Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 01:26 am BST

PDB ID	:	6HZH
Title	:	Apo structure of TP domain from Chlamydia trachomatis penicillin-binding protein 3
Authors	:	Bellini, D.; Koekemoer, L.; Newman, H.; Dowson, C.G.
Deposited on	:	2018-10-23
Resolution	:	1.83 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 following versions of software and data (see references ⓘ) were used in the production of this report:

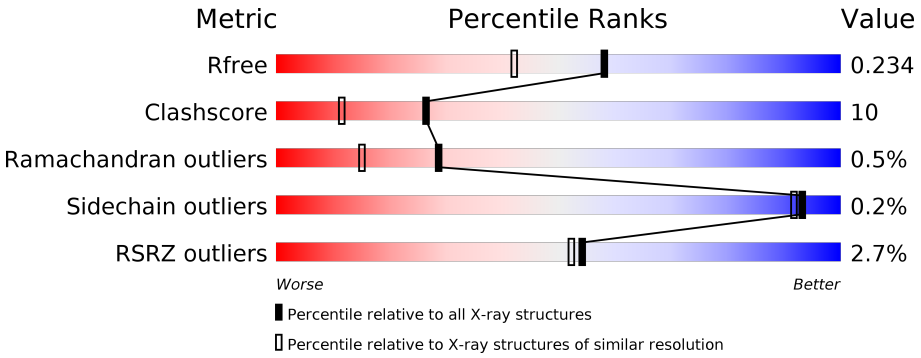
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

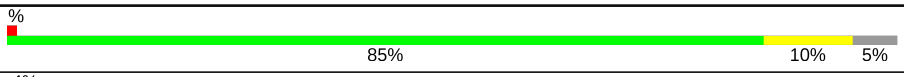
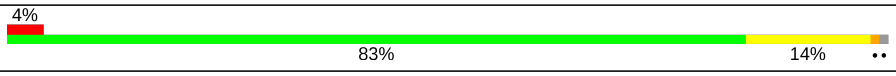
The reported resolution of this entry is 1.83 Å.

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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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 on 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	346	
1	B	346	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5150 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 Penicillin-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2444	1534	415	487	8			
1	B	342	Total	C	N	O	S	0	0	0
			2536	1590	428	509	9			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	261	GLY	-	expression tag	UNP A0A0E9FXJ8
A	262	PRO	-	expression tag	UNP A0A0E9FXJ8
A	263	GLY	-	expression tag	UNP A0A0E9FXJ8
A	264	TYR	-	expression tag	UNP A0A0E9FXJ8
A	265	GLN	-	expression tag	UNP A0A0E9FXJ8
A	266	ASP	-	expression tag	UNP A0A0E9FXJ8
A	267	PRO	-	expression tag	UNP A0A0E9FXJ8
A	?	-	ASP	deletion	UNP A0A0E9FXJ8
A	?	-	SER	deletion	UNP A0A0E9FXJ8
A	?	-	ASP	deletion	UNP A0A0E9FXJ8
A	?	-	SER	deletion	UNP A0A0E9FXJ8
A	?	-	PRO	deletion	UNP A0A0E9FXJ8
A	?	-	ASN	deletion	UNP A0A0E9FXJ8
A	?	-	PRO	deletion	UNP A0A0E9FXJ8
A	?	-	SER	deletion	UNP A0A0E9FXJ8
A	?	-	ASN	deletion	UNP A0A0E9FXJ8
A	?	-	LEU	deletion	UNP A0A0E9FXJ8
A	?	-	ASP	deletion	UNP A0A0E9FXJ8
A	?	-	SER	deletion	UNP A0A0E9FXJ8
A	?	-	ALA	deletion	UNP A0A0E9FXJ8
A	?	-	ASP	deletion	UNP A0A0E9FXJ8
A	?	-	VAL	deletion	UNP A0A0E9FXJ8
A	?	-	SER	deletion	UNP A0A0E9FXJ8
A	311	PRO	ASN	engineered mutation	UNP A0A0E9FXJ8
A	312	GLY	TRP	engineered mutation	UNP A0A0E9FXJ8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	261	GLY	-	expression tag	UNP A0A0E9FXJ8
B	262	PRO	-	expression tag	UNP A0A0E9FXJ8
B	263	GLY	-	expression tag	UNP A0A0E9FXJ8
B	264	TYR	-	expression tag	UNP A0A0E9FXJ8
B	265	GLN	-	expression tag	UNP A0A0E9FXJ8
B	266	ASP	-	expression tag	UNP A0A0E9FXJ8
B	267	PRO	-	expression tag	UNP A0A0E9FXJ8
B	?	-	ASP	deletion	UNP A0A0E9FXJ8
B	?	-	SER	deletion	UNP A0A0E9FXJ8
B	?	-	ASP	deletion	UNP A0A0E9FXJ8
B	?	-	SER	deletion	UNP A0A0E9FXJ8
B	?	-	PRO	deletion	UNP A0A0E9FXJ8
B	?	-	ASN	deletion	UNP A0A0E9FXJ8
B	?	-	PRO	deletion	UNP A0A0E9FXJ8
B	?	-	SER	deletion	UNP A0A0E9FXJ8
B	?	-	ASN	deletion	UNP A0A0E9FXJ8
B	?	-	LEU	deletion	UNP A0A0E9FXJ8
B	?	-	ASP	deletion	UNP A0A0E9FXJ8
B	?	-	SER	deletion	UNP A0A0E9FXJ8
B	?	-	ALA	deletion	UNP A0A0E9FXJ8
B	?	-	ASP	deletion	UNP A0A0E9FXJ8
B	?	-	VAL	deletion	UNP A0A0E9FXJ8
B	?	-	SER	deletion	UNP A0A0E9FXJ8
B	311	PRO	ASN	engineered mutation	UNP A0A0E9FXJ8
B	312	GLY	TRP	engineered mutation	UNP A0A0E9FXJ8

