Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	6JOY
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 (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 (1)) were used in the production of this report:

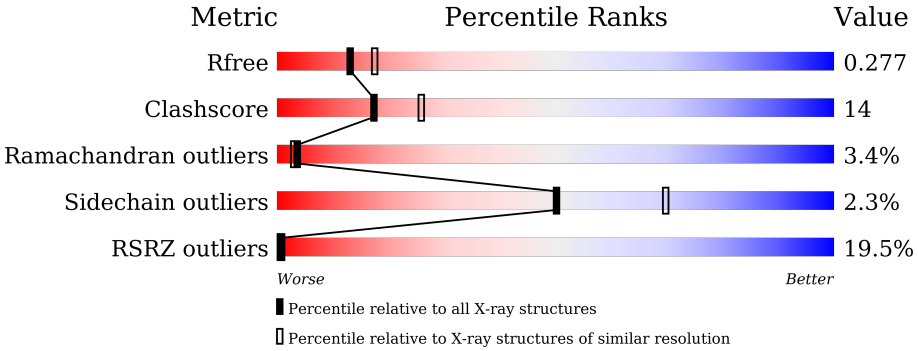
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.39 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 <=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	19% 75% 21% •

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	621	5132	3333	871	909	19	1	0	0

- Molecule 2 is water.

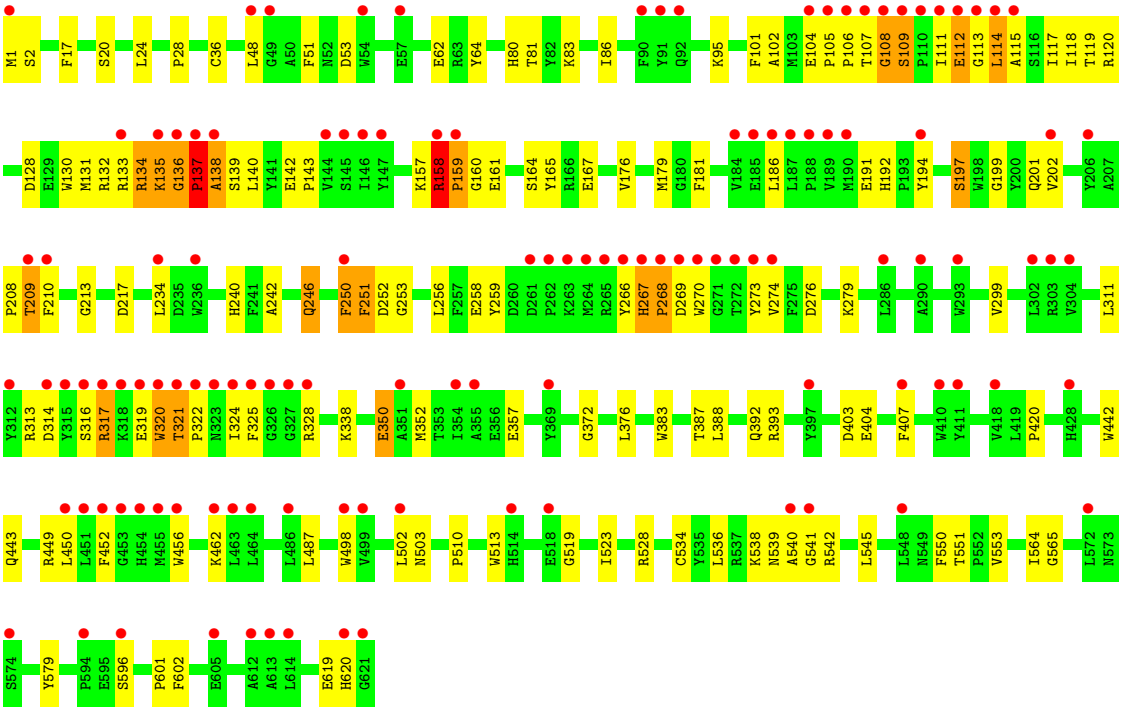
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	156	156	156	0	0

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: 1,4-alpha-glucan branching enzyme GlgB

Chain A:



4 Data and refinement statistics (i)

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 34.85 – 2.39	Depositor EDS
% Data completeness (in resolution range)	96.7 (31.42-2.39) 97.8 (34.85-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.247 , 0.278 0.246 , 0.277	Depositor DCC
R_{free} test set	3247 reflections (5.06%)	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 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	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.*

[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)

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	0.48	1/5336 (0.0%)	0.64	0/7280

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	534	CYS	CB-SG	-6.83	1.70	1.82

There are no bond angle outliers.

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 (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	5132	0	4771	137	0
2	A	156	0	0	11	1
All	All	5288	0	4771	137	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 14.

