



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:27 AM UTC

PDB ID : 6NLY / pdb_00006nly
Title : Fragment of human mitochondrial Alanyl-tRNA Synthetase C-Ala domain
Authors : Kuhle, B.; Schimmel, P.
Deposited on : 2019-01-09
Resolution : 2.31 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

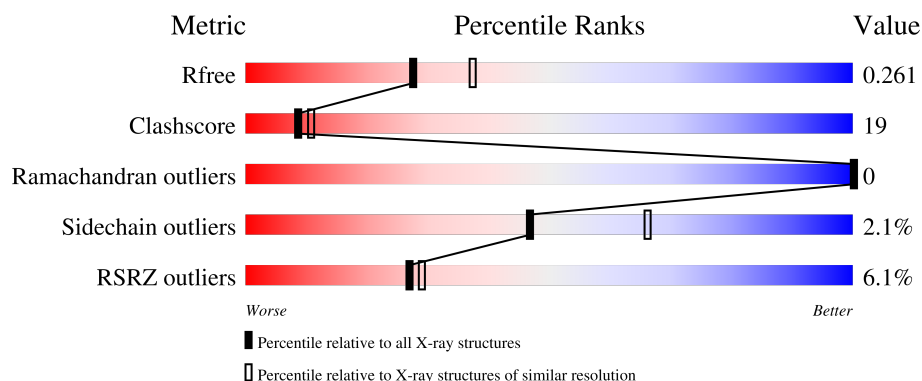
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	192	7% 72% 21% • 6%
1	B	192	8% 60% 30% • 7%
1	C	192	4% 65% 26% • 8%
1	D	192	4% 67% 26% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5425 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 Alanine-tRNA ligase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	178	Total	C	N	O	S	0	0	0
			1339	836	244	249	10			
1	A	181	Total	C	N	O	S	0	0	0
			1357	847	247	253	10			
1	C	176	Total	C	N	O	S	0	0	0
			1324	827	240	247	10			
1	D	182	Total	C	N	O	S	0	0	0
			1384	863	258	253	10			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	986	LEU	-	expression tag	UNP Q5JTZ9
B	987	GLU	-	expression tag	UNP Q5JTZ9
B	988	HIS	-	expression tag	UNP Q5JTZ9
B	989	HIS	-	expression tag	UNP Q5JTZ9
B	990	HIS	-	expression tag	UNP Q5JTZ9
B	991	HIS	-	expression tag	UNP Q5JTZ9
B	992	HIS	-	expression tag	UNP Q5JTZ9
B	993	HIS	-	expression tag	UNP Q5JTZ9
A	986	LEU	-	expression tag	UNP Q5JTZ9
