



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:28 PM EDT

PDB ID : 4K3C / pdb_00004k3c
Title : The crystal structure of BamA from Haemophilus ducreyi lacking POTRA domains 1-3
Authors : Noinaj, N.; Lukacik, P.; Chang, H.; Easley, N.; Buchanan, S.K.
Deposited on : 2013-04-10
Resolution : 2.91 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

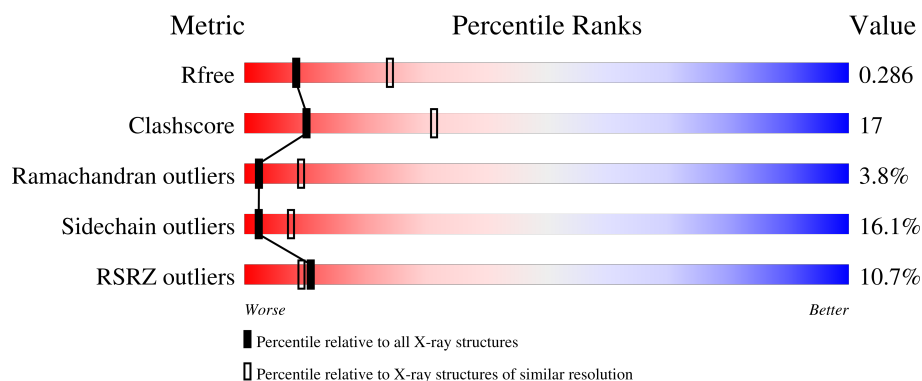
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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}	180053	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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 $\leq 5\%$. 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	532	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3959 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	532	Total	C	N	O	S	0	0	0
			3947	2484	686	770	7			

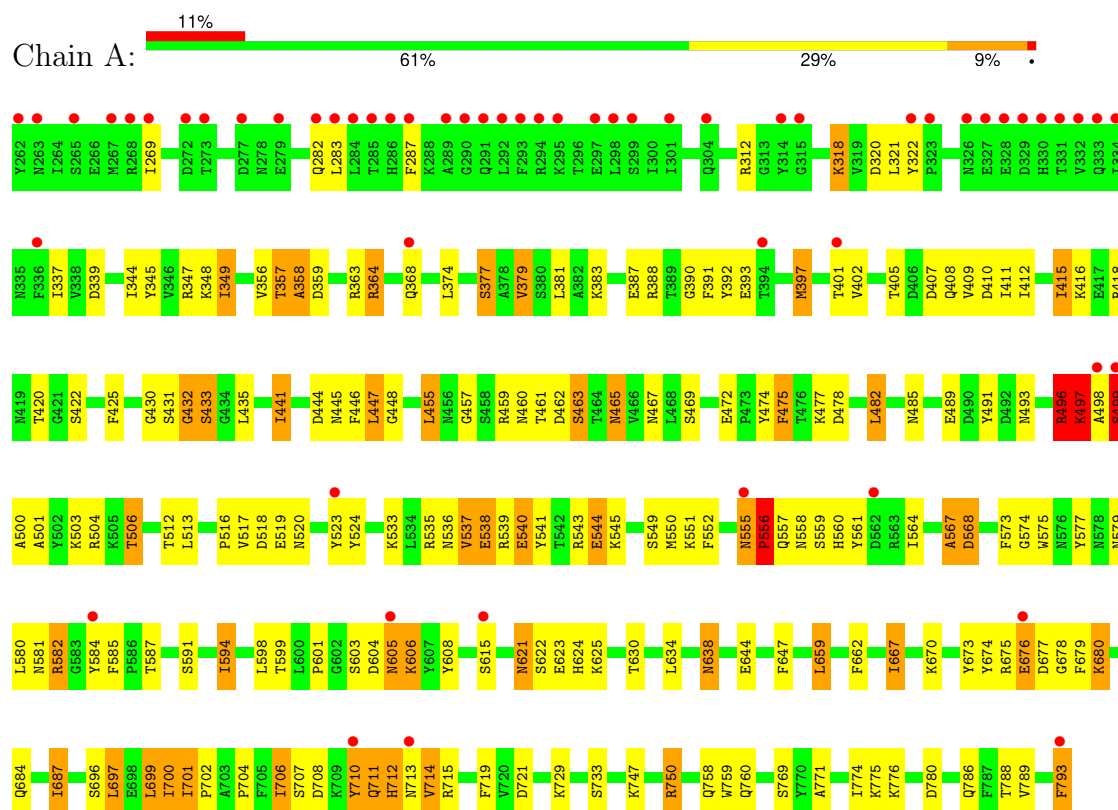
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	O	0	0
			12	12		

