL) (formula: C₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	2	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	734	Total	O	0	0
			734	734		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	82.78Å 195.40Å 117.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.92 – 1.79 46.93 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.92-1.79) 99.5 (46.93-1.79)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 1.78Å)	Xtrriage
Refinement program	PHENIX dev_1647	Depositor
R, R_{free}	0.174 , 0.207 0.175 , 0.207	Depositor DCC
R_{free} test set	4492 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtrriage
Anisotropy	0.418	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6130	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: OXL, GOL

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	A	0.38	0/5320	0.55	0/7221

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	A	5208	0	5126	130	0
2	A	78	104	104	16	0
3	A	6	0	0	0	0
4	A	734	0	0	31	4
All	All	6026	104	5230	131	4

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 12.

All (131) 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)
1:A:16:LEU:HD12	1:A:288:GLY:HA2	1.37	1.03
1:A:570[B]:ARG:NH2	4:A:904:HOH:O	2.11	0.84
1:A:511[B]:ASP:OD1	4:A:901:HOH:O	1.97	0.81
1:A:591:ILE:HD12	1:A:618:MET:SD	2.19	0.81
1:A:196:PRO:HA	2:A:802:GOL:H2	1.63	0.80
1:A:492:VAL:HG12	1:A:493:MET:HE2	1.62	0.79
1:A:492:VAL:HG12	1:A:493:MET:CE	2.12	0.79
1:A:155:TYR:N	2:A:802:GOL:O2	2.12	0.78
1:A:197[B]:ILE:HD11	1:A:239:GLY:CA	2.14	0.77
1:A:197[B]:ILE:HD11	1:A:239:GLY:HA3	1.66	0.77
1:A:454:GLU:O	1:A:495:ARG:NH1	2.18	0.76
1:A:564:ASN:OD1	4:A:902:HOH:O	2.04	0.75
1:A:154:ALA:HA	2:A:802:GOL:H31	1.69	0.73
1:A:36:THR:HG22	1:A:52:THR:HG22	1.70	0.72
1:A:589:ASP:OD1	1:A:592[B]:ARG:NH2	2.24	0.71
1:A:503:MET:HE3	1:A:521:ASP:HB2	1.73	0.69
2:A:802:GOL:O1	4:A:903:HOH:O	2.11	0.69
1:A:383[B]:ARG:NH1	4:A:911:HOH:O	2.25	0.69
1:A:31:CYS:HB3	1:A:57:PHE:CD2	2.28	0.68
1:A:195[B]:SER:OG	1:A:198:ASN:OD1	2.12	0.68
1:A:421[A]:MET:SD	1:A:432:LEU:HD23	2.34	0.68
1:A:369:PHE:HB2	2:A:808:GOL:H32	1.74	0.68
1:A:37:ILE:HB	4:A:1548:HOH:O	1.94	0.67
1:A:452:VAL:CG1	1:A:493:MET:HE3	2.26	0.65
1:A:154:ALA:HA	2:A:802:GOL:C3	2.25	0.65
1:A:472:THR:HG22	4:A:1377:HOH:O	1.98	0.64
1:A:272[B]:MET:HE3	1:A:288:GLY:HA2	1.80	0.64
1:A:16:LEU:CD1	1:A:288:GLY:HA2	2.21	0.63
1:A:439:THR:HG22	4:A:1247:HOH:O	1.97	0.63