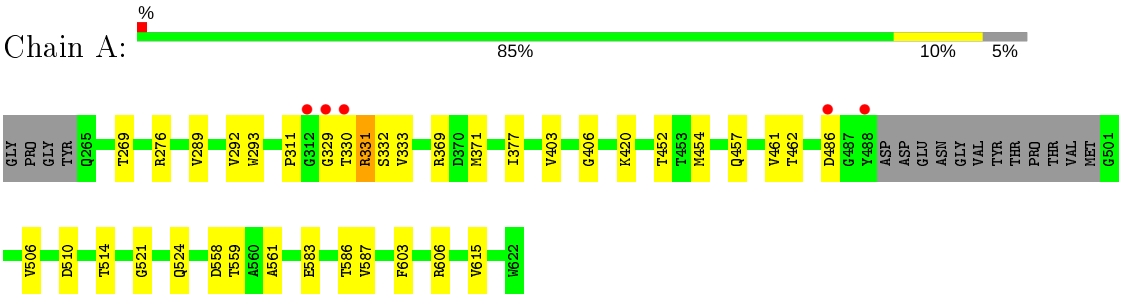
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	103	Total O 103 103	0	0
2	B	67	Total O 67 67	0	0

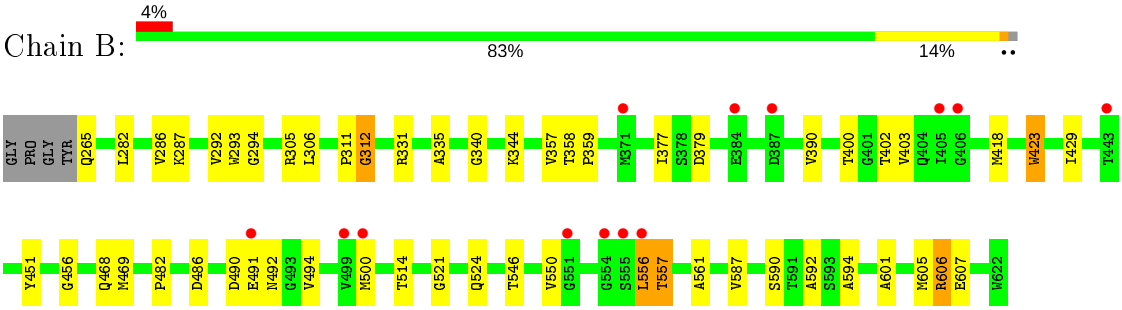
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Penicillin-binding protein



