



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2017 – 08:41 AM EDT

PDB ID : 2PME
Title : The Apo crystal Structure of the glycyl-tRNA synthetase
Authors : Xie, W.
Deposited on : unknown
Resolution : 2.90 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
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

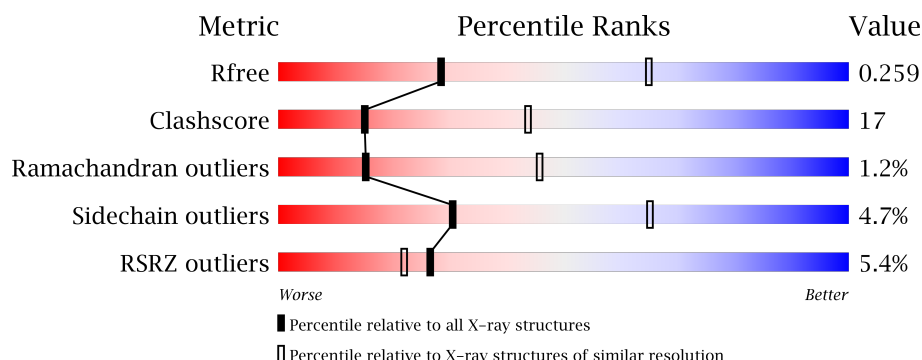
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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 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	693	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4258 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 Glycyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	0	0
			4136	2632	715	766	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	686	LEU	-	CLONING ARTIFACT	UNP P41250
A	687	GLU	-	CLONING ARTIFACT	UNP P41250
A	688	HIS	-	CLONING ARTIFACT	UNP P41250
A	689	HIS	-	CLONING ARTIFACT	UNP P41250
A	690	HIS	-	CLONING ARTIFACT	UNP P41250
A	691	HIS	-	CLONING ARTIFACT	UNP P41250
A	692	HIS	-	CLONING ARTIFACT	UNP P41250
A	693	HIS	-	CLONING ARTIFACT	UNP P41250

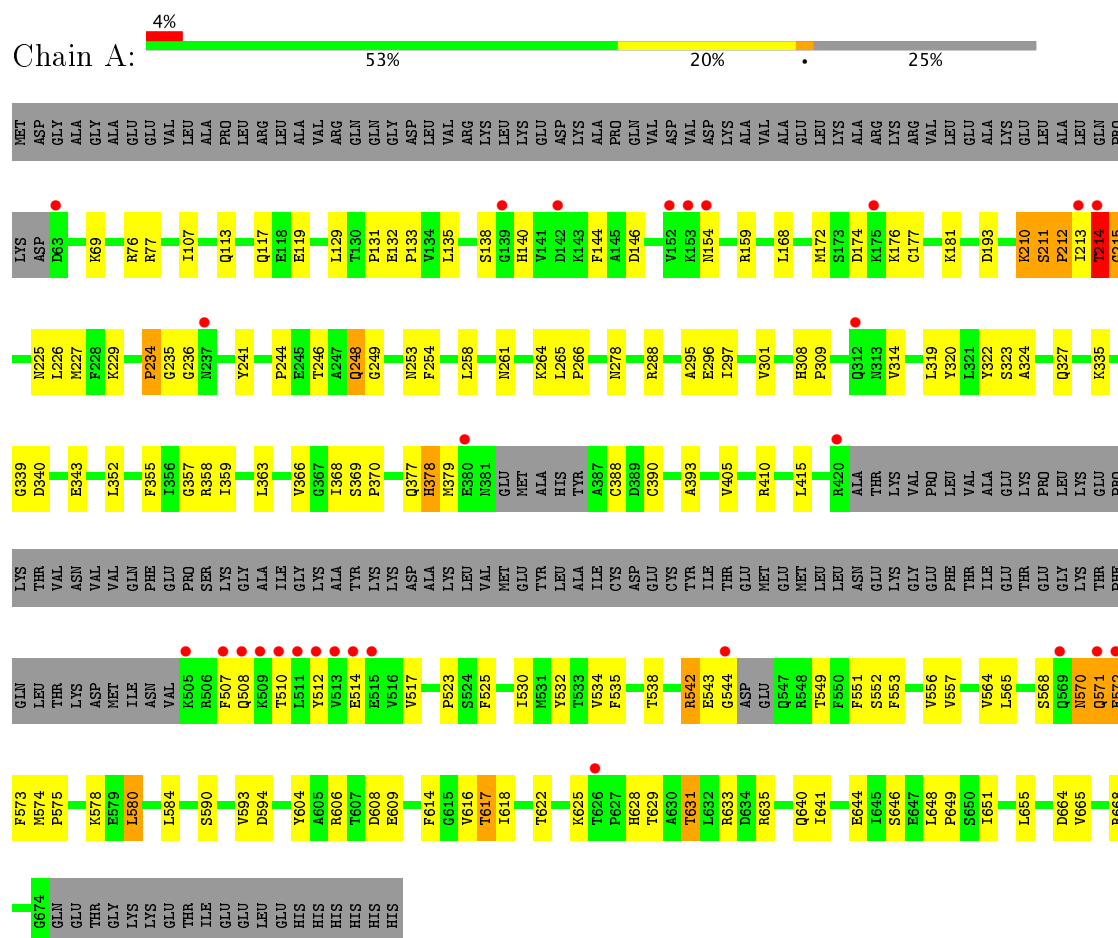
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	122	Total	O	0	0
			122	122		

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: Glycyl-tRNA synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	91.74Å 91.74Å 247.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.83 – 2.90 36.83 – 2.90	Depositor EDS
% Data completeness (in resolution range)	77.3 (36.83-2.90) 77.4 (36.83-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.230 , 0.271 0.223 , 0.259	Depositor DCC
R_{free} test set	978 reflections (5.51%)	DCC
Wilson B-factor (Å ²)	60.1	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4258	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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	0.24	0/4229	0.43	0/5711

