Full wwPDB X-ray Structure Validation Report

Jan 10, 2017 – 12:05 PM EST

PDB ID	:	5H9U
Title	:	Crystal structure of a thermostable methionine adenosyltransferase
Authors	:	Feng, Y.; Wang, W.
Deposited on	:	2015-12-29
Resolution	:	2.67 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

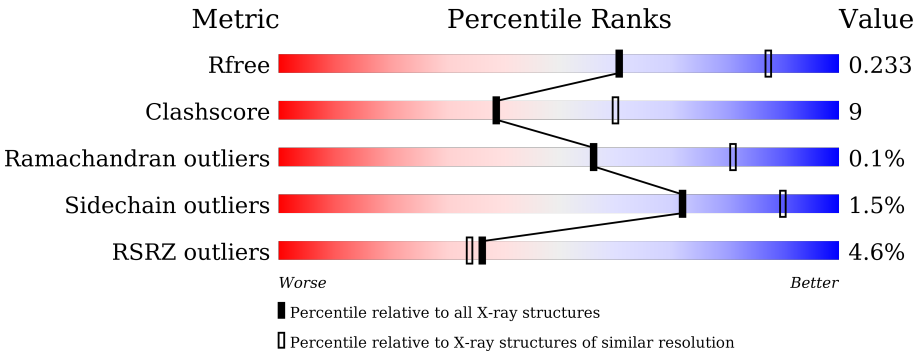
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.67 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}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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 <=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	413	4% 79% 16% 5%
1	B	413	3% 77% 18% • 5%
1	C	413	6% 77% 18% 5%
1	D	413	5% 73% 21% • 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12140 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 S-adenosylmethionine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	394	Total	C	N	O	S	0	0	0
			3035	1924	526	579	6			
1	A	394	Total	C	N	O	S	0	0	0
			3035	1924	526	579	6			
1	B	394	Total	C	N	O	S	0	0	0
			3035	1924	526	579	6			
1	D	394	Total	C	N	O	S	0	0	0
			3035	1924	526	579	6			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	MET	-	expression tag	UNP Q72I53
C	-16	GLY	-	expression tag	UNP Q72I53
C	-15	SER	-	expression tag	UNP Q72I53
C	-14	SER	-	expression tag	UNP Q72I53
C	-13	HIS	-	expression tag	UNP Q72I53
C	-12	HIS	-	expression tag	UNP Q72I53
C	-11	HIS	-	expression tag	UNP Q72I53
C	-10	HIS	-	expression tag	UNP Q72I53
C	-9	SER	-	expression tag	UNP Q72I53
C	-8	SER	-	expression tag	UNP Q72I53
C	-7	GLY	-	expression tag	UNP Q72I53
C	-6	LEU	-	expression tag	UNP Q72I53
C	-5	VAL	-	expression tag	UNP Q72I53
C	-4	PRO	-	expression tag	UNP Q72I53
C	-3	ARG	-	expression tag	UNP Q72I53
C	-2	GLY	-	expression tag	UNP Q72I53
C	-1	SER	-	expression tag	UNP Q72I53
C	0	HIS	-	expression tag	UNP Q72I53
A	-17	MET	-	expression tag	UNP Q72I53
A	-16	GLY	-	expression tag	UNP Q72I53
A	-15	SER	-	expression tag	UNP Q72I53

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	SER	-	expression tag	UNP Q72I53
A	-13	HIS	-	expression tag	UNP Q72I53
A	-12	HIS	-	expression tag	UNP Q72I53
A	-11	HIS	-	expression tag	UNP Q72I53
A	-10	HIS	-	expression tag	UNP Q72I53
A	-9	SER	-	expression tag	UNP Q72I53
A	-8	SER	-	expression tag	UNP Q72I53
A	-7	GLY	-	expression tag	UNP Q72I53
A	-6	LEU	-	expression tag	UNP Q72I53
A	-5	VAL	-	expression tag	UNP Q72I53
A	-4	PRO	-	expression tag	UNP Q72I53
A	-3	ARG	-	expression tag	UNP Q72I53
A	-2	GLY	-	expression tag	UNP Q72I53
A	-1	SER	-	expression tag	UNP Q72I53
A	0	HIS	-	expression tag	UNP Q72I53
B	-17	MET	-	expression tag	UNP Q72I53
B	-16	GLY	-	expression tag	UNP Q72I53
B	-15	SER	-	expression tag	UNP Q72I53
B	-14	SER	-	expression tag	UNP Q72I53
B	-13	HIS	-	expression tag	UNP Q72I53
B	-12	HIS	-	expression tag	UNP Q72I53
B	-11	HIS	-	expression tag	UNP Q72I53
B	-10	HIS	-	expression tag	UNP Q72I53
B	-9	SER	-	expression tag	UNP Q72I53
B	-8	SER	-	expression tag	UNP Q72I53
B	-7	GLY	-	expression tag	UNP Q72I53
B	-6	LEU	-	expression tag	UNP Q72I53
B	-5	VAL	-	expression tag	UNP Q72I53
B	-4	PRO	-	expression tag	UNP Q72I53
B	-3	ARG	-	expression tag	UNP Q72I53
B	-2	GLY	-	expression tag	UNP Q72I53
B	-1	SER	-	expression tag	UNP Q72I53
B	0	HIS	-	expression tag	UNP Q72I53
D	-17	MET	-	expression tag	UNP Q72I53
D	-16	GLY	-	expression tag	UNP Q72I53
D	-15	SER	-	expression tag	UNP Q72I53
D	-14	SER	-	expression tag	UNP Q72I53
D	-13	HIS	-	expression tag	UNP Q72I53
D	-12	HIS	-	expression tag	UNP Q72I53
D	-11	HIS	-	expression tag	UNP Q72I53
D	-10	HIS	-	expression tag	UNP Q72I53
D	-9	SER	-	expression tag	UNP Q72I53

