Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 05:19 AM EDT

PDB ID	:	6NLY
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:

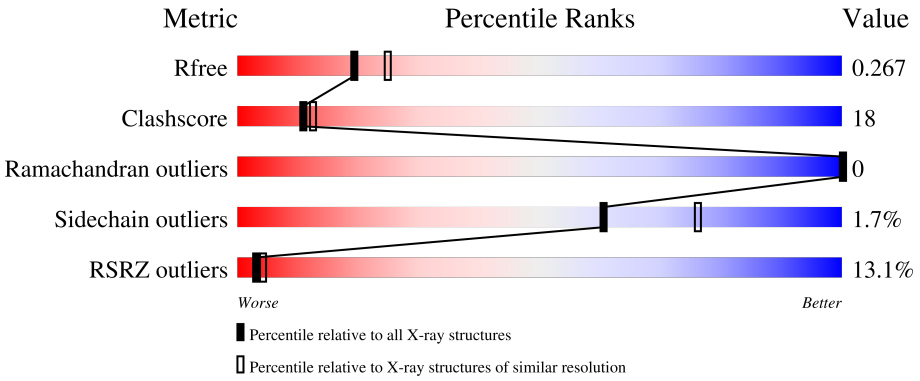
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 <=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	12% 72% 21% • 6%
1	B	192	16% 61% 30% • 7%
1	C	192	10% 67% 24% • 8%
1	D	192	11% 72% 22% • 5%

2 Entry composition (i)

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

Continued on next page...

Continued from previous page...

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

- Molecule 2 is water.

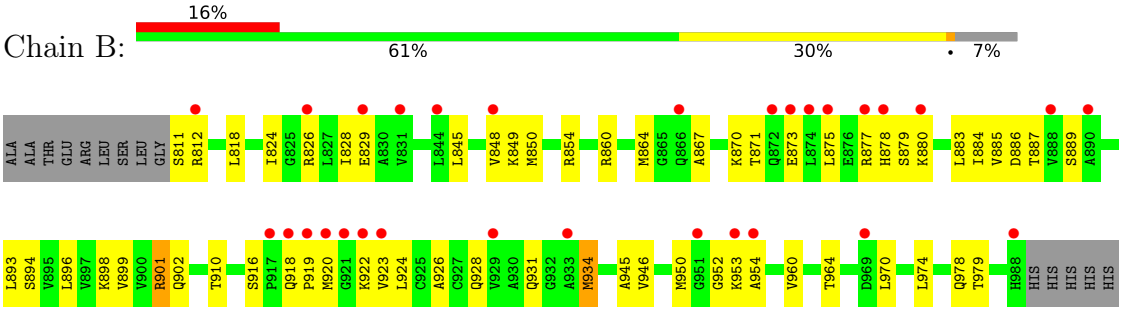
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	5	Total O 5 5	0	0
2	A	6	Total O 6 6	0	0
2	C	4	Total O 4 4	0	0
2	D	6	Total O 6 6	0	0

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.

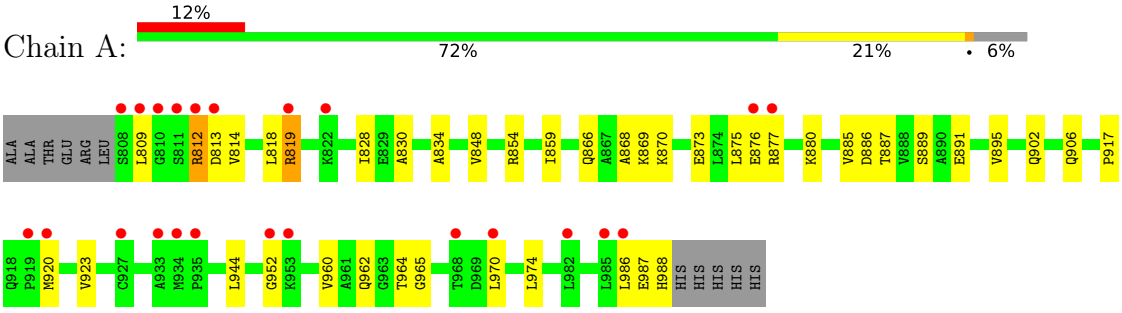
• Molecule 1: Alanine–tRNA ligase, mitochondrial

