



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:14 PM UTC

PDB ID : 4BMA / pdb_00004bma
Title : structural of Aspergillus fumigatus UDP-N-acetylglucosamine pyrophosphorylase
Authors : Fang, W.; Raimi, O.G.; HurtadoGuerrero, R.; vanAalten, D.M.F.
Deposited on : 2013-05-07
Resolution : 2.08 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

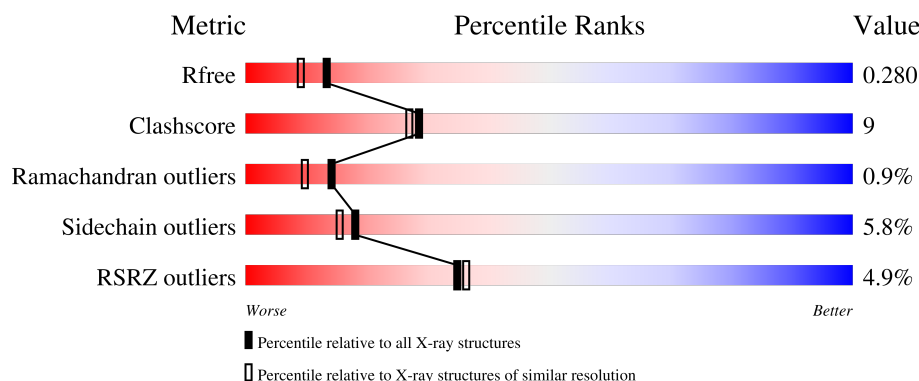
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	509	5% 76% 13% .. 9%
1	B	509	4% 68% 17% . 12%

2 Entry composition [i](#)

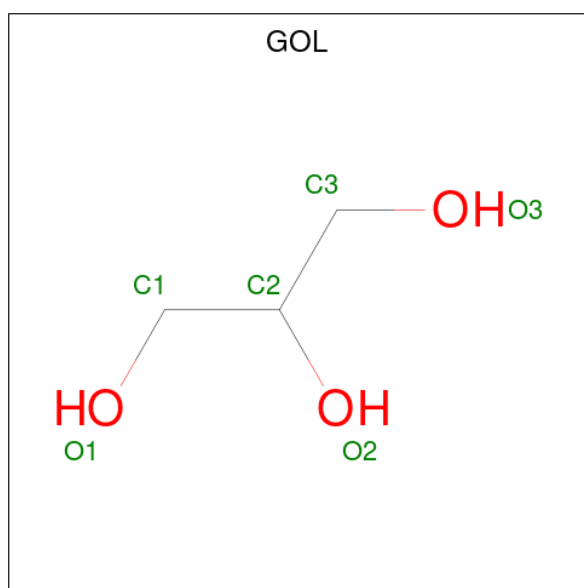
There are 3 unique types of molecules in this entry. The entry contains 7503 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UDP-N-ACETYLGLUCOSAMINE PYROPHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	1	0
			3651	2331	624	683	13			
1	B	447	Total	C	N	O	S	0	1	0
			3522	2251	603	653	15			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	155	Total	O	0	0
			155	155		

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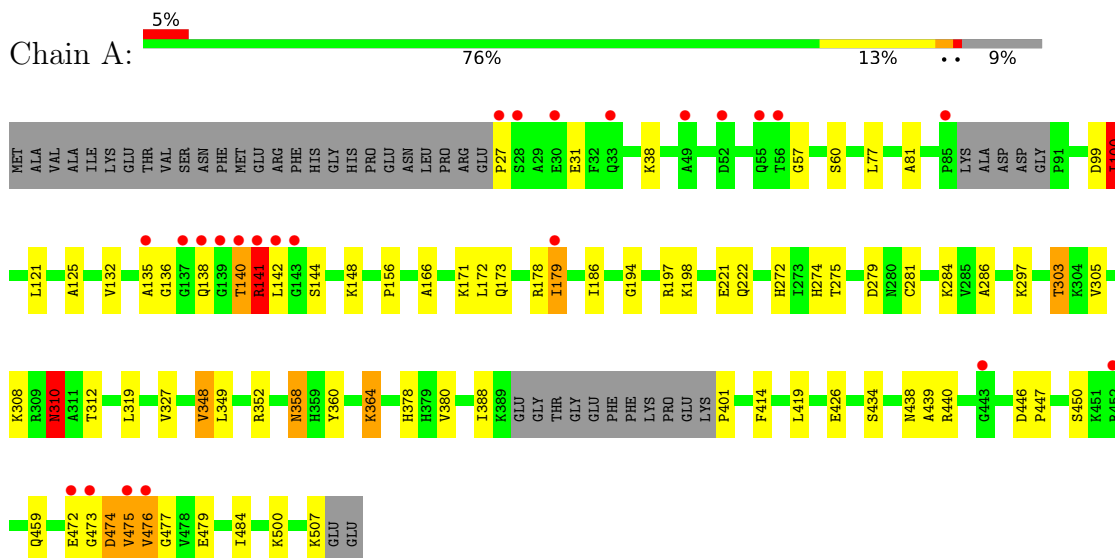
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	169	Total 169	O 169	0	0

