Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 06:59 PM BST

PDB ID	:	3L4T
Title	:	Crystal complex of N-terminal Human Maltase-Glucoamylase with BJ2661
Authors	:	Sim, L.; Rose, D.R.
Deposited on	:	2009-12-21
Resolution	:	1.90 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:

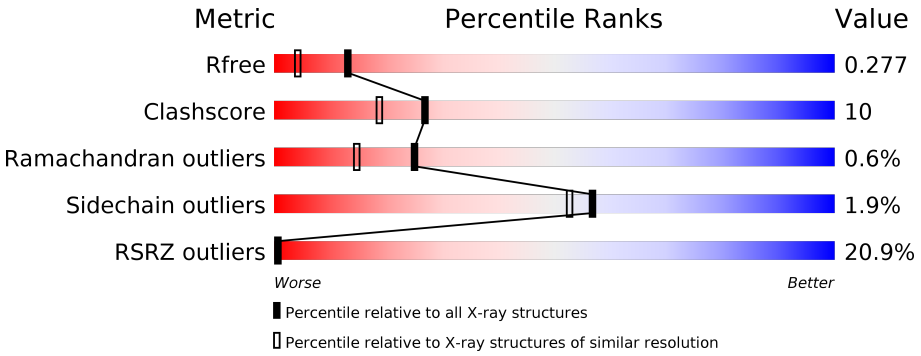
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	875	20% 80% 17%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7452 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.

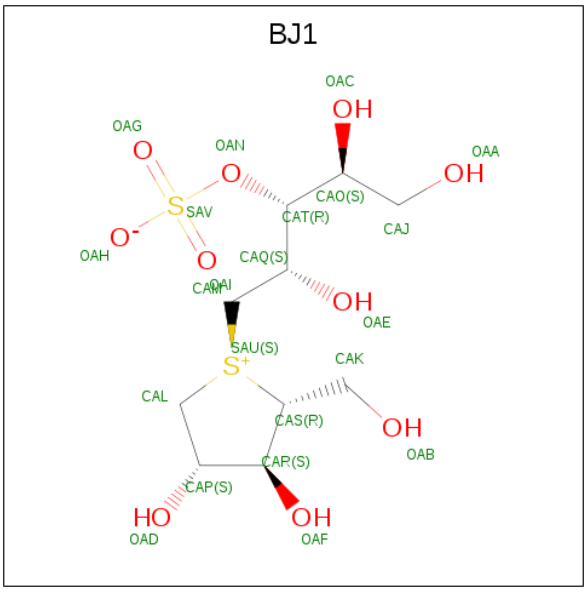
- Molecule 1 is a protein called Maltase-glucoamylase, intestinal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	856	Total	C	N	O	S	0	19	0
			6964	4466	1173	1295	30			

There are 8 discrepancies between the modelled and reference sequences:

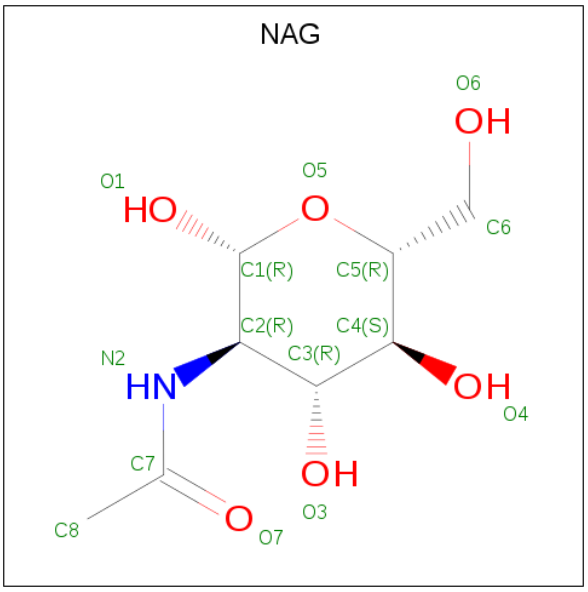
Chain	Residue	Modelled	Actual	Comment	Reference
A	772	ASP	ASN	variant	UNP O43451
A	869	ALA	-	expression tag	UNP O43451
A	870	HIS	-	expression tag	UNP O43451
A	871	HIS	-	expression tag	UNP O43451
A	872	HIS	-	expression tag	UNP O43451
A	873	HIS	-	expression tag	UNP O43451
A	874	HIS	-	expression tag	UNP O43451
A	875	HIS	-	expression tag	UNP O43451

- Molecule 2 is (1R,2S)-1-[(1S)-1,2-dihydroxyethyl]-3-[(2R,3S,4S)-3,4-dihydroxy-2-(hydroxymethyl)tetrahydrothiophenium-1-yl]-2-hydroxypropyl sulfate (three-letter code: BJ1) (formula: $C_{10}H_{20}O_{10}S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			22	10	10	2		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is water.

