Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:14 am BST

PDB ID	:	6FSU
Title	:	Crystal structure of E.coli BamA beta-barrel with a C-terminal extension
Authors	:	Zahn, M.; Hartmann, J.-B.; Hiller, S.
Deposited on	:	2018-02-20
Resolution	:	2.60 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:

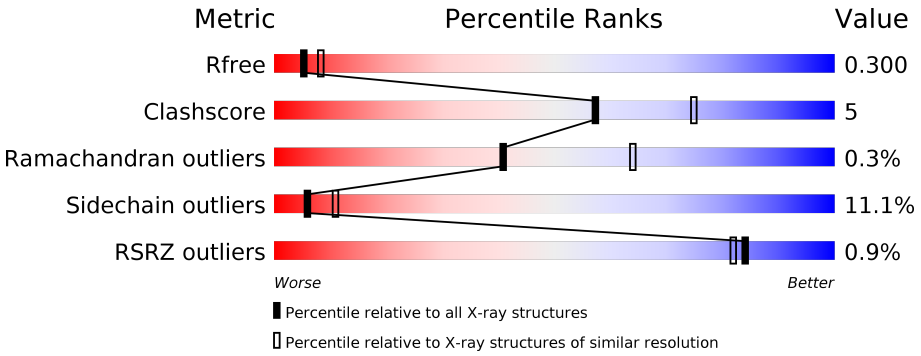
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	420	74% 15% • 8%
1	B	420	% 73% 17% • 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6195 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 Outer membrane protein assembly factor BamA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			3075	1958	497	610	10			
1	B	387	Total	C	N	O	S	0	0	0
			3067	1954	496	607	10			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	400	MET	-	initiating methionine	UNP P0A942
A	401	GLY	-	expression tag	UNP P0A942
A	402	SER	-	expression tag	UNP P0A942
A	403	SER	-	expression tag	UNP P0A942
A	404	HIS	-	expression tag	UNP P0A942
A	405	HIS	-	expression tag	UNP P0A942
A	406	HIS	-	expression tag	UNP P0A942
A	407	HIS	-	expression tag	UNP P0A942
A	408	HIS	-	expression tag	UNP P0A942
A	409	HIS	-	expression tag	UNP P0A942
A	410	SER	-	expression tag	UNP P0A942
A	411	SER	-	expression tag	UNP P0A942
A	412	GLY	-	expression tag	UNP P0A942
A	413	GLU	-	expression tag	UNP P0A942
A	414	ASN	-	expression tag	UNP P0A942
A	415	LEU	-	expression tag	UNP P0A942
A	416	TYR	-	expression tag	UNP P0A942
A	417	PHE	-	expression tag	UNP P0A942
A	418	GLN	-	expression tag	UNP P0A942
A	419	HIS	-	expression tag	UNP P0A942
A	420	MET	-	expression tag	UNP P0A942
A	690	SER	CYS	conflict	UNP P0A942
A	700	SER	CYS	conflict	UNP P0A942
A	811	MET	-	expression tag	UNP P0A942
A	812	GLU	-	expression tag	UNP P0A942

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Chain	Residue	Modelled	Actual	Comment	Reference
A	813	ASN	-	expression tag	UNP P0A942
A	814	VAL	-	expression tag	UNP P0A942
A	815	ALA	-	expression tag	UNP P0A942
A	816	LEU	-	expression tag	UNP P0A942
A	817	ASP	-	expression tag	UNP P0A942
A	818	PHE	-	expression tag	UNP P0A942
A	819	SER	-	expression tag	UNP P0A942
B	400	MET	-	initiating methionine	UNP P0A942
B	401	GLY	-	expression tag	UNP P0A942
B	402	SER	-	expression tag	UNP P0A942
B	403	SER	-	expression tag	UNP P0A942
B	404	HIS	-	expression tag	UNP P0A942
B	405	HIS	-	expression tag	UNP P0A942
B	406	HIS	-	expression tag	UNP P0A942
B	407	HIS	-	expression tag	UNP P0A942
B	408	HIS	-	expression tag	UNP P0A942
B	409	HIS	-	expression tag	UNP P0A942
B	410	SER	-	expression tag	UNP P0A942
B	411	SER	-	expression tag	UNP P0A942
B	412	GLY	-	expression tag	UNP P0A942
B	413	GLU	-	expression tag	UNP P0A942
B	414	ASN	-	expression tag	UNP P0A942
B	415	LEU	-	expression tag	UNP P0A942
B	416	TYR	-	expression tag	UNP P0A942
B	417	PHE	-	expression tag	UNP P0A942
B	418	GLN	-	expression tag	UNP P0A942
B	419	HIS	-	expression tag	UNP P0A942
B	420	MET	-	expression tag	UNP P0A942
B	690	SER	CYS	conflict	UNP P0A942
B	700	SER	CYS	conflict	UNP P0A942
B	811	MET	-	expression tag	UNP P0A942
B	812	GLU	-	expression tag	UNP P0A942
B	813	ASN	-	expression tag	UNP P0A942
B	814	VAL	-	expression tag	UNP P0A942
B	815	ALA	-	expression tag	UNP P0A942
B	816	LEU	-	expression tag	UNP P0A942
B	817	ASP	-	expression tag	UNP P0A942
B	818	PHE	-	expression tag	UNP P0A942
B	819	SER	-	expression tag	UNP P0A942

- Molecule 2 is water.

