



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:21 PM UTC

PDB ID : 6JOY / pdb_00006joy
Title : The X-ray Crystallographic Structure of Branching Enzyme from *Rhodothermus obamensis* STB05
Authors : Li, Z.F.; Ban, X.F.; Jiang, H.M.; Wang, Z.; Jin, T.C.; Li, C.M.; Gu, Z.B.
Deposited on : 2019-03-25
Resolution : 2.39 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

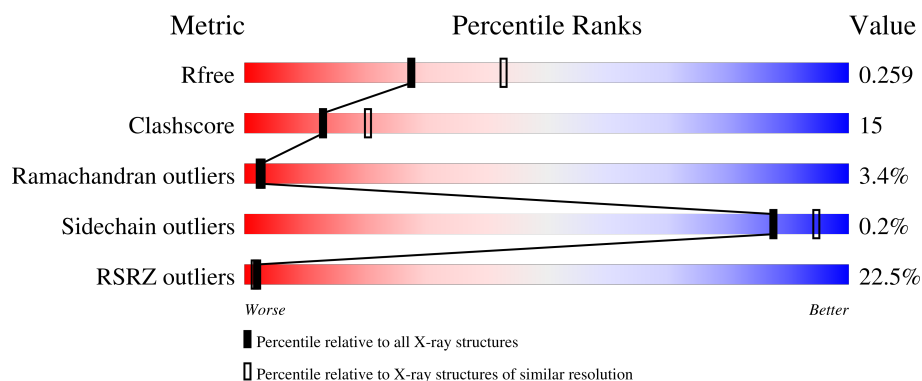
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	621	23% 74% 23% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5288 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 1,4-alpha-glucan branching enzyme GlgB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	621	Total	C	N	O	S	1	0	0
			5132	3333	871	909	19			

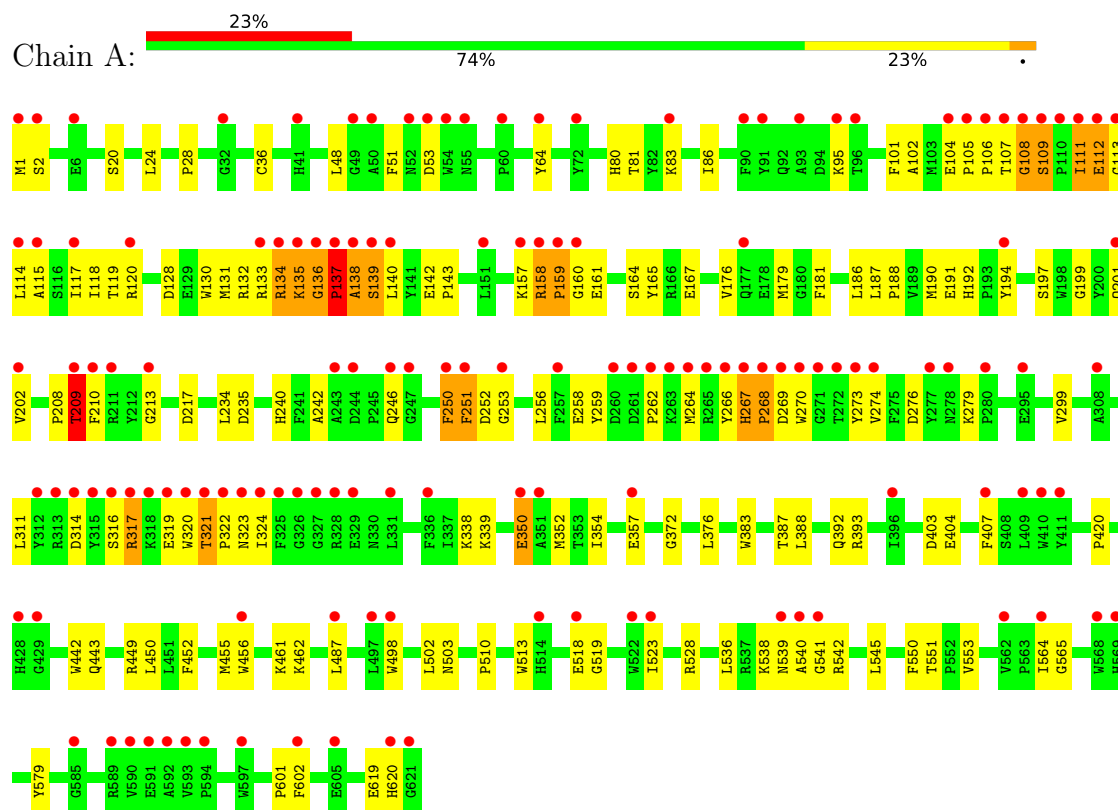
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	156	Total	O	0	0
			156	156		

