



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:45 PM UTC

PDB ID : 7O2N / pdb_00007o2n
Title : Crystal structure of B. subtilis UGPase YngB
Authors : Wu, C.
Deposited on : 2021-03-30
Resolution : 2.80 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
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

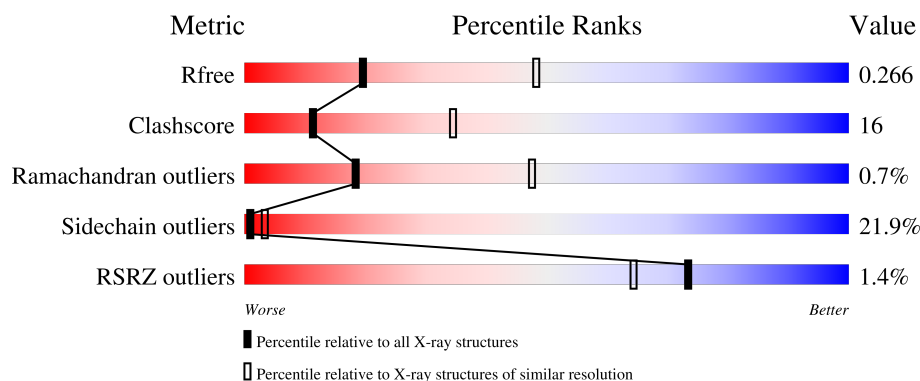
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	296	2% 59% 33% 6% ..
1	B	296	2% 61% 29% 6% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4383 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 Probable UTP--glucose-1-phosphate uridylyltransferase YngB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2193	1388	368	426	11			
1	B	289	Total	C	N	O	S	0	0	0
			2142	1349	369	413	11			

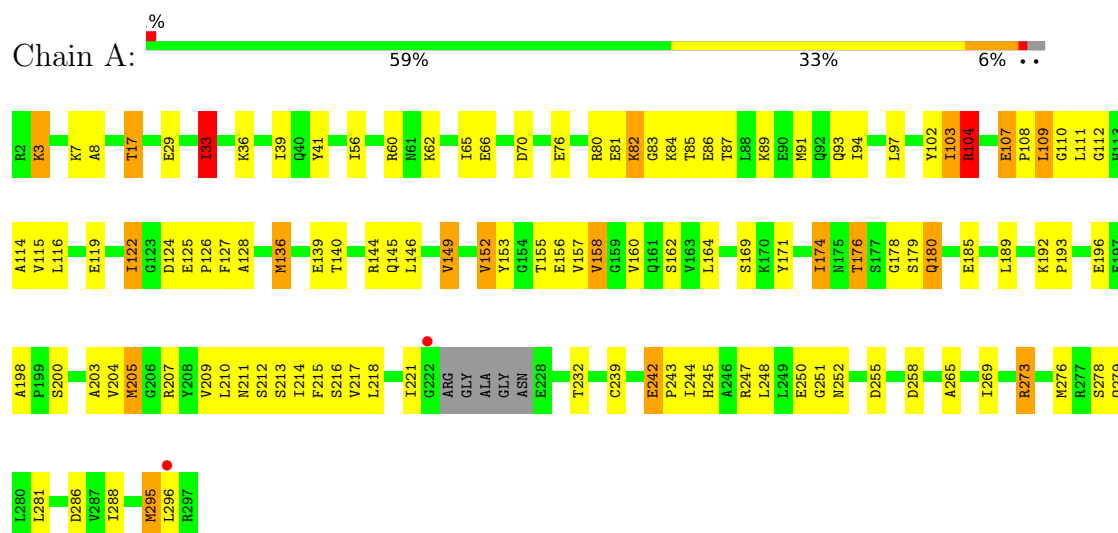
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	24	Total	O	0	0
			24	24		
2	B	24	Total	O	0	0
			24	24		