- Molecule 1: Penicillin-binding protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	105.44Å 105.44Å 118.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	72.34 – 1.83 72.34 – 1.83	Depositor EDS
% Data completeness (in resolution range)	67.2 (72.34-1.83) 67.4 (72.34-1.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.198 , 0.242 0.199 , 0.234	Depositor DCC
R_{free} test set	2362 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å^2)	29.8	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 40.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5150	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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

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	0.49	0/2490	0.60	0/3393
1	B	0.53	2/2585 (0.1%)	0.60	0/3526
All	All	0.51	2/5075 (0.0%)	0.60	0/6919

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	606	ARG	C-N	-12.31	1.05	1.34
1	B	423	TRP	CD2-CE2	5.06	1.47	1.41

There are no bond angle outliers.

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	2444	0	2426	39	0
1	B	2536	0	2506	64	0
2	A	103	0	0	2	1
2	B	67	0	0	3	1
All	All	5150	0	4932	102	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 10.

All (102) 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:550:VAL:HG22	1:B:556:LEU:CD2	1.74	1.17
1:B:550:VAL:CG2	1:B:556:LEU:CD2	2.27	1.12
1:B:550:VAL:CG2	1:B:556:LEU:HD21	1.84	1.08
1:A:269:THR:HG22	1:A:486:ASP:OD1	1.56	1.05
1:B:490:ASP:OD2	1:B:494:VAL:HB	1.54	1.04
1:A:406:GLY:HA3	1:A:454:MET:HE3	1.42	1.01
1:A:406:GLY:HA3	1:A:454:MET:CE	1.94	0.96
1:B:357:VAL:CG1	1:B:390:VAL:HG21	2.01	0.90
1:B:550:VAL:HG23	1:B:556:LEU:CD2	2.03	0.89
1:B:550:VAL:HG23	1:B:556:LEU:HD21	1.55	0.88
1:B:423:TRP:HE1	1:B:469:MET:HE2	1.37	0.86
1:B:550:VAL:HG22	1:B:556:LEU:CG	2.06	0.85
1:B:561:ALA:HB2	1:B:587:VAL:HG13	1.58	0.84
1:B:550:VAL:CG2	1:B:556:LEU:HD23	2.05	0.84
1:B:292:VAL:HG23	1:B:293:TRP:CD1	2.13	0.84
1:B:423:TRP:NE1	1:B:469:MET:HE2	1.98	0.77
1:B:550:VAL:HG22	1:B:556:LEU:HG	1.66	0.76
1:A:269:THR:CG2	1:A:486:ASP:OD1	2.33	0.76
1:A:329:GLY:HA3	2:A:794:HOH:O	1.85	0.75
1:A:330:THR:O	1:A:332:SER:N	2.20	0.74
1:B:403:VAL:HG13	1:B:451:TYR:CE1	2.24	0.72
1:B:306:LEU:HD12	1:B:429:ILE:HD11	1.73	0.71
1:A:403:VAL:HA	1:A:454:MET:CE	2.24	0.68
1:B:357:VAL:HG11	1:B:390:VAL:HG21	1.75	0.68
1:A:369:ARG:HG2	1:A:371:MET:HE1	1.75	0.68
1:B:490:ASP:OD2	1:B:494:VAL:CB	2.37	0.66
1:A:559:THR:HG21	1:A:586:THR:HG22	1.76	0.66
1:A:369:ARG:HB3	1:A:371:MET:HE3	1.80	0.62
1:B:423:TRP:HE1	1:B:469:MET:CE	2.12	0.61
1:A:311:PRO:C	1:A:329:GLY:H	2.03	0.60
1:B:491:GLU:O	1:B:492:ASN:CB	2.49	0.60
1:A:406:GLY:HA3	1:A:454:MET:HE1	1.84	0.59
1:A:369:ARG:HD3	1:A:371:MET:HE3	1.84	0.59
1:B:282:LEU:O	1:B:286:VAL:HG23	2.03	0.58
1:B:550:VAL:HG22	1:B:556:LEU:HD21	1.53	0.57
1:A:330:THR:O	1:A:333:VAL:N	2.29	0.56
1:B:587:VAL:HG22	1:B:592:ALA:HB2	1.87	0.56
1:A:289:VAL:CG1	1:A:587:VAL:HG12	2.35	0.56