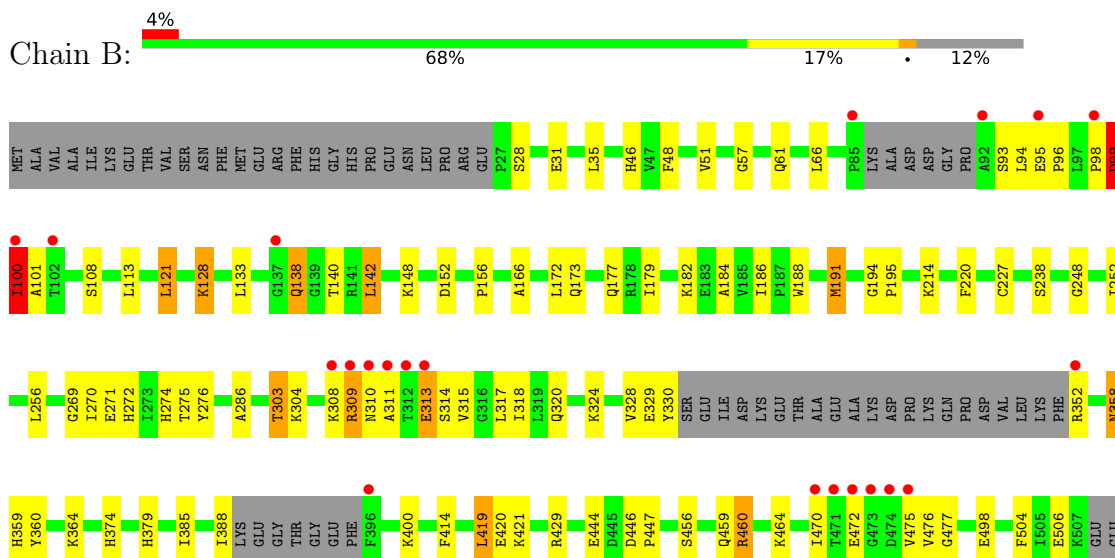
3 Residue-property plots

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: UDP-N-ACETYLGLUCOSAMINE PYROPHOSPHORYLASE



• Molecule 1: UDP-N-ACETYLGLUCOSAMINE PYROPHOSPHORYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.65Å 139.74Å 144.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.08 40.00 – 2.08	Depositor EDS
% Data completeness (in resolution range)	98.6 (40.00-2.08) 98.8 (40.00-2.08)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.212 , 0.265 (Not available) , 0.280	Depositor DCC
R_{free} test set	3453 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.560	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7503	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.16	1/3729 (0.0%)	1.16	10/5030 (0.2%)
1	B	1.27	10/3600 (0.3%)	1.22	8/4855 (0.2%)
All	All	1.22	11/7329 (0.2%)	1.19	18/9885 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	248	GLY	N-CA	6.50	1.52	1.45
1	B	270	ILE	N-CA	6.07	1.53	1.46
1	B	275	THR	N-CA	5.93	1.53	1.46
1	B	46	HIS	ND1-CE1	5.85	1.38	1.32
1	B	379	HIS	CG-CD2	5.60	1.42	1.35
1	B	379	HIS	CA-C	-5.47	1.46	1.52
1	B	304	LYS	N-CA	5.35	1.52	1.45
1	B	191	MET	N-CA	-5.13	1.39	1.46
1	B	379	HIS	CE1-NE2	5.12	1.37	1.32
1	B	374	HIS	CG-CD2	5.08	1.41	1.35
1	A	310	ASN	CA-C	5.02	1.58	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	ASP	N-CA-C	8.34	122.74	112.23
1	B	414	PHE	CA-C-N	-7.45	112.18	120.45
1	B	414	PHE	C-N-CA	-7.45	112.18	120.45
1	B	460	ARG	NE-CZ-NH1	-7.17	114.33	121.50
1	B	128	LYS	CD-CE-NZ	-7.04	89.38	111.90
1	A	135	ALA	N-CA-C	-6.47	102.60	110.88
1	A	414	PHE	CA-C-N	-6.20	113.24	120.12
1	A	414	PHE	C-N-CA	-6.20	113.24	120.12
1	B	179	ILE	CB-CA-C	-5.90	104.26	111.87
1	B	460	ARG	NE-CZ-NH2	5.77	124.39	119.20
1	A	125	ALA	N-CA-C	-5.69	105.60	112.54
1	A	60	SER	N-CA-C	5.59	117.05	111.07
1	A	166	ALA	N-CA-C	-5.51	105.35	111.36
1	A	327	VAL	N-CA-C	-5.33	100.64	108.11
1	A	100	ILE	CB-CG1-CD1	-5.20	102.89	113.80
1	B	269	GLY	N-CA-C	-5.19	107.09	115.08
1	A	303	THR	N-CA-CB	-5.12	102.00	111.53
1	A	57	GLY	N-CA-C	-5.05	106.67	112.73