Continued on next page...

Continued from previous page...

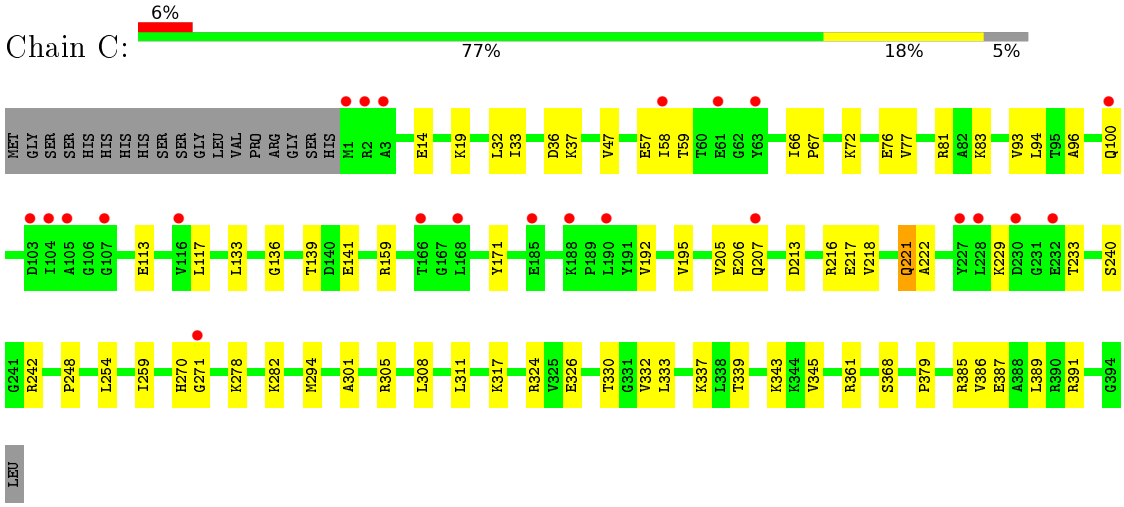
Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	SER	-	expression tag	UNP Q72I53
D	-7	GLY	-	expression tag	UNP Q72I53
D	-6	LEU	-	expression tag	UNP Q72I53
D	-5	VAL	-	expression tag	UNP Q72I53
D	-4	PRO	-	expression tag	UNP Q72I53
D	-3	ARG	-	expression tag	UNP Q72I53
D	-2	GLY	-	expression tag	UNP Q72I53
D	-1	SER	-	expression tag	UNP Q72I53
D	0	HIS	-	expression tag	UNP Q72I53

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 errors 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.

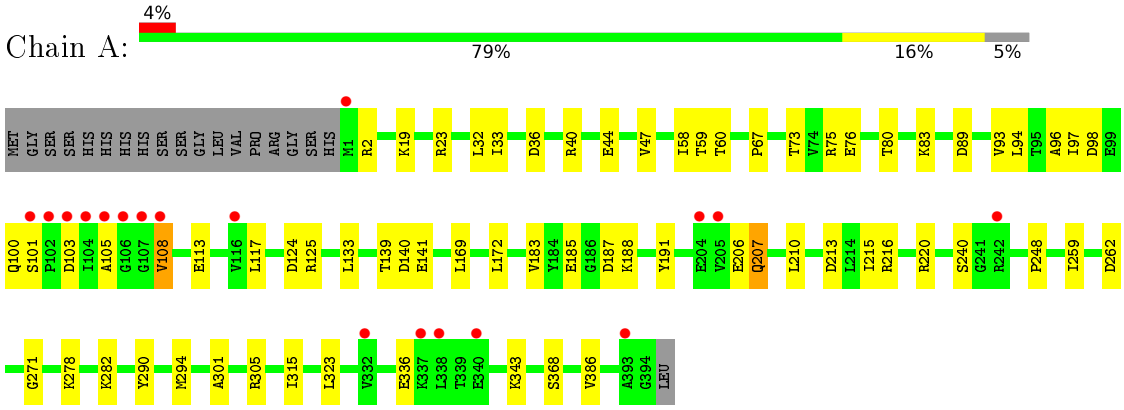
- Molecule 1: S-adenosylmethionine synthase