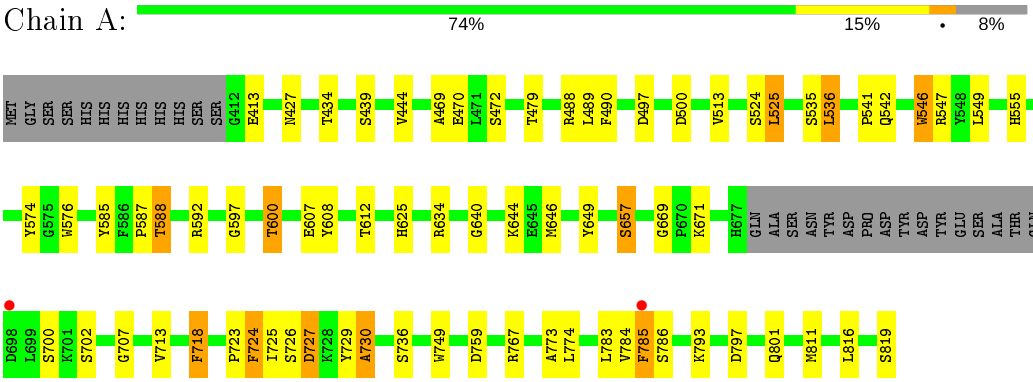
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	26	Total O 26 26	0	0
2	B	27	Total O 27 27	0	0

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.

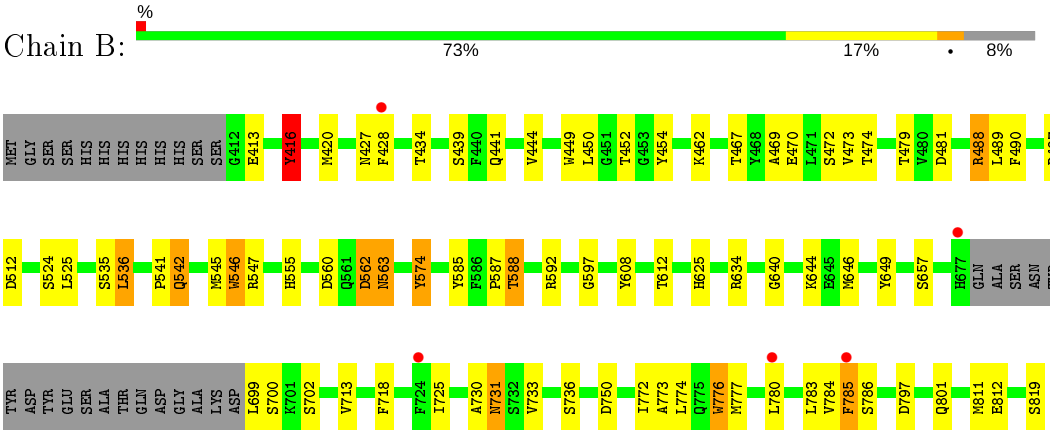
- Molecule 1: Outer membrane protein assembly factor BamA

Chain A:



- Molecule 1: Outer membrane protein assembly factor BamA

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	122.74Å 159.38Å 55.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.84 – 2.60 55.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (66.84-2.60) 99.8 (55.93-2.60)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.269 , 0.298 0.272 , 0.300	Depositor DCC
R_{free} test set	1747 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	38.1	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 35.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6195	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.26 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8085e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	1.03	5/3169 (0.2%)	1.07	12/4310 (0.3%)
1	B	1.03	2/3161 (0.1%)	1.09	11/4299 (0.3%)
All	All	1.03	7/6330 (0.1%)	1.08	23/8609 (0.3%)

