



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 04:20 AM EDT

PDB ID : 4L4Q
Title : Methionine Adenosyltransferase
Authors : Schlesier, J.; Siegrist, J.; Gerhardt, S.; Andexer, J.N.; Einsle, O.
Deposited on : 2013-06-09
Resolution : 2.00 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	:	2.37.1
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)	:	2.37.1

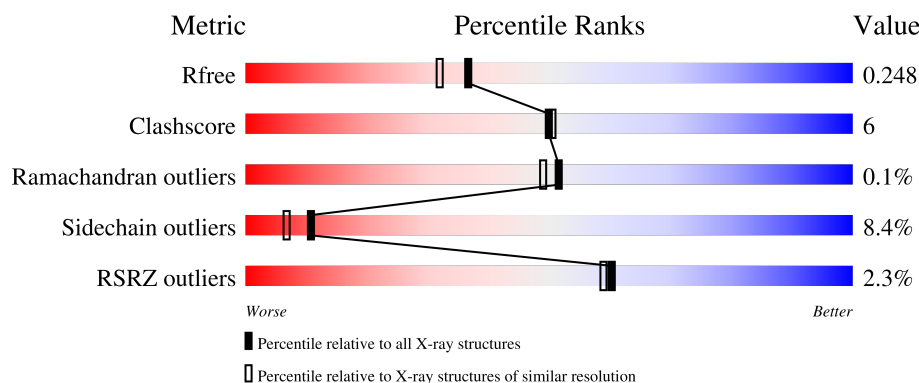
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	405	<div> <div>3%</div> <div>82%</div> <div>16%</div> <div>..</div> </div>
1	B	405	<div> <div>3%</div> <div>80%</div> <div>16%</div> <div>..</div> </div>
1	C	405	<div> <div>2%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>
1	D	405	<div> <div>%</div> <div>82%</div> <div>14%</div> <div>..</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13180 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	A	402	Total	C	N	O	S	0	1	0
			3130	1983	534	605	8			
1	B	401	Total	C	N	O	S	0	3	0
			3136	1985	535	608	8			
1	C	402	Total	C	N	O	S	0	1	0
			3130	1983	534	605	8			
1	D	402	Total	C	N	O	S	0	1	0
			3130	1983	534	605	8			

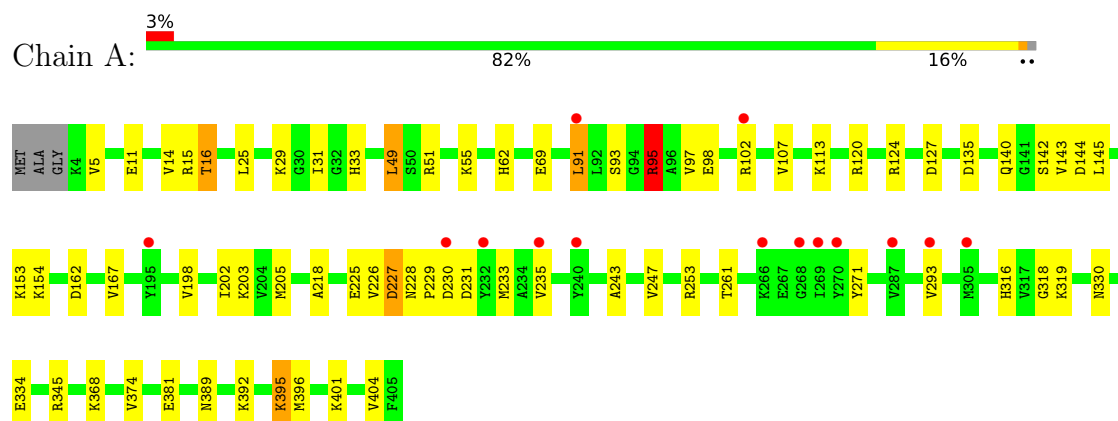
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	160	Total	O	0	0
			160	160		
2	B	179	Total	O	0	0
			179	179		
2	C	146	Total	O	0	0
			146	146		
2	D	169	Total	O	0	0
			169	169		