Chain C:



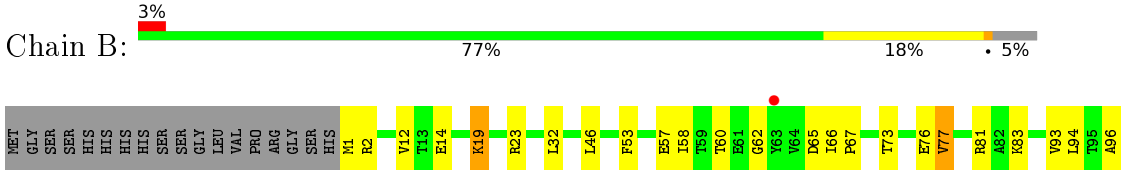
- Molecule 1: S-adenosylmethionine synthase

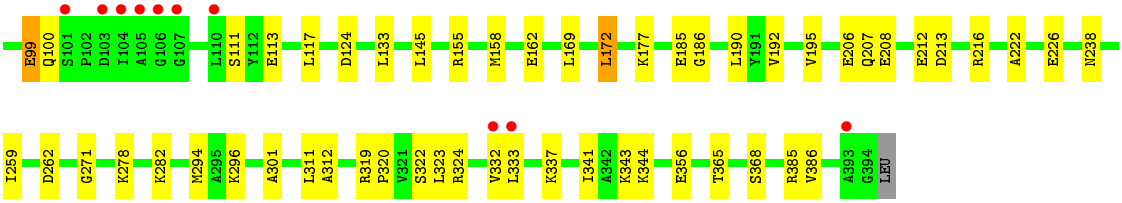
Chain A:



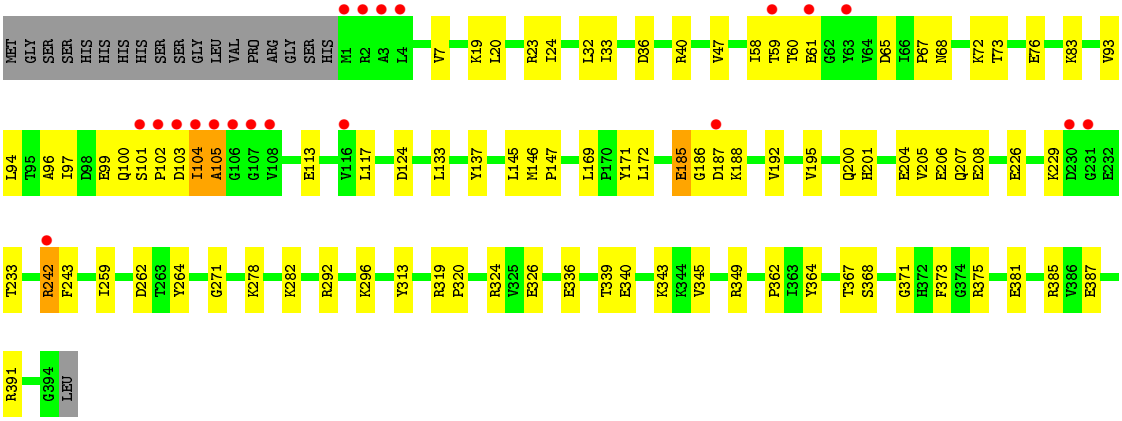
- Molecule 1: S-adenosylmethionine synthase

Chain B:





- Molecule 1: S-adenosylmethionine synthase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	230.02Å 77.05Å 96.79Å 90.00° 112.04° 90.00°	Depositor
Resolution (Å)	43.24 – 2.67 43.23 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.24-2.67) 99.6 (43.23-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.13 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.173 , 0.233 0.173 , 0.233	Depositor DCC
R_{free} test set	2262 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	45.6	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 58.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12140	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.32	0/3095	0.56	0/4208
1	B	0.33	0/3095	0.59	1/4208 (0.0%)
1	C	0.33	0/3095	0.59	0/4208
1	D	0.38	0/3095	0.62	0/4208
All	All	0.34	0/12380	0.59	1/16832 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	62	GLY	N-CA-C	-6.99	95.61	113.10

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	3035	0	3065	47	0
1	B	3035	0	3065	51	0
1	C	3035	0	3065	54	0
1	D	3035	0	3065	79	0
All	All	12140	0	12260	219	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 9.

