



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:11 PM EDT

PDB ID : 6NPS / pdb_00006nps
Title : Crystal structure of GH115 enzyme AxyAgu115A from *Amphibacillus xylanus*
Authors : Stogios, P.J.; Skarina, T.; Di Leo, R.; Yan, R.; Master, E.; Savchenko, A.
Deposited on : 2019-01-18
Resolution : 1.99 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

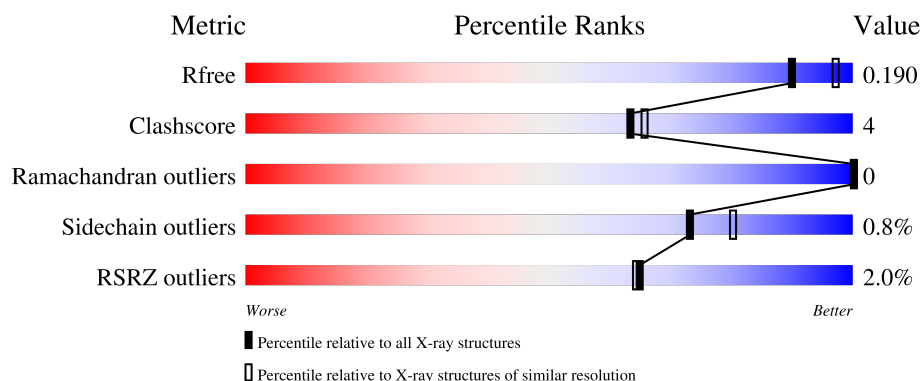
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

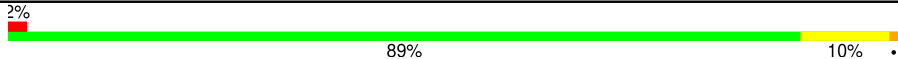
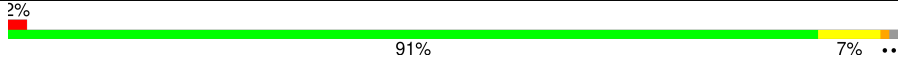
The reported resolution of this entry is 1.99 Å.

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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	968	
1	B	968	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17523 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 AxyAgu115A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	968	Total	C	N	O	S	0	4	0
			7797	4987	1295	1489	26			
1	B	958	Total	C	N	O	S	0	5	0
			7725	4945	1279	1475	26			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLN	-	expression tag	UNP K0J4X5
A	0	GLY	-	expression tag	UNP K0J4X5
A	79	ALA	LYS	engineered mutation	UNP K0J4X5
A	80	ALA	LYS	engineered mutation	UNP K0J4X5
A	81	ALA	GLU	engineered mutation	UNP K0J4X5
B	-1	GLN	-	expression tag	UNP K0J4X5
B	0	GLY	-	expression tag	UNP K0J4X5
B	79	ALA	LYS	engineered mutation	UNP K0J4X5
B	80	ALA	LYS	engineered mutation	UNP K0J4X5
B	81	ALA	GLU	engineered mutation	UNP K0J4X5

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	2	Total	Cl	0	0
			2	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	1
			12	6	6		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

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

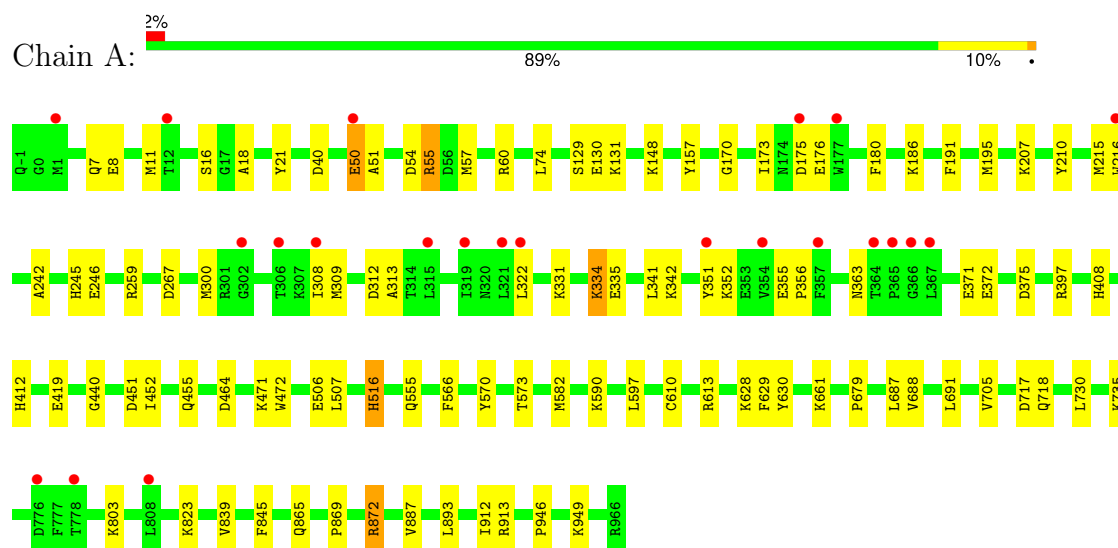
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	861	Total	O	0	15
			876	876		
4	B	976	Total	O	0	26
			1002	1002		