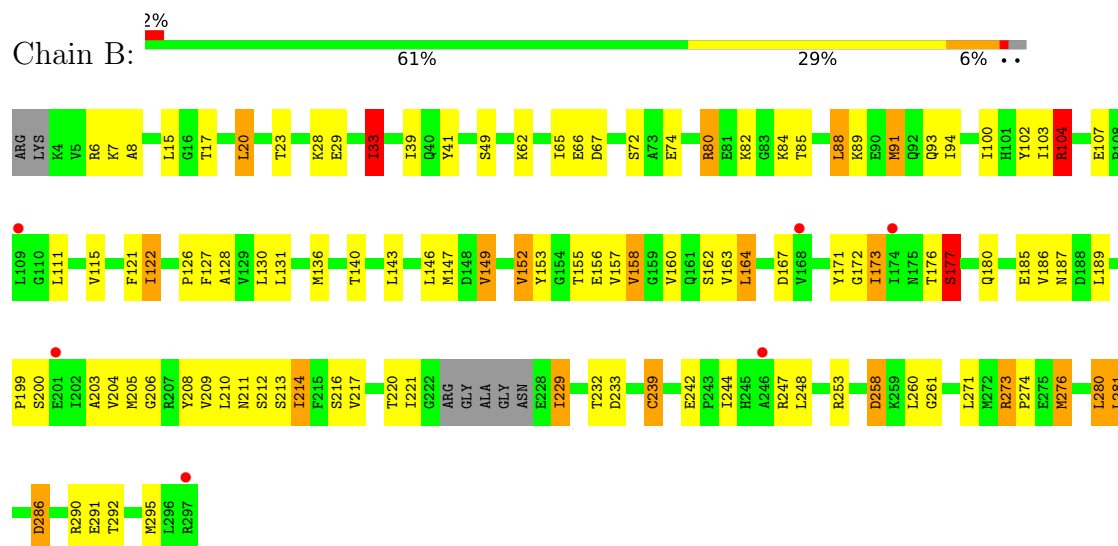
3 Residue-property plots

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: Probable UTP--glucose-1-phosphate uridylyltransferase YngB



- Molecule 1: Probable UTP--glucose-1-phosphate uridylyltransferase YngB



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.16Å 158.98Å 180.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.29 – 2.80 56.29 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (56.29-2.80) 99.8 (56.29-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.213 , 0.264 0.215 , 0.266	Depositor DCC
R_{free} test set	987 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	65.6	Xtriage
Anisotropy	0.773	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4383	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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

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	0.56	0/2227	1.30	6/3021 (0.2%)
1	B	0.55	0/2173	1.28	10/2951 (0.3%)
All	All	0.56	0/4400	1.29	16/5972 (0.3%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	ILE	CA-C-N	-11.38	109.08	122.63
1	A	33	ILE	C-N-CA	-11.38	109.08	122.63
1	B	33	ILE	CA-C-N	-10.91	109.64	122.63
1	B	33	ILE	C-N-CA	-10.91	109.64	122.63
1	A	17	THR	CA-CB-OG1	-10.75	93.47	109.60
1	B	258	ASP	CB-CA-C	-10.30	89.69	109.66
1	A	258	ASP	CA-CB-CG	8.70	121.30	112.60
1	A	273	ARG	CB-CA-C	7.37	117.47	110.17
1	B	273	ARG	CB-CA-C	6.42	117.17	109.85
1	B	286	ASP	CB-CA-C	6.26	122.68	110.67
1	B	286	ASP	CA-CB-CG	6.12	118.72	112.60
1	A	104	ARG	CG-CD-NE	-5.63	99.61	112.00
1	B	286	ASP	N-CA-CB	5.63	119.01	110.28
1	B	177	SER	N-CA-C	-5.48	107.14	113.88
1	B	104	ARG	CB-CG-CD	-5.15	99.45	111.30
1	B	6	ARG	CB-CA-C	5.05	118.43	109.75

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	2193	0	2148	78	0
1	B	2142	0	2081	65	0
2	A	24	0	0	3	0
2	B	24	0	0	1	0
All	All	4383	0	4229	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 16.

