



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:55 PM GMT

PDB ID : 4N75
Title : Structural Basis of BamA-mediate Outer Membrane Protein Biogenesis
Authors : Ni, D.C.
Deposited on : 2013-10-14
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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

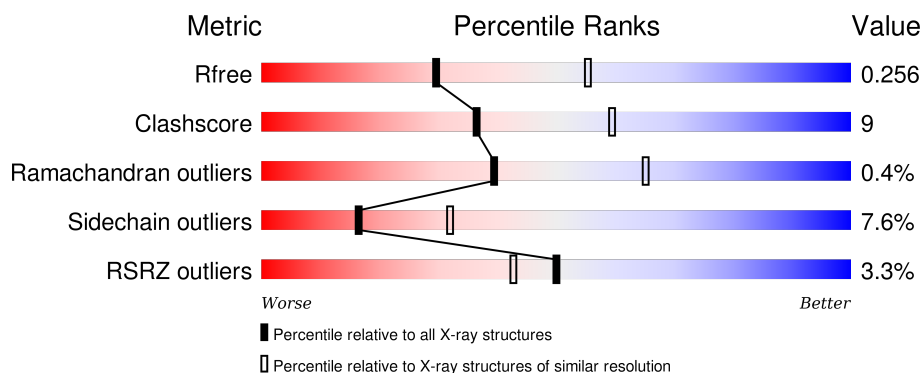
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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. 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	385	<div> <div>4%</div> <div>77%</div> <div>19%</div> <div>...</div> </div>
1	B	385	<div> <div>3%</div> <div>77%</div> <div>16%</div> <div>..</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5890 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	379	Total	C	N	O	S	0	0	0
			2947	1877	478	582	10			
1	B	370	Total	C	N	O	S	0	0	0
			2911	1856	471	574	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	426	MET	-	EXPRESSION TAG	UNP P0A940
B	426	MET	-	EXPRESSION TAG	UNP P0A940

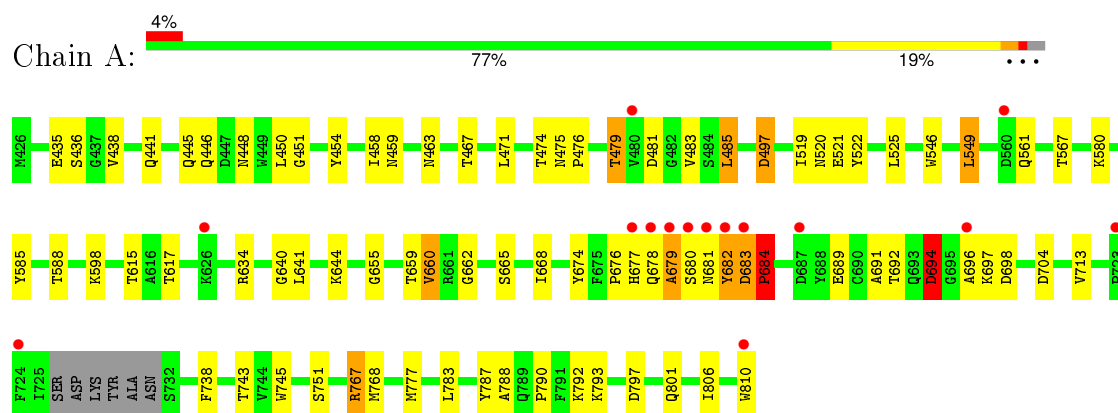
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	13	Total	O	0	0
			13	13		
2	B	19	Total	O	0	0
			19	19		

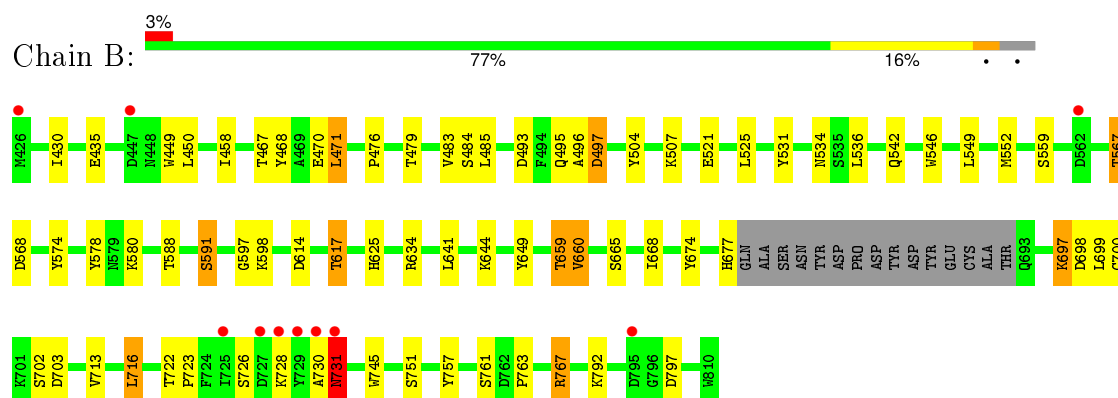
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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