All (219) 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:101:SER:HB3	1:D:103:ASP:OD1	1.38	1.21
1:D:101:SER:CB	1:D:103:ASP:OD1	2.03	1.05
1:D:101:SER:C	1:D:103:ASP:OD1	2.08	0.92
1:C:345:VAL:O	1:C:385:ARG:NH1	2.06	0.89
1:D:104:ILE:O	1:D:105:ALA:HB3	1.71	0.89
1:D:101:SER:CA	1:D:103:ASP:OD1	2.23	0.86
1:D:61:GLU:OE2	1:D:102:PRO:HD2	1.77	0.85
1:D:206:GLU:HG3	1:D:207:GLN:H	1.43	0.84
1:C:217:GLU:O	1:C:221:GLN:NE2	2.10	0.83
1:D:101:SER:OG	1:D:102:PRO:HD2	1.81	0.81
1:D:61:GLU:OE2	1:D:102:PRO:CD	2.28	0.81
1:D:101:SER:O	1:D:103:ASP:OD1	1.99	0.79
1:D:104:ILE:O	1:D:105:ALA:CB	2.28	0.79
1:D:101:SER:HB3	1:D:103:ASP:CG	2.04	0.78
1:A:187:ASP:OD2	1:A:305:ARG:NH2	2.17	0.77
1:B:81:ARG:HH12	1:B:83:LYS:HD2	1.53	0.74
1:B:99:GLU:C	1:B:100:GLN:HG3	2.06	0.74
1:C:213:ASP:OD1	1:C:216:ARG:NH2	2.20	0.74
1:B:356:GLU:OE1	1:B:385:ARG:NH2	2.18	0.74
1:D:185:GLU:O	1:D:187:ASP:N	2.24	0.71
1:D:387:GLU:O	1:D:391:ARG:HG3	1.89	0.71
1:C:240:SER:HB3	1:A:315:ILE:HG12	1.73	0.70
1:C:59:THR:OG1	1:C:100:GLN:OE1	2.08	0.70
1:D:19:LYS:NZ	1:D:262:ASP:OD1	2.22	0.70
1:C:159:ARG:HG2	1:C:221:GLN:NE2	2.07	0.69
1:C:57:GLU:HB3	1:C:100:GLN:NE2	2.08	0.68
1:A:23:ARG:NH1	1:A:76:GLU:OE1	2.27	0.68
1:A:19:LYS:NZ	1:A:262:ASP:OD1	2.22	0.67
1:A:75:ARG:NH1	1:A:89:ASP:OD1	2.28	0.67
1:A:323:LEU:HD23	1:A:343:LYS:HG2	1.76	0.67
1:A:278:LYS:HB3	1:A:282:LYS:HG3	1.76	0.67
1:D:278:LYS:HB3	1:D:282:LYS:HG3	1.77	0.66
1:B:323:LEU:HD23	1:B:343:LYS:HG2	1.77	0.66
1:D:206:GLU:HG3	1:D:207:GLN:N	2.11	0.65
1:A:100:GLN:OE1	1:A:105:ALA:HB2	1.95	0.65
1:A:75:ARG:HG2	1:A:80:THR:HG22	1.79	0.65
1:B:324:ARG:NH1	1:D:7:VAL:HG22	2.13	0.64
1:B:99:GLU:OE1	1:B:100:GLN:N	2.32	0.63
1:D:101:SER:O	1:D:104:ILE:O	2.17	0.63
1:D:229:LYS:H	1:D:233:THR:HG21	1.65	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:ARG:HH12	1:D:7:VAL:HG22	1.62	0.62
1:D:204:GLU:HG3	1:D:205:VAL:HG23	1.82	0.62
1:C:278:LYS:HB3	1:C:282:LYS:HG3	1.82	0.62
1:A:40:ARG:HD3	1:A:108:VAL:HG13	1.80	0.61
1:C:229:LYS:H	1:C:233:THR:HG21	1.66	0.60
1:A:67:PRO:HA	1:A:93:VAL:HG11	1.83	0.60
1:B:208:GLU:O	1:B:212:GLU:HG3	2.02	0.60
1:C:207:GLN:NE2	1:C:242:ARG:HG2	2.17	0.60
1:D:229:LYS:H	1:D:233:THR:CG2	2.14	0.60
1:C:324:ARG:NH1	1:C:326:GLU:OE2	2.34	0.59
1:B:158:MET:O	1:B:162:GLU:HG3	2.01	0.58
1:C:32:LEU:HD11	1:C:58:ILE:HD13	1.84	0.58
1:A:2:ARG:NH1	1:A:185:GLU:OE1	2.36	0.58
1:A:96:ALA:HB2	1:D:94:LEU:HD23	1.86	0.57
1:B:278:LYS:HB3	1:B:282:LYS:HG3	1.86	0.57
1:D:206:GLU:HG3	1:D:207:GLN:HG2	1.87	0.57
