Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:26 AM GMT

PDB ID	:	2X0H
Title	:	BTGH84 MICHAELIS COMPLEX
Authors	:	He, Y.; Davies, G.J.
Deposited on	:	2009-12-08
Resolution	:	2.21 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

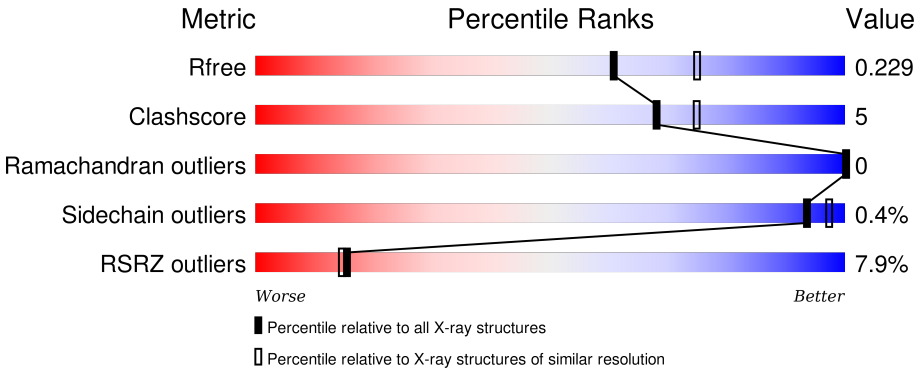
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4405 (2.24-2.20)
Clashscore	102246	5146 (2.24-2.20)
Ramachandran outliers	100387	5065 (2.24-2.20)
Sidechain outliers	100360	5066 (2.24-2.20)
RSRZ outliers	91569	4414 (2.24-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	737	7% 76% 9% 15%
1	B	737	6% 77% 9% 13%

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
3	GOL	B	1718	-	-	-	X
3	GOL	B	1719	-	-	-	X

2 Entry composition

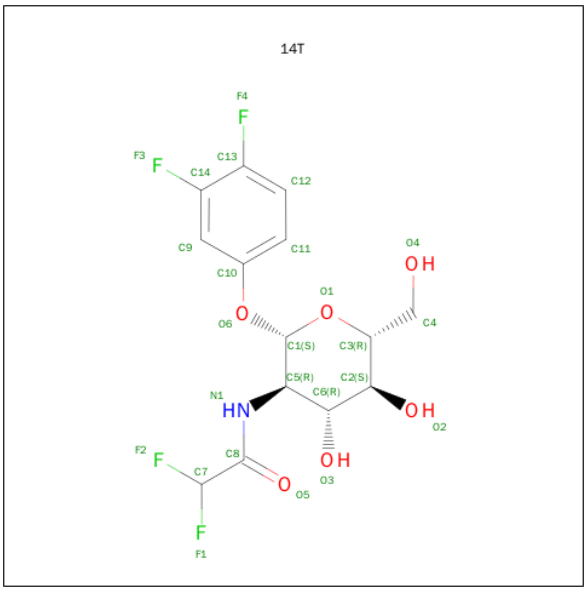
There are 5 unique types of molecules in this entry. The entry contains 11257 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 O-GLCNACASE BT_4395.

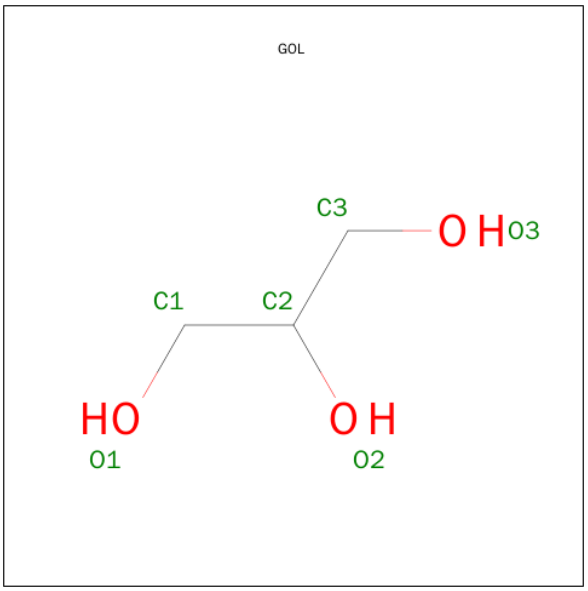
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	630	Total	C	N	O	S	0	3	0
			5168	3323	868	958	19			
1	B	642	Total	C	N	O	S	0	6	0
			5269	3373	896	981	19			