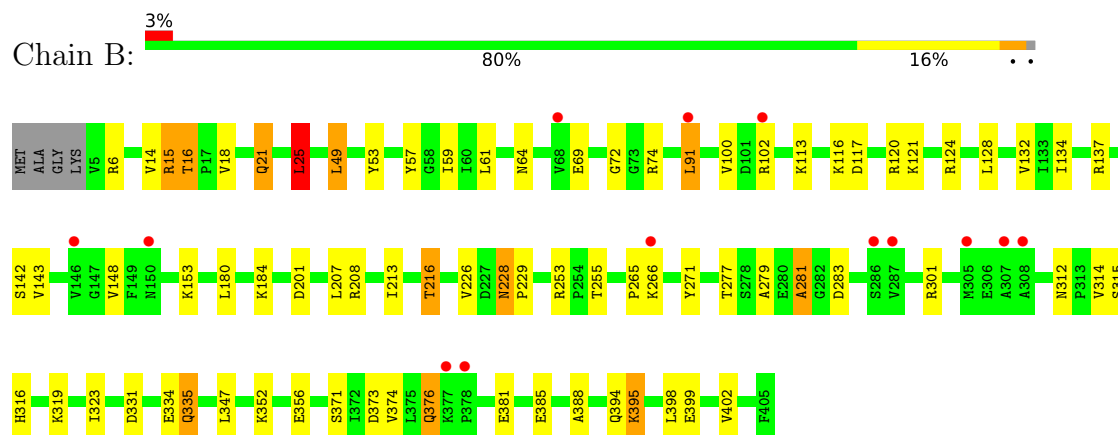
3 Residue-property plots [i](#)

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.

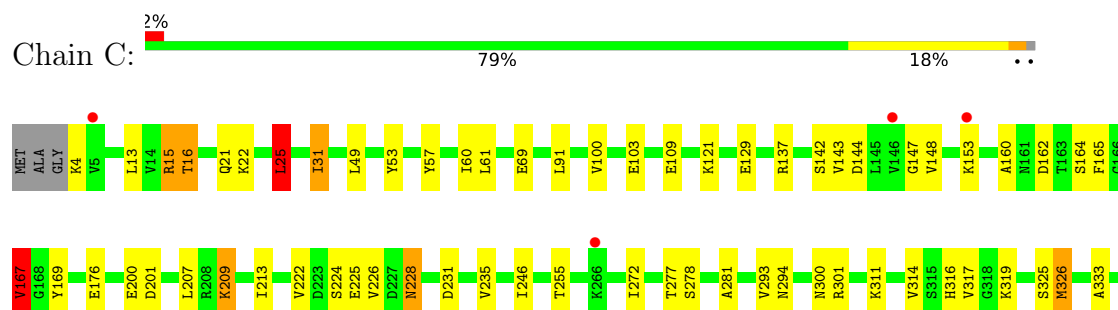
• Molecule 1: S-adenosylmethionine synthase

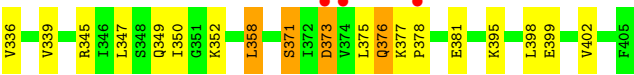


• Molecule 1: S-adenosylmethionine synthase

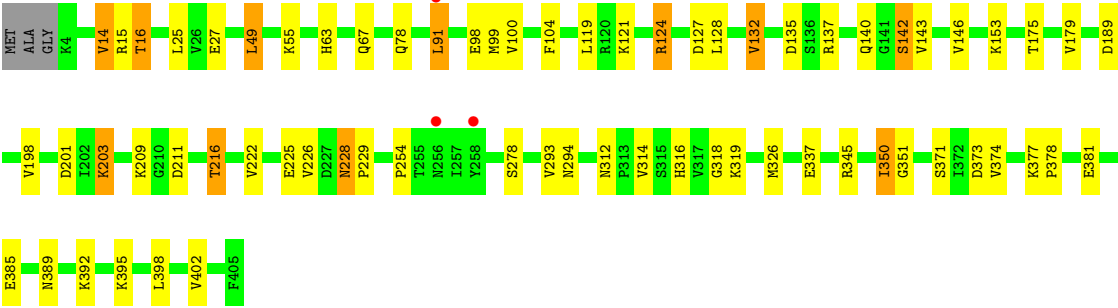
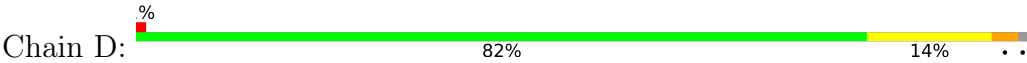