3 Residue-property plots

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: Outer membrane protein assembly factor BamA



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.78Å 88.16Å 244.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.91 19.95 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.95-2.91) 95.3 (19.95-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1042)	Depositor
R, R_{free}	0.220 , 0.270 0.244 , 0.286	Depositor DCC
R_{free} test set	2000 reflections (8.51%)	wwPDB-VP
Wilson B-factor (Å ²)	61.3	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3959	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.65	0/4034	1.07	16/5470 (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

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	500	ALA	N-CA-C	-13.09	95.60	110.91
1	A	517	VAL	N-CA-C	9.10	119.65	110.82
1	A	712	HIS	N-CA-C	-8.78	99.20	110.53
1	A	567	ALA	CA-C-N	6.99	134.29	121.70
1	A	567	ALA	C-N-CA	6.99	134.29	121.70
1	A	559	SER	N-CA-C	-5.86	102.64	110.55
1	A	432	GLY	N-CA-C	-5.82	100.12	111.12
1	A	606	LYS	N-CA-C	5.78	118.25	111.02
1	A	605	ASN	N-CA-C	5.75	123.05	110.80
1	A	622	SER	N-CA-C	-5.52	105.36	111.71
1	A	322	TYR	CA-C-N	5.27	126.09	120.13
1	A	322	TYR	C-N-CA	5.27	126.09	120.13
1	A	463	SER	N-CA-C	5.24	116.77	108.96
1	A	541	TYR	N-CA-C	5.17	116.60	110.97
1	A	667	ILE	N-CA-C	5.12	114.95	107.37
1	A	700	ILE	CB-CA-C	-5.04	105.78	111.23

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	497	LYS	Peptide
1	A	499	SER	Peptide
1	A	556	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	3947	0	3605	129	0
2	A	12	0	0	0	0
All	All	3959	0	3605	129	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 17.

