



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:31 AM UTC

PDB ID : 5ZTZ / pdb_00005ztz
Title : Proteobacterial origin of protein arginine methylation and regulation of Complex I assembly by MidA
Authors : Arold, S.T.; Swaminathan, K.; Hameed, U.F.S.
Deposited on : 2018-05-05
Resolution : 2.80 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

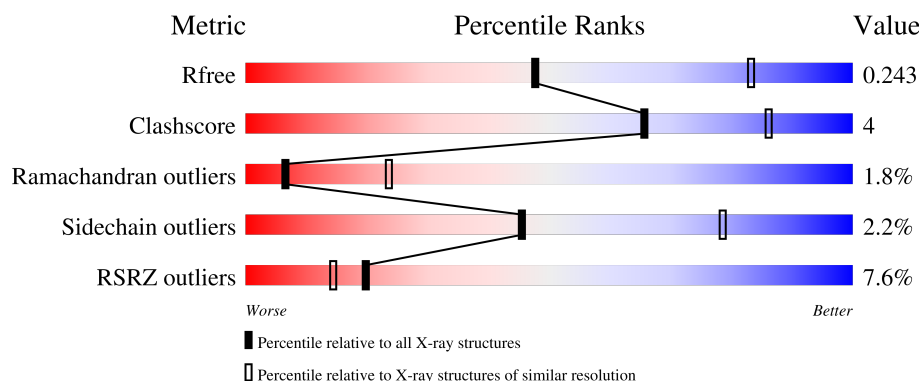
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	414	6% 86% 9% ..
1	B	414	7% 88% 8% .
1	C	414	9% 87% 8% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9622 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 Protein arginine methyltransferase NDUF7 homolog, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	Se	0	0	0
			3201	2067	520	600	3	11			
1	B	401	Total	C	N	O	S	Se	0	0	0
			3201	2067	520	600	3	11			
1	C	401	Total	C	N	O	S	Se	0	0	0
			3201	2067	520	600	3	11			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	GLY	-	expression tag	UNP Q54S83
A	72	PRO	-	expression tag	UNP Q54S83
A	73	LEU	-	expression tag	UNP Q54S83
A	74	GLY	-	expression tag	UNP Q54S83
A	75	SER	-	expression tag	UNP Q54S83
B	71	GLY	-	expression tag	UNP Q54S83
B	72	PRO	-	expression tag	UNP Q54S83
B	73	LEU	-	expression tag	UNP Q54S83
B	74	GLY	-	expression tag	UNP Q54S83
B	75	SER	-	expression tag	UNP Q54S83
C	71	GLY	-	expression tag	UNP Q54S83
C	72	PRO	-	expression tag	UNP Q54S83
C	73	LEU	-	expression tag	UNP Q54S83
C	74	GLY	-	expression tag	UNP Q54S83
C	75	SER	-	expression tag	UNP Q54S83

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	O	0	0
			4	4		

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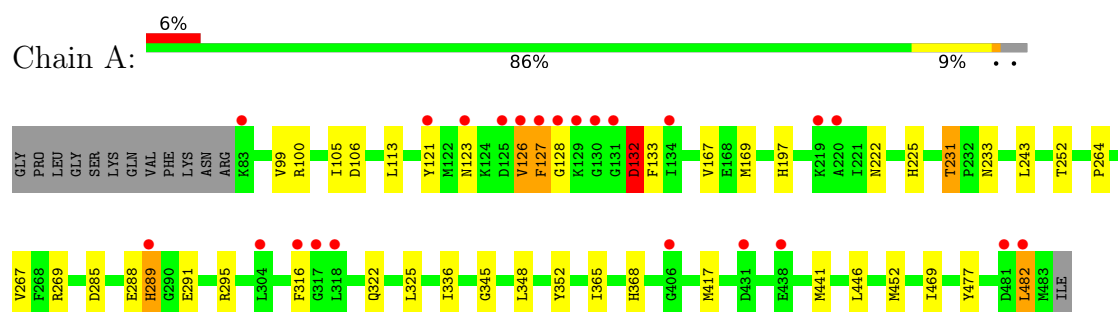
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	9	Total	O	0	0
			9	9		
2	C	6	Total	O	0	0
			6	6		