1:A:16:LEU:HD11	1:A:272[B]:MET:HE3	1.81	0.63
1:A:197[B]:ILE:HG12	1:A:198:ASN:N	2.14	0.63
1:A:281:THR:OG1	1:A:336:ARG:NH2	2.27	0.63
1:A:435:GLN:NE2	4:A:924:HOH:O	2.32	0.63
1:A:272[A]:MET:HE3	4:A:1083:HOH:O	1.99	0.63
1:A:334[A]:ARG:HG3	4:A:1213:HOH:O	1.99	0.62
1:A:17:THR:OG1	1:A:290:GLY:O	2.16	0.62
1:A:493:MET:CE	1:A:493:MET:HA	2.30	0.62
1:A:263[B]:ILE:HG12	4:A:1204:HOH:O	1.99	0.62
1:A:192[A]:VAL:HG13	1:A:203:THR:HG22	1.80	0.62
1:A:17:THR:N	1:A:290:GLY:HA2	2.15	0.61
1:A:133:ARG:NH1	4:A:927:HOH:O	2.33	0.61
1:A:29:PHE:HD2	1:A:37:ILE:HD11	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:VAL:HG11	1:A:493:MET:HE3	1.85	0.58
1:A:492:VAL:C	1:A:493:MET:HE2	2.24	0.58
1:A:565:ARG:HB3	2:A:813:GOL:H12	1.85	0.58
1:A:16:LEU:HD11	1:A:272[B]:MET:CE	2.33	0.58
1:A:596:TRP:CE2	1:A:624:GLU:HG3	2.39	0.58
1:A:32:SER:HB3	1:A:34:ASP:OD2	2.04	0.57
1:A:36:THR:HG22	1:A:52:THR:CG2	2.34	0.57
1:A:301:ALA:O	1:A:302:LEU:HD23	2.06	0.56
1:A:196:PRO:HA	2:A:802:GOL:C2	2.35	0.56
1:A:426:ASN:HA	4:A:906:HOH:O	2.07	0.55
1:A:16:LEU:HD11	1:A:272[B]:MET:SD	2.47	0.55
1:A:197[B]:ILE:HD11	1:A:239:GLY:N	2.22	0.55
1:A:15:GLU:O	1:A:290:GLY:HA3	2.08	0.55
1:A:365:THR:HG23	1:A:365:THR:O	2.07	0.54
1:A:5:VAL:HG21	1:A:263[A]:ILE:HG21	1.89	0.54
1:A:197[B]:ILE:HD13	4:A:1106:HOH:O	2.07	0.54
1:A:383[B]:ARG:HD3	4:A:1499:HOH:O	2.07	0.54
1:A:402:ARG:NH1	4:A:914:HOH:O	2.27	0.53
1:A:250:LEU:O	1:A:263[A]:ILE:HG22	2.09	0.53
1:A:565:ARG:HB3	2:A:813:GOL:C1	2.39	0.53
1:A:175:SER:OG	1:A:176:ASN:N	2.42	0.53
1:A:156[A]:ASP:OD1	1:A:156[A]:ASP:N	2.28	0.52
1:A:18:ALA:O	1:A:273[A]:THR:HG21	2.09	0.52
1:A:231:THR:HG1	1:A:270[B]:SER:HG	1.53	0.52
1:A:155:TYR:H	2:A:802:GOL:C2	2.21	0.52
1:A:16:LEU:CD1	1:A:272[B]:MET:HE3	2.38	0.52
1:A:306:LYS:HE2	4:A:1520:HOH:O	2.08	0.52
1:A:1:MET:CE	1:A:300:LEU:HD13	2.41	0.51
1:A:179:GLN:O	1:A:179:GLN:HG3	2.12	0.50
1:A:492:VAL:HG12	1:A:493:MET:HE3	1.91	0.50
1:A:69:LYS:HE3	1:A:372:LYS:O	2.12	0.50
1:A:272[B]:MET:HE3	1:A:288:GLY:CA	2.40	0.50
1:A:323:LEU:HD12	1:A:324:ASN:N	2.26	0.50
1:A:445:ASP:OD2	1:A:450:ARG:HG2	2.11	0.50
1:A:579:ALA:HB2	2:A:813:GOL:H2	1.93	0.49
1:A:40:TRP:CZ3	1:A:46:PRO:HG3	2.47	0.49
1:A:52:THR:O	1:A:53:LEU:HD23	2.13	0.49
1:A:383[B]:ARG:NH2	4:A:955:HOH:O	2.44	0.49
1:A:87:VAL:HG21	1:A:121:THR:HG21	1.95	0.49
1:A:195[B]:SER:HB3	1:A:235:TRP:CG	2.49	0.48
1:A:162:TYR:HE2	1:A:171[B]:LYS:HE3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263[A]:ILE:HD12	4:A:1288:HOH:O	2.14	0.48