- Molecule 2 is SUGAR (3,4-DIFLUOROPHENYL 2-DEOXY-2-[(DIFLUOROACETYL)AMINO]-BETA-D-GLUCOPYRANOSIDE) (three-letter code: 14T) (formula: $C_{14}H_{15}F_4NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			25	14	4	1	6		
2	B	1	Total	C	F	N	O	0	0
			25	14	4	1	6		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0

- Molecule 5 is water.

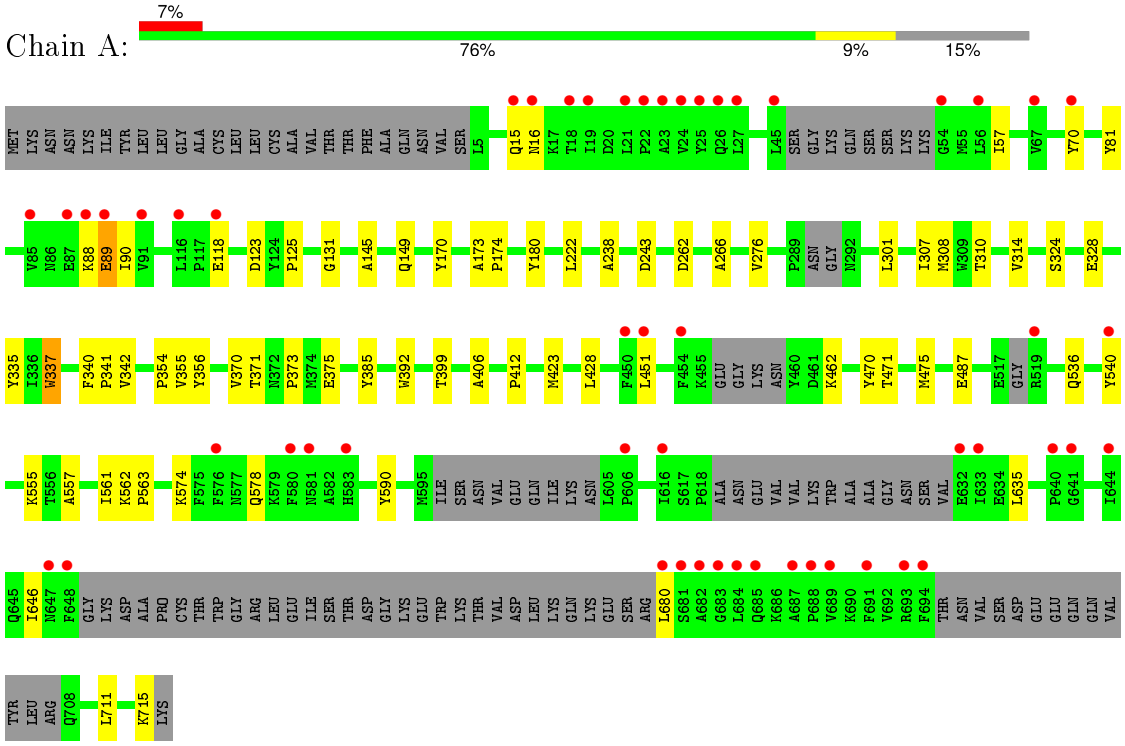
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	325	Total O 325 325	0	0
5	B	408	Total O 408 408	0	0