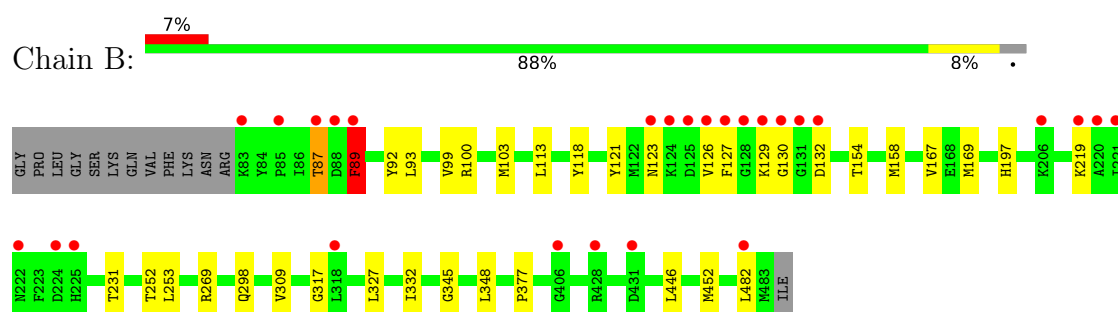
3 Residue-property plots [i](#)

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.

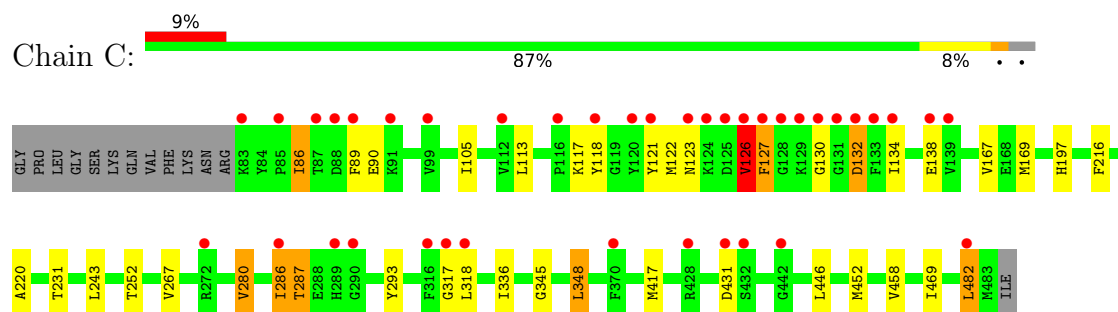
- Molecule 1: Protein arginine methyltransferase NDUFAF7 homolog, mitochondrial



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.01Å 105.63Å 201.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.53 – 2.80 100.53 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.8 (100.53-2.80) 96.8 (100.53-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0216	Depositor
R, R_{free}	0.215 , 0.235 0.223 , 0.243	Depositor DCC
R_{free} test set	2000 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9622	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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	0.50	0/3259	0.76	0/4381
1	B	0.52	0/3259	0.79	2/4381 (0.0%)
1	C	0.50	0/3259	0.78	2/4381 (0.0%)
All	All	0.51	0/9777	0.78	4/13143 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	86	ILE	N-CA-C	6.26	117.01	110.62
1	C	126	VAL	N-CA-C	6.12	122.07	109.34
1	B	87	THR	N-CA-C	5.42	119.44	113.21
1	B	89	PHE	CB-CA-C	5.35	119.99	109.72

There are no chirality outliers.

There are no planarity outliers.

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	3201	0	3234	23	0
1	B	3201	0	3234	27	0
1	C	3201	0	3234	27	0
2	A	4	0	0	0	0
2	B	9	0	0	0	0
2	C	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9622	0	9702	74	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 4.