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	99	ASP	Peptide

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	3651	0	3666	51	0
1	B	3522	0	3533	76	0
2	A	6	0	8	2	0
3	A	155	0	0	8	0
3	B	169	0	0	2	0
All	All	7503	0	7207	127	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 (127) 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:308:LYS:HA	1:B:309:ARG:CB	1.73	1.17
1:B:108:SER:HB2	3:B:2029:HOH:O	0.99	1.16
1:B:313:GLU:HG2	1:B:330:TYR:HB2	1.27	1.14
1:B:313:GLU:HB3	1:B:314:SER:HA	1.33	1.07
1:A:222:GLN:OE1	2:A:1508:GOL:H32	1.53	1.06
1:B:308:LYS:CA	1:B:309:ARG:HB3	1.85	1.05
1:A:274:HIS:HD2	1:A:286:ALA:H	1.06	1.02
1:B:310:ASN:HB2	1:B:311:ALA:HB3	1.41	0.99
1:B:308:LYS:HA	1:B:309:ARG:HB3	1.00	0.97
1:B:274:HIS:HD2	1:B:286:ALA:H	1.15	0.93
1:A:274:HIS:CD2	1:A:286:ALA:H	1.88	0.91
1:A:173:GLN:HE21	1:A:186:ILE:H	1.20	0.90
1:B:274:HIS:CD2	1:B:286:ALA:H	1.91	0.88
1:B:310:ASN:H	1:B:311:ALA:C	1.82	0.86
1:A:378:HIS:HD2	3:A:2123:HOH:O	1.58	0.85
1:B:313:GLU:CB	1:B:314:SER:HA	2.07	0.85
1:A:140:THR:HA	1:A:144:SER:O	1.77	0.85
1:B:313:GLU:HG2	1:B:330:TYR:CB	2.06	0.85
1:B:177:GLN:HE21	1:B:184:ALA:H	1.24	0.83
1:B:313:GLU:HB3	1:B:314:SER:CA	2.08	0.83
1:A:197:ARG:HH11	1:A:221:GLU:HG3	1.43	0.82
1:A:484:ILE:HD11	1:A:507:LYS:HA	1.64	0.79
1:A:310:ASN:HD22	1:A:312:THR:H	1.31	0.76
1:B:173:GLN:HE21	1:B:186:ILE:H	1.36	0.72
1:B:272:HIS:HD2	1:B:360:TYR:OH	1.72	0.71
1:A:173:GLN:NE2	1:A:186:ILE:H	1.90	0.70
1:B:310:ASN:N	1:B:311:ALA:C	2.51	0.69
1:B:98:PRO:C	1:B:100:ILE:HB	2.19	0.68
1:B:98:PRO:HB2	1:B:100:ILE:HB	1.75	0.68
1:B:456:SER:OG	1:B:460:ARG:NH1	2.27	0.67
1:A:27:PRO:HA	1:A:31:GLU:OE2	1.94	0.67
1:A:136:GLY:N	2:A:1508:GOL:O1	2.26	0.67
1:B:309:ARG:HA	1:B:310:ASN:ND2	2.11	0.66
1:A:274:HIS:HE1	1:A:358:ASN:HD21	1.43	0.64
1:B:274:HIS:HE1	1:B:358:ASN:ND2	1.96	0.64
1:A:100:ILE:O	1:A:297:LYS:HE2	1.97	0.63
1:A:148:LYS:HD3	1:A:279:ASP:HB3	1.80	0.63
1:B:98:PRO:O	1:B:101:ALA:N	2.28	0.62
1:A:284:LYS:HG2	3:A:2150:HOH:O	1.99	0.62