1:B:521:GLY:HA2	1:B:524:GLN:HG3	1.89	0.55
1:A:561:ALA:HB2	1:A:587:VAL:HG23	1.89	0.55
1:A:369:ARG:CG	1:A:371:MET:HE1	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:THR:O	1:A:331:ARG:C	2.45	0.54
1:B:556:LEU:O	1:B:557:THR:CG2	2.55	0.54
1:A:292:VAL:HG23	1:A:293:TRP:CD1	2.42	0.54
1:A:461:VAL:HG12	1:A:462:THR:O	2.08	0.53
1:A:289:VAL:HG11	1:A:587:VAL:HG12	1.91	0.53
1:B:306:LEU:CD1	1:B:429:ILE:CD1	2.87	0.53
1:B:556:LEU:O	1:B:557:THR:HG23	2.09	0.53
1:A:369:ARG:HD3	1:A:371:MET:CE	2.38	0.52
1:B:550:VAL:CA	1:B:556:LEU:HD23	2.39	0.52
1:B:306:LEU:CD1	1:B:429:ILE:HD11	2.39	0.51
1:B:491:GLU:O	1:B:492:ASN:HB2	2.12	0.50
1:A:403:VAL:HA	1:A:454:MET:HE1	1.93	0.50
1:B:403:VAL:HG13	1:B:451:TYR:CD1	2.46	0.50
1:B:606:ARG:O	1:B:607:GLU:C	2.46	0.50
1:A:558:ASP:OD1	1:A:583:GLU:O	2.30	0.50
1:A:369:ARG:CG	1:A:371:MET:CE	2.89	0.49
1:A:603:PHE:HD1	1:A:606:ARG:NH1	2.09	0.49
1:A:420:LYS:HB3	1:A:506:VAL:HG13	1.95	0.49
1:B:550:VAL:HG23	1:B:556:LEU:HD23	1.79	0.49
1:B:590:SER:O	1:B:594:ALA:HB3	2.13	0.49
1:B:561:ALA:CB	1:B:587:VAL:HG13	2.37	0.48
1:B:550:VAL:HA	1:B:556:LEU:HD23	1.96	0.48
1:A:403:VAL:HA	1:A:454:MET:HE2	1.93	0.47
1:B:556:LEU:C	1:B:557:THR:HG23	2.35	0.47
1:B:306:LEU:HD12	1:B:429:ILE:CD1	2.43	0.47
1:B:358:THR:HB	1:B:359:PRO:HD2	1.97	0.47
1:B:550:VAL:HG22	1:B:556:LEU:HD23	1.73	0.46
1:B:601:ALA:O	1:B:605:MET:HG2	2.16	0.46
1:B:358:THR:HB	1:B:359:PRO:CD	2.46	0.46
1:B:305:ARG:HD2	1:B:486:ASP:OD1	2.15	0.46
1:A:452:THR:HB	1:A:457:GLN:HB2	1.98	0.45
1:B:377:ILE:HG13	1:B:403:VAL:HG21	1.97	0.45
1:A:369:ARG:HB3	1:A:371:MET:CE	2.45	0.45
1:B:423:TRP:CE2	1:B:469:MET:HE2	2.52	0.45
1:A:311:PRO:C	1:A:329:GLY:N	2.69	0.44
1:B:491:GLU:O	1:B:492:ASN:CG	2.56	0.44
1:B:490:ASP:OD2	1:B:494:VAL:O	2.36	0.44
1:B:546:THR:HG23	1:B:587:VAL:O	2.18	0.44
1:A:521:GLY:HA2	1:A:524:GLN:HG3	2.00	0.44
1:B:344:LYS:HD3	1:B:402:THR:HG21	2.00	0.43
1:B:490:ASP:OD1	1:B:491:GLU:O	2.36	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:GLN:N	2:B:708:HOH:O	2.51	0.43
1:B:293:TRP:CE3	1:B:331:ARG:HD2	2.53	0.42
1:B:468:GLN:OE1	1:B:482:PRO:HD3	2.18	0.42
1:B:379:ASP:OD1	1:B:400:THR:HG23	2.20	0.42
1:B:418:MET:HE2	2:B:732:HOH:O	2.20	0.42
1:B:357:VAL:HG13	1:B:390:VAL:HG21	1.94	0.42
1:A:369:ARG:CD	1:A:371:MET:CE	2.98	0.42
1:B:306:LEU:HD11	1:B:429:ILE:CD1	2.50	0.42
1:A:510:ASP:O	1:A:514:THR:HG23	2.20	0.41
1:B:340:GLY:O	1:B:456:GLY:HA3	2.20	0.41
1:A:377:ILE:HG13	1:A:403:VAL:HG11	2.01	0.41
1:A:292:VAL:HG11	1:A:583:GLU:CD	2.41	0.41
1:B:311:PRO:C	1:B:312:GLY:O	2.58	0.41
1:A:311:PRO:O	1:A:329:GLY:N	2.44	0.41
1:A:276:ARG:HH12	1:B:287:LYS:HE2	1.86	0.41
1:B:500:MET:HG2	2:B:741:HOH:O	2.21	0.41
1:A:615:VAL:HG13	2:A:793:HOH:O	2.19	0.41
1:B:331:ARG:HD3	1:B:335:ALA:HB2	2.03	0.40
1:B:294:GLY:O	1:B:311:PRO:HD3	2.21	0.40
1:B:359:PRO:HG3	1:B:514:THR:HG23	2.04	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:793:HOH:O	2:B:707:HOH:O[3_655]	1.88	0.32