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	3
1	B	0	2
All	All	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	574	TYR	CG-CD2	-6.45	1.30	1.39
1	A	576	TRP	CE3-CZ3	5.65	1.48	1.38
1	A	657	SER	CB-OG	5.59	1.49	1.42
1	A	785	PHE	CG-CD2	5.52	1.47	1.38
1	B	785	PHE	CG-CD2	5.50	1.47	1.38
1	A	749	TRP	CB-CG	-5.16	1.41	1.50
1	A	707	GLY	C-O	5.12	1.31	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	592	ARG	NE-CZ-NH1	9.55	125.07	120.30
1	A	592	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	B	785	PHE	CB-CG-CD1	7.27	125.89	120.80
1	B	750	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	A	785	PHE	CB-CG-CD1	7.10	125.77	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	547	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	A	724	PHE	N-CA-C	-6.58	93.22	111.00
1	B	547	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	B	699	LEU	CA-CB-CG	6.01	129.12	115.30
1	B	797	ASP	CB-CG-OD1	5.86	123.58	118.30
1	B	776	TRP	CA-C-N	5.77	129.89	117.20
1	A	439	SER	CB-CA-C	-5.69	99.30	110.10
1	A	592	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	416	TYR	CA-CB-CG	5.55	123.95	113.40
1	A	767	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	776	TRP	N-CA-C	5.40	125.58	111.00
1	A	525	LEU	CB-CG-CD1	-5.30	101.99	111.00
1	B	776	TRP	O-C-N	-5.29	114.23	122.70
1	A	479	THR	N-CA-CB	5.29	120.34	110.30
1	A	797	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	497	ASP	CB-CG-OD1	5.15	122.94	118.30
1	B	497	ASP	CB-CG-OD1	5.06	122.85	118.30
1	A	759	ASP	CB-CG-OD1	5.00	122.81	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	562	ASP	Peptide
1	A	563	ASN	Peptide
1	A	723	PRO	Peptide
1	B	562	ASP	Peptide
1	B	563	ASN	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	3075	0	2809	21	0
1	B	3067	0	2805	37	0
2	A	26	0	0	0	0
2	B	27	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6195	0	5614	57	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 5.

All (57) 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:600:THR:HG21	1:A:607:GLU:HA	1.46	0.98
1:B:776:TRP:O	1:B:776:TRP:CD1	2.29	0.85
1:B:542:GLN:HE22	1:B:545:MET:CE	2.04	0.69
1:A:640:GLY:HA3	1:A:644:LYS:O	1.96	0.66
1:B:640:GLY:HA3	1:B:644:LYS:O	1.95	0.65
1:A:574:TYR:CZ	1:A:597:GLY:HA3	2.33	0.63
1:B:574:TYR:CZ	1:B:597:GLY:HA3	2.34	0.63
1:B:536:LEU:HD11	1:B:649:TYR:CD1	2.32	0.63
1:A:536:LEU:HD11	1:A:649:TYR:CD1	2.36	0.61
1:A:588:THR:CG2	1:A:625:HIS:ND1	2.65	0.59
1:B:449:TRP:O	1:B:452:THR:HG22	2.02	0.59
1:B:588:THR:CG2	1:B:625:HIS:ND1	2.66	0.59
1:B:725:ILE:HD13	1:B:733:VAL:HG11	1.85	0.58
1:B:462:LYS:CD	1:B:467:THR:HG22	2.34	0.58
1:B:452:THR:HG23	1:B:454:TYR:H	1.69	0.57
1:B:730:ALA:O	1:B:731:ASN:CB	2.53	0.56
1:B:730:ALA:O	1:B:731:ASN:HB3	2.04	0.56
1:B:608:TYR:CD2	1:B:646:MET:HG3	2.42	0.55
1:B:462:LYS:HD3	1:B:467:THR:HG22	1.87	0.55
1:A:608:TYR:CD2	1:A:646:MET:HG3	2.42	0.54
1:B:479:THR:HG22	1:B:481:ASP:N	2.25	0.52
1:B:479:THR:HG22	1:B:481:ASP:H	1.73	0.52
1:B:783:LEU:HD23	1:B:784:VAL:N	2.25	0.52
1:A:783:LEU:HD23	1:A:784:VAL:N	2.26	0.50
1:B:776:TRP:O	1:B:777:MET:C	2.45	0.50
1:B:736:SER:OG	1:B:773:ALA:HB3	2.13	0.49
1:A:727:ASP:CG	1:A:730:ALA:HB2	2.34	0.48
1:A:729:TYR:O	1:A:730:ALA:C	2.51	0.47
1:A:783:LEU:C	1:A:783:LEU:HD23	2.35	0.47
1:B:725:ILE:O	1:B:725:ILE:HG23	2.14	0.47
1:B:783:LEU:HD23	1:B:783:LEU:C	2.36	0.46
1:A:634:ARG:HB3	1:A:713:VAL:HB	1.98	0.46
1:B:725:ILE:HD13	1:B:733:VAL:CG1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:776:TRP:O	1:B:776:TRP:HD1	1.90	0.46
1:B:469:ALA:O	1:B:490:PHE:HA	2.16	0.46
1:A:736:SER:OG	1:A:773:ALA:HB3	2.16	0.45
1:A:469:ALA:O	1:A:490:PHE:HA	2.17	0.45
1:B:541:PRO:HA	1:B:546:TRP:CZ3	2.53	0.44
1:A:525:LEU:HD11	1:B:525:LEU:HD11	1.99	0.44
1:B:462:LYS:HD2	1:B:467:THR:HG22	2.00	0.43
1:B:634:ARG:HB3	1:B:713:VAL:HB	2.00	0.42
1:A:718:PHE:N	1:A:718:PHE:CD1	2.87	0.42
1:A:470:GLU:HA	1:A:489:LEU:O	2.19	0.42
1:A:669:GLY:O	1:A:671:LYS:HE3	2.20	0.42
1:B:473:VAL:O	1:B:474:THR:HG22	2.20	0.42
1:A:585:TYR:O	1:A:587:PRO:HD3	2.19	0.42
1:B:585:TYR:O	1:B:587:PRO:HD3	2.20	0.41
1:B:776:TRP:CG	1:B:776:TRP:O	2.73	0.41
1:A:725:ILE:HD12	1:A:729:TYR:HB2	2.01	0.41
1:A:541:PRO:HA	1:A:546:TRP:CZ3	2.54	0.41
1:B:470:GLU:HA	1:B:489:LEU:O	2.20	0.41
1:B:413:GLU:O	1:B:416:TYR:HB2	2.20	0.41
1:B:718:PHE:N	1:B:718:PHE:CD1	2.89	0.40
1:A:718:PHE:O	1:A:736:SER:HA	2.22	0.40
1:B:718:PHE:O	1:B:736:SER:HA	2.21	0.40
1:B:488:ARG:NH2	1:B:512:ASP:OD2	2.45	0.40
1:B:542:GLN:NE2	1:B:545:MET:SD	2.95	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	384/420 (91%)	365 (95%)	18 (5%)	1 (0%)	41 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	383/420 (91%)	363 (95%)	19 (5%)	1 (0%)	41 64
All	All	767/840 (91%)	728 (95%)	37 (5%)	2 (0%)	41 64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	730	ALA
1	B	731	ASN