A	987	GLU	-	expression tag	UNP Q5JTZ9
A	988	HIS	-	expression tag	UNP Q5JTZ9
A	989	HIS	-	expression tag	UNP Q5JTZ9
A	990	HIS	-	expression tag	UNP Q5JTZ9
A	991	HIS	-	expression tag	UNP Q5JTZ9
A	992	HIS	-	expression tag	UNP Q5JTZ9
A	993	HIS	-	expression tag	UNP Q5JTZ9
C	986	LEU	-	expression tag	UNP Q5JTZ9
C	987	GLU	-	expression tag	UNP Q5JTZ9
C	988	HIS	-	expression tag	UNP Q5JTZ9
C	989	HIS	-	expression tag	UNP Q5JTZ9
C	990	HIS	-	expression tag	UNP Q5JTZ9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	991	HIS	-	expression tag	UNP Q5J TZ9
C	992	HIS	-	expression tag	UNP Q5J TZ9
C	993	HIS	-	expression tag	UNP Q5J TZ9
D	986	LEU	-	expression tag	UNP Q5J TZ9
D	987	GLU	-	expression tag	UNP Q5J TZ9
D	988	HIS	-	expression tag	UNP Q5J TZ9
D	989	HIS	-	expression tag	UNP Q5J TZ9
D	990	HIS	-	expression tag	UNP Q5J TZ9
D	991	HIS	-	expression tag	UNP Q5J TZ9
D	992	HIS	-	expression tag	UNP Q5J TZ9
D	993	HIS	-	expression tag	UNP Q5J TZ9

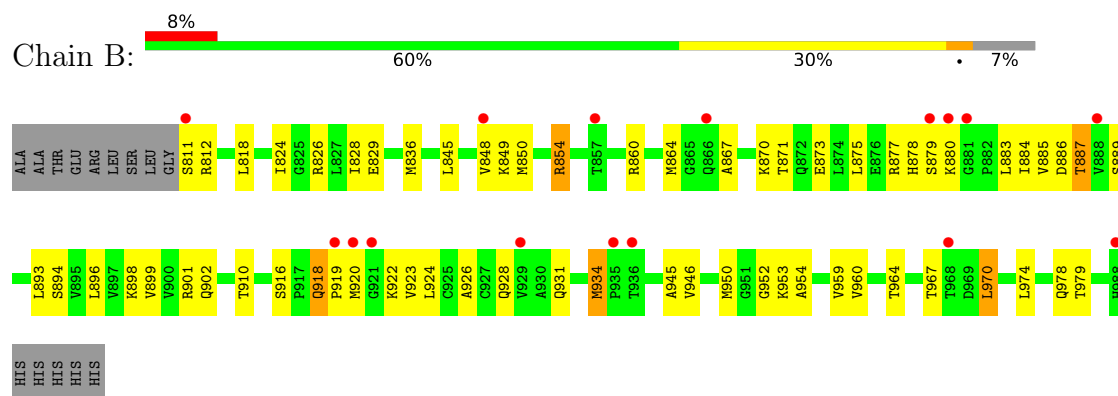
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	5	Total O 5 5	0	0
2	A	6	Total O 6 6	0	0
2	C	4	Total O 4 4	0	0
2	D	6	Total O 6 6	0	0

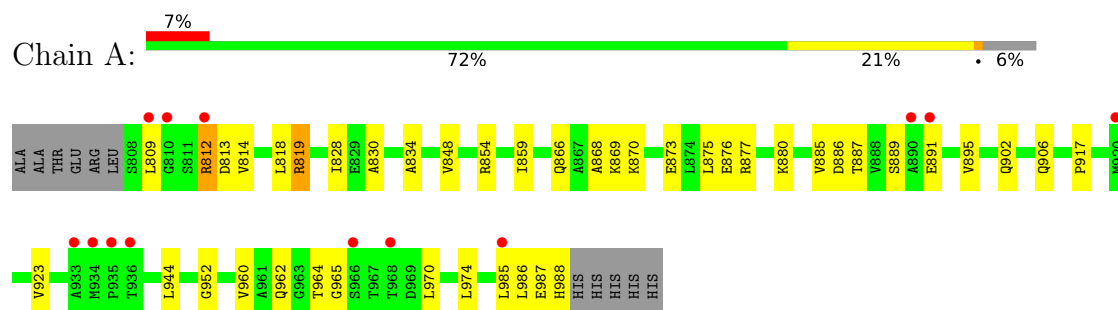
3 Residue-property plots [i](#)

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.