1:A:37:ILE:CG2	1:A:51:SER:HB2	2.42	0.48
1:A:229:PRO:HG2	2:A:805:GOL:H32	1.94	0.48
1:A:397:TYR:HE1	2:A:808:GOL:H12	1.78	0.48
1:A:268[A]:THR:HG23	1:A:269:GLY:O	2.14	0.48
1:A:1:MET:HE2	1:A:300:LEU:HD13	1.95	0.47
1:A:620:MET:HE1	4:A:1625:HOH:O	2.13	0.47
1:A:485:ARG:HE	2:A:809:GOL:C2	2.28	0.47
1:A:383[B]:ARG:HB2	4:A:906:HOH:O	2.15	0.47
1:A:6:LYS:HE2	4:A:1017:HOH:O	2.15	0.47
1:A:283:LEU:C	1:A:283:LEU:HD12	2.35	0.47
1:A:307:MET:SD	1:A:321:ASP:HA	2.56	0.45
1:A:322:ILE:O	1:A:322:ILE:HG22	2.16	0.45
1:A:554:LYS:NZ	4:A:940:HOH:O	2.39	0.45
1:A:155:TYR:HB3	4:A:1350:HOH:O	2.16	0.45
1:A:323:LEU:HD12	1:A:323:LEU:C	2.37	0.45
1:A:604:ARG:HD2	4:A:931:HOH:O	2.17	0.45
1:A:45[B]:GLU:HA	1:A:46:PRO:HD3	1.85	0.44
1:A:559[B]:GLN:NE2	4:A:953:HOH:O	2.44	0.44
1:A:607:LYS:HD2	4:A:1369:HOH:O	2.18	0.44
1:A:191:LYS:HE2	1:A:191:LYS:HB2	1.80	0.44
1:A:493:MET:N	1:A:493:MET:HE2	2.33	0.44
1:A:413[B]:ARG:HE	1:A:416:LEU:HD12	1.83	0.43
1:A:132:SER:HB2	1:A:134:ASN:OD1	2.18	0.43
1:A:262:LYS:NZ	4:A:966:HOH:O	2.49	0.43
1:A:122:ALA:HB1	1:A:148:VAL:HB	2.00	0.43
1:A:37:ILE:HG21	1:A:51:SER:HB2	1.99	0.43
1:A:37:ILE:HG23	1:A:51:SER:H	1.83	0.43
1:A:397:TYR:HE1	2:A:808:GOL:C1	2.31	0.43
1:A:81:ALA:HB2	1:A:110:LEU:HG	2.00	0.43
1:A:591:ILE:HD13	1:A:596:TRP:CH2	2.54	0.43
1:A:598:LYS:HG2	1:A:601[C]:ARG:NH2	2.34	0.43
1:A:367:HIS:HD2	4:A:1400:HOH:O	2.02	0.42
1:A:491:PRO:HD3	1:A:534:TYR:OH	2.19	0.42
1:A:2:ARG:HA	1:A:261[B]:SER:OG	2.19	0.42
1:A:503:MET:CE	1:A:521:ASP:HB2	2.46	0.42
1:A:409:PHE:CE1	1:A:412:LEU:HD13	2.55	0.42
1:A:598:LYS:HG2	1:A:601[C]:ARG:HH21	1.84	0.42
1:A:477[B]:GLN:NE2	1:A:531:SER:OG	2.47	0.42
1:A:37:ILE:HG23	1:A:51:SER:N	2.34	0.41
1:A:71:GLN:HG3	1:A:72:ALA:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:TYR:H	2:A:802:GOL:HO2	1.56	0.41
1:A:301:ALA:HB1	1:A:308:GLN:NE2	2.36	0.41
1:A:416:LEU:O	1:A:421[B]:MET:SD	2.79	0.41
1:A:540:LEU:HD13	1:A:540:LEU:C	2.41	0.40
1:A:306:LYS:HG2	4:A:1520:HOH:O	2.21	0.40
1:A:358:TYR:CD2	1:A:366:PRO:HB3	2.57	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1541:HOH:O	4:A:1541:HOH:O[3_755]	2.11	0.09
4:A:1220:HOH:O	4:A:1598:HOH:O[3_755]	2.13	0.07
4:A:1291:HOH:O	4:A:1612:HOH:O[4_566]	2.15	0.05
4:A:970:HOH:O	4:A:1170:HOH:O[4_566]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	A	665/771 (86%)	648 (97%)	16 (2%)	1 (0%)	47 33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	ILE