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	326/353 (92%)	289 (89%)	37 (11%)	6 10
1	B	325/353 (92%)	290 (89%)	35 (11%)	6 12
All	All	651/706 (92%)	579 (89%)	72 (11%)	6 11

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	413	GLU
1	A	427	ASN
1	A	434	THR
1	A	444	VAL
1	A	472	SER
1	A	488	ARG
1	A	500	ASP
1	A	513	VAL
1	A	524	SER
1	A	535	SER
1	A	536	LEU
1	A	542	GLN
1	A	546	TRP
1	A	549	LEU

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Mol	Chain	Res	Type
1	A	555	HIS
1	A	560	ASP
1	A	561	GLN
1	A	562	ASP
1	A	563	ASN
1	A	588	THR
1	A	600	THR
1	A	612	THR
1	A	657	SER
1	A	700	SER
1	A	702	SER
1	A	718	PHE
1	A	724	PHE
1	A	726	SER
1	A	727	ASP
1	A	774	LEU
1	A	785	PHE
1	A	786	SER
1	A	793	LYS
1	A	801	GLN
1	A	811	MET
1	A	816	LEU
1	A	819	SER
1	B	416	TYR
1	B	420	MET
1	B	427	ASN
1	B	428	PHE
1	B	434	THR
1	B	439	SER
1	B	441	GLN
1	B	444	VAL
1	B	450	LEU
1	B	472	SER
1	B	488	ARG
1	B	500	ASP
1	B	524	SER
1	B	535	SER
1	B	536	LEU
1	B	542	GLN
1	B	546	TRP
1	B	555	HIS
1	B	560	ASP

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Mol	Chain	Res	Type
1	B	562	ASP
1	B	563	ASN
1	B	588	THR
1	B	612	THR
1	B	657	SER
1	B	700	SER
1	B	702	SER
1	B	772	ILE
1	B	774	LEU
1	B	780	LEU
1	B	785	PHE
1	B	786	SER
1	B	801	GLN
1	B	811	MET
1	B	812	GLU
1	B	819	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	538	ASN
1	A	563	ASN
1	A	664	GLN
1	B	418	GLN
1	B	427	ASN
1	B	441	GLN
1	B	542	GLN
1	B	563	ASN
1	B	664	GLN
1	B	731	ASN

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 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

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, 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	388/420 (92%)	-0.25	2 (0%)	91	89	24, 42, 81, 117	0
1	B	387/420 (92%)	-0.13	5 (1%)	77	73	24, 43, 82, 121	0
All	All	775/840 (92%)	-0.19	7 (0%)	84	82	24, 42, 83, 121	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	724	PHE	4.4
1	B	785	PHE	3.5
1	A	785	PHE	3.2
1	A	698	ASP	2.7
1	B	677	HIS	2.4
1	B	428	PHE	2.4
1	B	780	LEU	2.1

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 carbohydrates 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.