Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 11:45 AM EDT

PDB ID	:	3CTT
Title	:	Crystal complex of N-terminal Human Maltase-Glucoamylase with Casuarine
Authors	:	Sim, L.; Rose, D.R.
Deposited on	:	2008-04-14
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

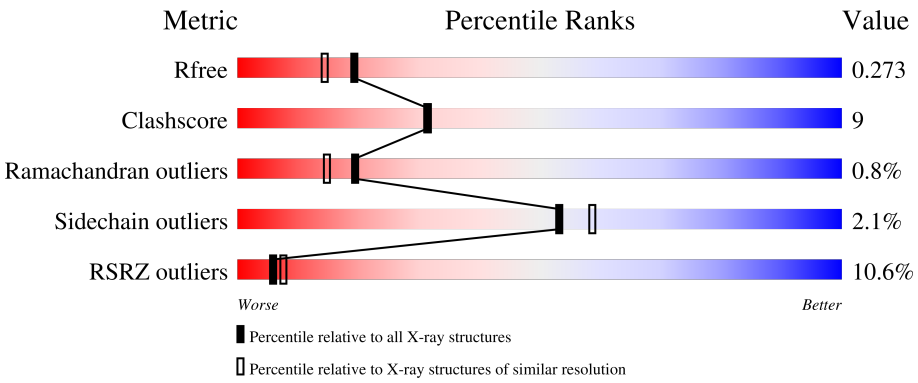
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.10 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))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 of 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	870	10% 81% 18% ••

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
5	GOL	A	3008	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7358 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.

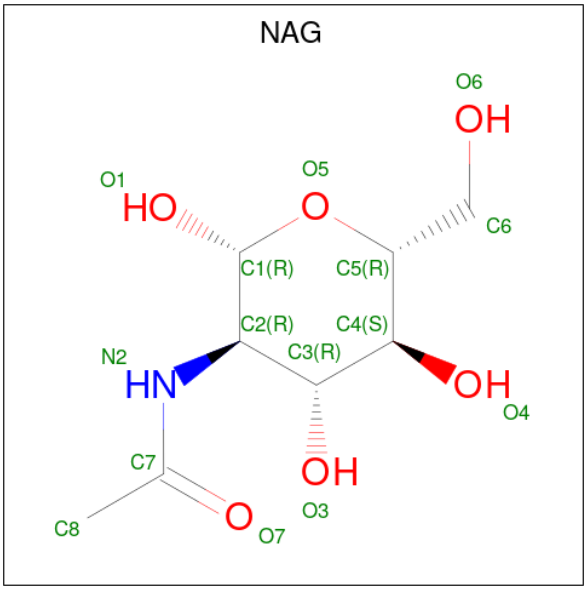
- Molecule 1 is a protein called Maltase-glucoamylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	862	6905	4403	1170	1306	26	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

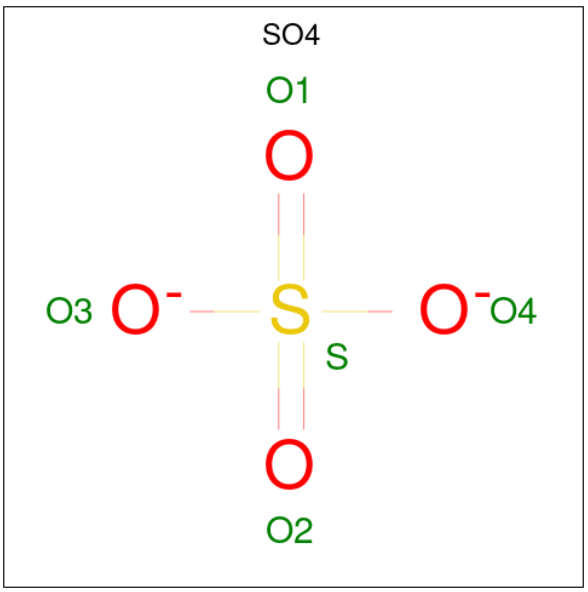
Chain	Residue	Modelled	Actual	Comment	Reference
A	869	ALA	-	expression tag	UNP O43451
A	870	HIS	-	expression tag	UNP O43451