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

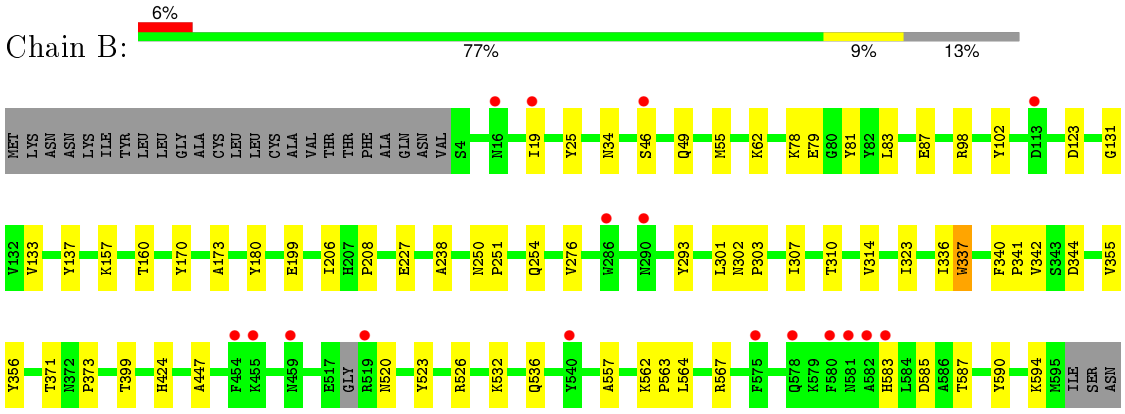
- Molecule 1: O-GLCNACASE BT_4395

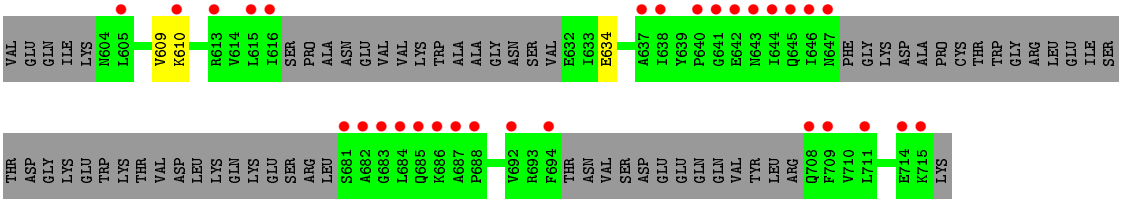
Chain A:



- Molecule 1: O-GLCNACASE BT_4395

Chain B:




VAL GLU GLN ILE LYS N604 L605 V609 K610 R613 V614 L615 I616 SER PRO ALA ASN GLU VAL VAL LYS TRP ALA ALA GLY ASN SER VAL E632 I633 E634 A637 I638 Y639 P640 G641 E642 N643 I644 Q645 I646 N647 PHE GLY LYS ASP ALA PRO CYS THR TRP GLY ARG LEU GLU ILE SER
THR ASP GLY LYS GLU TRP LYS THR VAL ASP LEU LYS GLN LYS GLU SER ARG LEU S681 A682 G683 L684 Q685 K686 A687 P688 V692 R693 F694 THR ASN VAL SER ASP GLU GLU GLN GLN VAL TYR LEU ARG Q708 F709 V710 L711 E714 K715 LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.63Å 163.15Å 224.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.08 – 2.21 45.08 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.08-2.21) 99.2 (45.08-2.21)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.96 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.194 , 0.226 0.201 , 0.229	Depositor DCC
R_{free} test set	4767 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	3 of 95737 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11257	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.53 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.5926e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, 14T

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	0.78	0/5297	0.68	0/7175
1	B	0.83	0/5402	0.72	0/7313
All	All	0.80	0/10699	0.70	0/14488

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

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	5168	0	5077	48	0
1	B	5269	0	5179	49	0
2	A	25	0	15	2	0
2	B	25	0	15	1	0
3	A	12	0	16	1	0
3	B	24	0	32	2	0
4	B	1	0	0	0	0
5	A	325	0	0	7	0
5	B	408	0	0	7	0
All	All	11257	0	10334	97	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 5.