All (74) 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:B:154:THR:HG22	1:B:158:MSE:HE2	1.46	0.94
1:C:89:PHE:HB2	1:C:118:TYR:CD2	2.13	0.84
1:A:222:ASN:HD22	1:A:225:HIS:CE1	2.04	0.76
1:A:133:PHE:HZ	1:A:365:ILE:HG21	1.51	0.75
1:B:158:MSE:HE1	1:B:253:LEU:HD21	1.69	0.74
1:B:158:MSE:CE	1:B:253:LEU:HD21	2.19	0.72
1:C:446:LEU:HA	1:C:452:MSE:HE3	1.72	0.71
1:C:267:VAL:HB	1:C:280:VAL:HG13	1.76	0.68
1:B:158:MSE:HE1	1:B:253:LEU:CD2	2.30	0.62
1:B:87:THR:O	1:B:87:THR:CG2	2.47	0.62
1:B:89:PHE:HB3	1:B:118:TYR:CG	2.35	0.61
1:C:446:LEU:HD23	1:C:452:MSE:CE	2.33	0.59
1:B:89:PHE:HB3	1:B:118:TYR:CD1	2.39	0.57
1:C:86:ILE:HA	1:C:293:TYR:CE2	2.39	0.57
1:A:169:MSE:HE1	1:A:243:LEU:HD13	1.87	0.57
1:B:446:LEU:HA	1:B:452:MSE:HE3	1.85	0.57
1:A:113:LEU:HD13	1:A:121:TYR:CE2	2.40	0.57
1:C:286:ILE:O	1:C:287:THR:O	2.23	0.57
1:C:127:PHE:CE2	1:C:132:ASP:HB2	2.39	0.56
1:B:113:LEU:HD13	1:B:121:TYR:CE2	2.41	0.56
1:B:87:THR:O	1:B:87:THR:HG22	2.06	0.55
1:C:113:LEU:HD13	1:C:121:TYR:CE2	2.41	0.55
1:C:127:PHE:HD1	1:C:127:PHE:N	2.05	0.54
1:A:446:LEU:HA	1:A:452:MSE:HE3	1.89	0.54
1:B:154:THR:CG2	1:B:158:MSE:HE2	2.30	0.53
1:B:89:PHE:HB2	1:B:118:TYR:CD2	2.44	0.53
1:B:309:VAL:HG11	1:B:327:LEU:CD2	2.39	0.53
1:C:446:LEU:HD23	1:C:452:MSE:HE1	1.91	0.53
1:C:127:PHE:N	1:C:127:PHE:CD1	2.76	0.53
1:B:269:ARG:HD3	1:B:298:GLN:HE21	1.73	0.52
1:A:106:ASP:OD1	1:A:264:PRO:HB2	2.10	0.52
1:B:169:MSE:HE2	1:B:332:ILE:HG21	1.91	0.51
1:B:99:VAL:HG23	1:B:100:ARG:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:THR:HG22	1:B:158:MSE:CE	2.30	0.51
1:C:169:MSE:HE1	1:C:243:LEU:HD13	1.92	0.50
1:B:89:PHE:CB	1:B:118:TYR:CG	2.95	0.50
1:C:105:ILE:HD12	1:C:267:VAL:HB	1.94	0.49
1:A:128:GLY:HA3	1:A:132:ASP:OD1	2.13	0.49
1:B:309:VAL:HG11	1:B:327:LEU:HD21	1.96	0.48
1:B:89:PHE:HE1	1:B:377:PRO:O	1.96	0.48
1:C:127:PHE:HD1	1:C:127:PHE:H	1.59	0.48
1:C:90:GLU:OE1	1:C:293:TYR:HB2	2.14	0.47
1:A:169:MSE:HE3	1:A:336:ILE:HD11	1.96	0.47
1:A:99:VAL:HG23	1:A:100:ARG:HG3	1.97	0.47
1:A:288:GLU:HG3	1:A:289:HIS:CE1	2.51	0.46
1:C:169:MSE:HE3	1:C:336:ILE:HD11	1.99	0.45
1:A:368:HIS:HB3	1:C:216:PHE:O	2.17	0.45
1:C:134:ILE:HG23	1:C:138:GLU:HB2	1.98	0.45
1:A:316:PHE:CD2	1:A:316:PHE:O	2.70	0.44
1:C:252:THR:O	1:C:345:GLY:HA3	2.18	0.44
1:C:446:LEU:HD23	1:C:452:MSE:HE3	2.00	0.43
1:A:269:ARG:CZ	1:A:322:GLN:OE1	2.67	0.43
1:B:89:PHE:CB	1:B:118:TYR:CD2	3.02	0.43
1:B:154:THR:O	1:B:158:MSE:HG3	2.18	0.43
1:A:352:TYR:CG	1:C:220:ALA:HB2	2.54	0.42
1:A:352:TYR:CD1	1:C:220:ALA:HB2	2.55	0.42
1:C:267:VAL:HG12	1:C:280:VAL:CG1	2.50	0.42
1:A:126:VAL:O	1:A:127:PHE:HD1	2.03	0.41
1:A:417:MSE:SE	1:A:469:ILE:HG22	2.70	0.41
1:A:167:VAL:HA	1:A:197:HIS:O	2.21	0.41
1:A:285:ASP:HA	1:A:295:ARG:HD3	2.02	0.41
1:A:231:THR:HG22	1:A:233:ASN:H	1.86	0.41
1:C:417:MSE:SE	1:C:469:ILE:HG22	2.70	0.41
1:A:252:THR:O	1:A:345:GLY:HA3	2.19	0.41
1:B:167:VAL:HA	1:B:197:HIS:O	2.21	0.41
1:C:267:VAL:HB	1:C:280:VAL:CG1	2.48	0.41
1:A:446:LEU:HD23	1:A:452:MSE:CE	2.51	0.41
1:A:105:ILE:HD12	1:A:267:VAL:HB	2.02	0.41
1:B:89:PHE:HA	1:B:92:TYR:HB3	2.03	0.41
1:C:348:LEU:HD22	1:C:458:VAL:CG1	2.51	0.40
1:B:252:THR:O	1:B:345:GLY:HA3	2.20	0.40
1:B:446:LEU:HD23	1:B:452:MSE:CE	2.51	0.40
1:B:93:LEU:HB3	1:B:103:MSE:HE1	2.03	0.40
1:C:167:VAL:HA	1:C:197:HIS:O	2.21	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	399/414 (96%)	375 (94%)	18 (4%)	6 (2%)	8	28
1	B	399/414 (96%)	374 (94%)	18 (4%)	7 (2%)	6	23
1	C	399/414 (96%)	374 (94%)	17 (4%)	8 (2%)	6	21
All	All	1197/1242 (96%)	1123 (94%)	53 (4%)	21 (2%)	6	23