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



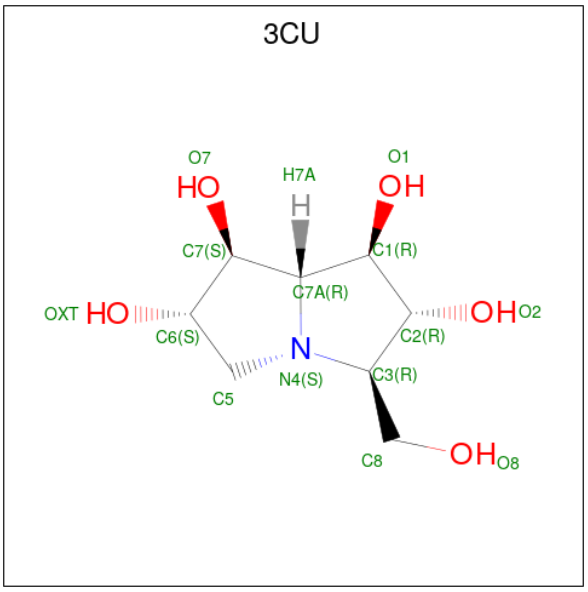
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



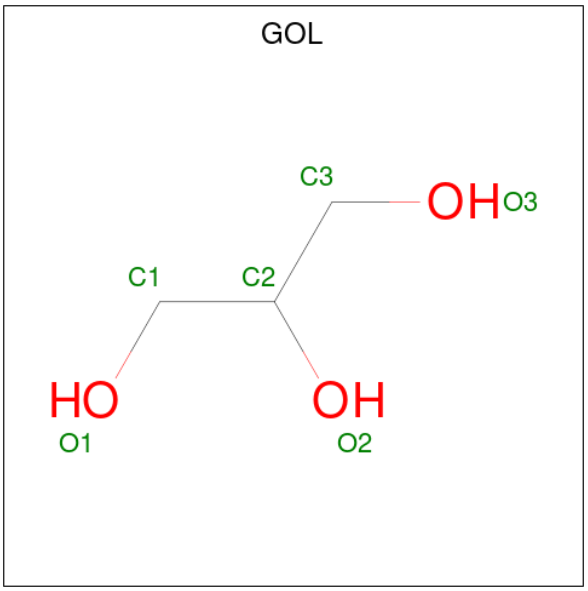
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is CASUARINE (three-letter code: 3CU) (formula: $C_8H_{15}NO_5$).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

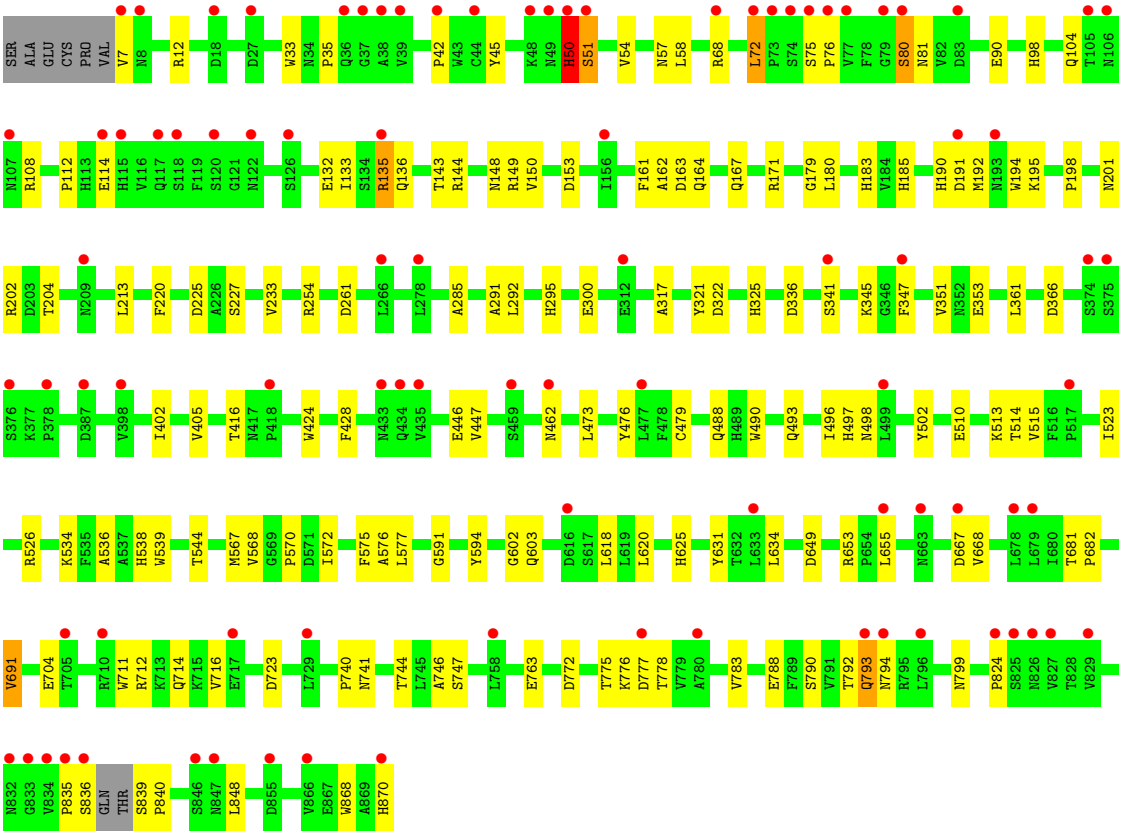
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	352	352	352	0	0