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:176:THR:HG22	1:A:178:GLY:H	1.39	0.87
1:B:136:MET:HE2	1:B:253:ARG:HB2	1.59	0.82
1:A:104:ARG:NH2	1:B:67:ASP:OD1	2.13	0.81
1:A:171:TYR:CE1	1:A:205:MET:HE1	2.17	0.80
1:B:91:MET:HE2	1:B:94:ILE:HD12	1.63	0.78
1:A:122:ILE:HD11	1:A:215:PHE:HZ	1.50	0.77
1:A:156:GLU:O	1:A:244:ILE:HG23	1.83	0.76
1:B:136:MET:CE	1:B:253:ARG:HB2	2.15	0.75
1:A:152:VAL:HG22	1:A:153:TYR:CD1	2.23	0.73
1:B:217:VAL:O	1:B:221:ILE:HG12	1.88	0.73
1:B:111:LEU:O	1:B:115:VAL:HG23	1.87	0.73
1:A:89:LYS:O	1:A:93:GLN:HG3	1.89	0.72
1:B:164:LEU:O	1:B:167:ASP:HB2	1.90	0.72
1:A:247:ARG:NH1	1:A:248:LEU:O	2.22	0.72
1:B:258:ASP:HB2	1:B:261:GLY:H	1.55	0.71
1:A:176:THR:CG2	1:A:178:GLY:O	2.37	0.71
1:A:205:MET:HA	1:A:205:MET:CE	2.21	0.71
1:B:247:ARG:NH1	1:B:248:LEU:O	2.24	0.70
1:A:176:THR:HG21	1:A:178:GLY:O	1.91	0.69
1:B:89:LYS:O	1:B:93:GLN:HG3	1.92	0.68
1:A:217:VAL:O	1:A:221:ILE:HG12	1.92	0.68
1:B:104:ARG:CG	1:B:104:ARG:HH11	2.07	0.66
1:B:214:ILE:HD13	1:B:214:ILE:O	1.95	0.65
1:A:205:MET:HA	1:A:205:MET:HE2	1.78	0.65
1:A:140:THR:HG22	1:A:145:GLN:HG3	1.80	0.64
1:B:104:ARG:HH11	1:B:104:ARG:HG2	1.64	0.62
1:B:88:LEU:O	1:B:88:LEU:HG	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:VAL:HG11	1:B:247:ARG:HB2	1.82	0.60
1:B:20:LEU:HD12	1:B:23:THR:OG1	2.01	0.60
1:B:173:ILE:HG21	1:B:199:PRO:HD2	1.82	0.60
1:B:271:LEU:HD21	1:B:281:LEU:HD13	1.82	0.60
1:A:122:ILE:HD11	1:A:215:PHE:CZ	2.34	0.59
1:A:152:VAL:CG2	1:A:153:TYR:CD1	2.85	0.59
1:A:7:LYS:HD2	1:A:125:GLU:OE1	2.02	0.59
1:A:140:THR:HG22	1:A:145:GLN:CG	2.33	0.58
1:A:149:VAL:HG11	1:A:247:ARG:HB2	1.86	0.58
1:A:180:GLN:HB3	2:A:316:HOH:O	2.02	0.58
1:A:7:LYS:HD3	1:A:122:ILE:HG22	1.84	0.58
1:A:107:GLU:HG2	1:A:109:LEU:HD21	1.85	0.58
1:B:91:MET:HE2	1:B:94:ILE:CD1	2.32	0.58
1:B:131:LEU:HD13	1:B:206:GLY:HA2	1.86	0.58
1:B:172:GLY:O	1:B:203:ALA:HA	2.04	0.57
1:B:7:LYS:NZ	1:B:121:PHE:O	2.37	0.56
1:B:239:CYS:HA	1:B:242:GLU:O	2.04	0.56
1:A:153:TYR:CD2	1:A:245:HIS:CD2	2.93	0.56
1:A:108:PRO:C	1:A:109:LEU:HD23	2.31	0.55
1:B:91:MET:HA	1:B:91:MET:CE	2.37	0.55