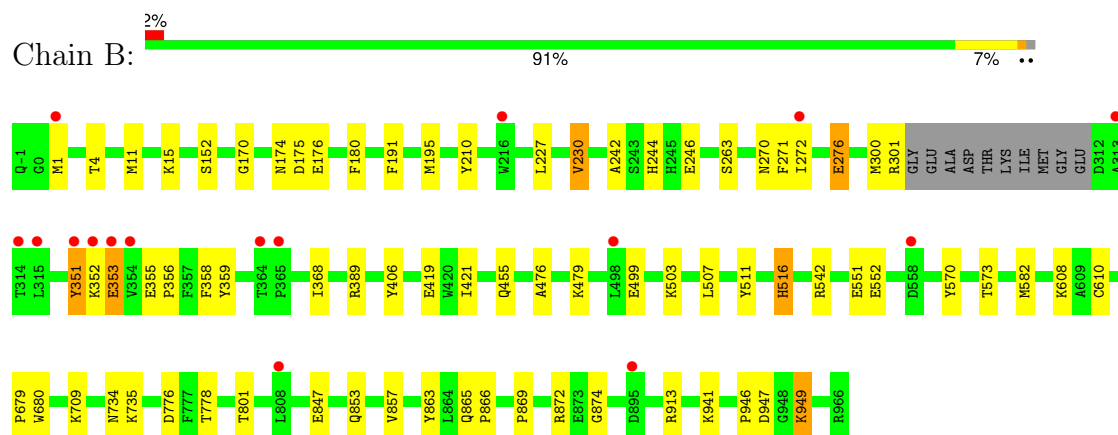
3 Residue-property plots [i](#)

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: AxyAgu115A



• Molecule 1: AxyAgu115A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.08Å 96.21Å 111.75Å 84.37° 78.37° 83.32°	Depositor
Resolution (Å)	47.64 – 1.99 47.64 – 1.99	Depositor EDS
% Data completeness (in resolution range)	94.6 (47.64-1.99) 94.6 (47.64-1.99)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.147 , 0.190 0.149 , 0.190	Depositor DCC
R_{free} test set	8161 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17523	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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: CL, 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	0.53	1/8005 (0.0%)	0.67	2/10870 (0.0%)
1	B	0.59	3/7935 (0.0%)	0.70	2/10778 (0.0%)
All	All	0.56	4/15940 (0.0%)	0.69	4/21648 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	516	HIS	C-O	-6.67	1.15	1.24
1	B	853[A]	GLN	CA-C	6.16	1.61	1.52
1	B	853[B]	GLN	CA-C	6.16	1.61	1.52
1	B	516	HIS	C-O	-5.56	1.16	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	ASN	N-CA-C	8.79	120.63	111.14
1	B	853[A]	GLN	CA-C-O	7.55	128.66	119.97
1	B	853[B]	GLN	CA-C-O	7.55	128.66	119.97
1	A	555	GLN	CA-CB-CG	-5.09	103.92	114.10

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	7797	0	7540	69	0
1	B	7725	0	7465	51	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	66	0	86	9	0
3	B	54	0	71	4	0
4	A	876	0	0	14	0
4	B	1002	0	0	8	0
All	All	17523	0	15162	122	0