5.3.2 Protein sidechains [i](#)

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	A	564/654 (86%)	559 (99%)	5 (1%)	78	75

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	THR
1	A	110	LEU
1	A	156[A]	ASP
1	A	156[B]	ASP
1	A	323	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

14 ligands are modelled in this entry.

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
2	GOL	A	813	-	5,5,5	0.39	0	5,5,5	0.53	0
2	GOL	A	804	-	5,5,5	0.36	0	5,5,5	0.21	0
2	GOL	A	814	-	5,5,5	0.54	0	5,5,5	0.69	0
2	GOL	A	808	-	5,5,5	0.50	0	5,5,5	0.33	0
2	GOL	A	801	-	5,5,5	0.25	0	5,5,5	0.37	0
3	OXL	A	812	-	0,5,5	0.00	-	0,6,6	0.00	-
2	GOL	A	802	-	5,5,5	0.42	0	5,5,5	0.59	0
2	GOL	A	805	-	5,5,5	0.35	0	5,5,5	0.21	0
2	GOL	A	806	-	5,5,5	0.36	0	5,5,5	0.48	0
2	GOL	A	809	-	5,5,5	0.38	0	5,5,5	0.17	0
2	GOL	A	811	-	5,5,5	0.36	0	5,5,5	0.21	0
2	GOL	A	810	-	5,5,5	0.36	0	5,5,5	0.30	0
2	GOL	A	803	-	5,5,5	0.39	0	5,5,5	0.14	0
2	GOL	A	807	-	5,5,5	0.42	0	5,5,5	0.17	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
2	GOL	A	813	-	-	2/4/4/4	-
2	GOL	A	804	-	-	2/4/4/4	-
2	GOL	A	814	-	-	0/4/4/4	-
2	GOL	A	808	-	-	2/4/4/4	-
2	GOL	A	801	-	-	0/4/4/4	-
3	OXL	A	812	-	-	0/0/4/4	-
2	GOL	A	802	-	-	2/4/4/4	-
2	GOL	A	805	-	-	2/4/4/4	-
2	GOL	A	806	-	-	2/4/4/4	-
2	GOL	A	809	-	-	2/4/4/4	-
2	GOL	A	811	-	-	3/4/4/4	-
2	GOL	A	810	-	-	2/4/4/4	-
2	GOL	A	803	-	-	4/4/4/4	-
2	GOL	A	807	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	813	GOL	O2-C2-C3-O3
2	A	804	GOL	O1-C1-C2-C3
2	A	808	GOL	C1-C2-C3-O3
2	A	802	GOL	O1-C1-C2-O2
2	A	802	GOL	O1-C1-C2-C3
2	A	805	GOL	O1-C1-C2-C3
2	A	806	GOL	O1-C1-C2-O2
2	A	806	GOL	O1-C1-C2-C3
2	A	810	GOL	O1-C1-C2-C3
2	A	803	GOL	O1-C1-C2-C3
2	A	810	GOL	O1-C1-C2-O2
2	A	803	GOL	O1-C1-C2-O2
2	A	803	GOL	O2-C2-C3-O3
2	A	807	GOL	O1-C1-C2-O2
2	A	813	GOL	C1-C2-C3-O3
2	A	809	GOL	O1-C1-C2-C3
2	A	803	GOL	C1-C2-C3-O3
2	A	807	GOL	O1-C1-C2-C3
2	A	809	GOL	O1-C1-C2-O2
2	A	808	GOL	O2-C2-C3-O3
2	A	805	GOL	O1-C1-C2-O2
2	A	804	GOL	O1-C1-C2-O2
2	A	811	GOL	O1-C1-C2-O2
2	A	811	GOL	O1-C1-C2-C3
2	A	811	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	813	GOL	3	0
2	A	808	GOL	3	0
2	A	802	GOL	8	0
2	A	805	GOL	1	0
2	A	809	GOL	1	0