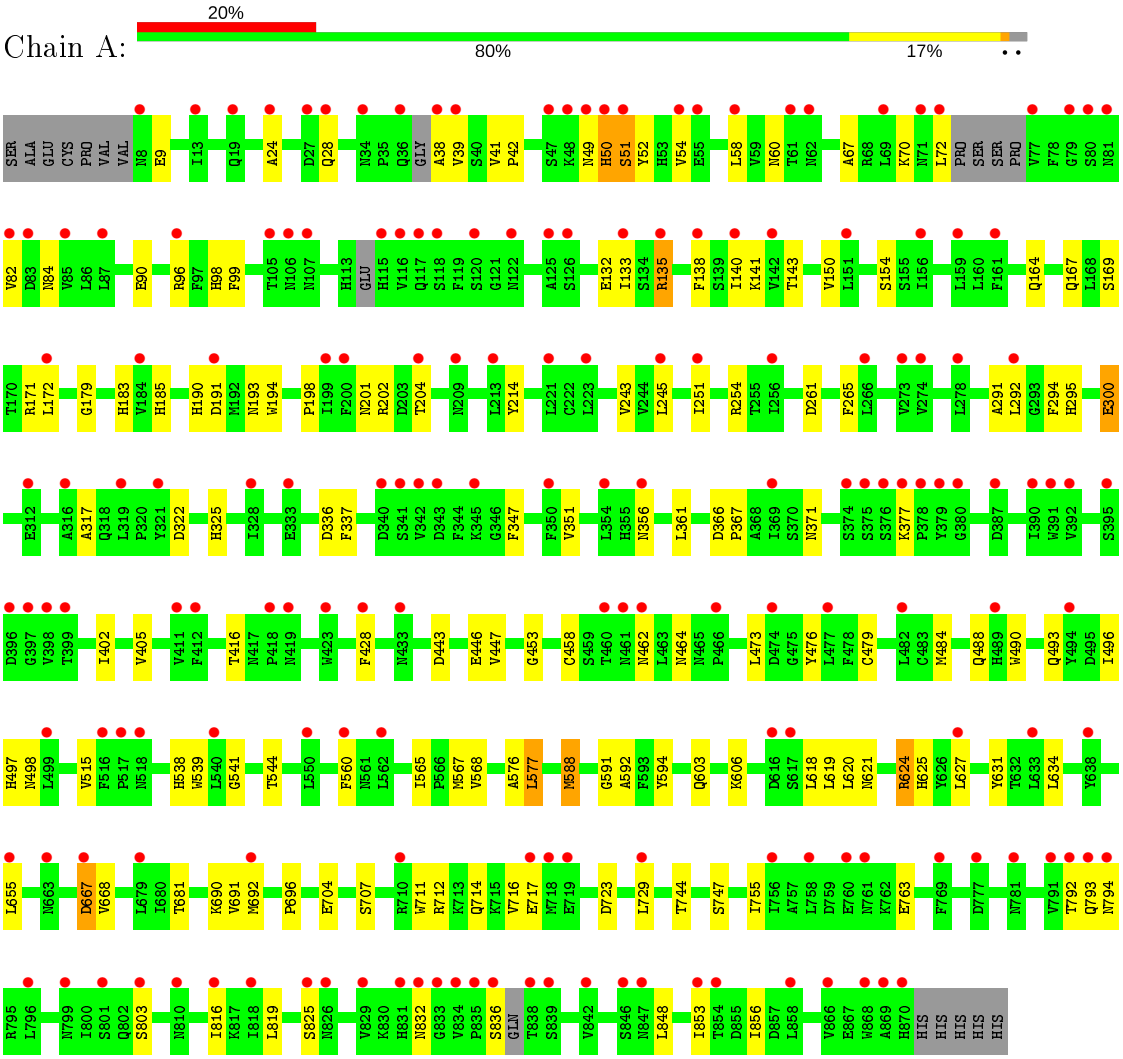
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	438	Total	O	0	0
			438	438		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

- Molecule 1: Maltase-glucoamylase, intestinal

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.78Å 108.44Å 110.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 1.90 18.96 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.3 (19.99-1.90) 95.3 (18.96-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.20 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.252 , 0.291 0.239 , 0.277	Depositor DCC
R_{free} test set	4206 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.55 , 71.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7452	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: NAG, BJ1

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	0.72	0/7215	0.75	2/9831 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	624	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	A	624	ARG	NE-CZ-NH2	-7.52	116.54	120.30

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	6964	0	6731	138	0
2	A	22	0	20	0	0
3	A	28	0	26	1	0
4	A	438	0	0	18	0
All	All	7452	0	6777	139	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 10.