1:B:308:LYS:HG2	1:B:309:ARG:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:ASN:CB	1:B:311:ALA:HB3	2.24	0.61
1:B:308:LYS:CA	1:B:309:ARG:CB	2.56	0.60
1:A:459:GLN:HE21	1:A:477:GLY:HA2	1.67	0.60
1:A:310:ASN:ND2	1:A:312:THR:H	1.99	0.60
1:B:98:PRO:HB2	1:B:100:ILE:CB	2.32	0.60
1:B:303:THR:OG1	1:B:359:HIS:HD2	1.84	0.60
1:B:320:GLN:HE21	1:B:419:LEU:HD21	1.68	0.58
1:B:191:MET:HB2	1:B:220:PHE:CZ	2.39	0.58
1:A:171:LYS:NZ	3:A:2061:HOH:O	2.37	0.57
1:A:272:HIS:HD2	1:A:360:TYR:OH	1.88	0.57
1:A:274:HIS:HD2	1:A:286:ALA:N	1.89	0.56
1:A:274:HIS:HE1	1:A:358:ASN:ND2	2.04	0.56
1:A:364:LYS:HG3	3:A:2121:HOH:O	2.05	0.56
1:B:113:LEU:HD21	3:B:2029:HOH:O	2.04	0.56
1:B:309:ARG:HG2	1:B:315:VAL:HG21	1.87	0.56
1:A:77:LEU:HD22	1:A:378:HIS:CD2	2.41	0.55
1:B:313:GLU:CG	1:B:330:TYR:CB	2.82	0.55
1:A:99:ASP:O	3:A:2023:HOH:O	2.18	0.54
1:B:99:ASP:N	1:B:100:ILE:HB	2.22	0.54
1:B:309:ARG:HB2	1:B:429:ARG:NH2	2.23	0.54
1:B:470:ILE:HD11	1:B:498:GLU:HG2	1.89	0.54
1:B:274:HIS:HE1	1:B:358:ASN:HD21	1.52	0.54
1:B:313:GLU:CG	1:B:330:TYR:HB2	2.19	0.54
1:A:274:HIS:CD2	1:A:286:ALA:N	2.68	0.54
1:A:378:HIS:CD2	3:A:2123:HOH:O	2.43	0.54
1:B:173:GLN:NE2	1:B:186:ILE:H	2.05	0.54
1:B:310:ASN:H	1:B:311:ALA:CA	2.21	0.53
1:B:48:PHE:HD1	1:B:51:VAL:HG21	1.74	0.53
1:A:446:ASP:HB2	1:A:447:PRO:CD	2.39	0.53
1:B:177:GLN:HG2	1:B:182:LYS:O	2.10	0.52
1:A:438:ASN:O	1:A:447:PRO:HD3	2.10	0.51
1:B:328:VAL:HG23	1:B:328:VAL:O	2.11	0.51
1:B:313:GLU:CB	1:B:314:SER:CA	2.80	0.51
1:A:148:LYS:CD	1:A:279:ASP:HB3	2.40	0.51
1:A:140:THR:C	1:A:142:LEU:H	2.18	0.50
1:B:142:LEU:HD11	1:B:148:LYS:HE2	1.94	0.50
1:B:35:LEU:HD21	1:B:66:LEU:HB2	1.94	0.49
1:B:142:LEU:HD12	1:B:142:LEU:N	2.28	0.49
1:A:360:TYR:C	1:A:360:TYR:CD1	2.91	0.48
1:A:281[B]:CYS:SG	1:A:434:SER:HB3	2.54	0.48
1:A:474:ASP:O	1:A:476:VAL:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ASP:H	1:B:100:ILE:HG12	1.78	0.48
1:B:166:ALA:HB2	1:B:188:TRP:CZ3	2.50	0.46
1:B:194:GLY:N	1:B:195:PRO:HD2	2.31	0.46
1:B:274:HIS:CD2	1:B:286:ALA:N	2.73	0.46
