



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:37 AM GMT

PDB ID : 4K3B
Title : The crystal structure of BamA from Neisseria gonorrhoeae
Authors : Noinaj, N.; Lukacik, P.; Chang, H.; Easley, N.; Buchanan, S.K.
Deposited on : 2013-04-10
Resolution : 3.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

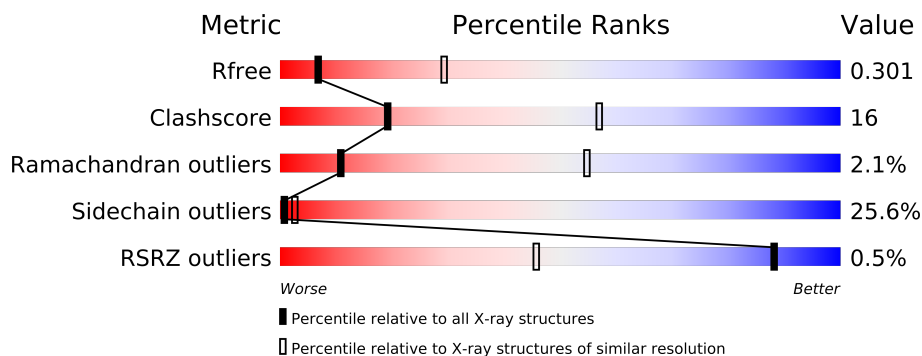
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance


The reported resolution of this entry is 3.20 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}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	792	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5759 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

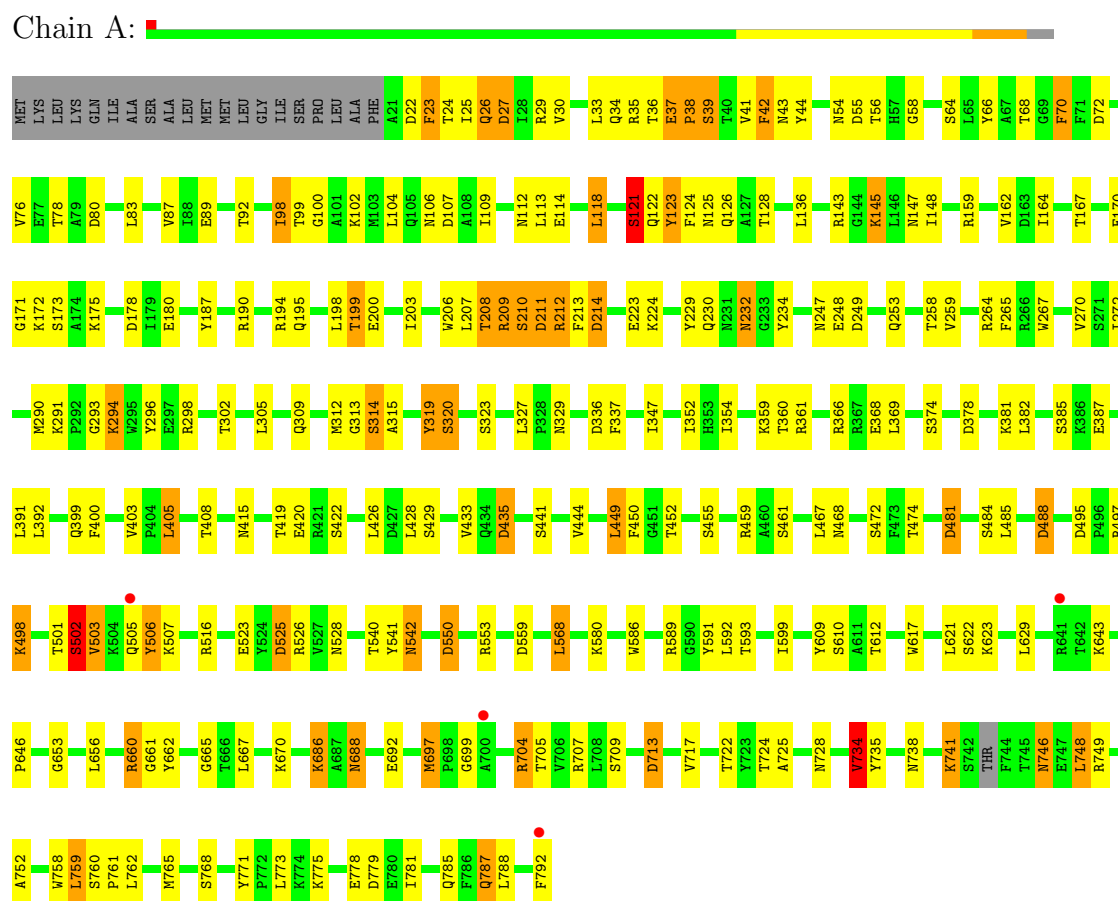
- Molecule 1 is a protein called Outer membrane protein assembly factor BamA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	771	5759	3639	985	1122	13	0	1	0