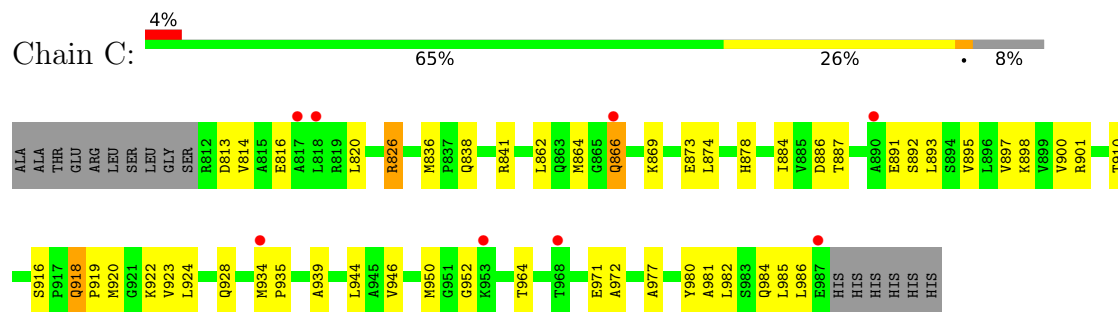
- Molecule 1: Alanine-tRNA ligase, mitochondrial



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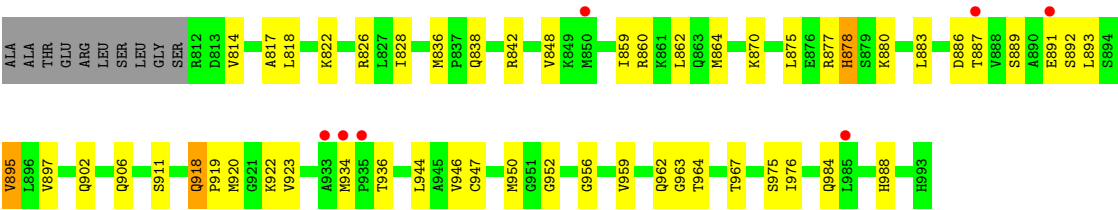


- Molecule 1: Alanine-tRNA ligase, mitochondrial



- Molecule 1: Alanine-tRNA ligase, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	103.22Å 317.23Å 54.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.02 – 2.31 38.02 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.1 (38.02-2.31) 99.3 (38.02-2.31)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 2.31Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.209 , 0.257 (Not available) , 0.261	Depositor DCC
R_{free} test set	2001 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.848	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5425	wwPDB-VP
Average B, all atoms (Å ²)	77.0	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 21.11 % 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 7.5256e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.54	0/1373	0.71	1/1857 (0.1%)
1	B	0.76	0/1355	0.92	5/1833 (0.3%)
1	C	0.61	0/1339	0.91	8/1812 (0.4%)
1	D	0.74	0/1405	0.88	8/1900 (0.4%)
All	All	0.67	0/5472	0.86	22/7402 (0.3%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	817	ALA	N-CA-C	-7.01	103.72	111.36
1	D	959	VAL	N-CA-C	6.57	118.55	111.58
1	D	956	GLY	N-CA-C	6.26	119.01	110.69
1	B	959	VAL	N-CA-C	6.16	116.94	110.72
1	B	918	GLN	CA-C-N	-5.95	114.14	120.03
1	B	918	GLN	C-N-CA	-5.95	114.14	120.03
1	D	878	HIS	N-CA-C	5.81	118.86	109.40
1	C	916	SER	CA-C-N	-5.67	114.13	119.85
1	C	916	SER	C-N-CA	-5.67	114.13	119.85
1	C	918	GLN	CA-C-N	-5.67	114.13	119.85
1	C	918	GLN	C-N-CA	-5.67	114.13	119.85
1	D	836	MET	CA-C-N	-5.66	113.95	119.78
1	D	836	MET	C-N-CA	-5.66	113.95	119.78
1	D	918	GLN	CA-C-N	-5.53	114.26	119.85
1	D	918	GLN	C-N-CA	-5.53	114.26	119.85
1	B	836	MET	CA-C-N	-5.47	114.15	119.78
1	B	836	MET	C-N-CA	-5.47	114.15	119.78
1	C	866	GLN	CA-CB-CG	-5.42	103.25	114.10
1	C	939	ALA	N-CA-C	5.24	116.99	111.28
1	C	836	MET	CA-C-N	-5.21	114.41	119.78
1	C	836	MET	C-N-CA	-5.21	114.41	119.78
1	A	985	LEU	N-CA-C	5.05	116.78	111.28

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	1357	0	1419	38	0
1	B	1339	0	1400	79	0
1	C	1324	0	1388	46	0
1	D	1384	0	1430	55	0
2	A	6	0	0	0	0
2	B	5	0	0	1	0
2	C	4	0	0	0	0
2	D	6	0	0	2	0
All	All	5425	0	5637	208	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 19.