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

All (122) 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:B:351:TYR:O	1:B:355:GLU:HG3	1.64	0.97
1:B:276:GLU:HA	1:B:276:GLU:OE2	1.93	0.67
1:A:351:TYR:CE2	1:A:352:LYS:HD2	2.30	0.66
1:A:191:PHE:HA	1:A:195:MET:HE3	1.78	0.66
1:A:372:GLU:HG2	4:A:1663:HOH:O	1.98	0.64
1:B:406:TYR:OH	3:B:1010:GOL:H32	1.98	0.64
1:A:839:VAL:HG11	1:A:887:VAL:HG11	1.80	0.63
1:A:661:LYS:NZ	4:A:1111:HOH:O	2.31	0.62
1:B:358:PHE:CZ	1:B:368:ILE:HD13	2.35	0.62
1:B:244:HIS:CD2	1:B:301:ARG:HD2	2.34	0.61
1:A:148:LYS:NZ	4:A:1118:HOH:O	2.33	0.60
1:A:570:TYR:OH	1:A:613[A]:ARG:NH2	2.34	0.60
1:B:542:ARG:NH1	4:B:1111:HOH:O	2.35	0.60
1:A:148:LYS:HE3	4:A:1729:HOH:O	2.02	0.60
1:A:455:GLN:NE2	4:A:1113:HOH:O	2.31	0.59
1:A:180:PHE:HB2	1:A:451:ASP:OD2	2.04	0.58
1:A:175:ASP:HB3	1:A:419:GLU:OE1	2.04	0.57
1:A:16:SER:CB	1:A:60:ARG:HE	2.18	0.57
1:A:7:GLN:HB3	1:A:11:MET:HE2	1.87	0.57
1:B:776:ASP:HB2	1:B:778:THR:HG23	1.85	0.56
1:B:865:GLN:HG2	1:B:866:PRO:HD2	1.85	0.56
1:A:215:MET:HG3	4:A:1184:HOH:O	2.05	0.56
1:B:352:LYS:HD2	1:B:389:ARG:NH2	2.20	0.56
1:A:215:MET:HE1	1:A:245:HIS:NE2	2.20	0.55
1:B:709:LYS:HG2	4:B:1825:HOH:O	2.05	0.55
1:B:191:PHE:HA	1:B:195:MET:HE3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LYS:NZ	3:A:1005:GOL:H31	2.23	0.54
1:A:54:ASP:HB3	1:A:57:MET:HG3	1.90	0.54
1:A:176:GLU:HB2	1:A:180:PHE:HB3	1.89	0.54
3:A:1008[B]:GOL:H31	4:A:1103:HOH:O	2.08	0.53
1:A:50:GLU:OE2	1:A:51:ALA:N	2.40	0.53
1:B:359:TYR:CE2	1:B:872:ARG:HD3	2.44	0.53
1:A:18:ALA:HB1	1:A:50:GLU:O	2.09	0.52
1:A:334:LYS:HD2	1:A:341:LEU:HD22	1.92	0.52
1:A:130:GLU:HB2	4:A:1632[B]:HOH:O	2.09	0.51
1:B:270:ASN:OD1	1:B:272:ILE:HG22	2.11	0.51
1:A:471:LYS:HD2	1:A:472:TRP:NE1	2.26	0.50
1:A:21:TYR:CE1	1:A:55:ARG:HG3	2.46	0.50
1:A:408:HIS:NE2	3:A:1008[B]:GOL:O3	2.34	0.50
1:B:542:ARG:NH2	4:B:1128:HOH:O	2.45	0.50
1:B:170:GLY:HA3	1:B:210:TYR:O	2.11	0.49
1:A:170:GLY:HA3	1:A:210:TYR:O	2.12	0.49