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

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	86.69Å 109.13Å 109.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.65 – 2.10 15.65 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.6 (15.65-2.10) 94.6 (15.65-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.58 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.225 , 0.278 0.216 , 0.273	Depositor DCC
R_{free} test set	2932 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	27.2	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.52 , 61.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7358	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, GOL, 3CU, SO4

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	0.67	0/7104	0.72	3/9690 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	50	HIS	N-CA-C	-5.51	96.11	111.00
1	A	653	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	72	LEU	CA-CB-CG	5.37	127.65	115.30

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	6905	0	6570	123	0
2	A	28	0	26	0	0
3	A	5	0	0	1	0
4	A	14	0	15	0	0
5	A	54	0	72	18	0
6	A	352	0	0	9	0
All	All	7358	0	6683	123	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 9.

All (123) 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:202:ARG:HG3	1:A:204:THR:HG23	1.16	1.14
1:A:667:ASP:HB2	6:A:4245:HOH:O	1.57	1.02
1:A:202:ARG:HG3	1:A:204:THR:CG2	1.93	0.97
1:A:171:ARG:HD2	5:A:3005:GOL:H12	1.46	0.96
1:A:98:HIS:HE1	1:A:261:ASP:OD1	1.53	0.92
1:A:202:ARG:CG	1:A:204:THR:HG23	2.03	0.89
1:A:300:GLU:HG3	1:A:603:GLN:HG3	1.60	0.82
1:A:135:ARG:HG2	1:A:135:ARG:HH11	1.45	0.81
1:A:776:LYS:O	1:A:777:ASP:HB2	1.83	0.78
1:A:202:ARG:CG	1:A:204:THR:CG2	2.61	0.78
1:A:740:PRO:HD2	5:A:3008:GOL:H12	1.65	0.78
1:A:183:HIS:HD2	1:A:185:HIS:NE2	1.84	0.76
1:A:201:ASN:H	1:A:498:ASN:HD21	1.35	0.75
1:A:201:ASN:O	1:A:497:HIS:HE1	1.70	0.74
1:A:58:LEU:HD23	5:A:3004:GOL:H11	1.69	0.73
1:A:681:THR:HG22	1:A:691:VAL:HG11	1.72	0.72
1:A:625:HIS:HE1	1:A:704:GLU:OE2	1.72	0.71
1:A:179:GLY:O	1:A:190:HIS:HE1	1.73	0.70
1:A:201:ASN:H	1:A:498:ASN:ND2	1.89	0.69
1:A:544:THR:CG2	1:A:577:LEU:HD22	2.23	0.68
1:A:712:ARG:H	1:A:714:GLN:HE21	1.43	0.67
1:A:57:ASN:HA	1:A:135:ARG:NH2	2.10	0.67
1:A:135:ARG:HB3	1:A:136:GLN:HE21	1.60	0.67