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	326/346 (94%)	321 (98%)	4 (1%)	1 (0%)	41 27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	340/346 (98%)	337 (99%)	1 (0%)	2 (1%)	25 12
All	All	666/692 (96%)	658 (99%)	5 (1%)	3 (0%)	29 15

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	331	ARG
1	B	312	GLY
1	B	557	THR

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	260/273 (95%)	260 (100%)	0	100 100
1	B	271/273 (99%)	270 (100%)	1 (0%)	91 88
All	All	531/546 (97%)	530 (100%)	1 (0%)	93 92

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

Mol	Chain	Res	Type
1	B	556	LEU

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

Mol	Chain	Res	Type
1	B	602	GLN

5.3.3 RNA (i)

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 carbohydrates 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	606:ARG	C	607:GLU	N	1.05

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, 95^{th} 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	330/346 (95%)	-0.20	5 (1%)	73	73	17, 27, 47, 76	0
1	B	342/346 (98%)	0.04	13 (3%)	40	37	20, 34, 64, 88	0
All	All	672/692 (97%)	-0.08	18 (2%)	54	52	17, 30, 59, 88	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	556	LEU	9.6
1	B	555	SER	7.4
1	B	491	GLU	5.2
1	A	312	GLY	4.4
1	B	499	VAL	3.9
1	A	329	GLY	3.6
1	B	554	GLY	3.6
1	A	488	TYR	3.4
1	B	500	MET	3.3
1	A	330	THR	3.1
1	B	443	THR	3.0
1	B	371	MET	3.0
1	B	384	GLU	2.7
1	B	551	GLY	2.5
1	B	406	GLY	2.5
1	B	387	ASP	2.2
1	A	486	ASP	2.1
1	B	405	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 (i)

There are no carbohydrates 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.