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: 1,4-alpha-glucan branching enzyme GlgB



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	125.67Å 125.67Å 205.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.42 – 2.39 31.42 – 2.39	Depositor EDS
% Data completeness (in resolution range)	96.7 (31.42-2.39) 97.8 (31.42-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.247 , 0.278 (Not available) , 0.259	Depositor DCC
R_{free} test set	3248 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5288	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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	0.41	0/5336	0.65	5/7280 (0.1%)

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	A	0	6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	139	SER	N-CA-C	-5.80	106.29	113.19
1	A	323	ASN	CB-CA-C	-5.39	109.90	117.23
1	A	111	ILE	CA-C-N	5.20	131.47	121.54
1	A	111	ILE	C-N-CA	5.20	131.47	121.54
1	A	209	THR	N-CA-CB	5.20	119.27	110.49

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	SER	Peptide
1	A	136	GLY	Peptide
1	A	137	PRO	Peptide
1	A	317	ARG	Peptide
1	A	350	GLU	Peptide
1	A	51	PHE	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	5132	0	4771	148	0
2	A	156	0	0	12	1
All	All	5288	0	4771	148	1

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 15.

All (148) 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:107:THR:HG23	1:A:114:LEU:HD21	1.37	1.06
1:A:107:THR:HA	1:A:114:LEU:CD2	1.89	1.02
1:A:134:ARG:O	1:A:136:GLY:N	1.95	0.99
1:A:137:PRO:HA	1:A:350:GLU:HG2	1.43	0.99
1:A:131:MET:SD	2:A:702:HOH:O	2.23	0.95
1:A:104:GLU:HG2	1:A:105:PRO:HD2	1.47	0.95
1:A:273:TYR:O	2:A:701:HOH:O	1.89	0.88
1:A:158:ARG:HH11	1:A:158:ARG:HB3	1.39	0.88
1:A:540:ALA:O	1:A:542:ARG:N	2.05	0.88
1:A:107:THR:HA	1:A:114:LEU:HD21	1.58	0.85
1:A:158:ARG:HB3	1:A:158:ARG:NH1	1.93	0.84
1:A:159:PRO:O	1:A:161:GLU:N	2.11	0.83
1:A:542:ARG:NH2	2:A:704:HOH:O	2.13	0.82
1:A:107:THR:CG2	1:A:114:LEU:HD21	2.11	0.81
1:A:551:THR:HG23	1:A:553:VAL:H	1.45	0.79
1:A:114:LEU:HD12	1:A:246:GLN:NE2	1.97	0.78
1:A:107:THR:C	1:A:111:ILE:HD12	2.09	0.77
1:A:83:LYS:NZ	2:A:705:HOH:O	2.17	0.76
1:A:104:GLU:HA	1:A:117:ILE:HD11	1.68	0.74
1:A:256:LEU:O	1:A:279:LYS:HE2	1.87	0.74
1:A:106:PRO:HB3	1:A:112:GLU:HG3	1.70	0.73
1:A:95:LYS:HE3	1:A:251:PHE:HA	1.72	0.72
1:A:262:PRO:HD2	1:A:264:MET:HE3	1.72	0.71
1:A:131:MET:HE1	1:A:134:ARG:NH2	2.06	0.71
1:A:352:MET:HE2	1:A:354:ILE:HD11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:NE	2:A:702:HOH:O	2.12	0.69
1:A:452:PHE:O	1:A:456:TRP:HD1	1.76	0.68
1:A:102:ALA:HB1	1:A:210:PHE:HE1	1.59	0.67