1:A:244:ILE:HG22	1:A:245:HIS:N	2.21	0.55
1:B:152:VAL:HG12	1:B:153:TYR:N	2.22	0.55
1:A:176:THR:HG23	1:A:185:GLU:H	1.71	0.55
1:A:244:ILE:CG2	1:A:245:HIS:N	2.70	0.55
1:A:153:TYR:CD2	1:A:245:HIS:NE2	2.75	0.54
1:B:229:ILE:H	1:B:229:ILE:HD12	1.72	0.54
1:B:131:LEU:H	1:B:131:LEU:HD12	1.73	0.54
1:A:70:ASP:CG	1:B:104:ARG:HD2	2.32	0.54
1:A:136:MET:HE1	1:A:251:GLY:C	2.33	0.54
1:A:239:CYS:HA	1:A:242:GLU:O	2.07	0.54
1:B:66:GLU:HG2	1:B:102:TYR:CE2	2.43	0.53
1:B:229:ILE:HD12	1:B:229:ILE:N	2.24	0.53
1:B:49:SER:O	1:B:147:MET:HE1	2.09	0.53
1:A:94:ILE:O	1:A:97:LEU:HD12	2.09	0.52
1:A:242:GLU:HG2	1:A:243:PRO:HD2	1.90	0.52
1:A:66:GLU:HA	1:A:102:TYR:OH	2.10	0.52
1:A:139:GLU:HB3	2:A:317:HOH:O	2.10	0.52
1:B:80:ARG:NH2	1:B:80:ARG:HB2	2.25	0.52
1:B:62:LYS:HB3	1:B:65:ILE:HD12	1.91	0.51
1:B:186:VAL:HB	1:B:244:ILE:HG13	1.93	0.51
1:A:171:TYR:HE1	1:A:205:MET:HE1	1.71	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:LEU:CD1	1:B:208:TYR:HE1	2.23	0.50
1:A:152:VAL:CG2	1:A:153:TYR:N	2.73	0.50
1:A:136:MET:HG3	1:A:207:ARG:NH2	2.26	0.50
1:A:103:ILE:HD12	1:B:100:ILE:O	2.11	0.50
1:B:130:LEU:HD21	1:B:143:LEU:HD13	1.94	0.49
1:B:91:MET:HA	1:B:91:MET:HE3	1.94	0.49
1:A:108:PRO:O	1:A:109:LEU:HD23	2.12	0.49
1:B:104:ARG:CG	1:B:104:ARG:NH1	2.73	0.49
1:B:273:ARG:NH1	2:B:303:HOH:O	2.45	0.49
1:A:153:TYR:CG	1:A:245:HIS:CD2	3.01	0.49
1:A:36:LYS:HB2	1:A:41:TYR:CE2	2.48	0.48
1:B:209:VAL:O	1:B:210:LEU:HD23	2.14	0.48
1:A:62:LYS:HB3	1:A:65:ILE:HD12	1.95	0.48
1:B:156:GLU:O	1:B:244:ILE:HB	2.13	0.47
1:A:33:ILE:HD13	1:A:33:ILE:HA	1.69	0.47
1:B:91:MET:HE3	1:B:91:MET:CA	2.45	0.47
1:A:70:ASP:OD2	1:B:104:ARG:HD2	2.15	0.47
1:A:205:MET:HA	1:A:205:MET:HE3	1.95	0.47
1:A:169:SER:O	1:A:192:LYS:HB2	2.15	0.46
1:A:179:SER:C	1:A:180:GLN:HG3	2.40	0.46
1:A:8:ALA:HA	1:A:128:ALA:O	2.15	0.46
1:B:177:SER:HB2	1:B:187:ASN:OD1	2.16	0.46
1:A:176:THR:HG22	1:A:178:GLY:O	2.14	0.46
1:A:126:PRO:HA	1:A:210:LEU:O	2.16	0.45
1:B:292:THR:HA	1:B:295:MET:HE2	1.97	0.45
1:B:171:TYR:HB3	1:B:203:ALA:HB1	1.99	0.45
1:A:86:GLU:HG2	1:A:87:THR:N	2.32	0.45
1:B:290:ARG:NH1	1:B:291:GLU:OE2	2.49	0.45