All (208) 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:D:822:LYS:HE2	1:D:826:ARG:NH2	1.60	1.14
1:B:901:ARG:NH2	1:B:960:VAL:HG11	1.65	1.10
1:D:822:LYS:CE	1:D:826:ARG:HH22	1.66	1.08
1:B:864:MET:HE3	1:B:902:GLN:NE2	1.72	1.03
1:A:812:ARG:NH1	1:A:813:ASP:OD1	1.92	1.02
1:D:822:LYS:HE2	1:D:826:ARG:HH22	0.88	1.02
1:A:812:ARG:HH11	1:A:812:ARG:HG3	1.24	0.97
1:B:860:ARG:HH11	1:B:860:ARG:HG3	1.30	0.96
1:A:854:ARG:HG2	1:A:854:ARG:HH21	1.32	0.94
1:B:918:GLN:HE21	1:B:924:LEU:CD1	1.83	0.92
1:B:931:GLN:OE1	1:B:931:GLN:N	2.03	0.91
1:B:934:MET:HE2	1:B:934:MET:H	1.38	0.88
1:D:822:LYS:HG2	1:D:826:ARG:NH2	1.90	0.87
1:D:860:ARG:NH1	1:D:864:MET:HE2	1.90	0.87
1:A:809:LEU:O	1:A:812:ARG:HG2	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:901:ARG:NH2	1:B:960:VAL:CG1	2.37	0.86
1:B:901:ARG:HH22	1:B:960:VAL:CG1	1.95	0.79
1:B:918:GLN:HE21	1:B:924:LEU:HD11	1.47	0.78
1:B:934:MET:HE2	1:B:934:MET:N	1.98	0.77
1:C:826:ARG:HG2	1:C:826:ARG:HH21	1.48	0.77
1:B:918:GLN:NE2	1:B:924:LEU:HD13	2.00	0.76
1:B:870:LYS:HE3	1:B:889:SER:O	1.84	0.76
1:B:864:MET:CE	1:B:902:GLN:NE2	2.48	0.75
1:B:918:GLN:NE2	1:B:924:LEU:CD1	2.49	0.75
1:B:864:MET:CE	1:B:902:GLN:HE21	1.99	0.75
1:D:822:LYS:HG2	1:D:826:ARG:HH21	1.51	0.74
1:B:901:ARG:HH22	1:B:960:VAL:CB	2.01	0.74
1:B:884:ILE:HG12	1:B:910:THR:HG21	1.70	0.73
1:D:878:HIS:O	1:D:880:LYS:NZ	2.20	0.73
1:B:860:ARG:HG3	1:B:860:ARG:NH1	2.00	0.72
1:D:952:GLY:HA3	1:D:964:THR:O	1.90	0.72
1:B:878:HIS:NE2	1:B:886:ASP:OD2	2.23	0.71
1:B:901:ARG:HH22	1:B:960:VAL:HB	1.56	0.71
1:A:917:PRO:HG3	1:A:970:LEU:HD11	1.73	0.70
1:D:962:GLN:HG3	2:D:1004:HOH:O	1.90	0.70
1:B:879:SER:HB3	2:B:1004:HOH:O	1.91	0.70
1:C:934:MET:HG3	1:C:935:PRO:HD2	1.73	0.69
1:B:826:ARG:O	1:B:829:GLU:HG3	1.93	0.69
1:D:822:LYS:HE2	1:D:826:ARG:CZ	2.23	0.68
1:B:896:LEU:C	1:B:896:LEU:HD23	2.17	0.68
1:A:812:ARG:NH1	1:A:812:ARG:HG3	2.00	0.68
1:B:896:LEU:CD2	1:B:926:ALA:HB3	2.23	0.68
1:B:867:ALA:O	1:B:871:THR:HG23	1.96	0.66
1:A:877:ARG:NH1	1:A:886:ASP:OD2	2.28	0.66
1:C:918:GLN:HE21	1:C:924:LEU:HD12	1.60	0.66
1:B:896:LEU:HD23	1:B:896:LEU:O	1.94	0.66
1:A:868:ALA:HA	1:A:902:GLN:HE22	1.60	0.66
1:C:814:VAL:HG21	1:C:866:GLN:NE2	2.10	0.66
1:C:891:GLU:OE1	1:C:891:GLU:N	2.19	0.66
1:C:814:VAL:HG21	1:C:866:GLN:HE22	1.60	0.65