All (97) 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:355:VAL:O	1:A:399:THR:HG23	1.76	0.85
1:B:536:GLN:HG2	1:B:590:TYR:CD1	2.17	0.79
1:B:355:VAL:O	1:B:399:THR:HG23	1.84	0.76
1:A:324:SER:O	1:A:328:GLU:HG3	1.91	0.70
1:B:563:PRO:O	1:B:567[B]:ARG:HG3	1.94	0.68
1:A:15:GLN:O	1:A:16:ASN:HB2	1.93	0.68
1:B:585:ASP:OD1	1:B:587:THR:HG23	1.97	0.65
1:B:46:SER:CA	5:B:2040:HOH:O	2.43	0.65
1:A:375:GLU:CD	5:A:2197:HOH:O	2.34	0.65
1:A:536:GLN:HG2	1:A:590:TYR:CD1	2.34	0.62
1:B:250:ASN:O	1:B:254:GLN:HG3	2.00	0.61
1:A:356:TYR:HB3	1:A:399:THR:HG21	1.82	0.61
1:B:583[B]:HIS:CD2	1:B:583[B]:HIS:O	2.54	0.61
1:B:532:LYS:O	1:B:536:GLN:HG3	2.01	0.60
1:A:354:PRO:HB2	1:A:399:THR:HG22	1.84	0.60
1:A:423[B]:MET:HE3	1:A:423[B]:MET:HA	1.83	0.59
1:A:562:LYS:HB3	1:A:563:PRO:HD3	1.85	0.57
1:A:646:ILE:O	1:A:680:LEU:HB2	2.03	0.57
1:B:520:ASN:OD1	1:B:523:TYR:N	2.36	0.57
1:A:555:LYS:HE3	5:A:2289:HOH:O	2.04	0.56
1:A:536:GLN:O	1:A:540[A]:TYR:HD2	1.89	0.54
3:A:1716:GOL:H2	5:A:2324:HOH:O	2.08	0.54
1:A:412:PRO:HD2	1:A:487:GLU:OE1	2.08	0.53
1:A:423[B]:MET:HA	1:A:423[B]:MET:CE	2.39	0.53
1:B:340:PHE:O	1:B:371:THR:OG1	2.25	0.53
1:B:447:ALA:HB1	1:B:564:LEU:CD1	2.39	0.52
1:A:342:VAL:HG23	5:A:2196:HOH:O	2.10	0.52
1:A:462:LYS:NZ	5:A:2252:HOH:O	2.43	0.52
1:A:243:ASP:OD2	2:A:1000:14T:H5	2.11	0.51
1:B:78:LYS:O	1:B:79:GLU:HB2	2.11	0.51
1:A:557:ALA:HB1	1:A:561:ILE:HB	1.92	0.50
1:B:356:TYR:HB3	1:B:399:THR:HG21	1.94	0.49
1:B:323:ILE:HD12	1:B:336:ILE:HD11	1.94	0.49
1:B:137:TYR:HB2	3:B:1718:GOL:H32	1.94	0.49
1:B:19:ILE:HD12	1:B:55:MET:CE	2.43	0.49
1:A:170:TYR:HB2	1:A:180:TYR:CE1	2.48	0.49
1:B:344:ASP:O	3:B:1718:GOL:H31	2.13	0.48
1:B:19:ILE:HD12	1:B:55:MET:HE1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:TYR:CE2	1:B:123:ASP:HB3	2.49	0.48
1:B:310:THR:HA	1:B:337:TRP:O	2.13	0.48
1:A:314:VAL:HG11	2:A:1000:14T:H9	1.96	0.47
1:B:238:ALA:HA	1:B:276:VAL:O	2.14	0.47
1:A:471:THR:O	1:A:475:MET:HG3	2.14	0.47
1:A:262:ASP:HA	1:A:266:ALA:HB3	1.98	0.46
1:A:15:GLN:HB2	1:A:118:GLU:HB3	1.96	0.46
1:B:81:TYR:CZ	1:B:123:ASP:HB3	2.50	0.46
1:A:145:ALA:O	1:A:149:GLN:HG2	2.15	0.46