1:A:20:SER:HB2	1:A:24:LEU:CD1	2.25	0.67
1:A:53:ASP:OD1	2:A:703:HOH:O	2.13	0.66
1:A:456:TRP:HH2	1:A:503:ASN:OD1	1.78	0.65
1:A:314:ASP:O	1:A:319:GLU:HG2	1.96	0.64
1:A:456:TRP:CH2	1:A:503:ASN:OD1	2.50	0.64
1:A:107:THR:HG22	1:A:107:THR:O	1.97	0.64
1:A:107:THR:CA	1:A:114:LEU:HD21	2.28	0.63
1:A:320:TRP:O	1:A:321:THR:HB	1.98	0.63
1:A:102:ALA:HB1	1:A:210:PHE:CE1	2.35	0.61
1:A:339:LYS:NZ	2:A:711:HOH:O	2.33	0.61
1:A:107:THR:HA	1:A:114:LEU:HD23	1.76	0.61
1:A:104:GLU:O	1:A:107:THR:OG1	2.15	0.60
1:A:267:HIS:HD2	1:A:268:PRO:HD2	1.67	0.60
1:A:133:ARG:C	1:A:135:LYS:H	2.09	0.60
1:A:158:ARG:HH11	1:A:158:ARG:CB	2.13	0.60
1:A:523:ILE:HD12	1:A:545:LEU:HD13	1.84	0.60
1:A:452:PHE:O	1:A:456:TRP:CD1	2.56	0.59
1:A:83:LYS:HE3	1:A:114:LEU:O	2.03	0.59
1:A:276:ASP:OD2	1:A:279:LYS:NZ	2.35	0.58
1:A:158:ARG:HG3	1:A:159:PRO:HD2	1.83	0.58
1:A:523:ILE:HD11	1:A:536:LEU:HG	1.85	0.58
1:A:80:HIS:HB2	1:A:118:ILE:HD12	1.85	0.58
1:A:131:MET:CE	1:A:134:ARG:NH2	2.66	0.58
1:A:20:SER:O	1:A:24:LEU:HD12	2.04	0.58
1:A:456:TRP:NE1	2:A:712:HOH:O	2.36	0.57
1:A:619:GLU:O	1:A:620:HIS:ND1	2.37	0.57
1:A:393:ARG:NH1	1:A:404:GLU:OE1	2.39	0.56
1:A:134:ARG:C	1:A:136:GLY:N	2.65	0.55
1:A:132:ARG:HD2	2:A:807:HOH:O	2.07	0.55
1:A:101:PHE:HB2	1:A:119:THR:CG2	2.38	0.54
1:A:210:PHE:HA	1:A:213:GLY:O	2.06	0.54
1:A:131:MET:SD	1:A:134:ARG:NH2	2.81	0.54
1:A:20:SER:HB2	1:A:24:LEU:HD12	1.89	0.54
1:A:208:PRO:O	1:A:209:THR:HG23	2.08	0.54
1:A:449:ARG:O	1:A:498:TRP:CZ3	2.62	0.53
1:A:134:ARG:O	1:A:134:ARG:HG2	2.08	0.53
1:A:137:PRO:HD2	1:A:139:SER:CA	2.39	0.53
1:A:2:SER:HB2	1:A:64:TYR:HE1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ALA:C	1:A:140:LEU:H	2.16	0.52
1:A:539:ASN:CG	1:A:540:ALA:H	2.17	0.52
1:A:316:SER:OG	1:A:317:ARG:N	2.42	0.52
1:A:498:TRP:HD1	1:A:579:TYR:CZ	2.28	0.51
1:A:107:THR:O	1:A:111:ILE:HD12	2.09	0.51
1:A:319:GLU:CD	1:A:320:TRP:H	2.18	0.51
1:A:2:SER:HB2	1:A:64:TYR:CE1	2.45	0.51
1:A:131:MET:HE1	1:A:134:ARG:HH22	1.75	0.51
1:A:1:MET:HG2	1:A:1:MET:O	2.11	0.51
1:A:81:THR:HB	1:A:115:ALA:CB	2.41	0.51
1:A:192:HIS:CG	1:A:199:GLY:HA2	2.46	0.51
1:A:250:PHE:CE2	1:A:253:GLY:HA2	2.46	0.50
1:A:352:MET:HG2	1:A:376:LEU:HD23	1.92	0.50
1:A:194:TYR:O	1:A:197:SER:HB3	2.10	0.50
1:A:165:TYR:HB2	1:A:217:ASP:HB3	1.93	0.50
1:A:197:SER:OG	1:A:201:GLN:HG2	2.11	0.50
1:A:138:ALA:C	1:A:140:LEU:N	2.70	0.50
1:A:234:LEU:HD11	1:A:299:VAL:HG11	1.93	0.49
1:A:133:ARG:C	1:A:135:LYS:N	2.69	0.49
1:A:104:GLU:HG2	1:A:105:PRO:CD	2.32	0.49
1:A:107:THR:HA	1:A:114:LEU:CG	2.40	0.49
1:A:131:MET:HA	2:A:702:HOH:O	2.11	0.49
1:A:133:ARG:O	1:A:135:LYS:N	2.46	0.49