1:B:854:ARG:CG	1:B:854:ARG:HH21	2.10	0.65
1:D:860:ARG:NH2	1:D:864:MET:HE3	2.11	0.65
1:B:883:LEU:HD11	1:B:885:VAL:HG23	1.79	0.65
1:D:934:MET:SD	1:D:988:HIS:HA	2.36	0.64
1:B:934:MET:H	1:B:934:MET:CE	2.09	0.64
1:C:826:ARG:HH21	1:C:826:ARG:CG	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:871:THR:HG22	1:B:899:VAL:HG13	1.78	0.64
1:B:864:MET:HE3	1:B:902:GLN:HE21	1.53	0.64
1:B:877:ARG:NH1	1:B:886:ASP:OD2	2.31	0.64
1:D:860:ARG:HH12	1:D:864:MET:HE2	1.60	0.64
1:B:893:LEU:HB2	1:B:924:LEU:HD23	1.80	0.63
1:D:946:VAL:HA	1:D:976:ILE:HD11	1.81	0.63
1:D:962:GLN:CG	2:D:1004:HOH:O	2.45	0.63
1:B:919:PRO:O	1:B:920:MET:HB2	1.98	0.62
1:B:880:LYS:O	1:B:880:LYS:HG2	1.99	0.62
1:D:877:ARG:NH2	1:D:886:ASP:OD2	2.32	0.62
1:B:870:LYS:HA	1:B:873:GLU:HG2	1.82	0.62
1:A:866:GLN:NE2	1:A:891:GLU:OE2	2.32	0.62
1:C:862:LEU:C	1:C:866:GLN:HE21	2.07	0.62
1:D:893:LEU:O	1:D:897:VAL:HG23	1.99	0.62
1:D:950:MET:HE2	1:D:967:THR:HG22	1.82	0.61
1:A:987:GLU:OE2	1:C:878:HIS:ND1	2.23	0.61
1:C:820:LEU:C	1:C:820:LEU:HD23	2.26	0.61
1:A:944:LEU:HD22	1:D:944:LEU:HD11	1.82	0.61
1:A:870:LYS:NZ	1:A:889:SER:O	2.30	0.60
1:D:946:VAL:HA	1:D:976:ILE:CD1	2.32	0.60
1:D:860:ARG:NH1	1:D:864:MET:CE	2.62	0.60
1:D:822:LYS:CG	1:D:826:ARG:NH2	2.63	0.60
1:D:814:VAL:HG12	1:D:862:LEU:HD23	1.82	0.60
1:C:891:GLU:H	1:C:891:GLU:CD	2.01	0.60
1:A:854:ARG:HH21	1:A:854:ARG:CG	2.12	0.59
1:B:901:ARG:NH2	1:B:960:VAL:CB	2.64	0.59
1:B:931:GLN:H	1:B:931:GLN:CD	2.00	0.58
1:C:982:LEU:O	1:C:986:LEU:HG	2.03	0.58
1:B:886:ASP:OD1	1:B:887:THR:N	2.32	0.58
1:A:854:ARG:HG2	1:A:854:ARG:NH2	2.07	0.58
1:C:864:MET:HE2	1:C:898:LYS:HE2	1.85	0.58
1:C:869:LYS:O	1:C:873:GLU:HG3	2.05	0.57
1:D:918:GLN:HB2	1:D:922:LYS:O	2.05	0.57
1:B:845:LEU:O	1:B:849:LYS:HG3	2.04	0.57
1:A:873:GLU:O	1:A:877:ARG:HG3	2.05	0.56
1:C:918:GLN:NE2	1:C:924:LEU:HD12	2.19	0.56
1:B:918:GLN:HG3	1:B:922:LYS:HE3	1.86	0.56
1:A:828:ILE:HG12	1:A:848:VAL:HG23	1.87	0.56
1:B:945:ALA:HB2	1:C:944:LEU:HD23	1.87	0.56
1:A:891:GLU:H	1:A:891:GLU:CD	2.13	0.56
1:A:880:LYS:NZ	1:A:906:GLN:O	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:813:ASP:HA	1:C:816:GLU:OE1	2.06	0.55
1:C:919:PRO:O	1:C:920:MET:HB2	2.07	0.55
1:A:866:GLN:O	1:A:870:LYS:HG3	2.06	0.55
1:D:892:SER:OG	1:D:895:VAL:HG12	2.06	0.55
1:B:824:ILE:O	1:B:828:ILE:HD12	2.08	0.54