All (129) 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:379:VAL:CG1	1:A:397:MET:HE1	1.69	1.23
1:A:379:VAL:HG13	1:A:397:MET:HE1	1.56	0.82
1:A:707:SER:HB2	1:A:708:ASP:HA	1.61	0.81
1:A:379:VAL:HG12	1:A:397:MET:HE1	1.62	0.81
1:A:621:ASN:HB3	1:A:624:HIS:H	1.43	0.80
1:A:675:ARG:H	1:A:678:GLY:HA2	1.46	0.80
1:A:379:VAL:CG1	1:A:397:MET:CE	2.56	0.79
1:A:497:LYS:C	1:A:499:SER:H	1.95	0.75
1:A:567:ALA:HA	1:A:568:ASP:HB2	1.69	0.73
1:A:496:ARG:HD3	1:A:498:ALA:HB3	1.70	0.73
1:A:379:VAL:HG13	1:A:397:MET:CE	2.19	0.73
1:A:392:TYR:CD1	1:A:415:ILE:HG13	2.23	0.72
1:A:630:THR:HG22	1:A:697:LEU:HD23	1.72	0.72
1:A:472:GLU:HG3	1:A:474:TYR:O	1.91	0.70
1:A:750:ARG:HD3	1:A:780:ASP:OD2	1.92	0.69
1:A:347:ARG:NH2	1:A:410:ASP:OD2	2.23	0.68
1:A:555:ASN:O	1:A:556:PRO:O	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:ASN:C	1:A:556:PRO:O	2.36	0.68
1:A:462:ASP:OD2	1:A:496:ARG:NH1	2.26	0.68
1:A:707:SER:CB	1:A:708:ASP:HA	2.23	0.68
1:A:667:ILE:HD12	1:A:750:ARG:HD2	1.76	0.67
1:A:584:TYR:CE1	1:A:760:GLN:HG3	2.32	0.65
1:A:712:HIS:O	1:A:713:ASN:HB2	1.97	0.64
1:A:556:PRO:C	1:A:558:ASN:H	2.05	0.64
1:A:706:ILE:HG21	1:A:714:VAL:HG11	1.79	0.64
1:A:706:ILE:HG22	1:A:707:SER:H	1.63	0.63
1:A:581:ASN:HD21	1:A:587:THR:HG23	1.67	0.60
1:A:497:LYS:HG2	1:A:498:ALA:H	1.67	0.60
1:A:359:ASP:OD1	1:A:363:ARG:NH2	2.34	0.60
1:A:552:PHE:CE2	1:A:564:ILE:HG23	2.37	0.59
1:A:368:GLN:HE22	1:A:374:LEU:HA	1.67	0.58
1:A:349:ILE:HD11	1:A:363:ARG:HE	1.67	0.58
1:A:674:TYR:HA	1:A:679:PHE:H	1.69	0.57
1:A:543:ARG:NE	1:A:687:ILE:HD11	2.19	0.57
1:A:625:LYS:HB3	1:A:702:PRO:HG3	1.85	0.57
1:A:379:VAL:HG11	1:A:397:MET:HE1	1.75	0.57
1:A:474:TYR:O	1:A:475:PHE:HB2	2.05	0.57
1:A:390:GLY:O	1:A:418:ARG:NE	2.28	0.57
1:A:489:GLU:OE2	1:A:504:ARG:NH1	2.37	0.56
1:A:320:ASP:HB2	1:A:337:ILE:HB	1.88	0.55
1:A:497:LYS:C	1:A:499:SER:N	2.61	0.54
1:A:318:LYS:HB2	1:A:339:ASP:HB3	1.89	0.54
1:A:707:SER:HB3	1:A:711:GLN:CD	2.33	0.53
1:A:539:ARG:HA	1:A:561:TYR:CE2	2.44	0.53
1:A:677:ASP:OD2	1:A:680:LYS:HD2	2.10	0.52
1:A:467:ASN:OD1	1:A:485:ASN:ND2	2.39	0.52
1:A:555:ASN:O	1:A:556:PRO:C	2.51	0.52
1:A:445:ASN:O	1:A:448:GLY:N	2.35	0.52
1:A:591:SER:HG	1:A:615:SER:HG	1.57	0.52
1:A:710:TYR:O	1:A:712:HIS:O	2.27	0.52
1:A:700:ILE:HD13	1:A:715:ARG:CZ	2.40	0.51
1:A:707:SER:HA	1:A:711:GLN:HB2	1.93	0.51
1:A:696:SER:OG	1:A:721:ASP:OD1	2.26	0.51
1:A:638:ASN:HD21	1:A:729:LYS:HE3	1.76	0.51
1:A:518:ASP:C	1:A:520:ASN:H	2.18	0.50
1:A:585:PHE:HE1	1:A:758:GLN:HE21	1.58	0.50
1:A:432:GLY:O	1:A:433:SER:HB2	2.11	0.50
1:A:524:TYR:CE2	1:A:574:GLY:HA3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:THR:HG22	1:A:358:ALA:N	2.26	0.49
1:A:568:ASP:H	1:A:603:SER:HA	1.77	0.49
1:A:402:VAL:O	1:A:405:THR:OG1	2.27	0.49
1:A:493:ASN:OD1	1:A:501:ALA:HA	2.11	0.49
1:A:523:TYR:CE1	1:A:575:TRP:CD1	3.01	0.49
1:A:750:ARG:HG2	1:A:776:LYS:HA	1.93	0.49