Chain B:



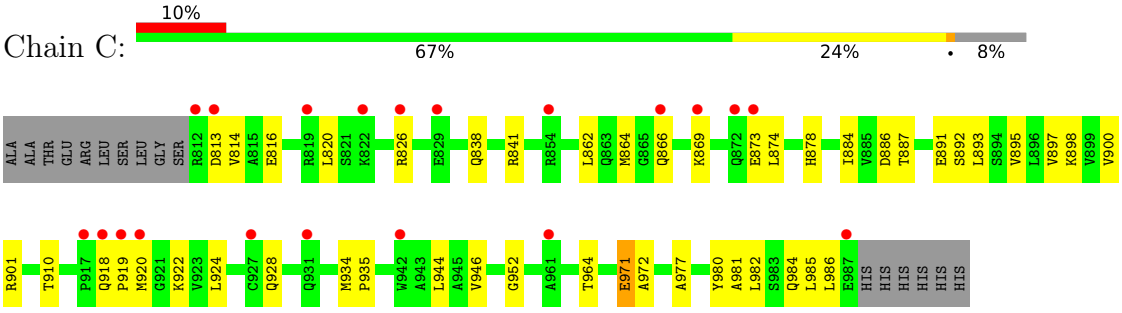
• Molecule 1: Alanine–tRNA ligase, mitochondrial

Chain A:



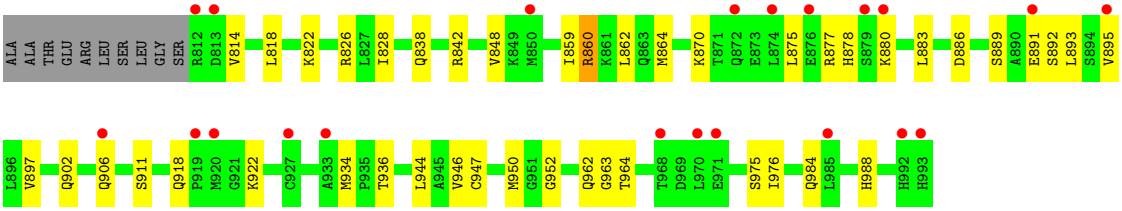
• Molecule 1: Alanine–tRNA ligase, mitochondrial

Chain C:



• Molecule 1: Alanine–tRNA ligase, mitochondrial

Chain D:


ALA ALA THR GLU ARG LEU SER LEU GLY SER R812 D813 V814 L818 K822 R826 L827 I828 Q838 R842 V848 K849 M850 I859 R860 K861 L862 Q863 M864 K870 T871 Q872 E873 L874 L875 E876 R877 H878 S879 K880 L883 D886 S889 A890 E891 S892 L893 S894 V895
L896 V897 Q902 Q906 S911 Q918 P919 M920 G921 K922 C927 A933 M934 P935 T936 L944 A945 V946 C947 M950 G951 G952 Q962 G963 T964 T968 D969 L970 E971 S975 I976 Q984 L985 H988 H992 H993

4 Data and refinement statistics (i)

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 38.45 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.1 (38.02-2.31) 99.4 (38.45-2.31)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.27 (at 2.31Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.209 , 0.257 0.227 , 0.267	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)	0.35 , 62.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.44	0/1373	0.61	0/1857
1	B	0.55	0/1355	0.70	0/1833
1	C	0.53	0/1339	0.74	0/1812
1	D	0.55	0/1405	0.65	0/1900
All	All	0.52	0/5472	0.68	0/7402

There are no bond length outliers.

There are no bond angle outliers.

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	37	0
1	B	1339	0	1400	79	0
1	C	1324	0	1388	43	0
1	D	1384	0	1430	52	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	201	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 18.