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	126	VAL
1	B	123	ASN
1	B	126	VAL
1	C	123	ASN
1	C	126	VAL
1	C	287	THR
1	A	291	GLU
1	A	482	LEU
1	B	130	GLY
1	B	317	GLY
1	C	286	ILE
1	C	317	GLY
1	A	132	ASP
1	B	129	LYS
1	B	132	ASP
1	B	482	LEU
1	C	132	ASP
1	C	482	LEU
1	A	477	TYR
1	C	130	GLY

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	352/352 (100%)	344 (98%)	8 (2%)	44	78
1	B	352/352 (100%)	347 (99%)	5 (1%)	59	85
1	C	352/352 (100%)	342 (97%)	10 (3%)	38	73
All	All	1056/1056 (100%)	1033 (98%)	23 (2%)	45	78

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	PHE
1	A	132	ASP
1	A	231	THR
1	A	289	HIS
1	A	325	LEU
1	A	348	LEU
1	A	441	MSE
1	A	482	LEU
1	B	89	PHE
1	B	127	PHE
1	B	219	LYS
1	B	231	THR
1	B	348	LEU
1	C	117	LYS
1	C	122	MSE
1	C	126	VAL
1	C	127	PHE
1	C	231	THR
1	C	280	VAL
1	C	318	LEU
1	C	348	LEU
1	C	431	ASP
1	C	482	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	ASN
1	A	233	ASN
1	A	257	GLN
1	A	289	HIS
1	A	298	GLN
1	A	335	GLN
1	A	410	GLN
1	B	225	HIS
1	B	257	GLN
1	B	298	GLN
1	B	335	GLN
1	B	433	ASN
1	C	225	HIS
1	C	257	GLN
1	C	335	GLN
1	C	363	GLN
1	C	410	GLN
1	C	421	HIS
1	C	433	ASN