1:A:504:ARG:HE	1:A:506:THR:CG2	2.25	0.49
1:A:524:TYR:CZ	1:A:574:GLY:HA3	2.48	0.48
1:A:435:LEU:O	1:A:459:ARG:NH1	2.46	0.48
1:A:604:ASP:O	1:A:606:LYS:N	2.45	0.48
1:A:676:GLU:HA	1:A:677:ASP:C	2.38	0.48
1:A:598:LEU:HD22	1:A:599:THR:N	2.29	0.47
1:A:598:LEU:HD23	1:A:608:TYR:HB3	1.97	0.47
1:A:713:ASN:O	1:A:759:TRP:HB2	2.15	0.47
1:A:387:GLU:O	1:A:388:ARG:HB3	2.15	0.47
1:A:460:ASN:HB2	1:A:463:SER:H	1.80	0.47
1:A:707:SER:HB3	1:A:711:GLN:NE2	2.30	0.47
1:A:550:MET:HE1	1:A:605:ASN:H	1.80	0.47
1:A:497:LYS:HG2	1:A:498:ALA:N	2.30	0.46
1:A:391:PHE:CE1	1:A:445:ASN:HB2	2.51	0.46
1:A:431:SER:OG	1:A:786:GLN:HA	2.14	0.46
1:A:556:PRO:C	1:A:558:ASN:N	2.71	0.46
1:A:349:ILE:O	1:A:363:ARG:NH1	2.49	0.46
1:A:535:ARG:O	1:A:536:ASN:HB3	2.15	0.46
1:A:568:ASP:HA	1:A:603:SER:HB3	1.97	0.45
1:A:491:TYR:CE2	1:A:493:ASN:HB2	2.51	0.45
1:A:357:THR:O	1:A:358:ALA:HB2	2.17	0.45
1:A:543:ARG:HG2	1:A:647:PHE:CG	2.52	0.44
1:A:699:LEU:HD13	1:A:701:ILE:HG22	1.99	0.44
1:A:430:GLY:HA3	1:A:788:THR:HG22	2.00	0.44
1:A:457:GLY:HA2	1:A:465:ASN:O	2.18	0.44
1:A:540:GLU:HB3	1:A:673:TYR:CD1	2.52	0.44
1:A:538:GLU:HA	1:A:560:HIS:CD2	2.52	0.44
1:A:441:ILE:HG22	1:A:455:LEU:HB3	2.00	0.44
1:A:544:GLU:HG3	1:A:679:PHE:HZ	1.83	0.43
1:A:391:PHE:CD1	1:A:445:ASN:HB2	2.53	0.43
1:A:598:LEU:HD22	1:A:599:THR:H	1.82	0.43
1:A:460:ASN:HB3	1:A:462:ASP:H	1.82	0.43
1:A:706:ILE:O	1:A:707:SER:OG	2.30	0.43
1:A:552:PHE:HE2	1:A:564:ILE:HG23	1.83	0.43
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:LEU:HD23	1:A:513:LEU:HD23	2.00	0.43
1:A:623:GLU:O	1:A:624:HIS:HB2	2.18	0.43
1:A:704:PRO:O	1:A:706:ILE:HG12	2.19	0.42
1:A:345:TYR:HD2	1:A:408:GLN:HG2	1.84	0.42
1:A:594:ILE:HA	1:A:594:ILE:HD13	1.83	0.42
1:A:621:ASN:HD22	1:A:621:ASN:HA	1.60	0.42
1:A:707:SER:CB	1:A:711:GLN:HB2	2.50	0.42
1:A:659:LEU:HD13	1:A:662:PHE:CD1	2.54	0.42
1:A:282:GLN:HA	1:A:283:LEU:HA	1.52	0.42
1:A:469:SER:HB3	1:A:485:ASN:HD22	1.85	0.42
1:A:520:ASN:O	1:A:577:TYR:HA	2.20	0.42
1:A:379:VAL:HG12	1:A:397:MET:CE	2.37	0.42
1:A:539:ARG:HA	1:A:561:TYR:CZ	2.55	0.41
1:A:670:LYS:HD2	1:A:684:GLN:O	2.19	0.41
1:A:446:PHE:HA	1:A:447:LEU:HA	1.75	0.41
1:A:496:ARG:HB3	1:A:497:LYS:H	1.53	0.41
1:A:551:LYS:HB3	1:A:551:LYS:HE3	1.81	0.41
1:A:415:ILE:HG12	1:A:416:LYS:N	2.34	0.41
1:A:582:ARG:HE	1:A:582:ARG:HB3	1.68	0.41
1:A:707:SER:CB	1:A:711:GLN:NE2	2.84	0.41
1:A:536:ASN:OD1	1:A:537:VAL:N	2.53	0.41
1:A:582:ARG:NH1	1:A:584:TYR:O	2.54	0.41
1:A:393:GLU:HG2	1:A:418:ARG:CB	2.51	0.40
1:A:401:THR:HA	1:A:409:VAL:HG12	2.03	0.40
1:A:503:LYS:HB2	1:A:535:ARG:HG2	2.03	0.40
1:A:704:PRO:C	1:A:706:ILE:H	2.29	0.40
1:A:545:LYS:HE3	1:A:545:LYS:HB2	1.86	0.40
1:A:377:SER:O	1:A:381:LEU:N	2.49	0.40
1:A:425:PHE:HB2	1:A:793:PHE:CD1	2.56	0.40
1:A:719:PHE:HZ	1:A:771:ALA:HB2	1.86	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	530/532 (100%)	459 (87%)	51 (10%)	20 (4%)	2 9