All (139) 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:204:THR:HG21	1:A:473:LEU:HD23	1.14	1.12
1:A:204:THR:CG2	1:A:473:LEU:HD23	1.83	1.09
1:A:729[B]:LEU:CD1	1:A:755[B]:ILE:HD11	1.80	1.09
1:A:692:MET:SD	1:A:717:GLU:HG2	1.97	1.04
1:A:479[A]:CYS:SG	4:A:4105:HOH:O	2.16	1.04
1:A:729[B]:LEU:HD13	1:A:755[B]:ILE:HD11	1.04	1.00
1:A:853[B]:ILE:CD1	1:A:856:ILE:HD12	1.92	0.99
1:A:853[B]:ILE:HD11	1:A:856:ILE:HD12	1.00	0.99
1:A:853[B]:ILE:HD11	1:A:856:ILE:CD1	1.93	0.98
1:A:729[B]:LEU:HD13	1:A:755[B]:ILE:CD1	1.97	0.94
1:A:204:THR:HG21	1:A:473:LEU:CD2	1.99	0.92
1:A:836:SER:HA	4:A:4429:HOH:O	1.73	0.88
1:A:712:ARG:H	1:A:714:GLN:HE21	1.25	0.83
1:A:38:ALA:N	1:A:41:VAL:HB	1.94	0.83
1:A:98:HIS:HE1	1:A:261:ASP:OD1	1.62	0.81
1:A:655[B]:LEU:HD12	1:A:668:VAL:HG11	1.63	0.80
1:A:150[B]:VAL:HG22	4:A:4173:HOH:O	1.82	0.79
1:A:143:THR:HG22	1:A:150[B]:VAL:HG12	1.65	0.79
1:A:141:LYS:HE3	1:A:150[B]:VAL:HG11	1.65	0.77
1:A:135:ARG:NH1	1:A:135:ARG:CB	2.48	0.76
1:A:836:SER:HB3	4:A:4389:HOH:O	1.84	0.76
1:A:300:GLU:HG3	1:A:603:GLN:HE21	1.50	0.76
1:A:141:LYS:HE3	1:A:150[B]:VAL:CG1	2.17	0.75
1:A:164:GLN:NE2	1:A:462:ASN:HD22	1.85	0.74
1:A:245:LEU:HD22	1:A:251[B]:ILE:HG12	1.68	0.73
1:A:493:GLN:HE21	1:A:497:HIS:HD2	1.40	0.69
1:A:204:THR:CG2	1:A:473:LEU:CD2	2.65	0.68
1:A:356:ASN:HB2	4:A:4424:HOH:O	1.94	0.68
1:A:167:GLN:NE2	1:A:254:ARG:HE	1.93	0.67
1:A:135:ARG:CG	1:A:135:ARG:HH11	2.07	0.67
1:A:729[B]:LEU:CD1	1:A:755[B]:ILE:CD1	2.63	0.67
1:A:488:GLN:HB2	1:A:496:ILE:HD11	1.77	0.66
1:A:164:GLN:HE22	1:A:462:ASN:HD22	1.41	0.66
1:A:183:HIS:HE1	1:A:198:PRO:O	1.78	0.65
1:A:295:HIS:HD2	1:A:325:HIS:NE2	1.94	0.64
1:A:135:ARG:CB	1:A:135:ARG:HH11	2.10	0.64
1:A:38:ALA:HA	1:A:39:VAL:C	2.19	0.63
1:A:201:ASN:H	1:A:498:ASN:ND2	1.97	0.63
1:A:621:ASN:OD1	1:A:624:ARG:NH2	2.31	0.63
1:A:90:GLU:OE1	1:A:98:HIS:HD2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ARG:NH1	1:A:135:ARG:HB2	2.13	0.62
1:A:493:GLN:NE2	1:A:497:HIS:HD2	1.98	0.61
1:A:135:ARG:HB3	1:A:135:ARG:CZ	2.30	0.61
1:A:476:TYR:HB2	1:A:479[A]:CYS:SG	2.41	0.61
3:A:2001:NAG:O4	4:A:4373:HOH:O	2.15	0.60
1:A:202:ARG:HG3	1:A:204:THR:HG23	1.83	0.60
1:A:446:GLU:N	1:A:447:VAL:HA	2.16	0.60
1:A:317:ALA:HB1	1:A:620:LEU:HD21	1.84	0.60
1:A:655[A]:LEU:HD23	1:A:696:PRO:HG3	1.84	0.59
1:A:24:ALA:O	1:A:28:GLN:HG3	2.03	0.58
1:A:98:HIS:CE1	1:A:261:ASP:OD1	2.52	0.58
1:A:681:THR:HG22	1:A:691:VAL:HG11	1.86	0.58
1:A:143:THR:CG2	1:A:150[B]:VAL:HG12	2.32	0.58
1:A:201:ASN:O	1:A:497:HIS:HE1	1.86	0.57
1:A:9:GLU:HB2	1:A:41:VAL:HG11	1.85	0.57
1:A:201:ASN:H	1:A:498:ASN:HD21	1.52	0.57
1:A:190:HIS:HD2	4:A:4010:HOH:O	1.86	0.57
1:A:711:TRP:CG	1:A:716:VAL:HG11	2.39	0.57
1:A:135:ARG:HG3	1:A:135:ARG:HH11	1.70	0.56
1:A:618:LEU:HD11	1:A:723:ASP:HB3	1.86	0.55
1:A:292:LEU:HD23	1:A:567:MET:CE	2.36	0.55
1:A:49:ASN:O	1:A:50:HIS:HB2	2.07	0.55
1:A:371:ASN:ND2	1:A:402:ILE:HD12	2.22	0.55
1:A:135:ARG:CZ	1:A:135:ARG:CB	2.85	0.54
1:A:135:ARG:HG3	4:A:4048:HOH:O	2.07	0.54
1:A:58:LEU:HD22	1:A:67:ALA:HB2	1.90	0.54
1:A:356:ASN:HB2	4:A:4426:HOH:O	2.08	0.53
1:A:619:LEU:C	1:A:619:LEU:HD23	2.29	0.53
1:A:691:VAL:HG23	4:A:4260:HOH:O	2.08	0.53
1:A:132:GLU:HG2	1:A:141:LYS:HB3	1.89	0.53
1:A:179:GLY:O	1:A:190:HIS:HE1	1.92	0.53