1:A:408:HIS:NE2	3:A:1008[A]:GOL:O3	2.29	0.48
1:B:271:PHE:HB2	1:B:300:MET:SD	2.53	0.48
1:B:1:MET:HA	1:B:1:MET:HE2	1.96	0.48
1:B:176:GLU:HB2	1:B:180:PHE:HB3	1.95	0.48
1:A:946:PRO:HG2	1:A:949:LYS:HG3	1.95	0.48
1:A:803:LYS:HE3	1:A:845:PHE:CZ	2.49	0.48
1:B:913:ARG:NH2	4:B:1104:HOH:O	2.28	0.48
1:A:207:LYS:HZ1	3:A:1005:GOL:H31	1.79	0.48
1:A:259:ARG:NE	1:A:267:ASP:OD2	2.38	0.48
1:A:309:MET:HB3	1:A:313:ALA:HB2	1.96	0.48
1:B:679:PRO:HB2	3:B:1006:GOL:H11	1.95	0.48
1:A:50:GLU:OE2	1:A:50:GLU:HA	2.14	0.48
1:A:173:ILE:HG12	1:A:452:ILE:HD11	1.96	0.47
1:A:397:ARG:HD2	4:A:1302:HOH:O	2.14	0.47
1:A:8:GLU:HA	1:A:11:MET:HE3	1.97	0.47
3:A:1008[A]:GOL:H31	4:A:1103:HOH:O	2.13	0.47
1:A:679:PRO:HB2	3:A:1004:GOL:H31	1.96	0.47
1:A:74:LEU:HD23	1:A:74:LEU:HA	1.78	0.47
1:A:40:ASP:OD2	1:A:129:SER:OG	2.30	0.46
1:A:590:LYS:HE3	4:A:1876:HOH:O	2.15	0.46
1:A:717:ASP:OD1	1:A:718:GLN:HG2	2.15	0.46
1:B:503:LYS:NZ	1:B:552:GLU:OE2	2.34	0.46
1:A:331:LYS:HE2	1:A:335:GLU:OE2	2.15	0.46
1:A:730:LEU:HD23	1:A:735:LYS:HG2	1.97	0.46
1:B:608:LYS:NZ	4:B:1140:HOH:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:SER:HB2	3:B:1009:GOL:H11	1.96	0.46
1:B:863:TYR:HB2	1:B:941:LYS:HB3	1.98	0.46
1:B:801:THR:HG22	1:B:847:GLU:HB3	1.97	0.46
1:B:175:ASP:HB3	1:B:419:GLU:OE1	2.16	0.45
1:B:499:GLU:HG2	4:B:1302:HOH:O	2.16	0.45
1:B:244:HIS:NE2	1:B:301:ARG:NH1	2.65	0.45
1:B:734:ASN:OD1	1:B:735:LYS:HG3	2.17	0.45
1:B:455:GLN:NE2	4:B:1132:HOH:O	2.47	0.45
1:B:242:ALA:HB1	1:B:246:GLU:HB2	1.98	0.45
1:A:371:GLU:H	1:A:371:GLU:CD	2.25	0.45
1:A:242:ALA:HB1	1:A:246:GLU:HB2	1.98	0.44
1:A:872[B]:ARG:HG2	4:A:1608:HOH:O	2.17	0.44
1:B:351:TYR:O	1:B:355:GLU:CG	2.50	0.44
1:B:11:MET:O	1:B:15:LYS:HG2	2.18	0.44
1:A:16:SER:HB2	1:A:60:ARG:HE	1.80	0.44
1:A:300:MET:HE2	1:A:308:ILE:HD11	2.00	0.44
1:A:131:LYS:HE3	1:A:157:TYR:OH	2.18	0.44
1:A:464:ASP:OD1	3:A:1005:GOL:H11	2.18	0.44
1:A:566:PHE:HA	1:A:570:TYR:HB3	2.00	0.44