• Molecule 1: S-adenosylmethionine synthase





● Molecule 1: S-adenosylmethionine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	134.84Å 57.79Å 236.43Å 90.00° 103.95° 90.00°	Depositor
Resolution (Å)	46.37 – 2.00 46.33 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.37-2.00) 99.9 (46.33-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.187 , 0.245 0.195 , 0.248	Depositor DCC
R_{free} test set	5999 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13180	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.44% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.94	0/3183	1.05	16/4309 (0.4%)
1	B	0.90	1/3189 (0.0%)	1.04	13/4318 (0.3%)
1	C	0.80	2/3183 (0.1%)	0.95	7/4309 (0.2%)
1	D	0.90	0/3183	1.00	9/4309 (0.2%)
All	All	0.89	3/12738 (0.0%)	1.01	45/17245 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	109	GLU	CD-OE1	-6.57	1.18	1.25
1	C	176	GLU	CD-OE2	6.04	1.32	1.25
1	B	216	THR	CB-CG2	-5.53	1.34	1.52

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	ARG	NE-CZ-NH2	-14.63	112.98	120.30
1	B	15	ARG	NE-CZ-NH1	12.64	126.62	120.30
1	A	95	ARG	NE-CZ-NH1	12.08	126.34	120.30
1	B	15	ARG	NE-CZ-NH2	-11.06	114.77	120.30
1	C	15	ARG	NE-CZ-NH1	9.96	125.28	120.30
1	C	137	ARG	NE-CZ-NH1	8.75	124.68	120.30
1	A	51	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	A	135	ASP	CB-CG-OD1	8.16	125.64	118.30
1	D	49	LEU	CB-CG-CD1	8.03	124.64	111.00
1	C	167	VAL	CB-CA-C	-7.77	96.64	111.40
1	B	137	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	C	15	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	B	124	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	D	135	ASP	CB-CG-OD1	7.31	124.88	118.30
1	D	132	VAL	CB-CA-C	-7.27	97.59	111.40
1	A	253	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	A	49	LEU	CB-CG-CD1	6.93	122.78	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	137	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	A	374	VAL	CB-CA-C	-6.36	99.31	111.40
1	A	167	VAL	CG1-CB-CG2	6.27	120.93	110.90
1	B	124	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	C	25	LEU	CA-CB-CG	6.17	129.50	115.30
1	B	49	LEU	CB-CG-CD1	6.08	121.33	111.00
1	B	137	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	B	91	LEU	CB-CG-CD2	5.98	121.16	111.00
1	C	326	MET	CG-SD-CE	-5.96	90.66	100.20
1	D	127	ASP	CB-CG-OD1	5.85	123.57	118.30
1	A	51	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	D	91	LEU	CA-CB-CG	5.69	128.38	115.30
1	A	91	LEU	CB-CG-CD2	5.68	120.66	111.00
1	D	374	VAL	CB-CA-C	-5.63	100.69	111.40
1	D	124	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	B	25	LEU	CA-CB-CG	5.53	128.01	115.30
1	B	208	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	401	LYS	CD-CE-NZ	-5.38	99.32	111.70
1	D	373	ASP	CB-CG-OD1	5.34	123.11	118.30
1	D	49	LEU	CA-CB-CG	5.33	127.57	115.30
1	A	120	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	B	132	VAL	CG1-CB-CG2	-5.20	102.58	110.90
1	A	167	VAL	CA-CB-CG1	5.17	118.65	110.90
1	B	253	ARG	NE-CZ-NH2	5.09	122.85	120.30
1	B	253	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	A	253	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	A	135	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	A	127	ASP	CB-CG-OD1	5.01	122.81	118.30

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	3130	0	3166	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3136	0	3164	40	0
1	C	3130	0	3166	52	0
1	D	3130	0	3166	35	0
2	A	160	0	0	3	0
2	B	179	0	0	4	0
2	C	146	0	0	6	0
2	D	169	0	0	4	0
All	All	13180	0	12662	147	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 6.