1:A:172:LEU:HD11	1:A:251[B]:ILE:HG13	1.90	0.52
1:A:402:ILE:HD11	4:A:4100:HOH:O	2.10	0.52
1:A:141:LYS:HE3	1:A:150[A]:VAL:HG22	1.90	0.52
1:A:183:HIS:HD2	1:A:185:HIS:NE2	2.08	0.52
1:A:667:ASP:HA	4:A:4196:HOH:O	2.09	0.51
1:A:351:VAL:HG22	1:A:361:LEU:HD22	1.91	0.51
1:A:135:ARG:NH1	1:A:135:ARG:CG	2.70	0.51
1:A:243:VAL:HG11	1:A:251[A]:ILE:HD11	1.92	0.51
1:A:96[B]:ARG:HE	1:A:265:PHE:HE1	1.57	0.50
1:A:191:ASP:HB3	1:A:193:ASN:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:VAL:CG1	1:A:251[A]:ILE:HD11	2.42	0.49
1:A:51:SER:OG	1:A:52:TYR:N	2.44	0.49
1:A:377:LYS:HG3	1:A:377:LYS:O	2.12	0.49
1:A:592:ALA:HB2	1:A:627[B]:LEU:HD12	1.94	0.49
1:A:453:GLY:HA3	1:A:458:CYS:SG	2.53	0.49
1:A:763:GLU:HG2	1:A:792:THR:HA	1.95	0.49
1:A:99:PHE:CE1	1:A:140[B]:ILE:HD12	2.48	0.48
1:A:591:GLY:HA2	1:A:594:TYR:CD2	2.49	0.48
1:A:183:HIS:CD2	1:A:185:HIS:NE2	2.81	0.48
1:A:294:PHE:CZ	1:A:588[A]:MET:HE3	2.49	0.48
1:A:38:ALA:HB3	4:A:4318:HOH:O	2.14	0.48
1:A:544:THR:CG2	1:A:577:LEU:HD22	2.45	0.47
1:A:711:TRP:CD1	1:A:716:VAL:HG11	2.50	0.47
1:A:356:ASN:CB	4:A:4426:HOH:O	2.63	0.47
1:A:42:PRO:HD3	1:A:194:TRP:CH2	2.50	0.47
1:A:300:GLU:HG3	1:A:603:GLN:NE2	2.23	0.47
1:A:38:ALA:N	1:A:41:VAL:CB	2.73	0.47
1:A:135:ARG:HB2	1:A:135:ARG:HH11	1.74	0.46
1:A:464:ASN:ND2	1:A:484:MET:H	2.14	0.46
1:A:204:THR:HG22	1:A:473:LEU:HD23	1.85	0.46
1:A:493:GLN:NE2	1:A:497:HIS:CD2	2.81	0.46
1:A:70:LYS:HE3	1:A:84:ASN:HD21	1.81	0.46
1:A:54:VAL:HG21	1:A:133[B]:ILE:HD11	1.98	0.46
1:A:138:PHE:CZ	1:A:140[B]:ILE:HG12	2.50	0.46
1:A:744:THR:HA	1:A:747:SER:OG	2.16	0.46
1:A:60:ASN:ND2	4:A:4146:HOH:O	2.49	0.45
1:A:625:HIS:HE1	1:A:704:GLU:OE1	2.00	0.45
1:A:538:HIS:O	1:A:568:VAL:HA	2.16	0.45
1:A:291:ALA:O	1:A:295:HIS:HE1	2.00	0.45
1:A:464:ASN:HD21	1:A:484:MET:H	1.63	0.44
1:A:366:ASP:HB3	4:A:4119:HOH:O	2.18	0.44
1:A:154:SER:HA	1:A:169:SER:O	2.18	0.44
1:A:214:TYR:CE2	1:A:541:GLY:HA3	2.52	0.44
1:A:141:LYS:HE3	1:A:150[B]:VAL:HG12	2.00	0.43
1:A:560:PHE:HD2	1:A:565:ILE:HD12	1.81	0.43
1:A:560:PHE:CD2	1:A:565:ILE:HD12	2.53	0.43
1:A:576:ALA:O	1:A:577:LEU:HB2	2.19	0.43
1:A:292:LEU:HD23	1:A:567:MET:HE1	2.01	0.42
1:A:367:PRO:HD3	1:A:443:ASP:O	2.19	0.42
1:A:317:ALA:CB	1:A:620:LEU:HD21	2.47	0.42
1:A:295:HIS:CD2	1:A:325:HIS:NE2	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655[B]:LEU:HD22	1:A:696:PRO:CG	2.50	0.42
1:A:96[B]:ARG:CZ	1:A:96[B]:ARG:HB2	2.48	0.42
1:A:150[B]:VAL:HG21	4:A:4204:HOH:O	2.19	0.41
1:A:371:ASN:HD22	1:A:402:ILE:HD12	1.83	0.41
1:A:631:TYR:HA	1:A:634:LEU:HG	2.01	0.41
1:A:793:GLN:O	1:A:794:ASN:HB2	2.20	0.41
1:A:171:ARG:HB3	4:A:4134:HOH:O	2.20	0.41
1:A:655[B]:LEU:HD22	1:A:696:PRO:HG2	2.02	0.41
1:A:135:ARG:NH1	1:A:135:ARG:HB3	2.34	0.41
1:A:141:LYS:HE3	1:A:150[A]:VAL:CG2	2.49	0.41
1:A:816:ILE:HB	1:A:853[B]:ILE:HG12	2.01	0.41
1:A:336:ASP:HB3	1:A:337:PHE:CD2	2.56	0.41
1:A:428:PHE:HB3	1:A:515:VAL:HG21	2.02	0.40
1:A:52:TYR:OH	1:A:82:VAL:O	2.34	0.40
1:A:755[B]:ILE:HD12	1:A:819:LEU:HD11	2.03	0.40
1:A:655[B]:LEU:HD12	1:A:668:VAL:CG1	2.44	0.40
1:A:416:THR:HB	1:A:490:TRP:CG	2.57	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	865/875 (99%)	824 (95%)	36 (4%)	5 (1%)	25 15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	832	ASN
1	A	51	SER
1	A	300	GLU