1:B:308:LYS:HB2	1:B:352:ARG:O	2.16	0.45
1:B:98:PRO:HB2	1:B:100:ILE:CG2	2.47	0.45
1:A:281[B]:CYS:SG	1:A:450:SER:HB3	2.56	0.45
1:B:156:PRO:HB2	1:B:504:PHE:HB2	1.99	0.45
1:A:132:VAL:O	1:A:275:THR:HG23	2.16	0.45
1:B:446:ASP:HB2	1:B:447:PRO:CD	2.47	0.45
1:A:472:GLU:OE1	1:A:500:LYS:HD3	2.17	0.44
1:B:252:ILE:O	1:B:256:LEU:HG	2.17	0.44
1:A:305:VAL:HG23	1:A:426:GLU:HA	2.00	0.44
1:B:303:THR:HG1	1:B:359:HIS:HD2	1.65	0.44
1:A:173:GLN:HE21	1:A:186:ILE:N	2.02	0.44
1:B:138:GLN:CG	1:B:140:THR:HG23	2.49	0.43
1:A:310:ASN:HD22	1:A:310:ASN:C	2.25	0.43
1:B:421:LYS:HD3	1:B:421:LYS:HA	1.84	0.43
1:A:473:GLY:O	1:A:475:VAL:N	2.51	0.43
1:B:313:GLU:HG3	1:B:315:VAL:H	1.84	0.43
1:A:308:LYS:HB3	1:A:352:ARG:HA	2.01	0.43
1:B:57:GLY:O	1:B:61:GLN:HG3	2.18	0.43
1:B:309:ARG:H	1:B:310:ASN:HA	1.84	0.43
1:A:440:ARG:HG3	1:A:447:PRO:HG2	2.00	0.43
1:B:459:GLN:HE21	1:B:477:GLY:HA2	1.84	0.43
1:A:348:VAL:HG13	1:A:352:ARG:HD3	2.00	0.42
1:B:504:PHE:CZ	1:B:506:GLU:HB2	2.55	0.42
1:A:171:LYS:CE	3:A:2060:HOH:O	2.68	0.42
1:B:313:GLU:HA	1:B:315:VAL:H	1.85	0.42
1:B:28:SER:OG	1:B:31:GLU:HG2	2.20	0.42
1:B:238:SER:HA	1:B:388:ILE:HD11	2.02	0.42
1:A:156:PRO:HD2	1:A:479:GLU:OE1	2.20	0.41
1:A:274:HIS:CE1	1:A:358:ASN:HD21	2.30	0.41
1:A:141:ARG:O	1:A:439:ALA:HB2	2.21	0.41
1:B:320:GLN:HA	1:B:324:LYS:O	2.20	0.41
1:A:81:ALA:HB1	1:A:380:VAL:HG23	2.03	0.41
1:B:128:LYS:HE2	1:B:271:GLU:OE2	2.21	0.41
1:B:133:LEU:HD13	1:B:276:TYR:CE2	2.56	0.41
1:B:272:HIS:CD2	1:B:360:TYR:OH	2.62	0.41
1:B:360:TYR:CD1	1:B:360:TYR:C	2.99	0.41
1:A:140:THR:C	1:A:142:LEU:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ILE:HD11	3:A:2031:HOH:O	2.20	0.41
1:B:227:CYS:HB3	1:B:385:ILE:HD13	2.03	0.41
1:B:138:GLN:HG2	1:B:140:THR:HG23	2.03	0.40
1:B:121:LEU:HD23	1:B:121:LEU:HA	1.78	0.40
1:B:310:ASN:HB2	1:B:311:ALA:CB	2.29	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	460/509 (90%)	438 (95%)	18 (4%)	4 (1%)	14	10
1	B	442/509 (87%)	423 (96%)	15 (3%)	4 (1%)	14	10
All	All	902/1018 (89%)	861 (96%)	33 (4%)	8 (1%)	14	10