1:A:191:GLU:OE1	1:A:209:THR:HG22	2.12	0.49
1:A:86:ILE:HG21	1:A:252:ASP:HA	1.95	0.48
1:A:498:TRP:CZ3	1:A:502:LEU:HD11	2.48	0.48
1:A:519:GLY:HA2	1:A:538:LYS:O	2.12	0.48
1:A:338:LYS:HE3	1:A:372:GLY:O	2.14	0.48
1:A:108:GLY:N	1:A:114:LEU:HG	2.30	0.47
1:A:510:PRO:HA	1:A:513:TRP:CD2	2.50	0.47
1:A:2:SER:CB	1:A:64:TYR:HE1	2.28	0.47
1:A:107:THR:HG21	1:A:191:GLU:CG	2.45	0.47
1:A:234:LEU:CD1	1:A:299:VAL:HG11	2.45	0.47
1:A:130:TRP:O	1:A:134:ARG:HB2	2.15	0.47
1:A:159:PRO:C	1:A:161:GLU:H	2.16	0.46
1:A:28:PRO:HG2	1:A:120:ARG:HG3	1.98	0.46
1:A:106:PRO:HB2	1:A:113:GLY:C	2.41	0.46
1:A:266:TYR:O	1:A:267:HIS:HB3	2.16	0.46
1:A:134:ARG:O	1:A:134:ARG:CG	2.64	0.45
1:A:456:TRP:HA	1:A:462:LYS:HE3	1.97	0.45
1:A:190:MET:HE3	1:A:190:MET:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:THR:HB	1:A:115:ALA:HB3	1.99	0.45
1:A:403:ASP:OD1	1:A:528:ARG:NH2	2.42	0.45
1:A:442:TRP:CE2	1:A:443:GLN:HG3	2.51	0.45
1:A:450:LEU:HD21	1:A:550:PHE:HA	1.98	0.44
1:A:101:PHE:HB2	1:A:119:THR:HG23	1.99	0.44
1:A:158:ARG:CG	1:A:159:PRO:HD2	2.47	0.44
1:A:250:PHE:HB3	1:A:251:PHE:H	1.59	0.44
1:A:314:ASP:O	1:A:316:SER:N	2.46	0.44
1:A:48:LEU:O	1:A:83:LYS:N	2.47	0.44
1:A:311:LEU:HD12	1:A:357:GLU:OE1	2.18	0.44
1:A:128:ASP:O	1:A:132:ARG:HG3	2.18	0.44
1:A:388:LEU:O	1:A:392:GLN:NE2	2.41	0.44
1:A:258:GLU:OE1	1:A:258:GLU:N	2.38	0.43
1:A:270:TRP:NE1	1:A:319:GLU:HA	2.33	0.43
1:A:518:GLU:H	1:A:518:GLU:CD	2.25	0.43
1:A:157:LYS:O	1:A:158:ARG:HG2	2.19	0.43
1:A:201:GLN:HB3	1:A:242:ALA:HB2	2.01	0.43
1:A:240:HIS:HE1	2:A:706:HOH:O	2.02	0.42
1:A:24:LEU:HA	1:A:36:CYS:HB3	2.01	0.42
1:A:106:PRO:O	1:A:114:LEU:HD23	2.20	0.42
1:A:142:GLU:O	1:A:461:LYS:NZ	2.50	0.42
1:A:456:TRP:CD1	1:A:456:TRP:N	2.88	0.42
1:A:455:MET:HE2	2:A:712:HOH:O	2.19	0.42
1:A:176:VAL:HG13	1:A:181:PHE:HB2	2.01	0.41
1:A:186:LEU:HD23	1:A:186:LEU:HA	1.84	0.41
1:A:403:ASP:O	1:A:407:PHE:HB2	2.20	0.41
1:A:487:LEU:HD13	1:A:487:LEU:HA	1.93	0.41
1:A:106:PRO:HD3	1:A:112:GLU:OE2	2.21	0.41
1:A:107:THR:CB	1:A:114:LEU:HD21	2.51	0.41
1:A:164:SER:OG	1:A:167:GLU:HG3	2.20	0.41
1:A:187:LEU:O	1:A:188:PRO:C	2.64	0.41
1:A:142:GLU:HB3	1:A:143:PRO:HD2	2.03	0.41
1:A:383:TRP:O	1:A:387:THR:OG1	2.24	0.41
1:A:259:TYR:CE2	1:A:274:VAL:HG23	2.56	0.40
1:A:601:PRO:HB2	1:A:602:PHE:CD1	2.55	0.40
1:A:449:ARG:O	1:A:498:TRP:HZ3	2.04	0.40
1:A:564:ILE:HG22	1:A:565:GLY:O	2.21	0.40
1:A:137:PRO:HD2	1:A:139:SER:HA	2.02	0.40
1:A:190:MET:HE1	1:A:235:ASP:O	2.21	0.40
1:A:179:MET:O	1:A:503:ASN:ND2	2.42	0.40
1:A:267:HIS:HD2	1:A:268:PRO:CD	2.32	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:781:HOH:O	2:A:850:HOH:O[3_444]	2.15	0.05