1:A:576:ALA:O	1:A:577:LEU:HB2	1.95	0.66
1:A:295:HIS:HD2	1:A:325:HIS:NE2	1.95	0.65
1:A:201:ASN:O	1:A:497:HIS:CE1	2.51	0.64
1:A:171:ARG:HD2	5:A:3005:GOL:C1	2.23	0.64
1:A:183:HIS:CD2	1:A:185:HIS:NE2	2.64	0.64
1:A:513:LYS:HE2	6:A:4163:HOH:O	1.98	0.64
1:A:778:THR:HG22	5:A:3007:GOL:H11	1.80	0.64
1:A:763:GLU:OE2	1:A:792:THR:HG23	1.98	0.63
1:A:135:ARG:HH11	1:A:135:ARG:CG	2.11	0.62
1:A:183:HIS:HE1	1:A:198:PRO:O	1.83	0.62
1:A:523:ILE:H	5:A:3002:GOL:H31	1.66	0.61
1:A:631:TYR:HA	1:A:634:LEU:HG	1.82	0.61
1:A:54:VAL:HG11	1:A:135:ARG:NH1	2.17	0.60
1:A:98:HIS:CE1	1:A:261:ASP:OD1	2.45	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:GLU:N	1:A:447:VAL:HA	2.17	0.59
1:A:57:ASN:HA	1:A:135:ARG:HH22	1.67	0.59
1:A:772:ASP:OD2	1:A:775:THR:OG1	2.15	0.58
1:A:536:ALA:HA	5:A:3002:GOL:H32	1.87	0.57
1:A:835:PRO:HA	1:A:836:SER:HB2	1.87	0.56
1:A:740:PRO:CD	5:A:3008:GOL:H12	2.36	0.56
1:A:291:ALA:O	1:A:295:HIS:HE1	1.89	0.56
1:A:58:LEU:CD2	5:A:3004:GOL:H11	2.35	0.56
1:A:204:THR:OG1	1:A:213:LEU:HD23	2.07	0.55
1:A:353:GLU:CD	5:A:3006:GOL:H2	2.25	0.55
1:A:402:ILE:HD11	6:A:4123:HOH:O	2.06	0.55
1:A:132:GLU:HG3	5:A:3009:GOL:H2	1.88	0.55
1:A:204:THR:CG2	1:A:473:LEU:HD23	2.38	0.54
1:A:353:GLU:HB3	5:A:3006:GOL:O2	2.07	0.54
1:A:488:GLN:HB2	1:A:496:ILE:HD11	1.90	0.54
1:A:493:GLN:NE2	1:A:497:HIS:HD2	2.05	0.54
1:A:90:GLU:OE1	1:A:98:HIS:HD2	1.92	0.52
1:A:682:PRO:O	1:A:691:VAL:HG21	2.09	0.52
1:A:295:HIS:CD2	1:A:325:HIS:NE2	2.78	0.52
1:A:351:VAL:HG22	1:A:361:LEU:HD22	1.91	0.52
1:A:317:ALA:HB1	1:A:620:LEU:HD21	1.91	0.51
1:A:618:LEU:HD11	1:A:723:ASP:HB3	1.93	0.51
1:A:591:GLY:HA2	1:A:594:TYR:CD2	2.46	0.51
1:A:741:ASN:HD22	1:A:746:ALA:HB1	1.75	0.51
1:A:691:VAL:HG23	6:A:4106:HOH:O	2.11	0.51
1:A:12:ARG:HD3	1:A:45:TYR:CD2	2.46	0.50
1:A:711:TRP:CG	1:A:716:VAL:HG11	2.47	0.50
1:A:794:ASN:ND2	1:A:870:HIS:CD2	2.80	0.50
1:A:740:PRO:O	5:A:3008:GOL:H32	2.11	0.50
1:A:655:LEU:HD22	1:A:668:VAL:HG11	1.93	0.50
1:A:424:TRP:CE2	1:A:428:PHE:HE2	2.30	0.49
1:A:133:ILE:H	5:A:3004:GOL:C3	2.26	0.49
1:A:149:ARG:NH2	1:A:225:ASP:OD2	2.46	0.49
1:A:741:ASN:ND2	1:A:746:ALA:HB1	2.27	0.49
1:A:794:ASN:HB3	1:A:868:TRP:O	2.12	0.48
1:A:132:GLU:HA	5:A:3009:GOL:H31	1.95	0.48
1:A:204:THR:HG22	1:A:473:LEU:HD23	1.94	0.48
1:A:81:ASN:HA	1:A:162:ALA:HA	1.94	0.48
1:A:794:ASN:HD21	1:A:870:HIS:HD2	1.62	0.48