3 Residue-property plots

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 ($RSRZ > 2$). 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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	59.52Å 270.21Å 190.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 49.66 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.8 (15.00-3.20) 98.6 (49.66-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1103)	Depositor
R, R_{free}	0.232 , 0.278 0.264 , 0.301	Depositor DCC
R_{free} test set	1977 reflections (7.64%)	DCC
Wilson B-factor (Å ²)	73.2	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 59.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 26156 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5759	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.59	0/5877	0.92	12/7985 (0.2%)

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	13

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	315	ALA	N-CA-C	-8.00	89.41	111.00
1	A	198	LEU	N-CA-C	-7.32	91.24	111.00
1	A	37	GLU	C-N-CD	6.11	141.23	128.40
1	A	542	ASN	N-CA-CB	-5.91	99.95	110.60
1	A	734	VAL	N-CA-C	-5.85	95.21	111.00
1	A	760	SER	C-N-CD	5.62	140.21	128.40
1	A	568	LEU	CA-CB-CG	5.48	127.90	115.30
1	A	748	LEU	CA-CB-CG	5.43	127.80	115.30
1	A	449	LEU	CA-CB-CG	5.30	127.48	115.30
1	A	80	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	118	LEU	N-CA-C	5.11	124.79	111.00
1	A	290	MET	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	A	121	SER	Peptide
1	A	265	PHE	Peptide
1	A	313	GLY	Peptide
1	A	314	SER	Peptide
1	A	319	TYR	Peptide
1	A	502	SER	Peptide
1	A	503	VAL	Peptide
1	A	728	ASN	Peptide
1	A	734	VAL	Peptide
1	A	735	TYR	Peptide
1	A	761	PRO	Peptide
1	A	99	THR	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5759	0	36	95	0
All	All	5759	0	36	95	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (95) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:497:ARG:NH1	1:A:541:TYR:CE2	1.71	1.59
1:A:41:VAL:O	1:A:43:ASN:N	1.67	1.27
1:A:497:ARG:NH1	1:A:541:TYR:CD2	2.15	1.14
1:A:145:LYS:NZ	1:A:173:SER:OG	1.80	1.13
1:A:38:PRO:O	1:A:41:VAL:N	1.85	1.09
1:A:41:VAL:O	1:A:44:TYR:N	1.86	1.08
1:A:145:LYS:HE3	1:A:172:LYS:O	1.61	1.00
1:A:368:GLU:OE2	1:A:392:LEU:CD2	2.13	0.97
1:A:41:VAL:C	1:A:43:ASN:N	2.22	0.91
1:A:22:ASP:OD1	1:A:23:PHE:N	2.06	0.88