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Mol	Chain	Res	Type
1	A	405	VAL

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	A	768/767 (100%)	753 (98%)	15 (2%)	55 51

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	135	ARG
1	A	322	ASP
1	A	347	PHE
1	A	539	TRP
1	A	577	LEU
1	A	588[A]	MET
1	A	588[B]	MET
1	A	606	LYS
1	A	667	ASP
1	A	690	LYS
1	A	707	SER
1	A	803	SER
1	A	825	SER
1	A	848	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	62	ASN
1	A	84	ASN
1	A	98	HIS
1	A	107	ASN

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Mol	Chain	Res	Type
1	A	115	HIS
1	A	130	GLN
1	A	148	ASN
1	A	164	GLN
1	A	167	GLN
1	A	183	HIS
1	A	190	HIS
1	A	239	ASN
1	A	295	HIS
1	A	357	ASN
1	A	464	ASN
1	A	465	ASN
1	A	488	GLN
1	A	493	GLN
1	A	497	HIS
1	A	498	ASN
1	A	603	GLN
1	A	625	HIS
1	A	669	HIS
1	A	714	GLN
1	A	739	GLN
1	A	802	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 monosaccharides in this entry.

5.6 Ligand geometry

3 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	$\#\|Z\| > 2$
3	NAG	A	2001	1	14,14,15	0.69	0	17,19,21	1.65	4 (23%)
2	BJ1	A	1001	-	17,22,22	1.01	1 (5%)	20,32,32	1.44	5 (25%)
3	NAG	A	2002	1	14,14,15	0.41	0	17,19,21	1.42	1 (5%)

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
3	NAG	A	2001	1	-	5/6/23/26	0/1/1/1
2	BJ1	A	1001	-	-	2/20/37/37	0/1/1/1
3	NAG	A	2002	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	BJ1	OAN-SAV	-2.92	1.48	1.57

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2002	NAG	C1-O5-C5	4.63	118.47	112.19
2	A	1001	BJ1	CAL-CAP-CAR	-2.93	103.81	106.41
3	A	2001	NAG	C8-C7-N2	2.80	120.84	116.10
2	A	1001	BJ1	OAN-CAT-CAQ	2.70	111.19	106.43
3	A	2001	NAG	O7-C7-C8	-2.57	117.29	122.06
3	A	2001	NAG	O5-C1-C2	-2.39	107.51	111.29
2	A	1001	BJ1	OAN-CAT-CAO	2.38	110.64	106.43
3	A	2001	NAG	C1-O5-C5	2.17	115.13	112.19
2	A	1001	BJ1	CAP-CAR-CAS	-2.15	103.94	106.71
2	A	1001	BJ1	OAF-CAR-CAP	-2.11	106.95	112.04