1:A:135:ARG:CG	1:A:135:ARG:NH1	2.75	0.47
1:A:783:VAL:HG11	5:A:3007:GOL:H2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:GLN:NE2	1:A:462:ASN:HD22	2.12	0.47
1:A:167:GLN:NE2	1:A:254:ARG:HE	2.12	0.46
1:A:572:ILE:HD13	1:A:591:GLY:HA3	1.97	0.46
1:A:68:ARG:HE	1:A:104:GLN:HE22	1.64	0.46
1:A:7:VAL:HG23	6:A:4143:HOH:O	2.15	0.46
1:A:68:ARG:HG2	1:A:104:GLN:NE2	2.31	0.46
1:A:135:ARG:HB3	1:A:136:GLN:HG2	1.98	0.46
1:A:225:ASP:OD1	1:A:227:SER:OG	2.24	0.46
1:A:799:ASN:HB2	6:A:4269:HOH:O	2.16	0.45
1:A:625:HIS:HD2	3:A:4001:SO4:O3	1.99	0.45
1:A:570:PRO:HD2	1:A:594:TYR:CD2	2.52	0.45
1:A:544:THR:HG23	1:A:577:LEU:HD22	1.99	0.45
1:A:625:HIS:CE1	1:A:704:GLU:OE2	2.61	0.45
1:A:794:ASN:ND2	1:A:870:HIS:HD2	2.15	0.45
1:A:416:THR:HB	1:A:490:TRP:CG	2.52	0.44
1:A:143:THR:HG22	1:A:150:VAL:HA	1.99	0.44
1:A:164:GLN:HE22	1:A:462:ASN:HB2	1.82	0.44
1:A:285:ALA:HB2	1:A:534:LYS:O	2.18	0.44
1:A:336:ASP:OD2	1:A:366:ASP:O	2.36	0.43
1:A:114:GLU:HB3	1:A:502:TYR:OH	2.19	0.43
1:A:220:PHE:CE2	1:A:233:VAL:HB	2.54	0.43
1:A:33:TRP:CE2	1:A:35:PRO:HG3	2.54	0.43
1:A:341:SER:O	1:A:345:LYS:HB2	2.18	0.43
1:A:75:SER:HA	1:A:76:PRO:HD3	1.86	0.43
1:A:202:ARG:HG2	1:A:204:THR:CG2	2.48	0.42
1:A:514:THR:HG22	6:A:4272:HOH:O	2.18	0.42
1:A:183:HIS:HB2	1:A:185:HIS:CD2	2.54	0.42
1:A:515:VAL:HG22	6:A:4272:HOH:O	2.19	0.42
1:A:292:LEU:HD23	1:A:567:MET:CE	2.49	0.42
1:A:108:ARG:HH12	1:A:163:ASP:HA	1.83	0.42
1:A:192:MET:HB2	6:A:4187:HOH:O	2.18	0.42
1:A:740:PRO:HG2	5:A:3008:GOL:H12	2.02	0.42
1:A:538:HIS:O	1:A:568:VAL:HA	2.19	0.42
1:A:476:TYR:HB2	1:A:479:CYS:SG	2.60	0.42
1:A:510:GLU:O	1:A:513:LYS:HB2	2.20	0.41
1:A:42:PRO:HD3	1:A:194:TRP:CZ3	2.55	0.41
1:A:144:ARG:O	1:A:148:ASN:HA	2.21	0.41
1:A:744:THR:HA	1:A:747:SER:OG	2.21	0.41
1:A:153:ASP:OD2	5:A:3005:GOL:O3	2.25	0.41
1:A:526:ARG:O	1:A:538:HIS:CE1	2.74	0.40
1:A:50:HIS:CD2	1:A:51:SER:N	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:GLN:HE21	1:A:497:HIS:HD2	1.69	0.40
1:A:575:PHE:CE1	1:A:602:GLY:HA2	2.56	0.40
1:A:112:PRO:HG2	1:A:490:TRP:CE3	2.56	0.40
1:A:839:SER:HA	1:A:840:PRO:HD2	1.96	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	858/870 (99%)	810 (94%)	41 (5%)	7 (1%)	19 15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	SER
1	A	793	GLN
1	A	50	HIS
1	A	191	ASP
1	A	180	LEU
1	A	80	SER
1	A	405	VAL