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	619/621 (100%)	559 (90%)	39 (6%)	21 (3%)	3 2

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	SER
1	A	112	GLU
1	A	134	ARG
1	A	135	LYS
1	A	160	GLY
1	A	209	THR
1	A	251	PHE
1	A	321	THR
1	A	322	PRO
1	A	541	GLY
1	A	137	PRO
1	A	138	ALA
1	A	158	ARG
1	A	159	PRO
1	A	202	VAL
1	A	420	PRO
1	A	268	PRO
1	A	269	ASP
1	A	267	HIS
1	A	324	ILE

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Mol	Chain	Res	Type
1	A	108	GLY

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	527/527 (100%)	526 (100%)	1 (0%)	87	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	250	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	227	GLN
1	A	267	HIS
1	A	428	HIS
1	A	504	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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

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	621/621 (100%)	1.79	140 (22%) 2 2	44, 54, 100, 159	1 (0%)

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	107	THR	19.6
1	A	320	TRP	17.2
1	A	324	ILE	15.5
1	A	271	GLY	14.5
1	A	268	PRO	14.2
1	A	137	PRO	14.0
1	A	210	PHE	13.6
1	A	105	PRO	13.5
1	A	110	PRO	12.5
1	A	322	PRO	12.0
1	A	325	PHE	11.9
1	A	108	GLY	11.9
1	A	262	PRO	11.7
1	A	270	TRP	11.3
1	A	321	THR	10.2
1	A	266	TYR	10.1
1	A	113	GLY	9.8
1	A	263	LYS	9.5
1	A	114	LEU	9.4
1	A	315	TYR	9.4
1	A	318	LYS	9.4
1	A	319	GLU	9.4
1	A	1	MET	9.3
1	A	267	HIS	8.9
1	A	273	TYR	8.8
1	A	327	GLY	8.5
1	A	136	GLY	8.2