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	215	GLY	Peptide
1	A	625	LYS	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	4136	0	4039	137	0
2	A	122	0	0	14	0
All	All	4258	0	4039	137	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 (137) 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:542:ARG:HG2	1:A:542:ARG:HH11	1.12	1.06
1:A:622:THR:HA	2:A:808:HOH:O	1.57	1.03
1:A:507:PHE:CE2	1:A:517:VAL:HG22	2.02	0.93
1:A:617:THR:HG23	1:A:631:THR:HG23	1.50	0.91
1:A:225:ASN:OD1	2:A:799:HOH:O	1.91	0.89
1:A:542:ARG:CG	1:A:542:ARG:HH11	1.90	0.84
1:A:140:HIS:HB3	1:A:227:MET:CE	2.10	0.81
1:A:212:PRO:HD2	1:A:213:ILE:H	1.45	0.81
1:A:314:VAL:HG11	1:A:357:GLY:HA3	1.62	0.80
1:A:210:LYS:O	1:A:211:SER:O	2.00	0.80
1:A:629:THR:N	2:A:808:HOH:O	2.17	0.77
1:A:633:ARG:HG3	1:A:640:GLN:HG2	1.65	0.76
1:A:553:PHE:O	1:A:635:ARG:NH2	2.18	0.76
1:A:140:HIS:CB	1:A:227:MET:HE1	2.16	0.75
1:A:140:HIS:HB3	1:A:227:MET:HE1	1.69	0.75
1:A:227:MET:SD	2:A:790:HOH:O	2.45	0.74
1:A:265:LEU:HB2	1:A:266:PRO:HD3	1.70	0.73
1:A:534:VAL:O	1:A:538:THR:HB	1.91	0.70
1:A:538:THR:HG23	1:A:552:SER:N	2.06	0.70
1:A:172:MET:HE1	2:A:780:HOH:O	1.90	0.69
1:A:571:GLN:O	1:A:573:PHE:N	2.26	0.69
1:A:664:ASP:O	1:A:668:ARG:HD2	1.93	0.67
1:A:538:THR:HG23	1:A:552:SER:H	1.59	0.67
1:A:140:HIS:O	2:A:799:HOH:O	2.12	0.66
1:A:248:GLN:NE2	2:A:700:HOH:O	2.28	0.66
1:A:144:PHE:CD2	1:A:144:PHE:O	2.49	0.65
1:A:227:MET:CE	1:A:244:PRO:HG3	2.26	0.65
1:A:542:ARG:NH1	1:A:542:ARG:HG2	1.94	0.65
1:A:69:LYS:NZ	2:A:804:HOH:O	2.29	0.64
1:A:113:GLN:HA	1:A:117:GLN:HG3	1.78	0.64
1:A:507:PHE:CD2	1:A:517:VAL:HG22	2.33	0.64
1:A:227:MET:HE2	1:A:244:PRO:HG3	1.79	0.63
1:A:648:LEU:HD23	1:A:651:ILE:HD11	1.81	0.63
1:A:213:ILE:O	1:A:214:THR:C	2.37	0.63
1:A:565:LEU:CD2	1:A:594:ASP:HB3	2.29	0.62
1:A:131:PRO:HB2	1:A:133:PRO:HD2	1.80	0.62
1:A:212:PRO:CD	1:A:213:ILE:H	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LYS:C	1:A:211:SER:O	2.38	0.61