1:A:173:ALA:HA	1:A:174:PRO:HA	1.65	0.46
1:B:83:LEU:C	1:B:83:LEU:HD23	2.36	0.46
1:A:340:PHE:O	1:A:371:THR:OG1	2.34	0.46
1:A:81:TYR:CZ	1:A:123:ASP:HB3	2.51	0.46
1:A:125:PRO:HB3	1:A:392:TRP:CE3	2.51	0.46
1:A:635:LEU:HD11	1:A:711:LEU:CD2	2.47	0.45
1:A:301:LEU:HD23	1:A:307:ILE:HD11	1.99	0.45
1:B:314:VAL:HG11	2:B:1000:14T:H9	1.98	0.45
1:A:308:MET:HA	1:A:335:TYR:O	2.16	0.45
1:B:424:HIS:O	1:B:557:ALA:HA	2.17	0.44
1:B:206:ILE:HG23	1:B:208:PRO:HD3	1.99	0.44
1:B:562:LYS:N	1:B:563:PRO:CD	2.80	0.44
1:B:609:VAL:O	1:B:610:LYS:HD3	2.17	0.44
1:A:354:PRO:HD2	5:A:2244:HOH:O	2.17	0.44
1:B:567[B]:ARG:NH2	5:B:2377:HOH:O	2.50	0.44
1:B:594:LYS:HB2	1:B:634:GLU:HB3	1.99	0.44
1:A:310:THR:HA	1:A:337:TRP:O	2.18	0.44
1:B:173:ALA:HB2	5:B:2186:HOH:O	2.17	0.44
1:A:385:TYR:CD2	1:A:406:ALA:HB2	2.52	0.44
1:B:25:TYR:CE2	1:B:49:GLN:HG3	2.53	0.43
1:A:341:PRO:HD2	1:A:373:PRO:HA	2.01	0.43
1:A:238:ALA:HA	1:A:276:VAL:O	2.18	0.43
1:A:70:TYR:OH	1:A:89:GLU:OE2	2.37	0.43
1:A:131:GLY:O	1:A:370:VAL:HA	2.19	0.43
1:B:251:PRO:HB3	1:B:293:TYR:CD1	2.54	0.43
1:A:555:LYS:CE	5:A:2289:HOH:O	2.66	0.43
1:A:371:THR:HG23	1:A:371:THR:O	2.19	0.42
1:B:131:GLY:HA3	1:B:160:THR:O	2.19	0.42
1:A:574:LYS:O	1:A:578:GLN:HG3	2.19	0.42
1:B:562:LYS:HB3	1:B:563:PRO:HD3	2.01	0.42
1:B:341:PRO:HD2	1:B:373:PRO:HA	2.01	0.42
1:B:102:TYR:CE1	1:B:157:LYS:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:ALA:HB1	1:B:564:LEU:HD12	2.02	0.41
1:A:536:GLN:HG2	1:A:590:TYR:CG	2.55	0.41
1:A:81:TYR:CE2	1:A:123:ASP:HB3	2.56	0.41
1:A:470:TYR:HE1	1:B:526:ARG:NH1	2.18	0.41
1:B:170:TYR:HB2	1:B:180:TYR:CE1	2.56	0.41
1:B:34:ASN:OD1	1:B:34:ASN:C	2.59	0.41
1:B:227:GLU:HB2	5:B:2196:HOH:O	2.21	0.41
1:B:98:ARG:HG3	1:B:199:GLU:HB3	2.03	0.41
1:A:428:LEU:N	1:A:428:LEU:HD12	2.36	0.41
1:B:87:GLU:HG2	5:B:2099:HOH:O	2.20	0.40
1:B:342:VAL:HG23	5:B:2278:HOH:O	2.21	0.40
1:B:301:LEU:HD12	1:B:307:ILE:HD11	2.02	0.40
1:A:57:ILE:HG12	1:A:90:ILE:HB	2.04	0.40
1:A:222:LEU:C	1:A:222:LEU:HD23	2.41	0.40
1:B:133:VAL:HG13	1:B:133:VAL:O	2.22	0.40
1:A:451:LEU:HD12	1:A:451:LEU:HA	1.83	0.40
1:B:62:LYS:HD2	5:B:2082:HOH:O	2.21	0.40
1:B:302:ASN:HA	1:B:303:PRO:HD3	1.95	0.40