1:A:440:GLY:HA2	3:A:1003:GOL:H12	1.99	0.43
1:A:688:VAL:HB	1:A:691:LEU:HD12	1.99	0.43
1:A:186:LYS:HD2	1:A:630:TYR:CG	2.54	0.43
1:B:421:ILE:HD13	1:B:421:ILE:HG21	1.81	0.43
1:B:680:TRP:CZ2	3:B:1006:GOL:H12	2.54	0.43
1:B:946:PRO:HD2	1:B:949:LYS:HE2	2.00	0.43
1:A:16:SER:HB3	1:A:60:ARG:HE	1.84	0.42
1:A:355:GLU:HB3	1:A:356:PRO:HD3	1.99	0.42
1:B:227:LEU:O	1:B:230[A]:VAL:HG13	2.19	0.42
1:B:244:HIS:NE2	1:B:301:ARG:CZ	2.83	0.42
1:B:353:GLU:O	1:B:356:PRO:HD2	2.19	0.42
1:A:582:MET:HB2	1:A:610:CYS:HB3	2.02	0.42
1:A:597:LEU:HD23	1:A:705:VAL:HG12	2.02	0.42
1:A:687:LEU:C	1:A:687:LEU:HD23	2.45	0.42
1:B:476:ALA:HB1	1:B:479:LYS:HG3	2.01	0.42
1:B:507:LEU:HD22	1:B:573:THR:HG21	2.02	0.42
1:A:506:GLU:OE2	4:A:1102:HOH:O	2.22	0.42
1:A:342:LYS:HG2	1:A:375:ASP:OD1	2.19	0.42
1:A:628:LYS:HD3	1:A:629:PHE:CZ	2.55	0.42
1:B:174:ASN:CG	1:B:175:ASP:H	2.28	0.42
1:A:913:ARG:NH1	4:A:1101:HOH:O	2.22	0.41
1:A:507:LEU:HD22	1:A:573:THR:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:823:LYS:HD2	1:A:912:ILE:HB	2.02	0.41
1:B:869:PRO:HG2	1:B:874:GLY:HA2	2.01	0.41
1:B:353:GLU:H	1:B:353:GLU:HG2	1.49	0.41
1:B:551:GLU:OE1	1:B:570:TYR:OH	2.21	0.41
1:B:175:ASP:HB2	4:B:1447:HOH:O	2.20	0.41
1:A:216:TRP:HH2	1:A:412:HIS:CD2	2.38	0.41
1:A:869:PRO:HG3	1:A:893:LEU:HD11	2.03	0.41
1:B:4:THR:HG22	1:B:152:SER:OG	2.21	0.41
1:B:582:MET:HB2	1:B:610:CYS:HB3	2.02	0.41
1:A:322:LEU:HD23	1:A:322:LEU:HA	1.82	0.40
1:B:776:ASP:CB	1:B:778:THR:HG23	2.51	0.40
1:A:312:ASP:OD2	1:A:312:ASP:N	2.54	0.40
1:B:776:ASP:OD1	1:B:776:ASP:N	2.55	0.40
1:B:857:VAL:HG12	1:B:947:ASP:HB2	2.03	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	970/968 (100%)	940 (97%)	30 (3%)	0	100	100
1	B	959/968 (99%)	931 (97%)	28 (3%)	0	100	100
All	All	1929/1936 (100%)	1871 (97%)	58 (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	840/836 (100%)	833 (99%)	7 (1%)	73	80
1	B	834/836 (100%)	826 (99%)	8 (1%)	68	75
All	All	1674/1672 (100%)	1659 (99%)	15 (1%)	73	78