1:D:58:ILE:HD12	1:D:97:ILE:HG21	1.87	0.57
1:A:32:LEU:HD11	1:A:58:ILE:HD13	1.86	0.56
1:A:59:THR:HA	1:A:100:GLN:O	2.05	0.56
1:B:365:THR:O	1:B:368:SER:OG	2.18	0.56
1:D:345:VAL:O	1:D:385:ARG:NH1	2.37	0.56
1:B:32:LEU:HD11	1:B:58:ILE:HD13	1.87	0.56
1:C:83:LYS:N	1:C:83:LYS:HD3	2.20	0.56
1:D:364:TYR:O	1:D:367:THR:OG1	2.19	0.56
1:A:83:LYS:HD3	1:A:83:LYS:N	2.21	0.56
1:A:23:ARG:HG2	1:A:73:THR:CG2	2.36	0.55
1:D:242:ARG:NH1	1:D:242:ARG:HG3	2.20	0.55
1:A:301:ALA:HA	1:A:386:VAL:HG13	1.89	0.55
1:B:14:GLU:HG3	1:B:77:VAL:HG22	1.88	0.55
1:A:33:ILE:HA	1:A:36:ASP:O	2.07	0.55
1:C:339:THR:HG22	1:C:343:LYS:HE2	1.88	0.55
1:D:192:VAL:HG11	1:D:195:VAL:HG13	1.89	0.54
1:A:206:GLU:CD	1:A:207:GLN:H	2.09	0.54
1:B:23:ARG:HG2	1:B:73:THR:CG2	2.37	0.54
1:C:301:ALA:HA	1:C:386:VAL:HG13	1.89	0.54
1:D:33:ILE:HA	1:D:36:ASP:O	2.08	0.54
1:A:113:GLU:HA	1:A:117:LEU:HB2	1.90	0.54
1:D:32:LEU:HD11	1:D:58:ILE:HD13	1.90	0.54
1:D:171:TYR:CG	1:D:205:VAL:HG21	2.43	0.54
1:A:98:ASP:CG	1:A:100:GLN:HE21	2.11	0.53
1:B:32:LEU:HD22	1:B:60:THR:HG21	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ASP:OD1	1:B:216:ARG:NH2	2.43	0.52
1:B:81:ARG:NH1	1:B:83:LYS:HD2	2.24	0.52
1:C:133:LEU:O	1:C:271:GLY:HA3	2.09	0.52
1:B:99:GLU:O	1:B:100:GLN:HG3	2.09	0.52
1:A:47:VAL:HG12	1:A:248:PRO:HB3	1.92	0.51
1:B:185:GLU:HB2	1:B:190:LEU:HD11	1.91	0.51
1:C:206:GLU:CD	1:C:207:GLN:H	2.13	0.51
1:C:216:ARG:NH1	1:C:217:GLU:OE2	2.43	0.51
1:D:324:ARG:NH2	1:D:326:GLU:OE2	2.34	0.51
1:A:113:GLU:HG3	1:A:124:ASP:HB3	1.93	0.51
1:B:259:ILE:HD11	1:D:259:ILE:HD11	1.93	0.51
1:B:2:ARG:NH1	1:B:185:GLU:OE2	2.44	0.50
1:D:339:THR:HG22	1:D:343:LYS:HE2	1.92	0.50
1:B:12:VAL:HG12	1:B:177:LYS:HG2	1.93	0.50
1:C:57:GLU:HB3	1:C:100:GLN:HE22	1.73	0.50
1:A:94:LEU:HD23	1:D:96:ALA:HB2	1.92	0.50
1:C:305:ARG:H	1:C:330:THR:HB	1.76	0.49
1:D:58:ILE:HG22	1:D:99:GLU:HG3	1.95	0.49
1:D:103:ASP:CG	1:D:104:ILE:H	2.15	0.49
1:D:137:TYR:CE2	1:D:147:PRO:HG3	2.47	0.49
1:D:113:GLU:HA	1:D:117:LEU:HB2	1.93	0.49
1:C:81:ARG:HD2	1:C:83:LYS:HZ3	1.78	0.49
1:C:14:GLU:HG3	1:C:77:VAL:HG22	1.95	0.49
1:B:133:LEU:O	1:B:271:GLY:HA3	2.13	0.48
1:C:33:ILE:HA	1:C:36:ASP:O	2.14	0.48
1:D:103:ASP:OD2	1:D:104:ILE:HG23	2.13	0.48
1:D:40:ARG:HB2	1:D:59:THR:HB	1.96	0.48
1:C:171:TYR:CG	1:C:205:VAL:HG21	2.48	0.48
1:D:61:GLU:OE1	1:D:101:SER:OG	2.24	0.48
1:A:140:ASP:OD2	1:A:305:ARG:HG2	2.14	0.48
1:A:98:ASP:OD2	1:A:100:GLN:NE2	2.44	0.48
1:B:155:ARG:NH1	1:B:222:ALA:O	2.47	0.48
1:D:133:LEU:O	1:D:271:GLY:HA3	2.12	0.48