All (147) 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:294:ASN:CA	1:D:326:MET:HE1	2.00	0.92
1:D:294:ASN:HA	1:D:326:MET:HE1	1.54	0.88
1:B:316:HIS:HD2	1:B:319:LYS:H	1.22	0.87
1:A:25:LEU:HD22	1:B:347:LEU:HD11	1.56	0.86
1:C:293:VAL:HG23	1:C:326:MET:HE3	1.57	0.84
1:A:316:HIS:HD2	1:A:318:GLY:H	1.32	0.77
1:C:316:HIS:HD2	1:C:319:LYS:H	1.31	0.74
1:C:165:PHE:CE2	1:C:167:VAL:HG22	2.22	0.73
1:C:294:ASN:N	1:C:326:MET:HE1	2.04	0.73
1:B:316:HIS:CD2	1:B:319:LYS:H	2.06	0.73
1:D:316:HIS:HD2	1:D:318:GLY:H	1.36	0.72
1:C:293:VAL:HG23	1:C:326:MET:CE	2.19	0.72
1:C:129:GLU:HG3	2:C:585:HOH:O	1.92	0.68
1:C:333:ALA:HA	1:C:339:VAL:HG11	1.76	0.66
1:D:228:ASN:HB2	1:D:229:PRO:HD2	1.79	0.65
1:D:294:ASN:HB3	1:D:326:MET:CE	2.27	0.65
1:A:69:GLU:HG2	1:B:69:GLU:HG2	1.80	0.64
1:B:64:ASN:HB3	2:B:677:HOH:O	1.96	0.64
1:C:160:ALA:O	1:C:350:ILE:O	2.16	0.64
1:A:98:GLU:CG	1:A:140:GLN:HG3	2.27	0.64
1:C:164:SER:HB2	1:C:317:VAL:CG2	2.28	0.64
1:C:281:ALA:HB3	2:C:561:HOH:O	1.99	0.62
1:C:57:TYR:CZ	1:C:100:VAL:HG11	2.35	0.62
1:A:98:GLU:HG2	1:A:140:GLN:HG3	1.80	0.62
1:A:69:GLU:CG	1:B:69:GLU:HG2	2.29	0.61
1:B:312:ASN:OD1	1:B:314:VAL:HG12	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:ASN:HB2	1:D:229:PRO:CD	2.30	0.61
1:B:331:ASP:O	1:B:335:GLN:HB2	2.01	0.61
1:B:117:ASP:OD1	1:B:120:ARG:NH2	2.30	0.61
1:D:99:MET:HB2	1:D:142:SER:OG	2.01	0.60
1:A:389:ASN:HB3	1:A:392:LYS:HD2	1.83	0.60
1:A:162:ASP:OD1	2:A:584:HOH:O	2.17	0.59
1:D:294:ASN:CB	1:D:326:MET:HE1	2.32	0.59
1:C:371:SER:OG	1:C:373:ASP:OD1	2.22	0.57
1:C:294:ASN:CA	1:C:326:MET:HE1	2.34	0.57
1:C:16:THR:CG2	1:D:14:VAL:HG13	2.35	0.56
1:B:53:TYR:CD1	1:B:61:LEU:HD12	2.40	0.56
1:C:336:VAL:O	1:C:339:VAL:HG12	2.05	0.56
1:D:98:GLU:HG2	1:D:140:GLN:HG3	1.87	0.56
1:C:316:HIS:CD2	1:C:319:LYS:H	2.19	0.56
1:C:294:ASN:HB3	1:C:326:MET:CE	2.36	0.55
1:D:201:ASP:OD2	1:D:278[A]:SER:OG	2.14	0.55
1:D:121:LYS:NZ	2:D:589:HOH:O	2.40	0.55
1:D:294:ASN:HB3	1:D:326:MET:HE2	1.90	0.54
1:A:124:ARG:NH2	1:A:198:VAL:O	2.41	0.54
1:A:113:LYS:HD3	2:A:645:HOH:O	2.07	0.54