1:B:91:MET:HE3	1:B:91:MET:N	2.32	0.45
1:A:3:LYS:HE2	1:A:3:LYS:HB2	1.80	0.44
1:A:174:ILE:HA	1:A:189:LEU:CD1	2.47	0.44
1:A:209:VAL:O	1:A:210:LEU:HD23	2.16	0.44
1:B:247:ARG:HG3	1:B:248:LEU:O	2.17	0.44
1:A:144:ARG:HH11	1:A:144:ARG:HG3	1.82	0.44
1:B:276:MET:O	1:B:280:LEU:HB2	2.17	0.44
1:A:158:VAL:HG12	1:A:160:VAL:HG13	1.99	0.44
1:B:66:GLU:HA	1:B:102:TYR:OH	2.17	0.44
1:B:211:ASN:O	1:B:214:ILE:HG22	2.17	0.44
1:B:122:ILE:HG13	1:B:127:PHE:HB3	1.99	0.44
1:A:56:ILE:HD12	1:A:102:TYR:CE1	2.53	0.44
1:B:152:VAL:CG1	1:B:153:TYR:N	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:HD12	1:A:189:LEU:HA	1.82	0.43
1:A:242:GLU:HG2	1:A:243:PRO:CD	2.49	0.43
1:A:111:LEU:HA	1:A:114:ALA:HB3	2.01	0.43
1:A:33:ILE:HB	1:A:41:TYR:CE2	2.54	0.43
1:A:174:ILE:HA	1:A:189:LEU:HD12	2.01	0.43
1:B:8:ALA:HA	1:B:128:ALA:O	2.19	0.42
1:B:273:ARG:HA	1:B:274:PRO:HD2	1.88	0.42
1:A:265:ALA:O	1:A:269:ILE:HG12	2.19	0.42
1:B:80:ARG:CZ	1:B:80:ARG:CB	2.97	0.42
1:A:83:GLY:O	1:A:85:THR:N	2.53	0.42
1:B:199:PRO:O	1:B:200:SER:HB3	2.19	0.42
1:A:107:GLU:HG2	1:A:109:LEU:HD11	2.01	0.42
1:A:119:GLU:HA	1:A:215:PHE:CZ	2.54	0.42
1:A:193:PRO:HG2	1:A:198:ALA:HB2	2.02	0.42
1:A:252:ASN:HA	2:A:307:HOH:O	2.19	0.42
1:A:295:MET:HE2	1:A:295:MET:HB3	1.73	0.42
1:B:239:CYS:SG	1:B:244:ILE:HG12	2.60	0.42
1:B:33:ILE:HB	1:B:41:TYR:CE2	2.55	0.42
1:A:122:ILE:HD12	1:A:127:PHE:CG	2.55	0.41
1:A:211:ASN:O	1:A:214:ILE:HG22	2.20	0.41
1:B:158:VAL:HG12	1:B:160:VAL:HG13	2.02	0.41
1:B:258:ASP:HB2	1:B:261:GLY:N	2.28	0.41
1:B:126:PRO:HA	1:B:210:LEU:O	2.20	0.41
1:A:140:THR:CG2	1:A:145:GLN:HG2	2.51	0.41
1:A:171:TYR:HB3	1:A:203:ALA:HB1	2.02	0.41
1:B:205:MET:HA	1:B:205:MET:HE2	2.03	0.41
1:A:112:GLY:H	1:A:115:VAL:HG23	1.86	0.41
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.83	0.40
1:A:152:VAL:HG22	1:A:153:TYR:N	2.36	0.40
1:A:110:GLY:C	1:A:111:LEU:O	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	287/296 (97%)	257 (90%)	28 (10%)	2 (1%)	18	47
1	B	285/296 (96%)	253 (89%)	30 (10%)	2 (1%)	18	47
All	All	572/592 (97%)	510 (89%)	58 (10%)	4 (1%)	18	47