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 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 ⓘ

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	390/414 (94%)	0.29	23 (5%) 28 21	26, 43, 81, 138	0
1	B	390/414 (94%)	0.28	27 (6%) 23 16	20, 38, 90, 154	0
1	C	390/414 (94%)	0.49	39 (10%) 12 9	27, 46, 102, 172	0
All	All	1170/1242 (94%)	0.35	89 (7%) 20 14	20, 43, 96, 172	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	482	LEU	5.9
1	C	126	VAL	5.7
1	A	126	VAL	5.7
1	A	482	LEU	5.7
1	B	126	VAL	5.5
1	B	127	PHE	5.2
1	A	134	ILE	5.2
1	B	129	LYS	5.1
1	C	134	ILE	5.0
1	A	127	PHE	5.0
1	C	129	LYS	4.7
1	B	128	GLY	4.5
1	C	127	PHE	4.5
1	A	130	GLY	4.3
1	C	130	GLY	4.3
1	B	130	GLY	4.1
1	C	131	GLY	4.1
1	B	224	ASP	4.1
1	C	83	LYS	4.1
1	A	316	PHE	4.0
1	C	482	LEU	3.7
1	C	125	ASP	3.7
1	C	128	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	286	ILE	3.5
1	B	132	ASP	3.4
1	C	87	THR	3.4
1	B	220	ALA	3.3
1	C	133	PHE	3.3
1	A	129	LYS	3.3
1	C	99	VAL	3.2
1	B	221	ILE	3.2
1	B	431	ASP	3.1
1	A	125	ASP	3.0
1	B	225	HIS	3.0
1	B	123	ASN	3.0
1	C	132	ASP	3.0
1	C	316	PHE	2.9
1	C	124	LYS	2.9
1	A	220	ALA	2.9
1	B	131	GLY	2.8
1	B	406	GLY	2.8
1	C	121	TYR	2.8
1	C	138	GLU	2.7
1	C	289	HIS	2.7
1	C	431	ASP	2.7
1	B	89	PHE	2.7
1	A	289	HIS	2.7
1	B	206	LYS	2.7
1	B	124	LYS	2.6
1	C	85	PRO	2.6
1	B	219	LYS	2.5
1	C	290	GLY	2.5
1	C	370	PHE	2.5
1	B	222	ASN	2.5
1	A	121	TYR	2.5
1	A	123	ASN	2.5
1	C	123	ASN	2.5
1	A	304	LEU	2.4
1	A	128	GLY	2.4
1	C	318	LEU	2.4
1	C	317	GLY	2.4
1	B	125	ASP	2.4
1	C	88	ASP	2.4
1	C	432	SER	2.4
1	B	83	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	131	GLY	2.3
1	C	89	PHE	2.3
1	B	87	THR	2.3
1	A	317	GLY	2.3
1	A	318	LEU	2.3
1	A	431	ASP	2.3
1	A	481	ASP	2.3
1	A	83	LYS	2.2
1	B	88	ASP	2.2
1	A	406	GLY	2.2
1	A	219	LYS	2.2
1	B	318	LEU	2.2
1	C	116	PRO	2.2
1	C	272	ARG	2.1
1	C	91	LYS	2.1
1	B	428	ARG	2.1
1	C	428	ARG	2.1
1	C	139	VAL	2.1
1	C	120	TYR	2.1
1	A	438	GLU	2.0
1	C	118	TYR	2.0
1	C	112	VAL	2.0
1	B	85	PRO	2.0
1	C	442	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 oligosaccharides 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.