1:A:229:LYS:HG2	1:A:241:TYR:HE2	1.67	0.60
1:A:608:ASP:OD2	1:A:633:ARG:NH2	2.34	0.58
1:A:510:THR:CG2	1:A:514:GLU:HB3	2.34	0.57
1:A:571:GLN:C	1:A:573:PHE:H	2.07	0.57
1:A:213:ILE:O	1:A:214:THR:O	2.23	0.57
1:A:571:GLN:O	1:A:574:MET:N	2.34	0.57
1:A:574:MET:O	1:A:578:LYS:HB2	2.04	0.57
1:A:530:ILE:O	1:A:534:VAL:HG23	2.05	0.57
1:A:146:ASP:OD1	1:A:159:ARG:NH2	2.37	0.56
1:A:229:LYS:HG2	1:A:241:TYR:CE2	2.41	0.56
1:A:608:ASP:CG	1:A:633:ARG:HH22	2.09	0.56
1:A:210:LYS:O	1:A:211:SER:C	2.45	0.55
1:A:246:THR:HB	1:A:296:GLU:HG3	1.88	0.55
1:A:168:LEU:O	1:A:172:MET:HB2	2.06	0.54
1:A:571:GLN:C	1:A:573:PHE:N	2.61	0.54
1:A:622:THR:O	1:A:628:HIS:HD2	1.92	0.53
1:A:314:VAL:CG1	1:A:357:GLY:HA3	2.33	0.53
1:A:664:ASP:O	1:A:668:ARG:CD	2.57	0.53
1:A:378:HIS:HB3	2:A:695:HOH:O	2.08	0.53
1:A:77:ARG:HH22	1:A:606:ARG:HB3	1.74	0.53
1:A:378:HIS:H	1:A:378:HIS:CD2	2.25	0.52
1:A:510:THR:HG22	1:A:514:GLU:HB3	1.90	0.52
1:A:323:SER:O	1:A:327:GLN:HG3	2.09	0.52
1:A:324:ALA:HB1	1:A:379:MET:HB3	1.92	0.52
1:A:249:GLY:O	1:A:253:ASN:ND2	2.33	0.52
1:A:132:GLU:N	1:A:133:PRO:CD	2.73	0.51
1:A:322:TYR:CE2	1:A:327:GLN:HG2	2.45	0.51
1:A:543:GLU:O	1:A:544:GLY:C	2.49	0.51
1:A:608:ASP:OD1	1:A:633:ARG:NH2	2.44	0.50
1:A:172:MET:CE	2:A:780:HOH:O	2.55	0.50
1:A:574:MET:N	1:A:575:PRO:CD	2.74	0.49
1:A:556:VAL:HG13	1:A:557:VAL:HG23	1.95	0.49
1:A:140:HIS:HB3	1:A:227:MET:HE3	1.94	0.49
1:A:378:HIS:N	1:A:378:HIS:CD2	2.81	0.49
1:A:568:SER:HB3	1:A:570:ASN:HB3	1.95	0.49
1:A:355:PHE:O	1:A:359:ILE:HG13	2.13	0.48
1:A:261:ASN:O	1:A:264:LYS:HG2	2.14	0.48
1:A:507:PHE:CE2	1:A:517:VAL:CG2	2.89	0.48
1:A:107:ILE:HD13	1:A:366:VAL:HG13	1.97	0.47
1:A:510:THR:HG23	1:A:512:TYR:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:VAL:HG12	1:A:534:VAL:HG21	1.97	0.47
1:A:542:ARG:NH1	1:A:542:ARG:CG	2.58	0.47
1:A:174:ASP:OD1	1:A:176:LYS:HG2	2.16	0.46
1:A:234:PRO:O	1:A:236:GLY:N	2.49	0.46
1:A:369:SER:HA	1:A:370:PRO:HD3	1.77	0.46