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	LYS
1	B	84	LYS
1	B	82	LYS
1	A	82	LYS

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	229/252 (91%)	179 (78%)	50 (22%)	1	3
1	B	219/252 (87%)	171 (78%)	48 (22%)	1	3
All	All	448/504 (89%)	350 (78%)	98 (22%)	1	3

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	17	THR
1	A	29	GLU
1	A	33	ILE
1	A	39	ILE
1	A	60	ARG
1	A	76	GLU
1	A	80	ARG
1	A	81	GLU

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Mol	Chain	Res	Type
1	A	82	LYS
1	A	91	MET
1	A	103	ILE
1	A	104	ARG
1	A	107	GLU
1	A	109	LEU
1	A	122	ILE
1	A	124	ASP
1	A	136	MET
1	A	146	LEU
1	A	149	VAL
1	A	152	VAL
1	A	155	THR
1	A	157	VAL
1	A	158	VAL
1	A	162	SER
1	A	164	LEU
1	A	174	ILE
1	A	176	THR
1	A	180	GLN
1	A	196	GLU
1	A	200	SER
1	A	204	VAL
1	A	205	MET
1	A	212	SER
1	A	213	SER
1	A	216	SER
1	A	218	LEU
1	A	232	THR
1	A	242	GLU
1	A	250	GLU
1	A	255	ASP
1	A	273	ARG
1	A	276	MET
1	A	278	SER
1	A	279	GLN
1	A	281	LEU
1	A	286	ASP
1	A	288	ILE
1	A	295	MET
1	A	296	LEU
1	B	15	LEU

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Mol	Chain	Res	Type
1	B	17	THR
1	B	20	LEU
1	B	28	LYS
1	B	29	GLU
1	B	33	ILE
1	B	39	ILE
1	B	72	SER
1	B	74	GLU
1	B	80	ARG
1	B	85	THR
1	B	88	LEU
1	B	91	MET
1	B	103	ILE
1	B	104	ARG
1	B	107	GLU
1	B	122	ILE
1	B	140	THR
1	B	146	LEU
1	B	149	VAL
1	B	152	VAL
1	B	155	THR
1	B	157	VAL
1	B	158	VAL
1	B	162	SER
1	B	163	VAL
1	B	164	LEU
1	B	173	ILE
1	B	176	THR
1	B	177	SER
1	B	180	GLN
1	B	185	GLU
1	B	189	LEU
1	B	204	VAL
1	B	212	SER
1	B	213	SER
1	B	214	ILE
1	B	216	SER
1	B	220	THR
1	B	229	ILE
1	B	232	THR
1	B	233	ASP
1	B	239	CYS

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Mol	Chain	Res	Type
1	B	260	LEU
1	B	276	MET
1	B	280	LEU
1	B	281	LEU
1	B	286	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	182	HIS
1	A	211	ASN
1	B	93	GLN
1	B	211	ASN
1	B	279	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	291/296 (98%)	-0.26	2 (0%) 84 77	37, 67, 100, 121	0
1	B	289/296 (97%)	0.10	6 (2%) 63 54	39, 75, 125, 161	0
All	All	580/592 (97%)	-0.08	8 (1%) 73 64	37, 70, 120, 161	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	246	ALA	2.6
1	A	222	GLY	2.3
1	B	297	ARG	2.3
1	A	296	LEU	2.3
1	B	109	LEU	2.1
1	B	174	ILE	2.1
1	B	201	GLU	2.0
1	B	168	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.