1:B:312:ASN:ND2	1:B:315:SER:OG	2.41	0.53
1:C:294:ASN:HB3	1:C:326:MET:HE2	1.88	0.53
1:A:69:GLU:HG2	1:B:69:GLU:CG	2.38	0.53
1:C:15:ARG:HD2	2:C:540:HOH:O	2.09	0.53
1:B:395:LYS:HD3	1:B:399:GLU:OE1	2.09	0.53
1:C:349:GLN:OE1	1:C:358:LEU:HD23	2.08	0.52
1:C:201:ASP:OD2	1:C:278[A]:SER:OG	2.10	0.52
1:C:162:ASP:OD1	1:C:162:ASP:C	2.48	0.52
1:C:143:VAL:HG21	1:C:148:VAL:CG2	2.40	0.52
1:D:294:ASN:N	1:D:326:MET:HE1	2.25	0.52
1:A:203:LYS:NZ	2:A:609:HOH:O	2.42	0.52
1:A:227:ASP:OD1	1:A:231:ASP:OD2	2.28	0.52
1:D:316:HIS:HD2	1:D:318:GLY:N	2.05	0.51
1:A:14:VAL:HG13	1:B:16:THR:CG2	2.40	0.51
1:B:100:VAL:O	1:B:100:VAL:HG23	2.11	0.51
1:D:146:VAL:HG23	2:D:665:HOH:O	2.09	0.51
1:C:164:SER:CB	1:C:317:VAL:CG2	2.88	0.51
1:B:228:ASN:HB2	1:B:229:PRO:CD	2.42	0.50
1:D:316:HIS:CD2	1:D:318:GLY:H	2.25	0.50
1:C:167:VAL:HG13	1:C:345:ARG:HG2	1.94	0.50
1:D:294:ASN:CB	1:D:326:MET:CE	2.90	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:TYR:CD1	1:C:61:LEU:HD12	2.47	0.49
1:B:57:TYR:CZ	1:B:100:VAL:HG21	2.47	0.49
1:A:231:ASP:O	1:A:235:VAL:HG23	2.13	0.49
1:D:216:THR:HG23	2:D:571:HOH:O	2.13	0.48
1:A:15:ARG:HB2	1:B:15:ARG:HD2	1.96	0.48
1:C:69:GLU:OE1	1:D:67:GLN:HB3	2.14	0.47
1:C:21:GLN:NE2	1:C:300:ASN:HD22	2.12	0.47
1:C:53:TYR:CE1	1:C:61:LEU:HD12	2.49	0.47
1:B:213:ILE:O	1:B:255:THR:HA	2.15	0.47
1:D:211:ASP:O	1:D:254:PRO:HD2	2.13	0.47
1:C:201:ASP:HB2	1:C:277:THR:HA	1.96	0.47
1:D:137:ARG:HD2	2:D:594:HOH:O	2.14	0.47
1:B:319:LYS:O	1:B:323:ILE:HG13	2.15	0.47
1:C:165:PHE:CZ	1:C:167:VAL:HG22	2.49	0.47
1:A:62:HIS:O	1:A:97:VAL:HG23	2.15	0.47
1:C:15:ARG:HG2	1:D:15:ARG:HB3	1.97	0.47
1:A:316:HIS:HD2	1:A:318:GLY:N	2.08	0.46
1:B:201:ASP:HB2	1:B:277:THR:HA	1.98	0.46
1:C:144:ASP:OD2	1:C:147:GLY:N	2.43	0.46
1:B:228:ASN:HB2	1:B:229:PRO:HD2	1.98	0.46
1:C:347:LEU:HD21	1:D:25:LEU:HD22	1.96	0.46
1:C:209:LYS:HD2	2:C:555:HOH:O	2.16	0.46
1:D:337:GLU:OE2	1:D:337:GLU:HA	2.16	0.46
1:D:377:LYS:HB3	1:D:378:PRO:HD3	1.97	0.45
1:A:330:ASN:O	1:A:334:GLU:HG2	2.15	0.45
1:D:27:GLU:OE2	1:D:203:LYS:HE3	2.17	0.45