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	PHE
1	A	357	THR
1	A	497	LYS
1	A	556	PRO
1	A	557	GLN
1	A	568	ASP
1	A	676	GLU
1	A	358	ALA
1	A	433	SER
1	A	475	PHE
1	A	496	ARG
1	A	580	LEU
1	A	706	ILE
1	A	269	ILE
1	A	499	SER
1	A	377	SER
1	A	364	ARG
1	A	537	VAL
1	A	555	ASN
1	A	516	PRO

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	379/445 (85%)	318 (84%)	61 (16%)	2 8

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	312	ARG
1	A	318	LYS
1	A	344	ILE
1	A	348	LYS
1	A	349	ILE
1	A	356	VAL
1	A	364	ARG
1	A	379	VAL
1	A	383	LYS
1	A	397	MET
1	A	407	ASP
1	A	411	ILE
1	A	412	ILE
1	A	415	ILE
1	A	420	THR
1	A	422	SER
1	A	441	ILE
1	A	444	ASP
1	A	447	LEU
1	A	455	LEU
1	A	461	THR
1	A	465	ASN
1	A	477	LYS
1	A	478	ASP
1	A	482	LEU
1	A	496	ARG
1	A	497	LYS
1	A	506	THR
1	A	512	THR
1	A	519	GLU
1	A	533	LYS
1	A	538	GLU
1	A	540	GLU
1	A	544	GLU
1	A	549	SER
1	A	573	PHE
1	A	579	ASN
1	A	582	ARG
1	A	594	ILE
1	A	601	PRO
1	A	621	ASN
1	A	634	LEU
1	A	638	ASN

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Mol	Chain	Res	Type
1	A	644	GLU
1	A	659	LEU
1	A	680	LYS
1	A	687	ILE
1	A	697	LEU
1	A	699	LEU
1	A	701	ILE
1	A	710	TYR
1	A	711	GLN
1	A	714	VAL
1	A	733	SER
1	A	747	LYS
1	A	750	ARG
1	A	769	SER
1	A	774	ILE
1	A	775	LYS
1	A	789	VAL
1	A	793	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	465	ASN
1	A	485	ASN
1	A	548	ASN
1	A	621	ASN
1	A	711	GLN
1	A	712	HIS
1	A	760	GLN

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 [i](#)

There are no oligosaccharides 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 ⓘ

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	532/532 (100%)	0.50	57 (10%) 11 9	30, 60, 189, 230	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	TYR	6.5
1	A	293	PHE	6.4
1	A	267	MET	5.1
1	A	272	ASP	5.0
1	A	328	GLU	4.9
1	A	292	LEU	4.9
1	A	277	ASP	4.5
1	A	498	ALA	4.4
1	A	331	THR	4.4
1	A	273	THR	4.3
1	A	301	ILE	4.2
1	A	285	THR	4.1
1	A	334	ILE	4.1
1	A	713	ASN	4.1
1	A	710	TYR	4.1
1	A	329	ASP	4.0
1	A	327	GLU	3.9
1	A	284	LEU	3.8
1	A	289	ALA	3.8
1	A	401	THR	3.7
1	A	268	ARG	3.6
1	A	330	HIS	3.6
1	A	265	SER	3.5
1	A	287	PHE	3.3
1	A	315	GLY	3.2
1	A	333	GLN	3.1
1	A	263	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	282	GLN	3.1
1	A	290	GLY	3.0
1	A	394	THR	3.0
1	A	294	ARG	3.0
1	A	336	PHE	2.9
1	A	323	PRO	2.9
1	A	269	ILE	2.9
1	A	523	TYR	2.9
1	A	326	ASN	2.9
1	A	279	GLU	2.8
1	A	291	GLN	2.8
1	A	314	TYR	2.8
1	A	286	HIS	2.8
1	A	605	ASN	2.7
1	A	555	ASN	2.7
1	A	298	LEU	2.5
1	A	615	SER	2.3
1	A	332	VAL	2.2
1	A	322	TYR	2.2
1	A	283	LEU	2.2
1	A	562	ASP	2.2
1	A	499	SER	2.2
1	A	584	TYR	2.2
1	A	295	LYS	2.2
1	A	676	GLU	2.2
1	A	368	GLN	2.2
1	A	304	GLN	2.1
1	A	793	PHE	2.1
1	A	297	GLU	2.1
1	A	299	SER	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 ⓘ

There are no oligosaccharides 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.