There are no symmetry-related clashes.

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	615/737 (83%)	596 (97%)	19 (3%)	0	100	100
1	B	636/737 (86%)	616 (97%)	20 (3%)	0	100	100
All	All	1251/1474 (85%)	1212 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	559/647 (86%)	555 (99%)	4 (1%)	88 94
1	B	570/647 (88%)	569 (100%)	1 (0%)	95 98
All	All	1129/1294 (87%)	1124 (100%)	5 (0%)	93 97

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

Mol	Chain	Res	Type
1	A	88	LYS
1	A	89	GLU
1	A	337	TRP
1	A	715	LYS
1	B	337	TRP

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

Mol	Chain	Res	Type
1	A	156	ASN
1	A	252	GLN
1	A	254	GLN
1	A	274	GLN
1	A	433	HIS
1	A	529	ASN
1	A	608	GLN
1	B	11	GLN
1	B	15	GLN
1	B	156	ASN
1	B	433	HIS
1	B	459	ASN
1	B	529	ASN
1	B	581	ASN
1	B	708	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\#\|Z\| > 2$
2	14T	A	1000	-	25,26,26	1.03	2 (8%)	32,37,37	2.13	6 (18%)
3	GOL	A	1716	-	5,5,5	0.37	0	5,5,5	1.10	0
3	GOL	A	1717	-	5,5,5	0.32	0	5,5,5	0.38	0
2	14T	B	1000	-	25,26,26	0.96	2 (8%)	32,37,37	1.84	5 (15%)
3	GOL	B	1717	-	5,5,5	0.33	0	5,5,5	0.16	0
3	GOL	B	1718	-	5,5,5	0.43	0	5,5,5	0.69	0
3	GOL	B	1719	-	5,5,5	0.41	0	5,5,5	0.76	0
3	GOL	B	1720	-	5,5,5	0.45	0	5,5,5	0.67	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	14T	A	1000	-	-	0/14/34/34	0/2/2/2
3	GOL	A	1716	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1717	-	-	0/4/4/4	0/0/0/0
2	14T	B	1000	-	-	0/14/34/34	0/2/2/2
3	GOL	B	1717	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1718	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1719	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1720	-	-	0/4/4/4	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	14T	O6-C1	2.16	1.44	1.41
2	B	1000	14T	O6-C1	2.20	1.44	1.41
2	B	1000	14T	C1-C5	2.51	1.57	1.53
2	A	1000	14T	C1-C5	3.17	1.58	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1000	14T	C6-C5-N1	-3.21	104.01	110.66
2	A	1000	14T	O1-C1-O6	-3.19	99.88	108.39
2	B	1000	14T	O1-C1-C5	2.32	115.82	110.78
2	B	1000	14T	C5-N1-C8	2.42	127.00	123.18
2	A	1000	14T	C5-N1-C8	3.16	128.16	123.18
2	B	1000	14T	C1-C5-N1	3.41	117.43	111.01
2	B	1000	14T	C1-O1-C3	3.79	121.10	113.75
2	A	1000	14T	C1-C5-N1	3.94	118.43	111.01
2	A	1000	14T	C1-O1-C3	4.92	123.28	113.75
2	B	1000	14T	C10-O6-C1	7.03	128.35	117.87
2	A	1000	14T	C10-O6-C1	7.37	128.85	117.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	14T	2	0
3	A	1716	GOL	1	0
2	B	1000	14T	1	0