1:A:988:HIS:NE2	1:D:976:ILE:HG22	2.22	0.54
1:A:819:ARG:O	1:A:819:ARG:HD3	2.07	0.54
1:B:952:GLY:HA3	1:B:964:THR:O	2.09	0.53
1:C:901:ARG:HD3	1:C:928:GLN:HE22	1.73	0.53
1:B:946:VAL:O	1:B:950:MET:HG3	2.08	0.53
1:C:981:ALA:O	1:C:985:LEU:HG	2.09	0.52
1:C:874:LEU:O	1:C:878:HIS:HB2	2.09	0.52
1:D:946:VAL:O	1:D:950:MET:HG3	2.09	0.52
1:A:814:VAL:HG21	1:A:866:GLN:NE2	2.24	0.51
1:D:860:ARG:HH12	1:D:864:MET:CE	2.22	0.51
1:C:892:SER:OG	1:C:895:VAL:HG23	2.09	0.51
1:A:873:GLU:O	1:A:876:GLU:HG2	2.10	0.51
1:B:896:LEU:HD22	1:B:926:ALA:HB3	1.90	0.51
1:B:877:ARG:NH1	1:B:886:ASP:CG	2.68	0.51
1:B:850:MET:C	1:B:850:MET:SD	2.94	0.51
1:C:826:ARG:CG	1:C:826:ARG:NH2	2.72	0.51
1:D:828:ILE:HG12	1:D:848:VAL:HG12	1.92	0.51
1:B:928:GLN:HG3	1:B:960:VAL:HG12	1.93	0.50
1:D:822:LYS:CE	1:D:826:ARG:NH2	2.45	0.50
1:D:891:GLU:CD	1:D:891:GLU:H	2.20	0.49
1:B:896:LEU:HD22	1:B:926:ALA:CB	2.41	0.49
1:B:828:ILE:CD1	1:B:848:VAL:HG12	2.42	0.49
1:D:947:CYS:SG	1:D:963:GLY:HA3	2.53	0.49
1:D:870:LYS:HE3	1:D:889:SER:O	2.13	0.49
1:B:826:ARG:CZ	1:B:829:GLU:HG2	2.43	0.48
1:B:893:LEU:HB2	1:B:924:LEU:CD2	2.42	0.48
1:B:828:ILE:HG13	1:B:848:VAL:CG1	2.43	0.48
1:A:869:LYS:O	1:A:873:GLU:HG3	2.13	0.48
1:A:988:HIS:CD2	1:D:976:ILE:HG22	2.49	0.48
1:B:974:LEU:O	1:B:978:GLN:HG2	2.14	0.48
1:D:822:LYS:HE2	1:D:826:ARG:NH1	2.29	0.48
1:B:828:ILE:HG13	1:B:848:VAL:HG12	1.96	0.47
1:D:891:GLU:CD	1:D:891:GLU:N	2.72	0.47
1:C:884:ILE:HG13	1:C:910:THR:HG21	1.96	0.47
1:C:923:VAL:HG21	1:C:950:MET:HE1	1.96	0.47
1:D:923:VAL:HG11	1:D:950:MET:HE1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:877:ARG:HB3	1:B:878:HIS:CD2	2.50	0.47
1:B:877:ARG:NH1	1:B:886:ASP:OD1	2.46	0.47
1:B:950:MET:HE2	1:B:967:THR:HG22	1.97	0.47
1:C:862:LEU:O	1:C:866:GLN:HG3	2.15	0.46
1:B:896:LEU:C	1:B:896:LEU:CD2	2.87	0.46
1:C:864:MET:CE	1:C:898:LYS:HE2	2.44	0.46
1:C:923:VAL:HG11	1:C:950:MET:HE1	1.97	0.46
1:B:894:SER:O	1:B:898:LYS:HG3	2.16	0.46
1:B:896:LEU:HD12	1:B:916:SER:HB2	1.97	0.46
1:D:828:ILE:CG1	1:D:848:VAL:HG12	2.46	0.46
1:B:871:THR:HG21	1:B:902:GLN:HB2	1.97	0.46
1:B:854:ARG:CG	1:B:854:ARG:NH2	2.72	0.45
1:C:893:LEU:O	1:C:897:VAL:HG23	2.16	0.45
1:C:918:GLN:HE21	1:C:924:LEU:CD1	2.29	0.45
1:D:936:THR:OG1	1:D:984:GLN:NE2	2.49	0.45
1:B:918:GLN:HB2	1:B:922:LYS:O	2.16	0.45
1:B:979:THR:HG22	1:C:980:TYR:CD1	2.51	0.45