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:435:ASP:OD1	1:A:435:ASP:N	2.13	0.81
1:A:208:THR:O	1:A:209:ARG:CB	2.29	0.80
1:A:488:ASP:OD2	1:A:516:ARG:NH2	2.14	0.80
1:A:495:ASP:OD2	1:A:498:LYS:NZ	2.15	0.79
1:A:230:GLN:NE2	1:A:234:TYR:O	2.17	0.77
1:A:199:THR:OG1	1:A:210:SER:OG	2.04	0.74
1:A:72:ASP:N	1:A:89:GLU:O	2.21	0.73
1:A:145:LYS:CE	1:A:172:LYS:O	2.36	0.73
1:A:145:LYS:HG2	1:A:171:GLY:N	2.04	0.72
1:A:208:THR:O	1:A:209:ARG:CG	2.41	0.69
1:A:291:LYS:O	1:A:293:GLY:N	2.27	0.68
1:A:41:VAL:O	1:A:42:PHE:C	2.34	0.67
1:A:30:VAL:CG2	1:A:42:PHE:CE1	2.80	0.64
1:A:200:GLU:O	1:A:211:ASP:OD2	2.16	0.64
1:A:378:ASP:OD2	1:A:381:LYS:NZ	2.32	0.63
1:A:55:ASP:O	1:A:58:GLY:N	2.32	0.62
1:A:653:GLY:O	1:A:665:GLY:N	2.33	0.62
1:A:403:VAL:O	1:A:405:LEU:N	2.33	0.62
1:A:550:ASP:OD1	1:A:553:ARG:NH1	2.33	0.61
1:A:329:ASN:ND2	1:A:336:ASP:OD2	2.34	0.60
1:A:622:SER:OG	1:A:623:LYS:N	2.34	0.60
1:A:41:VAL:O	1:A:43:ASN:CA	2.47	0.60
1:A:92:THR:O	1:A:162:VAL:N	2.36	0.59
1:A:660:ARG:NH2	1:A:692:GLU:OE2	2.36	0.58
1:A:580:LYS:O	1:A:591:TYR:N	2.37	0.57
1:A:39:SER:C	1:A:41:VAL:N	2.59	0.56
1:A:661:GLY:N	1:A:785:GLN:OE1	2.40	0.55
1:A:327:LEU:N	1:A:336:ASP:O	2.40	0.55
1:A:481:ASP:OD1	1:A:481:ASP:N	2.40	0.54
1:A:247:ASN:OD1	1:A:248:GLU:N	2.41	0.54
1:A:697:MET:O	1:A:699:GLY:N	2.40	0.54
1:A:713:ASP:OD1	1:A:713:ASP:N	2.41	0.54
1:A:497:ARG:CZ	1:A:541:TYR:CE2	2.77	0.54
1:A:523:GLU:OE1	1:A:523:GLU:N	2.42	0.53
1:A:124:PHE:CG	1:A:125:ASN:N	2.76	0.53
1:A:686:LYS:NZ	1:A:688:ASN:OD1	2.42	0.52
1:A:752:ALA:O	1:A:771:TYR:N	2.43	0.52
1:A:788:LEU:CD1	1:A:788:LEU:N	2.73	0.52
1:A:143:ARG:CG	1:A:143:ARG:NH2	2.73	0.52
1:A:488:ASP:N	1:A:488:ASP:OD1	2.43	0.51
1:A:209:ARG:O	1:A:212:ARG:CG	2.59	0.51
1:A:38:PRO:CD	1:A:39:SER:N	2.73	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:187:TYR:OH	1:A:232:ASN:OD1	2.29	0.50
1:A:38:PRO:O	1:A:41:VAL:CB	2.59	0.50
1:A:38:PRO:CG	1:A:39:SER:N	2.73	0.50
1:A:102:LYS:N	1:A:170:GLU:OE1	2.45	0.50
1:A:382:LEU:O	1:A:385:SER:N	2.45	0.50
1:A:121:SER:O	1:A:123:TYR:N	2.44	0.49
1:A:501:THR:OG1	1:A:502:SER:N	2.45	0.49
1:A:38:PRO:O	1:A:41:VAL:CG2	2.61	0.49
1:A:506:TYR:CD1	1:A:506:TYR:C	2.86	0.49
1:A:41:VAL:O	1:A:43:ASN:C	2.50	0.48
1:A:147:ASN:ND2	1:A:249:ASP:O	2.46	0.48
1:A:749:ARG:NE	1:A:779:ASP:OD2	2.47	0.48
1:A:360:THR:OG1	1:A:361:ARG:N	2.45	0.48
1:A:208:THR:C	1:A:209:ARG:CG	2.80	0.48
1:A:497:ARG:NH1	1:A:541:TYR:CZ	2.62	0.48
1:A:267:TRP:N	1:A:294:LYS:O	2.47	0.47
1:A:213:PHE:CD1	1:A:214:ASP:N	2.82	0.47
1:A:145:LYS:CG	1:A:171:GLY:N	2.76	0.47
1:A:232:ASN:O	1:A:264:ARG:NH2	2.48	0.47
1:A:662:TYR:O	1:A:785:GLN:NE2	2.48	0.47
1:A:320:SER:OG	1:A:320:SER:O	2.31	0.46
1:A:98:ILE:O	1:A:106:ASN:ND2	2.48	0.46
1:A:495:ASP:O	1:A:497:ARG:O	2.34	0.46
1:A:741:LYS:N	1:A:746:ASN:N	2.64	0.46
1:A:38:PRO:O	1:A:41:VAL:CA	2.61	0.46
1:A:724:THR:OG1	1:A:725:ALA:N	2.49	0.45
1:A:429:SER:O	1:A:441:SER:N	2.49	0.45
1:A:787:GLN:C	1:A:788:LEU:CD1	2.85	0.45
1:A:758:TRP:CD1	1:A:759:LEU:N	2.86	0.43
1:A:26:GLN:O	1:A:27:ASP:CB	2.67	0.43
1:A:415:ASN:OD1	1:A:415:ASN:N	2.51	0.43
1:A:540:THR:O	1:A:542:ASN:N	2.52	0.43
1:A:525:ASP:N	1:A:525:ASP:OD1	2.52	0.43
1:A:758:TRP:O	1:A:765:MET:N	2.53	0.42
1:A:617:TRP:N	1:A:629:LEU:O	2.52	0.42
1:A:54:ASN:OD1	1:A:55:ASP:N	2.52	0.42
1:A:312:MET:O	1:A:314:SER:N	2.53	0.42
1:A:497:ARG:C	1:A:498:LYS:CG	2.87	0.42
1:A:145:LYS:NZ	1:A:172:LYS:O	2.54	0.41
1:A:70:PHE:N	1:A:70:PHE:CD1	2.89	0.41
1:A:586:TRP:NE1	1:A:704:ARG:O	2.54	0.41
1:A:697:MET:C	1:A:699:GLY:N	2.74	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:420:GLU:O	1:A:422:SER:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	768/792 (97%)	619 (81%)	133 (17%)	16 (2%)	11 55