- Molecule 1: Outer membrane protein assembly factor BamA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	118.49Å 159.88Å 56.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.27 – 2.60 38.61 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.2 (36.27-2.60) 91.3 (38.61-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.205 , 0.253 0.209 , 0.256	Depositor DCC
R_{free} test set	1915 reflections (6.28%)	DCC
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	6 of 31854 reflections (0.019%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5890	wwPDB-VP
Average B, all atoms (Å ²)	51.0	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 31.44 % 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 1.1073e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.57	2/3037 (0.1%)	0.77	9/4139 (0.2%)
1	B	0.50	0/3000	0.68	2/4083 (0.0%)
All	All	0.54	2/6037 (0.0%)	0.73	11/8222 (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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	684	PRO	N-CD	11.88	1.64	1.47
1	A	697	LYS	C-N	9.23	1.55	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	697	LYS	CB-CA-C	11.34	133.07	110.40
1	A	684	PRO	CA-N-CD	-8.09	100.17	111.50
1	B	731	ASN	CB-CA-C	-7.20	96.01	110.40
1	A	694	ASP	N-CA-C	-7.11	91.81	111.00
1	A	450	LEU	CA-CB-CG	6.77	130.88	115.30
1	A	698	ASP	CB-CA-C	-6.65	97.10	110.40
1	B	702	SER	N-CA-CB	-6.62	100.57	110.50
1	A	697	LYS	O-C-N	6.40	132.94	122.70
1	A	697	LYS	CA-C-N	-6.02	103.96	117.20
1	A	689	GLU	N-CA-C	5.62	126.18	111.00
1	A	694	ASP	CB-CA-C	5.07	120.55	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	676	PRO	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	2947	0	2660	62	0
1	B	2911	0	2666	45	0
2	A	13	0	0	0	0
2	B	19	0	0	1	0
All	All	5890	0	5326	106	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 9.