3	B	1718	GOL	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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	630/737 (85%)	0.13	53 (8%)	14 13	22, 37, 74, 94	0
1	B	642/737 (87%)	-0.02	47 (7%)	18 17	19, 35, 77, 113	0
All	All	1272/1474 (86%)	0.05	100 (7%)	15 15	19, 36, 76, 113	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	646	ILE	6.7
1	B	682	ALA	5.9
1	A	454	PHE	5.7
1	A	688	PRO	5.0
1	B	685	GLN	4.9
1	B	644	ILE	4.7
1	B	605	LEU	4.6
1	B	687	ALA	4.4
1	B	610	LYS	4.3
1	B	694	PHE	4.3
1	B	709	PHE	4.3
1	B	645	GLN	4.2
1	B	681	SER	4.2
1	A	22	PRO	4.2
1	B	647	ASN	4.1
1	B	455	LYS	4.1
1	A	54	GLY	4.0
1	A	641	GLY	3.9
1	B	684	LEU	3.9
1	A	682	ALA	3.9
1	A	689	VAL	3.9
1	A	694	PHE	3.6
1	B	686	LYS	3.6
1	A	25	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	519	ARG	3.4
1	B	286	TRP	3.3
1	A	16	ASN	3.3
1	B	641	GLY	3.3
1	A	680	LEU	3.3
1	A	687	ALA	3.3
1	B	643	ASN	3.3
1	A	116	LEU	3.3
1	A	88	LYS	3.2
1	A	26	GLN	3.2
1	A	648	PHE	3.0
1	B	642	GLU	3.0
1	A	580	PHE	3.0
1	B	688	PRO	3.0
1	A	23	ALA	3.0
1	B	616	ILE	3.0
1	A	56	LEU	2.9
1	B	16	ASN	2.9
1	A	691	PHE	2.9
1	B	581	ASN	2.9
1	A	583	HIS	2.8
1	B	692	VAL	2.8
1	A	684	LEU	2.8
1	B	683	GLY	2.8
1	A	21	LEU	2.7
1	A	632	GLU	2.7
1	A	685	GLN	2.6
1	B	708	GLN	2.6
1	A	87	GLU	2.6
1	A	15	GLN	2.6
1	A	633	ILE	2.6
1	B	540	TYR	2.5
1	A	693	ARG	2.5
1	B	711	LEU	2.5
1	A	91	VAL	2.5
1	A	644	ILE	2.5
1	B	638	ILE	2.5
1	A	451	LEU	2.5
1	B	640	PRO	2.5
1	A	19	ILE	2.5
1	A	89	GLU	2.4
1	A	450	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	45	LEU	2.4
1	B	583[A]	HIS	2.4
1	A	70	TYR	2.4
1	B	715	LYS	2.4
1	A	18	THR	2.3
1	B	582	ALA	2.3
1	A	85	VAL	2.3
1	B	46	SER	2.3
1	B	714	GLU	2.3
1	B	19	ILE	2.2
1	A	647	ASN	2.2
1	A	118	GLU	2.2
1	B	454	PHE	2.2
1	B	459	ASN	2.2
1	A	519	ARG	2.2
1	A	581	ASN	2.2
1	B	113	ASP	2.1
1	A	24	VAL	2.1
1	A	640	PRO	2.1
1	A	616	ILE	2.1
1	A	683	GLY	2.1
1	B	290	ASN	2.1
1	B	575	PHE	2.1
1	A	540[A]	TYR	2.1
1	B	578	GLN	2.1
1	A	67	VAL	2.1
1	B	580	PHE	2.1
1	B	613	ARG	2.1
1	B	637	ALA	2.0
1	A	606	PRO	2.0
1	A	27	LEU	2.0
1	A	576	PHE	2.0
1	B	615	LEU	2.0
1	A	681	SER	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	B	1718	6/6	0.83	0.29	9.84	43,45,49,50	0
3	GOL	B	1719	6/6	0.93	0.15	2.12	47,53,53,57	0
2	14T	A	1000	25/25	0.96	0.15	1.68	29,37,57,59	9
3	GOL	A	1717	6/6	0.92	0.14	1.15	52,57,58,60	0
2	14T	B	1000	25/25	0.95	0.17	1.13	28,34,57,61	9
3	GOL	A	1716	6/6	0.90	0.12	0.68	40,47,49,52	0
3	GOL	B	1720	6/6	0.85	0.17	0.33	47,49,50,52	0
4	CA	B	1716	1/1	0.99	0.09	-0.34	30,30,30,30	1
3	GOL	B	1717	6/6	0.94	0.31	-	63,66,66,67	0

6.5 Other polymers (i)

There are no such residues in this entry.