1:A:388:CYS:HB3	1:A:410:ARG:HG3	1.98	0.46
1:A:538:THR:HG22	1:A:551:PHE:HD2	1.80	0.46
1:A:308:HIS:HA	1:A:309:PRO:HD3	1.80	0.46
1:A:261:ASN:O	1:A:264:LYS:CG	2.65	0.45
1:A:628:HIS:HA	2:A:808:HOH:O	2.16	0.45
1:A:177:CYS:SG	1:A:181:LYS:HB3	2.56	0.44
1:A:327:GLN:NE2	1:A:377:GLN:O	2.50	0.44
1:A:644:GLU:HG3	1:A:646:SER:H	1.81	0.44
1:A:614:PHE:CZ	1:A:655:LEU:HB3	2.53	0.44
1:A:212:PRO:CD	1:A:213:ILE:N	2.76	0.44
1:A:140:HIS:CB	1:A:227:MET:CE	2.82	0.44
1:A:339:GLY:O	1:A:343:GLU:HG3	2.18	0.44
1:A:295:ALA:HB3	1:A:525:PHE:HB2	2.00	0.44
1:A:320:TYR:HA	1:A:335:LYS:HA	1.99	0.44
1:A:532:TYR:HA	1:A:535:PHE:CD1	2.52	0.44
1:A:608:ASP:CG	1:A:633:ARG:NH2	2.71	0.44
1:A:507:PHE:HE2	1:A:517:VAL:HG13	1.82	0.44
1:A:193:ASP:N	1:A:193:ASP:OD2	2.51	0.44
1:A:144:PHE:CE2	1:A:226:LEU:HB2	2.53	0.43
1:A:358:ARG:HD3	2:A:705:HOH:O	2.18	0.43
1:A:565:LEU:HD23	1:A:594:ASP:HB3	1.99	0.43
1:A:378:HIS:CE1	1:A:390:CYS:HB2	2.53	0.43
1:A:648:LEU:N	1:A:649:PRO:CD	2.82	0.43
1:A:211:SER:HB3	1:A:215:GLY:HA2	2.00	0.43
1:A:564:VAL:HG22	1:A:593:VAL:HA	2.00	0.42
1:A:580:LEU:HD12	1:A:618:ILE:HD11	2.00	0.42
1:A:210:LYS:HB3	1:A:210:LYS:HE3	1.86	0.42
1:A:543:GLU:HB2	2:A:805:HOH:O	2.19	0.42
1:A:144:PHE:O	1:A:144:PHE:CG	2.71	0.42
1:A:211:SER:OG	1:A:212:PRO:CD	2.67	0.42
1:A:340:ASP:HA	1:A:343:GLU:CD	2.40	0.42
1:A:227:MET:HE3	1:A:244:PRO:HG3	2.02	0.42
1:A:288:ARG:NH1	2:A:764:HOH:O	2.53	0.42
1:A:340:ASP:O	1:A:343:GLU:HB2	2.20	0.42
1:A:510:THR:HG21	1:A:514:GLU:HB3	2.01	0.42
1:A:565:LEU:HD22	1:A:594:ASP:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:PHE:CE2	1:A:517:VAL:HG13	2.55	0.42
1:A:77:ARG:HD3	1:A:77:ARG:HA	1.79	0.42
1:A:542:ARG:NH2	1:A:635:ARG:O	2.53	0.41
1:A:140:HIS:HB2	1:A:227:MET:HE1	1.99	0.41
1:A:604:TYR:OH	1:A:617:THR:HG22	2.20	0.41
1:A:641:ILE:HD13	1:A:665:VAL:CG1	2.50	0.41
1:A:363:LEU:HB3	1:A:368:ILE:HD12	2.02	0.41
1:A:258:LEU:HD22	1:A:508:GLN:HG2	2.03	0.41
1:A:622:THR:O	1:A:628:HIS:CD2	2.72	0.41