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

Mol	Chain	Res	Type
1	A	50	GLU
1	A	55	ARG
1	A	334	LYS
1	A	516	HIS
1	A	865	GLN
1	A	872[A]	ARG
1	A	872[B]	ARG
1	B	230[A]	VAL
1	B	230[B]	VAL
1	B	276	GLU
1	B	351	TYR
1	B	353	GLU
1	B	511	TYR
1	B	516	HIS
1	B	949	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	HIS
1	A	586	ASN
1	A	838	GLN
1	B	187	ASN
1	B	318	ASN
1	B	490	GLN
1	B	491	GLN
1	B	586	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 3 are monoatomic - leaving 20 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	$\# Z > 2$
3	GOL	B	1008	-	5,5,5	1.12	0	5,5,5	0.95	0
3	GOL	B	1004	-	5,5,5	1.41	1 (20%)	5,5,5	0.77	0
3	GOL	A	1009	-	5,5,5	1.02	0	5,5,5	0.99	0
3	GOL	B	1009	-	5,5,5	1.58	1 (20%)	5,5,5	0.89	0
3	GOL	A	1005	-	5,5,5	1.06	0	5,5,5	1.08	0
3	GOL	A	1011	-	5,5,5	1.10	0	5,5,5	0.83	0
3	GOL	B	1006	-	5,5,5	0.96	0	5,5,5	1.00	0
3	GOL	A	1010	-	5,5,5	1.18	1 (20%)	5,5,5	0.97	0
3	GOL	A	1004	-	5,5,5	1.14	0	5,5,5	0.87	0
3	GOL	A	1006	-	5,5,5	1.01	0	5,5,5	1.08	0
3	GOL	B	1007	-	5,5,5	1.02	0	5,5,5	1.04	0
3	GOL	B	1003	-	5,5,5	1.26	1 (20%)	5,5,5	0.97	0
3	GOL	A	1007	-	5,5,5	1.16	0	5,5,5	0.88	0
3	GOL	A	1002	-	5,5,5	1.06	0	5,5,5	0.96	0
3	GOL	B	1010	-	5,5,5	1.40	1 (20%)	5,5,5	0.93	0
3	GOL	A	1008[A]	-	5,5,5	1.23	0	5,5,5	1.17	0
3	GOL	B	1011	-	5,5,5	1.13	1 (20%)	5,5,5	0.98	0
3	GOL	A	1003	-	5,5,5	0.96	0	5,5,5	1.30	1 (20%)
3	GOL	B	1005	-	5,5,5	0.98	0	5,5,5	0.98	0
3	GOL	A	1008[B]	-	5,5,5	1.28	0	5,5,5	1.12	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
3	GOL	B	1008	-	-	4/4/4/4	-
3	GOL	B	1004	-	-	0/4/4/4	-
3	GOL	A	1009	-	-	3/4/4/4	-
3	GOL	B	1009	-	-	2/4/4/4	-
3	GOL	A	1005	-	-	0/4/4/4	-
3	GOL	A	1011	-	-	0/4/4/4	-
3	GOL	B	1006	-	-	2/4/4/4	-
3	GOL	A	1010	-	-	4/4/4/4	-
3	GOL	A	1004	-	-	0/4/4/4	-
3	GOL	A	1006	-	-	2/4/4/4	-
3	GOL	B	1007	-	-	0/4/4/4	-
3	GOL	B	1003	-	-	2/4/4/4	-
3	GOL	A	1007	-	-	2/4/4/4	-
3	GOL	A	1002	-	-	2/4/4/4	-
3	GOL	B	1010	-	-	4/4/4/4	-
3	GOL	A	1008[A]	-	-	2/4/4/4	-
3	GOL	B	1011	-	-	2/4/4/4	-
3	GOL	A	1003	-	-	2/4/4/4	-
3	GOL	B	1005	-	-	0/4/4/4	-
3	GOL	A	1008[B]	-	-	2/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1009	GOL	C1-C2	2.99	1.63	1.51
3	B	1010	GOL	C1-C2	2.49	1.61	1.51
3	B	1004	GOL	O2-C2	-2.37	1.36	1.43
3	B	1011	GOL	C1-C2	2.06	1.59	1.51
3	B	1003	GOL	C3-C2	2.06	1.59	1.51
3	A	1010	GOL	C3-C2	2.01	1.59	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	GOL	C3-C2-C1	-2.18	103.79	111.80