All (201) 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: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:D:822:LYS:HG2	1:D:826:ARG:NH2	1.90	0.87
1:A:809:LEU:O	1:A:812:ARG:HG2	1.74	0.86
1:B:901:ARG:NH2	1:B:960:VAL:CG1	2.37	0.86
1:B:864:MET:HE1	1:B:902:GLN:HE21	1.46	0.81
1:B:901:ARG:HH22	1:B:960:VAL:CG1	1.95	0.79
1:B:934:MET:HE2	1:B:934:MET:H	1.47	0.79
1:B:918:GLN:HE21	1:B:924:LEU:HD11	1.47	0.78
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:D:860:ARG:NH1	1:D:864:MET:HE2	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:D:860:ARG:CZ	1:D:864:MET:HE2	2.16	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:864:MET:HE3	1:B:902:GLN:NE2	2.06	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:934:MET:HE2	1:B:934:MET:N	2.09	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:B:883:LEU:HD11	1:B:885:VAL:HG23	1.79	0.65
1:B:934:MET:H	1:B:934:MET:CE	2.09	0.64
1:D:934:MET:SD	1:D:988:HIS:HA	2.36	0.64
1:C:826:ARG:HH21	1:C:826:ARG:CG	2.10	0.64
1:B:871:THR:HG22	1:B:899:VAL:HG13	1.78	0.64
1:B:896:LEU:HD23	1:B:896:LEU:C	2.17	0.64
1:B:877:ARG:NH1	1:B:886:ASP:OD2	2.31	0.64
1:B:893:LEU:HB2	1:B:924:LEU:HD23	1.80	0.63
1:D:860:ARG:NH1	1:D:864:MET:CE	2.62	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:D:893:LEU:O	1:D:897:VAL:HG23	1.99	0.62
1:A:987:GLU:OE2	1:C:878:HIS:ND1	2.23	0.61
1:A:944:LEU:HD22	1:D:944:LEU:HD11	1.82	0.61
1:D:946:VAL:HA	1:D:976:ILE:CD1	2.32	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: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: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:862:LEU:C	1:C:866:GLN:HE21	2.07	0.57
1:C:869:LYS:O	1:C:873:GLU:HG3	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:820:LEU:C	1:C:820:LEU:HD23	2.26	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:880:LYS:NZ	1:A:906:GLN:O	2.35	0.55
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:B:931:GLN:H	1:B:931:GLN:CD	2.00	0.54
1:A:988:HIS:NE2	1:D:976:ILE:HG22	2.22	0.54
1:D:875:LEU:CD2	1:D:880:LYS:HZ2	2.21	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:860:ARG:HH12	1:D:864:MET:CE	2.22	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: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:A:891:GLU:H	1:A:891:GLU:CD	2.13	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:864:MET:HE1	1:B:902:GLN:NE2	2.16	0.47
1:C:884:ILE:HG13	1:C:910:THR:HG21	1.96	0.47
1:C:864:MET:CE	1:C:898:LYS:HE2	2.44	0.47
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:C:862:LEU:O	1:C:866:GLN:HG3	2.15	0.46
1:B:877:ARG:NH1	1:B:886:ASP:CG	2.68	0.46
1:B:850:MET:C	1:B:850:MET:SD	2.94	0.46
1:B:934:MET:N	1:B:934:MET:CE	2.73	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:870:LYS:NZ	1:A:889:SER:O	2.30	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:D:891:GLU:CD	1:D:891:GLU:H	2.20	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: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:D:875:LEU:HD22	1:D:880:LYS:HZ2	1.82	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:891:GLU:H	1:C:891:GLU:CD	2.01	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:D:860:ARG:NH2	1:D:864:MET:HE2	2.33	0.43
1:B:875:LEU:HD23	1:B:875:LEU:HA	1.87	0.43
1:D:891:GLU:CD	1:D:891:GLU:N	2.72	0.43
1:C:864:MET:HE1	1:C:898:LYS:HE2	2.00	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:D:875:LEU:HD23	1:D:880:LYS:HZ2	1.84	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:B:896:LEU:CD2	1:B:896:LEU:C	2.87	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:D:860:ARG:NH2	1:D:864:MET:CE	2.83	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: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: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: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 (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	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 (i)

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%)	141 (97%)	5 (3%)	37	51
1	B	144/155 (93%)	141 (98%)	3 (2%)	53	70
1	C	142/155 (92%)	141 (99%)	1 (1%)	84	92
1	D	148/155 (96%)	147 (99%)	1 (1%)	84	92
All	All	580/620 (94%)	570 (98%)	10 (2%)	60	76