All (106) 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:682:TYR:CD1	1:A:684:PRO:HD3	1.69	1.26
1:B:588:THR:HG21	1:B:625:HIS:HB3	1.36	1.06
1:A:682:TYR:HD1	1:A:684:PRO:HD3	0.85	1.00
1:A:682:TYR:HD1	1:A:684:PRO:CD	1.79	0.94
1:A:561:GLN:HB2	1:A:677:HIS:HE1	1.45	0.79
1:B:634:ARG:HB3	1:B:713:VAL:HG22	1.65	0.79
1:A:681:ASN:O	1:A:682:TYR:HD2	1.65	0.78
1:A:561:GLN:HB2	1:A:677:HIS:CE1	2.21	0.75
1:A:681:ASN:C	1:A:682:TYR:HD2	1.91	0.74
1:A:681:ASN:O	1:A:682:TYR:CD2	2.42	0.73
1:A:681:ASN:C	1:A:682:TYR:CD2	2.63	0.72
1:A:678:GLN:O	1:A:679:ALA:HB2	1.90	0.71
1:B:730:ALA:O	1:B:731:ASN:HB2	1.93	0.67
1:A:783:LEU:HG	1:A:806:ILE:HD12	1.77	0.67
1:A:682:TYR:CD1	1:A:684:PRO:CD	2.64	0.66
1:A:634:ARG:HB3	1:A:713:VAL:HG22	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:THR:HB	1:B:483:VAL:HB	1.79	0.65
1:A:668:ILE:HG23	1:A:767:ARG:HD2	1.79	0.64
1:A:680:SER:O	1:A:682:TYR:CE2	2.50	0.64
1:A:479:THR:HB	1:A:483:VAL:HB	1.78	0.64
1:B:534:ASN:HB2	1:B:567:THR:HG23	1.85	0.59
1:A:681:ASN:O	1:A:682:TYR:HB3	2.04	0.57
1:B:730:ALA:C	1:B:731:ASN:HD22	2.07	0.57
1:A:677:HIS:CG	1:A:678:GLN:H	2.23	0.57
1:B:699:LEU:HB2	1:B:757:TYR:OH	2.05	0.57
1:B:726:SER:O	1:B:728:LYS:N	2.37	0.56
1:B:588:THR:HG21	1:B:625:HIS:CB	2.25	0.56
1:A:681:ASN:O	1:A:682:TYR:CB	2.54	0.55
1:B:697:LYS:HZ2	1:B:698:ASP:H	1.55	0.54
1:B:703:ASP:OD1	1:B:703:ASP:N	2.41	0.54
1:B:591:SER:HB2	1:B:617:THR:HB	1.90	0.53
1:A:768:MET:HB2	1:A:792:LYS:HB2	1.90	0.53
1:B:731:ASN:N	1:B:731:ASN:HD22	2.08	0.52
1:A:655:GLY:HA2	1:A:660:VAL:HG13	1.91	0.52
1:A:678:GLN:O	1:A:679:ALA:CB	2.54	0.52
1:B:745:TRP:CE2	1:B:763:PRO:HB3	2.45	0.52
1:A:441:GLN:NE2	1:A:459:ASN:OD1	2.43	0.52
1:A:454:TYR:CE2	1:A:475:ASN:HB2	2.45	0.51
1:B:574:TYR:CZ	1:B:597:GLY:HA3	2.46	0.50
1:A:436:SER:HB3	1:A:463:ASN:OD1	2.11	0.50
1:A:783:LEU:HG	1:A:806:ILE:CD1	2.41	0.50
1:B:435:GLU:HG2	2:B:919:HOH:O	2.11	0.49
1:B:458:ILE:HG13	1:B:471:LEU:HD12	1.94	0.49
1:B:468:TYR:OH	1:B:470:GLU:OE1	2.28	0.49
1:A:446:GLN:HG3	1:A:448:ASN:O	2.12	0.49
1:A:525:LEU:HD11	1:B:525:LEU:HD11	1.95	0.48
1:A:497:ASP:OD1	1:A:497:ASP:N	2.30	0.48
1:A:677:HIS:CG	1:A:678:GLN:N	2.81	0.48
1:A:682:TYR:CD1	1:A:683:ASP:N	2.78	0.48
1:A:694:ASP:OD1	1:A:694:ASP:N	2.47	0.47
1:A:655:GLY:O	1:A:665:SER:HA	2.13	0.47
1:A:522:TYR:CZ	1:A:580:LYS:HE2	2.50	0.47
1:B:578:TYR:CZ	1:B:580:LYS:HB2	2.50	0.46
1:A:682:TYR:CG	1:A:683:ASP:N	2.82	0.46
1:B:614:ASP:OD1	1:B:634:ARG:HG3	2.15	0.46
1:B:552:MET:SD	1:B:644:LYS:HD2	2.55	0.46
1:B:730:ALA:O	1:B:731:ASN:CB	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ILE:HD11	1:A:471:LEU:HD12	1.96	0.46
1:B:458:ILE:CG1	1:B:471:LEU:HD12	2.45	0.46
1:B:493:ASP:OD2	1:B:507:LYS:HG2	2.16	0.46
1:A:479:THR:HG22	1:A:481:ASP:H	1.79	0.46
1:B:767:ARG:HD3	1:B:797:ASP:OD2	2.16	0.46
1:B:536:LEU:HD11	1:B:649:TYR:CD2	2.51	0.46
1:B:449:TRP:HA	1:B:450:LEU:HA	1.64	0.46
1:B:697:LYS:O	1:B:698:ASP:CB	2.64	0.45
1:A:522:TYR:CE1	1:A:580:LYS:HG3	2.51	0.45
1:B:668:ILE:HG23	1:B:767:ARG:HD2	1.99	0.44
1:B:668:ILE:HG23	1:B:767:ARG:NE	2.33	0.44
1:A:668:ILE:HG23	1:A:767:ARG:CD	2.46	0.43
1:B:697:LYS:HA	1:B:697:LYS:HD2	1.61	0.43
1:B:641:LEU:HA	1:B:641:LEU:HD23	1.86	0.43
1:A:792:LYS:HA	1:A:792:LYS:HD2	1.90	0.43
1:A:641:LEU:HA	1:A:641:LEU:HD23	1.70	0.43
1:B:496:ALA:HB3	1:B:504:TYR:H	1.84	0.43
1:A:680:SER:O	1:A:682:TYR:HE2	1.99	0.42
1:B:716:LEU:HA	1:B:716:LEU:HD22	1.84	0.42
1:B:668:ILE:HG23	1:B:767:ARG:CD	2.48	0.42
1:A:640:GLY:HA3	1:A:644:LYS:O	2.19	0.42
1:A:448:ASN:ND2	1:A:451:GLY:HA2	2.34	0.42
1:A:474:THR:O	1:A:476:PRO:HD3	2.19	0.42
1:A:520:ASN:HB2	1:A:521:GLU:OE1	2.19	0.42
1:A:787:TYR:HA	1:A:801:GLN:O	2.20	0.42
1:A:549:LEU:HD12	1:A:549:LEU:HA	1.91	0.42
1:A:522:TYR:CD1	1:A:580:LYS:HG3	2.55	0.42
1:A:522:TYR:CE2	1:A:580:LYS:HE2	2.55	0.42
1:B:722:THR:HA	1:B:723:PRO:HD3	1.93	0.42
1:A:585:TYR:CE2	1:A:777:MET:HB2	2.55	0.42
1:B:476:PRO:HA	1:B:484:SER:HB3	2.02	0.42
1:B:659:THR:OG1	1:B:660:VAL:N	2.53	0.41
1:A:692:THR:O	1:A:694:ASP:O	2.39	0.41
1:A:674:TYR:OH	1:A:704:ASP:OD2	2.21	0.41
1:A:692:THR:O	1:A:696:ALA:HB2	2.20	0.41
1:B:761:SER:O	1:B:763:PRO:HD3	2.21	0.41
1:B:697:LYS:HZ2	1:B:698:ASP:N	2.18	0.41
1:A:743:THR:HG23	1:A:745:TRP:HZ3	1.86	0.41
1:A:677:HIS:HB3	1:A:691:ALA:O	2.21	0.41
1:B:674:TYR:HB2	1:B:700:CYS:HB2	2.02	0.40
1:A:680:SER:O	1:A:682:TYR:CD2	2.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:SER:O	1:B:677:HIS:HB2	2.21	0.40
1:A:662:GLY:O	1:A:790:PRO:HG3	2.21	0.40
1:A:738:PHE:CZ	1:A:788:ALA:HB2	2.55	0.40
1:A:767:ARG:HD3	1:A:767:ARG:HH11	1.75	0.40
1:B:497:ASP:OD1	1:B:497:ASP:N	2.51	0.40
1:A:767:ARG:HD3	1:A:797:ASP:OD2	2.21	0.40
1:B:531:TYR:CE1	1:B:568:ASP:HB2	2.56	0.40
1:A:485:LEU:HA	1:A:485:LEU:HD23	1.90	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	375/385 (97%)	357 (95%)	15 (4%)	3 (1%)	24	46
1	B	366/385 (95%)	353 (96%)	13 (4%)	0	100	100
All	All	741/770 (96%)	710 (96%)	28 (4%)	3 (0%)	39	65