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	BJ1	CAJ-CAO-CAT-OAN
3	A	2001	NAG	C8-C7-N2-C2
3	A	2001	NAG	O7-C7-N2-C2
3	A	2001	NAG	C3-C2-N2-C7
3	A	2001	NAG	C4-C5-C6-O6
3	A	2001	NAG	O5-C5-C6-O6
2	A	1001	BJ1	CAQ-CAM-SAU-CAL

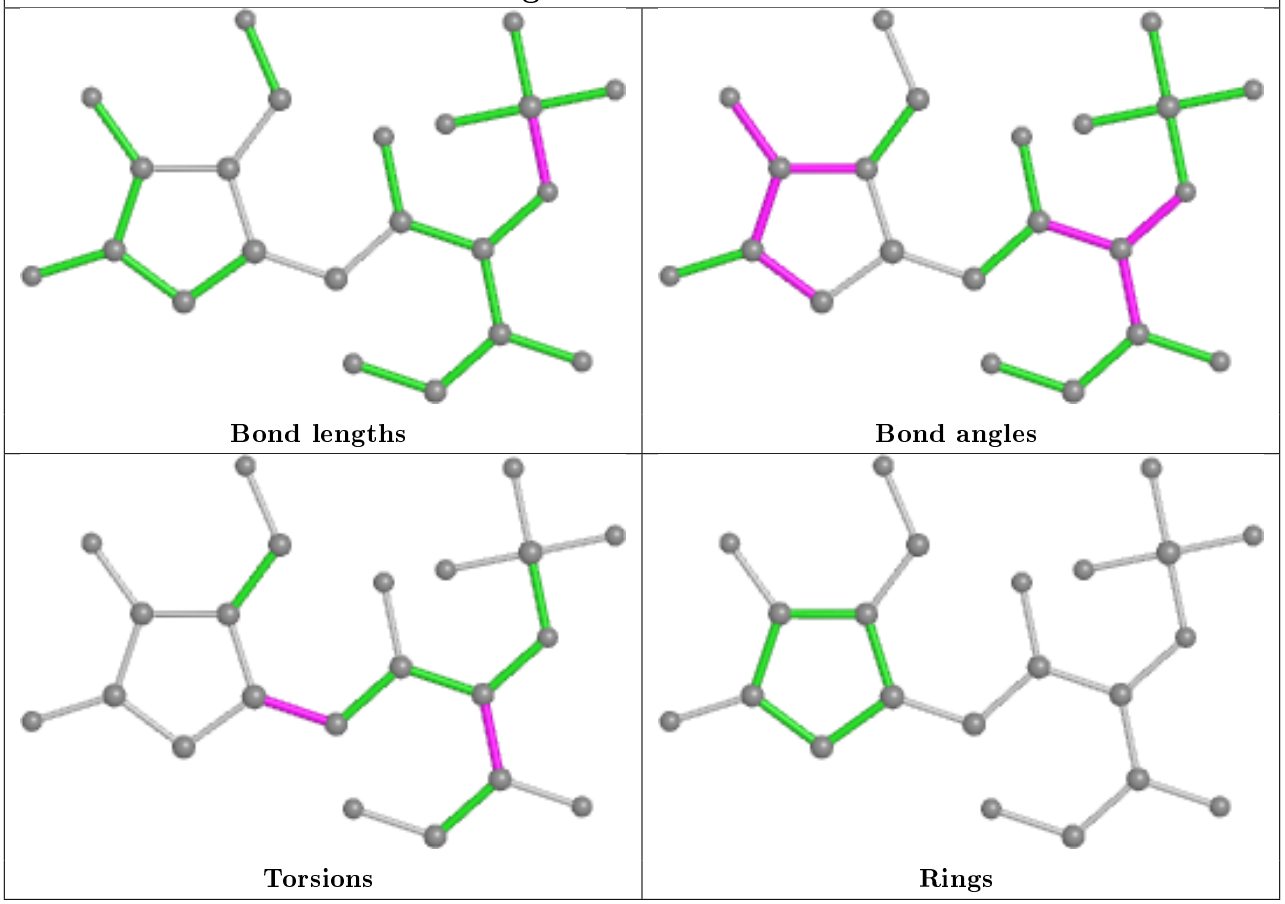
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand BJ1 A 1001