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Mol	Chain	Res	Type	RSRZ
1	A	326	GLY	8.2
1	A	272	THR	8.1
1	A	111	ILE	8.0
1	A	112	GLU	7.8
1	A	104	GLU	7.5
1	A	250	PHE	7.4
1	A	209	THR	7.3
1	A	106	PRO	7.2
1	A	138	ALA	7.0
1	A	269	ASP	6.9
1	A	621	GLY	6.8
1	A	264	MET	6.5
1	A	323	ASN	6.3
1	A	135	LYS	6.2
1	A	314	ASP	6.2
1	A	109	SER	6.0
1	A	261	ASP	6.0
1	A	90	PHE	5.9
1	A	274	VAL	5.4
1	A	429	GLY	5.3
1	A	159	PRO	5.2
1	A	317	ARG	4.7
1	A	265	ARG	4.6
1	A	2	SER	4.5
1	A	316	SER	4.5
1	A	115	ALA	4.4
1	A	456	TRP	4.3
1	A	407	PHE	4.2
1	A	64	TYR	4.2
1	A	194	TYR	4.2
1	A	350	GLU	4.1
1	A	133	ARG	4.0
1	A	313	ARG	3.9
1	A	158	ARG	3.8
1	A	54	TRP	3.8
1	A	246	GLN	3.7
1	A	585	GLY	3.6
1	A	91	TYR	3.6
1	A	569	HIS	3.6
1	A	620	HIS	3.6
1	A	50	ALA	3.5
1	A	160	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	72	TYR	3.4
1	A	410	TRP	3.3
1	A	134	ARG	3.3
1	A	411	TYR	3.2
1	A	605	GLU	3.2
1	A	523	ILE	3.2
1	A	540	ALA	3.1
1	A	257	PHE	3.1
1	A	211	ARG	3.1
1	A	336	PHE	3.0
1	A	52	ASN	3.0
1	A	278	ASN	3.0
1	A	6	GLU	3.0
1	A	428	HIS	3.0
1	A	260	ASP	2.9
1	A	328	ARG	2.9
1	A	201	GLN	2.9
1	A	357	GLU	2.9
1	A	53	ASP	2.9
1	A	49	GLY	2.8
1	A	213	GLY	2.8
1	A	498	TRP	2.8
1	A	597	TRP	2.8
1	A	96	THR	2.7
1	A	157	LYS	2.7
1	A	602	PHE	2.7
1	A	329	GLU	2.6
1	A	564	ILE	2.6
1	A	593	VAL	2.6
1	A	83	LYS	2.6
1	A	541	GLY	2.5
1	A	589	ARG	2.5
1	A	60	PRO	2.5
1	A	247	GLY	2.5
1	A	120	ARG	2.4
1	A	312	TYR	2.4
1	A	295	GLU	2.4
1	A	518	GLU	2.4
1	A	539	ASN	2.3
1	A	351	ALA	2.3
1	A	592	ALA	2.3
1	A	568	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	139	SER	2.3
1	A	590	VAL	2.3
1	A	202	VAL	2.3
1	A	497	LEU	2.3
1	A	522	TRP	2.3
1	A	594	PRO	2.2
1	A	95	LYS	2.2
1	A	308	ALA	2.2
1	A	331	LEU	2.2
1	A	396	ILE	2.2
1	A	409	LEU	2.2
1	A	32	GLY	2.2
1	A	93	ALA	2.2
1	A	487	LEU	2.1
1	A	514	HIS	2.1
1	A	253	GLY	2.1
1	A	151	LEU	2.1
1	A	251	PHE	2.1
1	A	280	PRO	2.1
1	A	140	LEU	2.1
1	A	562	VAL	2.1
1	A	41	HIS	2.1
1	A	277	TYR	2.1
1	A	177	GLN	2.0
1	A	55	ASN	2.0
1	A	244	ASP	2.0
1	A	591	GLU	2.0
1	A	243	ALA	2.0
1	A	117	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.