1:A:172:MET:HE2	1:A:172:MET:HB2	1.91	0.41
1:A:580:LEU:HD11	1:A:616:VAL:HG11	2.03	0.41
1:A:393:ALA:HB3	1:A:405:VAL:HB	2.03	0.41
1:A:594:ASP:OD1	1:A:594:ASP:C	2.59	0.41
1:A:135:LEU:HD13	1:A:227:MET:SD	2.61	0.40
1:A:254:PHE:CD1	1:A:415:LEU:HD11	2.56	0.40
1:A:297:ILE:HB	1:A:523:PRO:HD2	2.03	0.40
1:A:572:GLU:H	1:A:572:GLU:HG3	1.60	0.40
1:A:76:ARG:NH2	1:A:609:GLU:OE2	2.29	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	513/693 (74%)	476 (93%)	31 (6%)	6 (1%)	15	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	SER
1	A	214	THR
1	A	235	GLY

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Mol	Chain	Res	Type
1	A	572	GLU
1	A	212	PRO
1	A	234	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	446/600 (74%)	425 (95%)	21 (5%)	30	65

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	GLU
1	A	129	LEU
1	A	138	SER
1	A	154	ASN
1	A	210	LYS
1	A	214	THR
1	A	248	GLN
1	A	278	ASN
1	A	301	VAL
1	A	319	LEU
1	A	352	LEU
1	A	378	HIS
1	A	542	ARG
1	A	549	THR
1	A	570	ASN
1	A	571	GLN
1	A	580	LEU
1	A	584	LEU
1	A	590	SER
1	A	617	THR
1	A	631	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
1	A	169	GLN
1	A	206	ASN
1	A	261	ASN
1	A	278	ASN
1	A	570	ASN
1	A	571	GLN
1	A	628	HIS
1	A	640	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	521/693 (75%)	0.09	28 (5%) 26 22	20, 51, 96, 118	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	511	LEU	5.4
1	A	508	GLN	5.1
1	A	153	LYS	4.3
1	A	152	VAL	4.3
1	A	513	VAL	4.2
1	A	515	GLU	4.1
1	A	507	PHE	3.9
1	A	420	ARG	3.8
1	A	512	TYR	3.7
1	A	154	ASN	3.5
1	A	214	THR	3.4
1	A	510	THR	3.4
1	A	380	GLU	3.2
1	A	142	ASP	3.1
1	A	626	THR	3.0
1	A	572	GLU	3.0
1	A	509	LYS	2.7
1	A	63	ASP	2.6
1	A	505	LYS	2.6
1	A	569	GLN	2.6
1	A	571	GLN	2.5
1	A	514	GLU	2.5
1	A	175	LYS	2.3
1	A	237	ASN	2.3
1	A	213	ILE	2.2
1	A	312	GLN	2.1
1	A	544	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	139	GLY	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.