1:C:47:VAL:HG13	1:C:248:PRO:HG3	1.96	0.48
1:A:133:LEU:O	1:A:271:GLY:HA3	2.13	0.47
1:A:336:GLU:OE1	1:A:336:GLU:N	2.47	0.47
1:C:113:GLU:HA	1:C:117:LEU:HB2	1.96	0.47
1:A:213:ASP:OD1	1:A:216:ARG:NH2	2.45	0.47
1:D:242:ARG:HH11	1:D:242:ARG:HG3	1.78	0.47
1:D:137:TYR:HE2	1:D:147:PRO:HG3	1.77	0.47
1:B:207:GLN:NE2	1:B:238:ASN:HB2	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ARG:NH1	1:B:76:GLU:OE2	2.48	0.47
1:C:221:GLN:HG2	1:C:222:ALA:N	2.29	0.47
1:A:23:ARG:HG2	1:A:73:THR:HG23	1.97	0.47
1:B:1:MET:O	1:B:186:GLY:HA3	2.15	0.47
1:D:19:LYS:HD2	1:D:368:SER:O	2.15	0.47
1:B:169:LEU:HB2	1:B:172:LEU:HD22	1.97	0.46
1:B:294:MET:HE3	1:B:311:LEU:HD21	1.98	0.46
1:D:59:THR:HA	1:D:100:GLN:O	2.14	0.46
1:A:19:LYS:HD2	1:A:368:SER:O	2.15	0.46
1:C:47:VAL:CG1	1:C:248:PRO:HG3	2.45	0.46
1:C:259:ILE:HD11	1:A:259:ILE:HD11	1.97	0.46
1:C:229:LYS:O	1:C:233:THR:HG23	2.14	0.46
1:D:72:LYS:O	1:D:76:GLU:HG3	2.16	0.46
1:C:94:LEU:HD23	1:B:96:ALA:HB2	1.97	0.46
1:D:145:LEU:HD12	1:D:296:LYS:HG2	1.97	0.46
1:B:113:GLU:HA	1:B:117:LEU:HB2	1.97	0.46
1:C:345:VAL:HG21	1:C:389:LEU:HD23	1.97	0.46
1:B:19:LYS:NZ	1:B:262:ASP:OD1	2.48	0.46
1:D:83:LYS:H	1:D:83:LYS:HG3	1.55	0.46
1:C:139:THR:OG1	1:C:141:GLU:HG3	2.16	0.45
1:C:218:VAL:HA	1:C:221:GLN:NE2	2.31	0.45
1:D:146:MET:HE3	1:D:264:TYR:HE1	1.82	0.45
1:D:23:ARG:HG2	1:D:73:THR:CG2	2.47	0.45
1:B:192:VAL:HG11	1:B:195:VAL:HG13	1.98	0.45
1:C:332:VAL:HG12	1:C:333:LEU:HD12	1.97	0.45
1:D:201:HIS:CE1	1:D:243:PHE:H	2.35	0.45
1:A:94:LEU:CD2	1:D:96:ALA:HB2	2.47	0.45
1:D:375:ARG:O	1:D:381:GLU:HG3	2.17	0.45
1:D:242:ARG:HH11	1:D:242:ARG:CG	2.30	0.45
1:D:32:LEU:HD22	1:D:60:THR:HG21	1.98	0.45
1:D:61:GLU:OE2	1:D:102:PRO:HD3	2.13	0.45
1:B:65:ASP:OD1	1:B:67:PRO:HD2	2.17	0.44
1:A:207:GLN:OE1	1:A:210:LEU:HD23	2.17	0.44
1:D:371:GLY:O	1:D:375:ARG:NH1	2.48	0.44
1:A:58:ILE:HD12	1:A:97:ILE:HG21	1.99	0.44
1:B:226:GLU:HG2	1:B:226:GLU:H	1.53	0.44
1:D:20:LEU:O	1:D:24:ILE:HG13	2.17	0.44
1:C:259:ILE:HD12	1:C:270:HIS:CE1	2.53	0.44
1:A:60:THR:O	1:A:101:SER:HA	2.18	0.44
1:C:294:MET:HE1	1:C:311:LEU:HD11	2.00	0.44
1:B:332:VAL:HG12	1:B:333:LEU:HD12	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:LYS:O	1:B:341:ILE:HG13	2.18	0.44
1:D:65:ASP:OD2	1:D:68:ASN:HB2	2.18	0.44
1:A:290:TYR:O	1:A:294:MET:HG3	2.18	0.43
1:B:207:GLN:HE22	1:B:238:ASN:HB2	1.83	0.43
1:C:113:GLU:OE2	1:C:317:LYS:HA	2.17	0.43
1:D:19:LYS:HD3	1:D:19:LYS:HA	1.64	0.43
1:B:23:ARG:HG2	1:B:73:THR:HG23	2.00	0.43