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	474	ASP
1	B	96	PRO
1	B	309	ARG
1	A	194	GLY
1	B	100	ILE
1	A	141	ARG
1	B	95	GLU
1	A	179	ILE

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	395/431 (92%)	374 (95%)	21 (5%)	20	18
1	B	381/431 (88%)	357 (94%)	24 (6%)	16	13
All	All	776/862 (90%)	731 (94%)	45 (6%)	18	15

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LYS
1	A	100	ILE
1	A	121	LEU
1	A	138	GLN
1	A	140	THR
1	A	141	ARG
1	A	172	LEU
1	A	178	ARG
1	A	198	LYS
1	A	303	THR
1	A	310	ASN
1	A	319	LEU
1	A	348	VAL
1	A	349	LEU
1	A	358	ASN
1	A	364	LYS
1	A	388	ILE
1	A	401	PRO
1	A	419	LEU
1	A	475	VAL
1	A	476	VAL
1	B	93	SER
1	B	94	LEU
1	B	100	ILE
1	B	121	LEU
1	B	138	GLN
1	B	142	LEU

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Mol	Chain	Res	Type
1	B	152	ASP
1	B	172	LEU
1	B	214	LYS
1	B	303	THR
1	B	313	GLU
1	B	317	LEU
1	B	318	ILE
1	B	329	GLU
1	B	358	ASN
1	B	364	LYS
1	B	400	LYS
1	B	419	LEU
1	B	420	GLU
1	B	444	GLU
1	B	464	LYS
1	B	472	GLU
1	B	475	VAL
1	B	476	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	163	GLN
1	A	173	GLN
1	A	272	HIS
1	A	274	HIS
1	A	310	ASN
1	A	358	ASN
1	A	378	HIS
1	A	459	GLN
1	B	173	GLN
1	B	177	GLN
1	B	272	HIS
1	B	274	HIS
1	B	358	ASN
1	B	359	HIS
1	B	459	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	A	1508	-	5,5,5	0.28	0	5,5,5	1.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	1508	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1508	GOL	O1-C1-C2-C3
2	A	1508	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1508	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, 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	465/509 (91%)	0.22	24 (5%)	33 34	8, 19, 37, 79	1 (0%)
1	B	447/509 (87%)	0.06	21 (4%)	36 38	3, 16, 38, 65	1 (0%)
All	All	912/1018 (89%)	0.14	45 (4%)	35 36	3, 18, 38, 79	2 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	GLY	5.3
1	B	474	ASP	5.2
1	B	311	ALA	5.0
1	B	472	GLU	4.7
1	B	137	GLY	4.6
1	A	472	GLU	4.2
1	A	85	PRO	4.1
1	B	475	VAL	3.9
1	A	179	ILE	3.8
1	A	475	VAL	3.6
1	A	52	ASP	3.6
1	B	312	THR	3.5
1	A	33	GLN	3.3
1	B	85	PRO	3.2
1	A	473	GLY	3.1
1	A	452	ARG	3.1
1	B	98	PRO	3.1
1	B	471	THR	3.0
1	B	310	ASN	3.0
1	B	100	ILE	2.9
1	A	28	SER	2.8
1	B	473	GLY	2.7
1	A	49	ALA	2.6
1	B	313	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	102	THR	2.4
1	B	308	LYS	2.4
1	A	137	GLY	2.4
1	A	443	GLY	2.4
1	A	138	GLN	2.4
1	B	95	GLU	2.4
1	B	309	ARG	2.4
1	A	143	GLY	2.4
1	B	396	PHE	2.3
1	A	142	LEU	2.3
1	B	470	ILE	2.2
1	A	27	PRO	2.2
1	A	30	GLU	2.2
1	B	92	ALA	2.2
1	A	141	ARG	2.2
1	A	55	GLN	2.1
1	A	56	THR	2.1
1	A	476	VAL	2.1
1	A	140	THR	2.1
1	B	352	ARG	2.0
1	A	135	ALA	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($\text{\AA}^2$)	Q<0.9
2	GOL	A	1508	6/6	0.86	0.10	36,42,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.