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	679	ALA
1	A	682	TYR
1	A	683	ASP

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	303/322 (94%)	280 (92%)	23 (8%)	16	32
1	B	306/322 (95%)	283 (92%)	23 (8%)	17	33
All	All	609/644 (95%)	563 (92%)	46 (8%)	16	32

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	435	GLU
1	A	438	VAL
1	A	445	GLN
1	A	467	THR
1	A	479	THR
1	A	485	LEU
1	A	497	ASP
1	A	519	ILE
1	A	546	TRP
1	A	549	LEU
1	A	567	THR
1	A	588	THR
1	A	598	LYS
1	A	615	THR
1	A	617	THR
1	A	659	THR
1	A	660	VAL
1	A	684	PRO
1	A	694	ASP
1	A	751	SER
1	A	767	ARG
1	A	793	LYS
1	A	810	TRP
1	B	430	ILE
1	B	467	THR
1	B	471	LEU
1	B	485	LEU
1	B	495	GLN
1	B	497	ASP
1	B	521	GLU
1	B	542	GLN
1	B	546	TRP
1	B	549	LEU

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Mol	Chain	Res	Type
1	B	567	THR
1	B	591	SER
1	B	598	LYS
1	B	617	THR
1	B	659	THR
1	B	660	VAL
1	B	665	SER
1	B	697	LYS
1	B	716	LEU
1	B	731	ASN
1	B	751	SER
1	B	767	ARG
1	B	792	LYS

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	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, 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	379/385 (98%)	0.06	15 (3%) 42 34	22, 49, 97, 140	0
1	B	370/385 (96%)	-0.01	10 (2%) 58 51	21, 47, 83, 115	0
All	All	749/770 (97%)	0.02	25 (3%) 50 43	21, 48, 91, 140	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	680	SER	5.8
1	A	682	TYR	5.1
1	B	730	ALA	4.6
1	A	723	PRO	4.5
1	A	679	ALA	4.5
1	A	687	ASP	4.3
1	A	724	PHE	4.1
1	B	727	ASP	4.1
1	B	731	ASN	4.1
1	B	725	ILE	4.1
1	B	729	TYR	3.4
1	B	795	ASP	3.2
1	A	696	ALA	3.2
1	A	626	LYS	3.0
1	A	678	GLN	2.9
1	B	426	MET	2.9
1	B	562	ASP	2.8
1	A	677	HIS	2.8
1	A	560	ASP	2.5
1	B	447	ASP	2.5
1	B	728	LYS	2.4
1	A	683	ASP	2.2
1	A	681	ASN	2.1
1	A	480	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	810	TRP	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 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.