5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	633/771 (82%)	0.58	73 (11%) 4 3	20, 35, 79, 148	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	177	ALA	12.4
1	A	72	ALA	7.4
1	A	323	LEU	7.3
1	A	324	ASN	6.4
1	A	55	ALA	6.4
1	A	436	ALA	6.1
1	A	174	SER	5.9
1	A	176	ASN	5.6
1	A	66	SER	5.6
1	A	290	GLY	5.4
1	A	437	SER	5.2
1	A	54	ASP	5.2
1	A	56	TYR	4.9
1	A	178	LYS	4.8
1	A	71	GLN	4.7
1	A	37	ILE	4.6
1	A	175	SER	4.5
1	A	95	ARG	4.4
1	A	50	VAL	4.3
1	A	438	GLY	4.1
1	A	16	LEU	3.9
1	A	15	GLU	3.8
1	A	52	THR	3.6
1	A	36	THR	3.6
1	A	8	SER	3.5
1	A	57	PHE	3.4
1	A	322	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	291	GLY	3.3
1	A	321	ASP	3.3
1	A	33	ASP	3.3
1	A	35	GLN	3.3
1	A	70	THR	3.2
1	A	17	THR	3.2
1	A	365	THR	3.2
1	A	1	MET	3.1
1	A	38	HIS	3.1
1	A	289	SER	3.1
1	A	267	ASP	3.1
1	A	48	GLN	3.0
1	A	101	GLU	2.8
1	A	638	VAL	2.8
1	A	637	GLU	2.8
1	A	596	TRP	2.8
1	A	636	ASP	2.7
1	A	69	LYS	2.7
1	A	537	LYS	2.7
1	A	32	SER	2.7
1	A	459	THR	2.7
1	A	74	GLY	2.6
1	A	639	ASP	2.6
1	A	51	SER	2.6
1	A	535	VAL	2.6
1	A	626	ASN	2.6
1	A	137	LEU	2.6
1	A	538	ASP	2.5
1	A	53	LEU	2.5
1	A	326	ASN	2.5
1	A	625	LEU	2.5
1	A	327	ALA	2.4
1	A	100	ILE	2.3
1	A	236	ALA	2.3
1	A	361	THR	2.3
1	A	34	ASP	2.3
1	A	136	MET	2.3
1	A	568	VAL	2.3
1	A	623	LYS	2.3
1	A	173	LEU	2.2
1	A	592[A]	ARG	2.2
1	A	266	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	258	TRP	2.1
1	A	3	LEU	2.1
1	A	621	ALA	2.0
1	A	228	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95th 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	A	811	6/6	0.57	0.34	89,107,123,125	0
2	GOL	A	810	6/6	0.60	0.32	92,110,120,120	0
2	GOL	A	805	6/6	0.72	0.42	73,87,98,98	0
2	GOL	A	806	6/6	0.73	0.27	81,98,108,115	0
2	GOL	A	814	6/6	0.79	0.20	32,55,73,88	0
2	GOL	A	807	6/6	0.80	0.38	55,70,85,86	0
2	GOL	A	802	6/6	0.84	0.22	46,63,77,83	0
2	GOL	A	804	6/6	0.86	0.15	46,82,105,106	0
3	OXL	A	812	6/6	0.87	0.21	30,36,39,45	6
2	GOL	A	813	6/6	0.88	0.23	41,77,98,102	0
2	GOL	A	809	6/6	0.89	0.33	66,79,86,90	0
2	GOL	A	808	6/6	0.89	0.24	33,40,54,54	14
2	GOL	A	803	6/6	0.90	0.33	43,68,83,97	0
2	GOL	A	801	6/6	0.95	0.08	31,42,63,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.