1:C:96:ALA:HB2	1:B:94:LEU:HD23	1.99	0.43
1:C:254:LEU:HD11	1:A:44:GLU:HB3	2.00	0.43
1:C:387:GLU:OE1	1:C:391:ARG:NH1	2.52	0.43
1:D:124:ASP:OD1	1:D:349:ARG:NH1	2.41	0.43
1:A:183:VAL:HG21	1:A:191:TYR:CZ	2.54	0.43
1:C:192:VAL:HG11	1:C:195:VAL:HG23	2.01	0.43
1:D:33:ILE:HD11	1:D:362:PRO:CA	2.49	0.43
1:B:145:LEU:HD12	1:B:296:LYS:HG2	2.01	0.42
1:B:81:ARG:HH22	1:B:83:LYS:NZ	2.16	0.42
1:D:169:LEU:HB2	1:D:172:LEU:HD12	2.01	0.42
1:C:72:LYS:O	1:C:76:GLU:HG3	2.18	0.42
1:D:292:ARG:HG2	1:D:373:PHE:CD1	2.54	0.42
1:C:66:ILE:HB	1:C:67:PRO:HD3	2.02	0.42
1:C:83:LYS:HD3	1:C:83:LYS:H	1.83	0.42
1:D:200:GLN:HA	1:D:243:PHE:O	2.20	0.42
1:A:240:SER:OG	1:A:240:SER:O	2.32	0.42
1:D:33:ILE:HD11	1:D:362:PRO:HA	2.02	0.42
1:D:103:ASP:CG	1:D:104:ILE:N	2.73	0.42
1:D:192:VAL:O	1:D:233:THR:HG22	2.20	0.42
1:D:336:GLU:O	1:D:340:GLU:HG3	2.20	0.42
1:C:33:ILE:O	1:C:37:LYS:HG3	2.20	0.41
1:B:301:ALA:HA	1:B:386:VAL:HG13	2.02	0.41
1:B:319:ARG:HA	1:B:320:PRO:HD3	1.88	0.41
1:C:59:THR:HA	1:C:100:GLN:HB2	2.02	0.41
1:C:67:PRO:HA	1:C:93:VAL:HG11	2.02	0.41
1:B:312:ALA:HB3	1:B:322:SER:OG	2.20	0.41
1:B:344:LYS:HA	1:B:344:LYS:HD2	1.68	0.41
1:D:206:GLU:OE2	1:D:242:ARG:NH2	2.52	0.41
1:A:139:THR:OG1	1:A:141:GLU:HG3	2.20	0.41
1:A:19:LYS:HA	1:A:19:LYS:HD3	1.62	0.41
1:C:229:LYS:H	1:C:233:THR:CG2	2.32	0.41
1:C:333:LEU:HD23	1:C:337:LYS:CG	2.51	0.41
1:D:313:TYR:CE2	1:D:320:PRO:HG3	2.56	0.41
1:A:94:LEU:HD23	1:A:94:LEU:HA	1.87	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:PRO:HA	1:B:93:VAL:HG11	2.03	0.41
1:C:19:LYS:NZ	1:C:368:SER:O	2.40	0.41
1:D:242:ARG:NH1	1:D:242:ARG:CG	2.84	0.41
1:D:339:THR:O	1:D:343:LYS:HG3	2.21	0.41
1:A:2:ARG:HA	1:A:2:ARG:HD2	1.92	0.40
1:B:111:SER:OG	1:B:124:ASP:O	2.29	0.40
1:B:66:ILE:HB	1:B:67:PRO:HD3	2.02	0.40
1:D:67:PRO:HA	1:D:93:VAL:HG11	2.03	0.40
1:A:215:ILE:O	1:A:220:ARG:HG3	2.21	0.40
1:D:319:ARG:HA	1:D:320:PRO:HD3	1.90	0.40
1:C:96:ALA:HB2	1:B:94:LEU:CD2	2.51	0.40
1:A:169:LEU:HB2	1:A:172:LEU:HD12	2.04	0.40
1:B:46:LEU:HB3	1:B:53:PHE:HB3	2.04	0.40
1:C:136:GLY:O	1:C:308:LEU:HD12	2.21	0.40
1:C:361:ARG:NH2	1:C:379:PRO:HG3	2.36	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	392/413 (95%)	383 (98%)	9 (2%)	0	100	100
1	B	392/413 (95%)	383 (98%)	9 (2%)	0	100	100
1	C	392/413 (95%)	384 (98%)	8 (2%)	0	100	100
1	D	392/413 (95%)	384 (98%)	6 (2%)	2 (0%)	34	59
All	All	1568/1652 (95%)	1534 (98%)	32 (2%)	2 (0%)	56	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	186	GLY
1	D	105	ALA