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003	GOL	O1-C1-C2-C3
3	A	1006	GOL	O1-C1-C2-C3
3	A	1008[A]	GOL	O1-C1-C2-C3
3	A	1008[B]	GOL	O1-C1-C2-C3
3	A	1009	GOL	O1-C1-C2-O2
3	A	1009	GOL	O1-C1-C2-C3
3	B	1003	GOL	O1-C1-C2-O2
3	B	1003	GOL	O1-C1-C2-C3
3	B	1006	GOL	C1-C2-C3-O3
3	B	1009	GOL	O1-C1-C2-C3
3	B	1010	GOL	O1-C1-C2-C3
3	A	1003	GOL	O1-C1-C2-O2
3	B	1008	GOL	O2-C2-C3-O3
3	B	1009	GOL	O1-C1-C2-O2
3	B	1010	GOL	O1-C1-C2-O2
3	A	1002	GOL	O1-C1-C2-C3
3	A	1007	GOL	O1-C1-C2-C3
3	A	1010	GOL	O1-C1-C2-C3
3	A	1010	GOL	C1-C2-C3-O3
3	B	1008	GOL	O1-C1-C2-C3
3	B	1008	GOL	C1-C2-C3-O3
3	B	1010	GOL	C1-C2-C3-O3
3	B	1011	GOL	C1-C2-C3-O3
3	A	1006	GOL	O1-C1-C2-O2
3	A	1008[B]	GOL	O1-C1-C2-O2
3	B	1010	GOL	O2-C2-C3-O3
3	A	1002	GOL	O1-C1-C2-O2
3	A	1007	GOL	O1-C1-C2-O2
3	A	1008[A]	GOL	O1-C1-C2-O2
3	A	1010	GOL	O1-C1-C2-O2
3	A	1010	GOL	O2-C2-C3-O3
3	B	1006	GOL	O2-C2-C3-O3
3	A	1009	GOL	O2-C2-C3-O3
3	B	1011	GOL	O2-C2-C3-O3
3	B	1008	GOL	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1009	GOL	1	0
3	A	1005	GOL	3	0
3	B	1006	GOL	2	0
3	A	1004	GOL	1	0
3	B	1010	GOL	1	0
3	A	1008[A]	GOL	2	0
3	A	1003	GOL	1	0
3	A	1008[B]	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	968/968 (100%)	0.01	23 (2%) 59 59	22, 44, 78, 151	4 (0%)
1	B	958/968 (98%)	-0.15	16 (1%) 69 68	21, 39, 68, 145	5 (0%)
All	All	1926/1936 (99%)	-0.07	39 (2%) 65 64	21, 41, 73, 151	9 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	351	TYR	5.4
1	A	216	TRP	4.9
1	A	367	LEU	4.3
1	B	216	TRP	3.7
1	A	351	TYR	3.4
1	B	364	THR	3.3
1	A	366	GLY	3.3
1	A	321	LEU	3.2
1	B	808	LEU	3.2
1	A	354	VAL	3.1
1	B	365	PRO	3.1
1	A	365	PRO	3.1
1	A	177	TRP	3.0
1	A	322	LEU	2.9
1	A	175	ASP	2.9
1	A	776	ASP	2.8
1	B	315	LEU	2.7
1	B	272	ILE	2.7
1	A	50	GLU	2.7
1	B	313	ALA	2.6
1	A	308	ILE	2.6
1	A	778	THR	2.6
1	B	353	GLU	2.5
1	A	302	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	354	VAL	2.5
1	A	12	THR	2.5
1	A	364	THR	2.5
1	A	306	THR	2.5
1	A	357	PHE	2.4
1	B	314	THR	2.4
1	A	1	MET	2.4
1	A	319	ILE	2.4
1	B	498	LEU	2.2
1	B	1	MET	2.2
1	A	808	LEU	2.1
1	B	558	ASP	2.1
1	A	315	LEU	2.1
1	B	352	LYS	2.0
1	B	895	ASP	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 oligosaccharides 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
3	GOL	A	1006	6/6	0.65	0.15	102,107,108,110	0
3	GOL	A	1008[A]	6/6	0.67	0.25	61,66,68,68	6
3	GOL	A	1008[B]	6/6	0.67	0.25	60,65,68,69	6
3	GOL	B	1008	6/6	0.72	0.21	104,107,110,111	0
3	GOL	A	1002	6/6	0.75	0.09	90,97,98,99	0
3	GOL	B	1011	6/6	0.75	0.18	63,78,81,82	0
3	GOL	A	1003	6/6	0.78	0.14	80,82,93,97	0
3	GOL	A	1007	6/6	0.80	0.22	116,122,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	1007	6/6	0.81	0.12	92,96,96,97	0
3	GOL	A	1011	6/6	0.81	0.17	75,85,87,90	0
3	GOL	B	1010	6/6	0.81	0.21	39,79,82,82	0
3	GOL	B	1004	6/6	0.81	0.16	77,79,82,82	0
3	GOL	B	1009	6/6	0.83	0.21	68,79,82,84	0
3	GOL	A	1005	6/6	0.84	0.15	103,108,111,112	0
3	GOL	A	1004	6/6	0.84	0.11	74,83,84,86	0
3	GOL	A	1010	6/6	0.85	0.14	48,76,79,82	0
3	GOL	B	1005	6/6	0.86	0.10	82,93,94,100	0
3	GOL	A	1009	6/6	0.87	0.15	91,94,95,96	0
3	GOL	B	1006	6/6	0.88	0.11	73,85,89,90	0
3	GOL	B	1003	6/6	0.88	0.12	43,74,77,77	0
2	CL	B	1001	1/1	0.90	0.14	80,80,80,80	0
2	CL	B	1002	1/1	0.99	0.06	41,41,41,41	0
2	CL	A	1001	1/1	1.00	0.05	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.