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	36	THR
1	A	42	PHE
1	A	122	GLN
1	A	734	VAL
1	A	27	ASP
1	A	38	PRO
1	A	209	ARG
1	A	270	VAL
1	A	272	ILE
1	A	320	SER
1	A	369	LEU
1	A	738	ASN
1	A	741	LYS
1	A	503	VAL
1	A	37	GLU

5.3.2 Protein sidechains ⓘ

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	568/658 (86%)	423 (74%)	145 (26%)	1 3

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	PHE
1	A	24	THR
1	A	25	ILE
1	A	26	GLN
1	A	29	ARG
1	A	33	LEU
1	A	35	ARG
1	A	39	SER
1	A	56	THR
1	A	64	SER
1	A	66	TYR
1	A	68	THR
1	A	70	PHE
1	A	76	VAL
1	A	78	THR
1	A	83	LEU
1	A	87	VAL
1	A	98	ILE
1	A	104	LEU
1	A	107	ASP
1	A	109	ILE
1	A	112	ASN
1	A	113	LEU
1	A	114	GLU
1	A	118	LEU
1	A	121	SER
1	A	123	TYR
1	A	126	GLN
1	A	128	THR
1	A	136	LEU
1	A	145	LYS
1	A	148	ILE
1	A	159	ARG
1	A	164	ILE
1	A	167	THR
1	A	175	LYS

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Mol	Chain	Res	Type
1	A	178	ASP
1	A	180	GLU
1	A	190	ARG
1	A	194	ARG
1	A	195	GLN
1	A	199	THR
1	A	203	ILE
1	A	206	TRP
1	A	207	LEU
1	A	208	THR
1	A	210	SER
1	A	211	ASP
1	A	212	ARG
1	A	214	ASP
1	A	223	GLU
1	A	224	LYS
1	A	229	TYR
1	A	232	ASN
1	A	253	GLN
1	A	258	THR
1	A	259	VAL
1	A	294	LYS
1	A	296	TYR
1	A	298	ARG
1	A	302	THR
1	A	305	LEU
1	A	309	GLN
1	A	319	TYR
1	A	323	SER
1	A	337	PHE
1	A	347	ILE
1	A	352	ILE
1	A	354	ILE
1	A	359	LYS
1	A	366	ARG
1	A	374	SER
1	A	387	GLU
1	A	391	LEU
1	A	399	GLN
1	A	400	PHE
1	A	405	LEU
1	A	408	THR

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Mol	Chain	Res	Type
1	A	419	THR
1	A	426	LEU
1	A	428	LEU
1	A	433	VAL
1	A	435	ASP
1	A	444	VAL
1	A	449	LEU
1	A	450	PHE
1	A	452	THR
1	A	455	SER
1	A	459	ARG
1	A	461	SER
1	A	467	LEU
1	A	468	ASN
1	A	472	SER
1	A	474	THR
1	A	481	ASP
1	A	484	SER
1	A	485	LEU
1	A	488	ASP
1	A	498	LYS
1	A	502	SER
1	A	505	GLN
1	A	506	TYR
1	A	507	LYS
1	A	525	ASP
1	A	526	ARG
1	A	528	ASN
1	A	550	ASP
1	A	559	ASP
1	A	568	LEU
1	A	589	ARG
1	A	592	LEU
1	A	593	THR
1	A	599	ILE
1	A	609	TYR
1	A	610	SER
1	A	612	THR
1	A	621	LEU
1	A	643	LYS
1	A	646	PRO
1	A	656	LEU

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Mol	Chain	Res	Type
1	A	660	ARG
1	A	667	LEU
1	A	670	LYS
1	A	686	LYS
1	A	688	ASN
1	A	697	MET
1	A	704	ARG
1	A	705	THR
1	A	707	ARG
1	A	709	SER
1	A	713	ASP
1	A	717	VAL
1	A	722	THR
1	A	734	VAL
1	A	746	ASN
1	A	748	LEU
1	A	759	LEU
1	A	762	LEU
1	A	768	SER
1	A	773	LEU
1	A	775	LYS
1	A	778	GLU
1	A	781	ILE
1	A	787	GLN
1	A	792	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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	771/792 (97%)	-0.06	4 (0%)	88 46	56, 116, 173, 218	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	792	PHE	5.2
1	A	641	ARG	2.7
1	A	700	ALA	2.7
1	A	505	GLN	2.6

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 ⓘ

There are no such residues in this entry.