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	319/336 (95%)	314 (98%)	5 (2%)	70 89
1	B	319/336 (95%)	313 (98%)	6 (2%)	65 87
1	C	319/336 (95%)	318 (100%)	1 (0%)	94 99
1	D	319/336 (95%)	312 (98%)	7 (2%)	60 84
All	All	1276/1344 (95%)	1257 (98%)	19 (2%)	72 90

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	221	GLN
1	A	103	ASP
1	A	108	VAL
1	A	125	ARG
1	A	188	LYS
1	A	207	GLN
1	B	19	LYS
1	B	57	GLU
1	B	77	VAL
1	B	99	GLU
1	B	172	LEU
1	B	206	GLU
1	D	47	VAL
1	D	104	ILE
1	D	185	GLU
1	D	188	LYS
1	D	208	GLU
1	D	226	GLU
1	D	242	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	B	207	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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, 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	394/413 (95%)	0.06	18 (4%)	36	34	23, 45, 93, 175	0
1	B	394/413 (95%)	-0.09	11 (2%)	56	55	21, 41, 87, 208	0
1	C	394/413 (95%)	0.17	23 (5%)	26	24	21, 50, 94, 157	0
1	D	394/413 (95%)	0.09	20 (5%)	32	29	23, 47, 97, 190	0
All	All	1576/1652 (95%)	0.06	72 (4%)	36	34	21, 46, 93, 208	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	ALA	9.6
1	A	106	GLY	9.6
1	D	107	GLY	9.2
1	C	1	MET	8.2
1	D	1	MET	8.1
1	C	2	ARG	7.4
1	D	2	ARG	6.7
1	A	104	ILE	6.6
1	B	103	ASP	6.4
1	B	104	ILE	6.3
1	A	103	ASP	6.3
1	D	104	ILE	6.3
1	D	108	VAL	5.6
1	A	107	GLY	5.4
1	D	106	GLY	4.7
1	D	103	ASP	4.5
1	C	103	ASP	4.4
1	D	4	LEU	4.3
1	B	106	GLY	4.3
1	A	242	ARG	4.2
1	B	107	GLY	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	101	SER	4.0
1	A	116	VAL	4.0
1	C	100	GLN	3.9
1	B	105	ALA	3.7
1	A	340	GLU	3.5
1	C	232	GLU	3.5
1	D	3	ALA	3.5
1	A	1	MET	3.5
1	C	105	ALA	3.3
1	B	63	TYR	3.3
1	A	102	PRO	3.3
1	D	231	GLY	3.2
1	A	332	VAL	3.2
1	D	102	PRO	3.1
1	C	107	GLY	3.1
1	A	108	VAL	3.1
1	B	101	SER	3.1
1	C	63	TYR	3.0
1	A	393	ALA	2.9
1	D	63	TYR	2.8
1	C	230	ASP	2.7
1	C	3	ALA	2.7
1	C	207	GLN	2.7
1	D	230	ASP	2.7
1	B	332	VAL	2.6
1	B	333	LEU	2.6
1	D	59	THR	2.5
1	C	61	GLU	2.5
1	A	101	SER	2.5
1	B	393	ALA	2.5
1	A	205	VAL	2.4
1	C	168	LEU	2.4
1	C	116	VAL	2.3
1	C	104	ILE	2.3
1	C	188	LYS	2.3
1	C	227	TYR	2.3
1	D	105	ALA	2.3
1	C	185	GLU	2.2
1	A	337	LYS	2.2
1	C	166	THR	2.2
1	C	228	LEU	2.2
1	D	116	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	242	ARG	2.2
1	B	110	LEU	2.1
1	C	271	GLY	2.1
1	C	58	ILE	2.1
1	D	61	GLU	2.1
1	A	338	LEU	2.0
1	D	187	ASP	2.0
1	C	190	LEU	2.0
1	A	204	GLU	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.