1:A:812:ARG:NH1	1:A:812:ARG:CG	2.72	0.45
1:D:883:LEU:HD23	1:D:911:SER:HB2	1.99	0.45
1:B:828:ILE:HD11	1:B:848:VAL:HG12	1.99	0.45
1:C:820:LEU:HD23	1:C:820:LEU:O	2.16	0.45
1:A:988:HIS:CD2	1:D:976:ILE:CG2	3.00	0.44
1:C:886:ASP:OD1	1:C:887:THR:N	2.42	0.44
1:B:934:MET:N	1:B:934:MET:CE	2.73	0.44
1:A:818:LEU:HD23	1:A:859:ILE:HD13	1.99	0.44
1:C:900:VAL:HG12	1:C:928:GLN:HE21	1.83	0.44
1:A:923:VAL:N	1:A:965:GLY:O	2.50	0.44
1:A:952:GLY:HA3	1:A:964:THR:O	2.17	0.44
1:A:986:LEU:O	1:A:988:HIS:CD2	2.70	0.44
1:C:971:GLU:HG3	1:C:972:ALA:N	2.33	0.44
1:D:860:ARG:CZ	1:D:864:MET:CE	2.95	0.44
1:D:828:ILE:HG12	1:D:848:VAL:CG1	2.48	0.44
1:D:822:LYS:CG	1:D:826:ARG:HH22	2.29	0.44
1:D:838:GLN:HE21	1:D:842:ARG:NE	2.15	0.44
1:C:838:GLN:OE1	1:C:841:ARG:NH1	2.51	0.43
1:D:893:LEU:HD21	1:D:962:GLN:OE1	2.18	0.43
1:C:893:LEU:HD13	1:C:897:VAL:HG23	1.99	0.43
1:A:885:VAL:HG12	1:A:974:LEU:HD22	2.00	0.43
1:C:866:GLN:HG3	1:C:866:GLN:H	1.30	0.43
1:C:878:HIS:NE2	1:C:886:ASP:OD2	2.51	0.43
1:B:875:LEU:HD23	1:B:875:LEU:HA	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:819:ARG:HD3	1:A:819:ARG:C	2.42	0.43
1:D:902:GLN:O	1:D:906:GLN:HG3	2.19	0.43
1:B:979:THR:OG1	1:C:984:GLN:NE2	2.52	0.42
1:A:988:HIS:ND1	1:D:975:SER:OG	2.40	0.42
1:C:918:GLN:HB2	1:C:922:LYS:O	2.20	0.42
1:D:822:LYS:CD	1:D:826:ARG:HH22	2.26	0.42
1:B:923:VAL:HG21	1:B:970:LEU:HD11	2.00	0.42
1:A:830:ALA:O	1:A:834:ALA:HB2	2.20	0.42
1:A:891:GLU:OE2	1:A:895:VAL:HG21	2.19	0.42
1:A:886:ASP:OD1	1:A:887:THR:N	2.45	0.41
1:C:952:GLY:HA3	1:C:964:THR:O	2.19	0.41
1:D:818:LEU:HD23	1:D:859:ILE:HD13	2.03	0.41
1:A:875:LEU:HA	1:A:875:LEU:HD23	1.82	0.41
1:B:953:LYS:HE3	1:B:954:ALA:O	2.21	0.41
1:D:860:ARG:CZ	1:D:864:MET:HE3	2.50	0.41
1:C:918:GLN:NE2	1:C:924:LEU:CD1	2.83	0.41
1:D:875:LEU:HD22	1:D:880:LYS:NZ	2.36	0.41
1:D:860:ARG:HH22	1:D:864:MET:HE3	1.85	0.41
1:D:919:PRO:C	1:D:920:MET:HG2	2.45	0.41
1:B:928:GLN:HG3	1:B:960:VAL:CG1	2.51	0.40
1:B:811:SER:OG	1:B:812:ARG:N	2.55	0.40
1:C:946:VAL:HG21	1:C:977:ALA:HB2	2.02	0.40
1:C:814:VAL:HG21	1:C:866:GLN:CD	2.45	0.40
1:D:860:ARG:NH2	1:D:864:MET:CE	2.83	0.40
1:B:854:ARG:HH21	1:B:854:ARG:HG2	1.83	0.40
1:B:953:LYS:HD2	1:B:954:ALA:H	1.86	0.40
1:B:979:THR:HG21	1:C:984:GLN:HE21	1.86	0.40
1:B:828:ILE:HG23	1:B:845:LEU:HD11	2.03	0.40