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	856/875 (97%)	1.14	179 (20%) 1 1	17, 27, 43, 55	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	72	LEU	7.6
1	A	39	VAL	7.3
1	A	50	HIS	7.1
1	A	38	ALA	7.0
1	A	838	THR	6.6
1	A	375	SER	6.2
1	A	80	SER	6.1
1	A	36	GLN	6.0
1	A	377	LYS	6.0
1	A	374	SER	5.9
1	A	49	ASN	5.9
1	A	376	SER	5.9
1	A	834	VAL	5.8
1	A	120	SER	5.8
1	A	118	SER	5.6
1	A	77	VAL	5.6
1	A	826	ASN	5.5
1	A	48	LYS	5.2
1	A	794	ASN	5.2
1	A	846	SER	5.1
1	A	710	ARG	5.0
1	A	616	ASP	5.0
1	A	117	GLN	4.9
1	A	853[A]	ILE	4.9
1	A	833	GLY	4.8
1	A	477	LEU	4.8
1	A	777	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	832	ASN	4.5
1	A	8	ASN	4.5
1	A	106	ASN	4.4
1	A	717	GLU	4.4
1	A	793	GLN	4.4
1	A	105	THR	4.3
1	A	655[A]	LEU	4.2
1	A	433	ASN	4.2
1	A	342	VAL	4.2
1	A	836	SER	4.1
1	A	140[A]	ILE	4.0
1	A	847	ASN	4.0
1	A	79	GLY	4.0
1	A	316	ALA	4.0
1	A	369	ILE	3.9
1	A	858	LEU	3.9
1	A	829	VAL	3.9
1	A	27	ASP	3.8
1	A	758	LEU	3.8
1	A	482	LEU	3.8
1	A	13	ILE	3.7
1	A	866	VAL	3.7
1	A	223	LEU	3.6
1	A	419	ASN	3.6
1	A	28	GLN	3.6
1	A	396	ASP	3.5
1	A	760	GLU	3.5
1	A	835	PRO	3.5
1	A	387	ASP	3.5
1	A	133[A]	ILE	3.5
1	A	550	LEU	3.5
1	A	54	VAL	3.4
1	A	24	ALA	3.4
1	A	256	ILE	3.4
1	A	69	LEU	3.4
1	A	356	ASN	3.3
1	A	278	LEU	3.3
1	A	328	ILE	3.3
1	A	319	LEU	3.3
1	A	172	LEU	3.2
1	A	870	HIS	3.2
1	A	692	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	801	SER	3.2
1	A	71	ASN	3.2
1	A	718[A]	MET	3.2
1	A	839	SER	3.2
1	A	761	ASN	3.1
1	A	412	PHE	3.1
1	A	418	PRO	3.1
1	A	810	ASN	3.1
1	A	518	ASN	3.1
1	A	791	VAL	3.0
1	A	756	ILE	3.0
1	A	792	THR	3.0
1	A	796	LEU	3.0
1	A	125	ALA	2.9
1	A	462	ASN	2.9
1	A	116	VAL	2.9
1	A	266	LEU	2.9
1	A	122	ASN	2.8
1	A	562	LEU	2.8
1	A	312	GLU	2.8
1	A	85	VAL	2.8
1	A	627[B]	LEU	2.8
1	A	461	ASN	2.8
1	A	825	SER	2.8
1	A	474	ASP	2.8
1	A	719	GLU	2.8
1	A	489	HIS	2.8
1	A	58	LEU	2.8
1	A	34	ASN	2.7
1	A	126	SER	2.7
1	A	81	ASN	2.7
1	A	799	ASN	2.7
1	A	516	PHE	2.7
1	A	868	TRP	2.7
1	A	47	SER	2.7
1	A	51	SER	2.7
1	A	663	ASN	2.7
1	A	209	ASN	2.7
1	A	816	ILE	2.6
1	A	428	PHE	2.6
1	A	398	VAL	2.6
1	A	156	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	380	GLY	2.6
1	A	781	ASN	2.6
1	A	161	PHE	2.6
1	A	378	PRO	2.6
1	A	818	ILE	2.6
1	A	61	THR	2.6
1	A	204	THR	2.6
1	A	540	LEU	2.6
1	A	191	ASP	2.6
1	A	87	LEU	2.6
1	A	221	LEU	2.6
1	A	343	ASP	2.6
1	A	245	LEU	2.5
1	A	19	GLN	2.5
1	A	292	LEU	2.5
1	A	82	VAL	2.5
1	A	273	VAL	2.5
1	A	411	VAL	2.5
1	A	354	LEU	2.5
1	A	96[A]	ARG	2.5
1	A	667	ASP	2.5
1	A	397	GLY	2.4
1	A	390	ILE	2.4
1	A	159	LEU	2.4
1	A	379	TYR	2.4
1	A	135	ARG	2.4
1	A	854	THR	2.4
1	A	679	LEU	2.4
1	A	55	GLU	2.4
1	A	633[A]	LEU	2.4
1	A	729[A]	LEU	2.4
1	A	83	ASP	2.3
1	A	333	GLU	2.3
1	A	199	ILE	2.3
1	A	184	VAL	2.3
1	A	392	VAL	2.3
1	A	617	SER	2.3
1	A	213	LEU	2.3
1	A	138	PHE	2.2
1	A	62	ASN	2.2
1	A	340	ASP	2.2
1	A	517	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	341	SER	2.2
1	A	251[A]	ILE	2.2
1	A	869	ALA	2.2
1	A	460	THR	2.2
1	A	831	HIS	2.2
1	A	769	PHE	2.2
1	A	142	VAL	2.2
1	A	423	TRP	2.1
1	A	321	TYR	2.1
1	A	466	PRO	2.1
1	A	499	LEU	2.1
1	A	107	ASN	2.1
1	A	494	TYR	2.1
1	A	638	TYR	2.1
1	A	391	TRP	2.1
1	A	200	PHE	2.1
1	A	151	LEU	2.1
1	A	803	SER	2.1
1	A	399	THR	2.1
1	A	274	VAL	2.1
1	A	345	LYS	2.1
1	A	395	SER	2.0
1	A	560	PHE	2.0
1	A	115	HIS	2.0
1	A	842	VAL	2.0
1	A	350	PHE	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 monosaccharides in this entry.