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	818	LEU
1	B	901	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	934	MET
1	A	812	ARG
1	A	819	ARG
1	A	920	MET
1	A	960	VAL
1	A	962	GLN
1	C	971	GLU
1	D	860	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	866	GLN
1	B	902	GLN
1	B	918	GLN
1	B	928	GLN
1	A	852	GLN
1	A	902	GLN
1	A	918	GLN
1	A	928	GLN
1	C	856	ASN
1	C	866	GLN
1	C	928	GLN
1	C	978	GLN
1	C	984	GLN
1	D	838	GLN
1	D	840	GLN
1	D	872	GLN
1	D	984	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 monosaccharides 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, 95^{th} 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%)	1.09	23 (12%)	3	5	46, 70, 107, 132	0
1	B	178/192 (92%)	1.14	30 (16%)	1	2	52, 81, 119, 148	0
1	C	176/192 (91%)	0.94	20 (11%)	5	7	47, 71, 107, 137	0
1	D	182/192 (94%)	0.96	21 (11%)	4	7	49, 69, 106, 128	0
All	All	717/768 (93%)	1.03	94 (13%)	3	4	46, 72, 111, 148	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	809	LEU	9.5
1	A	808	SER	8.5
1	A	810	GLY	8.1
1	A	920	MET	6.3
1	D	920	MET	6.0
1	A	919	PRO	5.1
1	D	872	GLN	4.7
1	C	920	MET	4.5
1	B	920	MET	4.5
1	A	934	MET	4.2
1	B	969	ASP	4.1
1	A	811	SER	4.1
1	D	968	THR	4.0
1	C	917	PRO	4.0
1	B	812	ARG	4.0
1	C	919	PRO	3.9
1	D	876	GLU	3.9
1	B	919	PRO	3.9
1	B	923	VAL	3.8
1	A	812	ARG	3.6
1	C	918	GLN	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	888	VAL	3.6
1	D	993	HIS	3.5
1	A	813	ASP	3.5
1	D	919	PRO	3.5
1	B	917	PRO	3.4
1	D	970	LEU	3.3
1	C	813	ASP	3.2
1	B	875	LEU	3.2
1	B	954	ALA	3.2
1	B	826	ARG	3.2
1	B	872	GLN	3.1
1	C	829	GLU	3.1
1	B	890	ALA	3.0
1	B	929	VAL	3.0
1	D	880	LYS	3.0
1	D	992	HIS	3.0
1	B	921	GLY	3.0
1	C	987	GLU	3.0
1	A	986	LEU	2.9
1	B	874	LEU	2.9
1	A	935	PRO	2.9
1	D	927	CYS	2.8
1	B	933	ALA	2.8
1	B	918	GLN	2.8
1	A	933	ALA	2.7
1	C	866	GLN	2.7
1	C	819	ARG	2.7
1	B	953	LYS	2.6
1	A	876	GLU	2.6
1	C	872	GLN	2.6
1	C	873	GLU	2.6
1	B	877	ARG	2.6
1	A	822	LYS	2.6
1	A	952	GLY	2.5
1	A	970	LEU	2.5
1	D	874	LEU	2.5
1	C	942	TRP	2.5
1	D	971	GLU	2.4
1	A	985	LEU	2.4
1	B	829	GLU	2.4
1	B	922	LYS	2.4
1	D	813	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	933	ALA	2.4
1	A	927	CYS	2.4
1	A	877	ARG	2.3
1	D	891	GLU	2.3
1	C	812	ARG	2.3
1	B	831	VAL	2.3
1	C	869	LYS	2.3
1	B	866	GLN	2.3
1	D	850	MET	2.3
1	D	895	VAL	2.3
1	D	906	GLN	2.3
1	C	822	LYS	2.2
1	B	873	GLU	2.2
1	D	812	ARG	2.2
1	D	879	SER	2.2
1	B	951	GLY	2.2
1	A	953	LYS	2.2
1	A	968	THR	2.2
1	B	880	LYS	2.1
1	C	826	ARG	2.1
1	B	988	HIS	2.1
1	B	848	VAL	2.1
1	B	878	HIS	2.1
1	C	927	CYS	2.1
1	C	931	GLN	2.0
1	A	982	LEU	2.0
1	C	854	ARG	2.0
1	D	985	LEU	2.0
1	C	961	ALA	2.0
1	B	844	LEU	2.0
1	A	819	ARG	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 monosaccharides 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.