All (137) 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: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:107:THR:C	1:A:111:ILE:HD12	2.09	0.72
1:A:95:LYS:HE3	1:A:251:PHE:HA	1.72	0.72
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:133:ARG:C	1:A:135:LYS:H	2.09	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
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:2:SER:HB2	1:A:64:TYR:CE1	2.45	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:134:ARG:C	1:A:136:GLY:N	2.65	0.50
1:A:352:MET:HG2	1:A:376:LEU:HD23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:234:LEU:HD11	1:A:299:VAL:HG11	1.93	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:138:ALA:C	1:A:140:LEU:H	2.16	0.47
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:539:ASN:CG	1:A:540:ALA:H	2.17	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:319:GLU:CD	1:A:320:TRP:H	2.18	0.46
1:A:28:PRO:HG2	1:A:120:ARG:HG3	1.98	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:138:ALA:C	1:A:140:LEU:N	2.70	0.45
1:A:456:TRP:HA	1:A:462:LYS:HE3	1.97	0.45
1:A:81:THR:HB	1:A:115:ALA:HB3	1.99	0.45
1:A:133:ARG:C	1:A:135:LYS:N	2.69	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:456:TRP:NE1	2:A:712:HOH:O	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:456:TRP:CD1	1:A:456:TRP:N	2.88	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:106:PRO:HB2	1:A:113:GLY:C	2.41	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: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:456:TRP:CE2	2:A:712:HOH:O	2.75	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 3

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
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%)	515 (98%)	12 (2%)	50 70

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	PHE
1	A	62	GLU
1	A	114	LEU
1	A	158	ARG
1	A	197	SER
1	A	246	GLN
1	A	250	PHE
1	A	313	ARG
1	A	320	TRP
1	A	325	PHE
1	A	328	ARG
1	A	596	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	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)

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 (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	621/621 (100%)	1.39	121 (19%) 1 0	44, 54, 100, 159	1 (0%)

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	324	ILE	19.4
1	A	107	THR	17.5
1	A	320	TRP	17.3
1	A	268	PRO	15.8
1	A	323	ASN	15.6
1	A	326	GLY	14.3
1	A	266	TYR	13.5
1	A	315	TYR	13.2
1	A	321	THR	13.2
1	A	271	GLY	12.9
1	A	264	MET	12.5
1	A	325	PHE	12.4
1	A	322	PRO	12.2
1	A	267	HIS	12.2
1	A	262	PRO	11.7
1	A	137	PRO	11.4
1	A	270	TRP	11.4
1	A	269	ASP	11.4
1	A	1	MET	11.3
1	A	113	GLY	11.3
1	A	110	PRO	11.3
1	A	108	GLY	10.7
1	A	263	LYS	10.7
1	A	210	PHE	10.6
1	A	319	GLU	9.7
1	A	327	GLY	9.6
1	A	265	ARG	9.4

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Mol	Chain	Res	Type	RSRZ
1	A	317	ARG	9.2
1	A	318	LYS	9.1
1	A	272	THR	8.4
1	A	105	PRO	8.4
1	A	90	PHE	6.7
1	A	114	LEU	6.7
1	A	314	ASP	6.5
1	A	135	LYS	6.4
1	A	273	TYR	6.3
1	A	91	TYR	5.9
1	A	111	ILE	5.8
1	A	316	SER	5.7
1	A	463	LEU	5.0
1	A	261	ASP	4.8
1	A	250	PHE	4.6
1	A	209	THR	4.2
1	A	620	HIS	4.2
1	A	184	VAL	4.2
1	A	410	TRP	4.1
1	A	104	GLU	3.9
1	A	354	ILE	3.8
1	A	456	TRP	3.8
1	A	407	PHE	3.7
1	A	274	VAL	3.6
1	A	187	LEU	3.5
1	A	138	ALA	3.5
1	A	146	ILE	3.5
1	A	109	SER	3.4
1	A	411	TYR	3.3
1	A	464	LEU	3.3
1	A	614	LEU	3.3
1	A	499	VAL	3.3
1	A	158	ARG	3.3
1	A	498	TRP	3.3
1	A	502	LEU	3.2
1	A	572	LEU	3.2
1	A	613	ALA	3.2
1	A	189	VAL	3.1
1	A	190	MET	3.1
1	A	462	LYS	3.1
1	A	115	ALA	3.1
1	A	54	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	303	ARG	3.1
1	A	540	ALA	3.0
1	A	369	TYR	3.0
1	A	304	VAL	3.0
1	A	621	GLY	3.0
1	A	455	MET	3.0
1	A	451	LEU	2.9
1	A	147	TYR	2.9
1	A	312	TYR	2.9
1	A	106	PRO	2.9
1	A	452	PHE	2.8
1	A	286	LEU	2.8
1	A	186	LEU	2.7
1	A	236	TRP	2.7
1	A	328	ARG	2.7
1	A	48	LEU	2.7
1	A	351	ALA	2.7
1	A	541	GLY	2.6
1	A	302	LEU	2.6
1	A	185	GLU	2.6
1	A	136	GLY	2.6
1	A	112	GLU	2.6
1	A	234	LEU	2.6
1	A	594	PRO	2.6
1	A	144	VAL	2.5
1	A	612	ALA	2.5
1	A	92	GLN	2.5
1	A	293	TRP	2.5
1	A	355	ALA	2.5
1	A	514	HIS	2.5
1	A	453	GLY	2.4
1	A	290	ALA	2.4
1	A	194	TYR	2.4
1	A	206	TYR	2.4
1	A	133	ARG	2.4
1	A	574	SER	2.4
1	A	450	LEU	2.4
1	A	596	SER	2.3
1	A	518	GLU	2.3
1	A	49	GLY	2.3
1	A	486	LEU	2.3
1	A	57	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	159	PRO	2.2
1	A	397	TYR	2.2
1	A	145	SER	2.1
1	A	428	HIS	2.1
1	A	188	PRO	2.1
1	A	454	HIS	2.1
1	A	548	LEU	2.1
1	A	418	VAL	2.1
1	A	202	VAL	2.1
1	A	605	GLU	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.