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	755/762 (99%)	739 (98%)	16 (2%)	53 59

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	80	SER
1	A	135	ARG
1	A	161	PHE
1	A	195	LYS
1	A	321	TYR
1	A	322	ASP
1	A	347	PHE
1	A	539	TRP
1	A	649	ASP
1	A	691	VAL
1	A	788	GLU
1	A	790	SER
1	A	793	GLN
1	A	824	PRO
1	A	848	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	50	HIS
1	A	53	HIS
1	A	62	ASN
1	A	98	HIS
1	A	104	GLN
1	A	107	ASN
1	A	136	GLN
1	A	148	ASN
1	A	164	GLN
1	A	167	GLN
1	A	183	HIS
1	A	190	HIS
1	A	193	ASN
1	A	239	ASN
1	A	295	HIS
1	A	464	ASN

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Mol	Chain	Res	Type
1	A	493	GLN
1	A	497	HIS
1	A	498	ASN
1	A	625	HIS
1	A	628	ASN
1	A	669	HIS
1	A	714	GLN
1	A	739	GLN
1	A	793	GLN
1	A	794	ASN
1	A	802	GLN
1	A	810	ASN
1	A	870	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

13 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	$\#\|Z\| > 2$
5	GOL	A	3005	-	5,5,5	0.37	0	5,5,5	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	A	3007	-	5,5,5	0.47	0	5,5,5	0.49	0
2	NAG	A	2001	1	14,14,15	0.63	0	17,19,21	1.37	1 (5%)
5	GOL	A	3008	-	5,5,5	0.52	0	5,5,5	0.52	0
5	GOL	A	3002	-	5,5,5	0.50	0	5,5,5	0.49	0
2	NAG	A	2002	1	14,14,15	0.61	0	17,19,21	1.50	2 (11%)
5	GOL	A	3001	-	5,5,5	0.51	0	5,5,5	0.59	0
3	SO4	A	4001	-	4,4,4	0.17	0	6,6,6	0.34	0
5	GOL	A	3006	-	5,5,5	0.33	0	5,5,5	0.32	0
4	3CU	A	1001	-	15,15,15	0.83	0	18,23,23	1.53	4 (22%)
5	GOL	A	3004	-	5,5,5	0.34	0	5,5,5	0.68	0
5	GOL	A	3009	-	5,5,5	0.44	0	5,5,5	0.74	0
5	GOL	A	3003	-	5,5,5	0.39	0	5,5,5	0.40	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
5	GOL	A	3005	-	-	1/4/4/4	-
5	GOL	A	3007	-	-	2/4/4/4	-
2	NAG	A	2001	1	-	0/6/23/26	0/1/1/1
5	GOL	A	3008	-	-	0/4/4/4	-
5	GOL	A	3002	-	-	2/4/4/4	-
2	NAG	A	2002	1	-	0/6/23/26	0/1/1/1
5	GOL	A	3001	-	-	0/4/4/4	-
5	GOL	A	3006	-	-	1/4/4/4	-
4	3CU	A	1001	-	-	0/2/34/34	0/2/2/2
5	GOL	A	3004	-	-	2/4/4/4	-
5	GOL	A	3009	-	-	1/4/4/4	-
5	GOL	A	3003	-	-	0/4/4/4	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2002	NAG	C1-O5-C5	4.09	117.73	112.19
2	A	2002	NAG	O5-C1-C2	-3.47	105.81	111.29
2	A	2001	NAG	C1-O5-C5	3.38	116.77	112.19
4	A	1001	3CU	C2-C1-C7A	-3.16	98.59	102.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1001	3CU	C1-C2-C3	-2.71	98.09	102.45
4	A	1001	3CU	C2-C3-N4	-2.37	100.96	104.58
4	A	1001	3CU	C5-N4-C7A	2.16	109.41	105.59