6.4 Ligands (i)

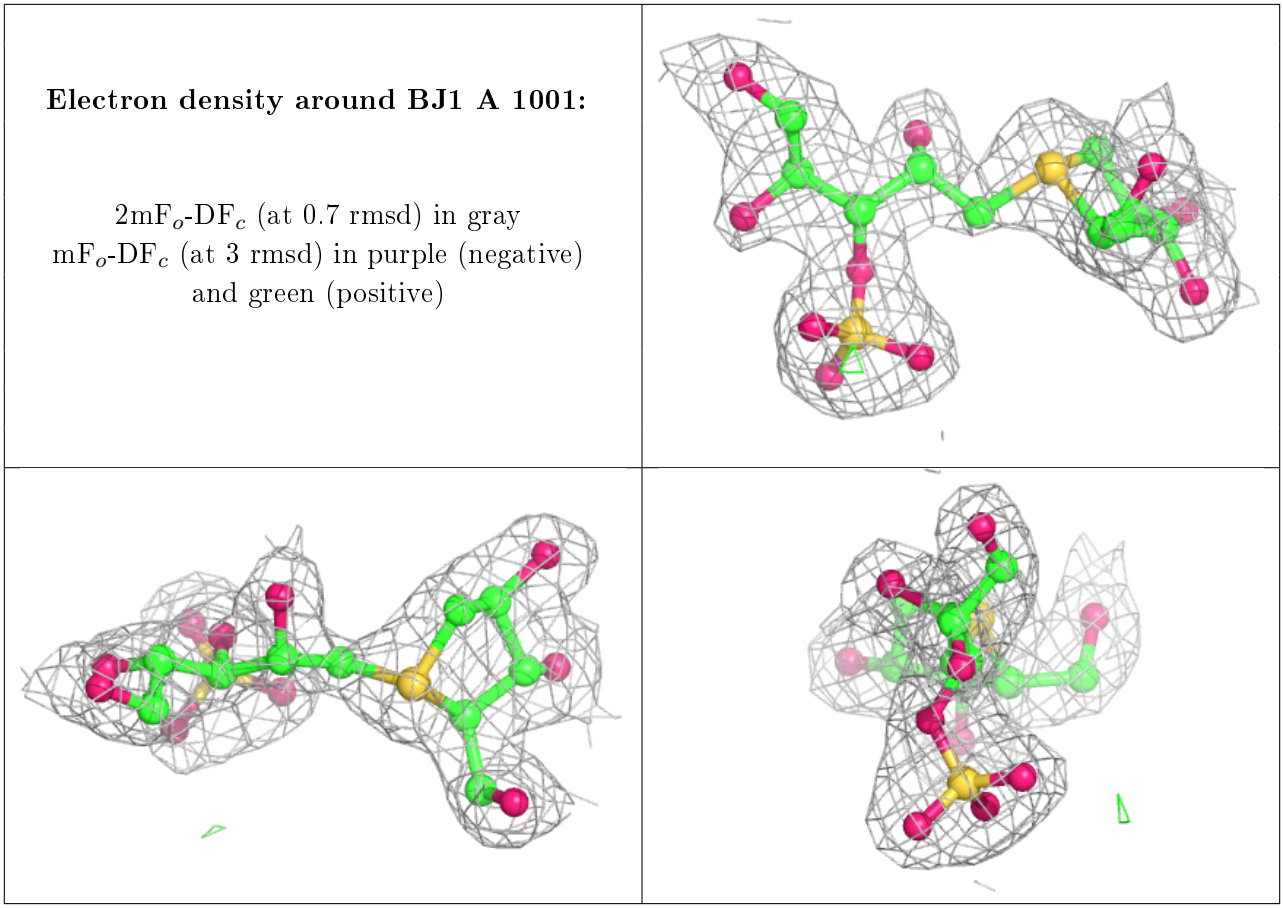
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	A	2001	14/15	0.77	0.22	34,37,41,44	0
3	NAG	A	2002	14/15	0.81	0.18	37,38,40,40	0
2	BJ1	A	1001	22/22	0.91	0.15	25,31,36,37	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BJ1 A 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.