1:B:924:LEU:HD12	1:B:924:LEU:N	2.37	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	179/192 (93%)	178 (99%)	1 (1%)	0	100	100
1	B	176/192 (92%)	175 (99%)	1 (1%)	0	100	100
1	C	174/192 (91%)	170 (98%)	4 (2%)	0	100	100
1	D	180/192 (94%)	179 (99%)	1 (1%)	0	100	100
All	All	709/768 (92%)	702 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	146/155 (94%)	142 (97%)	4 (3%)	39	58
1	B	144/155 (93%)	139 (96%)	5 (4%)	32	48
1	C	142/155 (92%)	141 (99%)	1 (1%)	76	87
1	D	148/155 (96%)	146 (99%)	2 (1%)	59	76
All	All	580/620 (94%)	568 (98%)	12 (2%)	47	66

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	818	LEU
1	B	854	ARG
1	B	887	THR
1	B	934	MET
1	B	970	LEU
1	A	812	ARG
1	A	819	ARG
1	A	960	VAL
1	A	962	GLN
1	C	826	ARG
1	D	887	THR
1	D	895	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	866	GLN
1	B	918	GLN
1	B	928	GLN
1	A	852	GLN
1	A	866	GLN
1	A	902	GLN
1	A	906	GLN
1	A	918	GLN
1	A	928	GLN
1	A	949	HIS
1	C	856	ASN
1	C	866	GLN
1	C	902	GLN
1	C	928	GLN
1	C	978	GLN
1	C	984	GLN
1	D	838	GLN
1	D	872	GLN
1	D	984	GLN
1	D	988	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	181/192 (94%)	0.62	13 (7%) 21 23	46, 70, 107, 132	0
1	B	178/192 (92%)	0.82	16 (8%) 15 16	52, 81, 119, 148	0
1	C	176/192 (91%)	0.59	8 (4%) 38 40	47, 71, 107, 137	0
1	D	182/192 (94%)	0.60	7 (3%) 44 46	49, 69, 106, 128	0
All	All	717/768 (93%)	0.66	44 (6%) 27 29	46, 72, 111, 148	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	809	LEU	6.9
1	C	987	GLU	5.0
1	A	934	MET	3.8
1	C	890	ALA	3.7
1	B	988	HIS	3.2
1	A	933	ALA	3.2
1	A	920	MET	3.1
1	C	818	LEU	2.9
1	C	866	GLN	2.8
1	B	881	GLY	2.8
1	A	935	PRO	2.8
1	A	968	THR	2.8
1	D	934	MET	2.8
1	A	810	GLY	2.7
1	B	919	PRO	2.7
1	B	880	LYS	2.7
1	D	985	LEU	2.7
1	A	891	GLU	2.6
1	A	812	ARG	2.6
1	A	890	ALA	2.6
1	B	811	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	933	ALA	2.6
1	B	936	THR	2.6
1	D	891	GLU	2.5
1	B	921	GLY	2.5
1	D	935	PRO	2.4
1	C	934	MET	2.4
1	A	985	LEU	2.4
1	C	817	ALA	2.4
1	B	879	SER	2.3
1	B	968	THR	2.3
1	D	850	MET	2.2
1	B	857	THR	2.2
1	B	866	GLN	2.2
1	B	888	VAL	2.2
1	A	936	THR	2.2
1	C	953	LYS	2.1
1	A	966	SER	2.1
1	C	968	THR	2.1
1	B	848	VAL	2.1
1	B	929	VAL	2.1
1	B	920	MET	2.0
1	D	887	THR	2.0
1	B	935	PRO	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.