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	3007	GOL	C1-C2-C3-O3
5	A	3002	GOL	C1-C2-C3-O3
5	A	3004	GOL	C1-C2-C3-O3
5	A	3009	GOL	O1-C1-C2-C3
5	A	3007	GOL	O2-C2-C3-O3
5	A	3002	GOL	O2-C2-C3-O3
5	A	3004	GOL	O2-C2-C3-O3
5	A	3006	GOL	O2-C2-C3-O3
5	A	3005	GOL	C1-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3005	GOL	3	0
5	A	3007	GOL	2	0
5	A	3008	GOL	4	0
5	A	3002	GOL	2	0
3	A	4001	SO4	1	0
5	A	3006	GOL	2	0
5	A	3004	GOL	3	0
5	A	3009	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 (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	862/870 (99%)	0.58	91 (10%) 6 7	11, 21, 35, 57	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	GLN	8.0
1	A	73	PRO	7.0
1	A	50	HIS	6.6
1	A	375	SER	6.4
1	A	105	THR	6.2
1	A	38	ALA	5.8
1	A	118	SER	5.7
1	A	826	ASN	5.5
1	A	120	SER	5.4
1	A	835	PRO	5.1
1	A	793	GLN	5.1
1	A	191	ASP	5.0
1	A	836	SER	5.0
1	A	710	ARG	4.9
1	A	106	ASN	4.7
1	A	825	SER	4.7
1	A	418	PRO	4.3
1	A	374	SER	4.3
1	A	80	SER	4.2
1	A	37	GLY	4.1
1	A	48	LYS	4.1
1	A	72	LEU	4.1
1	A	847	ASN	4.0
1	A	347	PHE	3.9
1	A	8	ASN	3.8
1	A	517	PRO	3.6
1	A	499	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	79	GLY	3.5
1	A	49	ASN	3.5
1	A	7	VAL	3.4
1	A	209	ASN	3.3
1	A	777	ASP	3.3
1	A	117	GLN	3.2
1	A	376	SER	3.2
1	A	832	ASN	3.2
1	A	387	ASP	3.2
1	A	193	ASN	3.1
1	A	126	SER	3.0
1	A	135	ARG	3.0
1	A	824	PRO	3.0
1	A	114	GLU	2.9
1	A	44	CYS	2.9
1	A	667	ASP	2.9
1	A	77	VAL	2.8
1	A	433	ASN	2.8
1	A	74	SER	2.8
1	A	115	HIS	2.7
1	A	68	ARG	2.7
1	A	107	ASN	2.7
1	A	122	ASN	2.7
1	A	833	GLY	2.7
1	A	796	LEU	2.7
1	A	27	ASP	2.7
1	A	266	LEU	2.6
1	A	398	VAL	2.5
1	A	794	ASN	2.5
1	A	278	LEU	2.5
1	A	717	GLU	2.5
1	A	341	SER	2.5
1	A	870	HIS	2.5
1	A	477	LEU	2.5
1	A	76	PRO	2.5
1	A	462	ASN	2.5
1	A	39	VAL	2.4
1	A	633	LEU	2.4
1	A	616	ASP	2.4
1	A	51	SER	2.4
1	A	312	GLU	2.3
1	A	705	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	729	LEU	2.2
1	A	42	PRO	2.2
1	A	18	ASP	2.2
1	A	156	ILE	2.2
1	A	435	VAL	2.2
1	A	829	VAL	2.2
1	A	834	VAL	2.2
1	A	866	VAL	2.2
1	A	75	SER	2.2
1	A	846	SER	2.1
1	A	378	PRO	2.1
1	A	758	LEU	2.1
1	A	83	ASP	2.1
1	A	679	LEU	2.1
1	A	663	ASN	2.1
1	A	678	LEU	2.0
1	A	855	ASP	2.0
1	A	655	LEU	2.0
1	A	434	GLN	2.0
1	A	459	SER	2.0
1	A	780	ALA	2.0
1	A	827	VAL	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, 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
5	GOL	A	3006	6/6	0.41	0.28	66,67,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	A	2001	14/15	0.68	0.38	35,39,41,43	0
5	GOL	A	3009	6/6	0.77	0.26	40,42,42,43	0
5	GOL	A	3007	6/6	0.79	0.20	41,44,44,46	0
5	GOL	A	3008	6/6	0.83	0.17	39,42,43,43	0
5	GOL	A	3002	6/6	0.84	0.15	26,31,32,36	0
2	NAG	A	2002	14/15	0.85	0.15	26,28,33,36	0
5	GOL	A	3004	6/6	0.88	0.11	33,36,38,40	0
5	GOL	A	3001	6/6	0.90	0.14	24,28,29,30	0
5	GOL	A	3005	6/6	0.92	0.24	27,38,42,42	0
5	GOL	A	3003	6/6	0.94	0.09	31,32,32,34	0
4	3CU	A	1001	14/14	0.95	0.09	15,17,19,19	0
3	SO4	A	4001	5/5	0.96	0.17	36,36,37,39	0

6.5 Other polymers (i)

There are no such residues in this entry.