1:A:395:LYS:HD2	1:A:396:MET:N	2.32	0.45
1:B:25:LEU:CD1	1:B:207:LEU:HD13	2.46	0.44
2:C:540:HOH:O	1:D:16:THR:HG23	2.16	0.44
1:C:373:ASP:HA	1:C:376:GLN:HE21	1.82	0.44
1:A:243:ALA:O	1:A:247:VAL:HG23	2.17	0.44
1:B:180:LEU:HD11	1:B:184:LYS:HE2	1.98	0.44
1:D:119:LEU:HB3	1:D:128:LEU:HD21	1.98	0.44
1:A:228:ASN:HD22	1:A:230:ASP:H	1.64	0.44
1:D:175:THR:O	1:D:179:VAL:HG23	2.18	0.44
1:C:373:ASP:HA	1:C:376:GLN:NE2	2.33	0.44
1:C:395:LYS:O	1:C:399:GLU:HG3	2.17	0.44
1:A:15:ARG:HB3	1:B:15:ARG:HG2	1.99	0.43
1:B:228:ASN:C	1:B:228:ASN:HD22	2.22	0.43
1:C:13:LEU:CD1	1:C:15:ARG:HD3	2.48	0.43
1:C:31:ILE:HG22	1:C:200:GLU:HB3	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ILE:HD13	1:B:148:VAL:HG12	2.00	0.43
1:D:124:ARG:NH2	1:D:198:VAL:O	2.51	0.43
1:A:316:HIS:CD2	1:A:318:GLY:H	2.21	0.43
1:B:352:LYS:HE3	1:B:356:GLU:OE1	2.19	0.43
1:B:74:ARG:NH1	2:B:508:HOH:O	2.52	0.42
1:D:389:ASN:HB3	1:D:392:LYS:HD2	2.01	0.42
1:A:16:THR:HG23	2:B:531:HOH:O	2.18	0.42
1:A:98:GLU:HB3	1:A:107:VAL:HG21	2.00	0.42
1:A:145:LEU:HA	1:A:145:LEU:HD12	1.80	0.42
1:B:15:ARG:HD2	2:B:531:HOH:O	2.18	0.42
1:B:116:LYS:HG3	1:B:134:ILE:HD12	2.00	0.42
1:D:350:ILE:HD13	1:D:351:GLY:H	1.84	0.42
1:B:153:LYS:N	1:B:153:LYS:HD2	2.34	0.42
1:A:11:GLU:OE1	1:B:21[B]:GLN:NE2	2.52	0.42
1:C:25:LEU:CD1	1:C:207:LEU:HD13	2.50	0.42
1:C:375:LEU:O	1:C:378:PRO:HD2	2.19	0.42
1:A:29:LYS:HD3	1:A:33:HIS:CE1	2.55	0.42
1:A:202:ILE:HA	1:A:218:ALA:O	2.19	0.42
1:C:311:LYS:HD3	1:C:316:HIS:CE1	2.55	0.42
1:C:293:VAL:C	1:C:326:MET:HE1	2.40	0.42
1:C:231:ASP:O	1:C:235:VAL:HG23	2.20	0.42
1:D:63:HIS:O	1:D:312:ASN:HB3	2.20	0.41
1:C:224:SER:HB3	2:C:531:HOH:O	2.19	0.41
1:C:228:ASN:C	1:C:228:ASN:HD22	2.23	0.41
1:C:377:LYS:HB3	1:C:378:PRO:HD3	2.02	0.41
1:B:64:ASN:OD1	1:B:64:ASN:N	2.53	0.41
1:B:72:GLY:HA2	1:B:279:ALA:O	2.20	0.41
1:C:60:ILE:HD11	1:C:398:LEU:HD11	2.02	0.41
1:B:6:ARG:NH2	1:B:388:ALA:HA	2.35	0.41
1:A:228:ASN:HB2	1:A:229:PRO:HD2	2.03	0.41
1:A:293:VAL:HG22	1:A:404:VAL:HA	2.03	0.41
1:B:120:ARG:HG3	1:B:128:LEU:HG	2.03	0.41
1:A:95:ARG:NH2	1:B:281:ALA:O	2.53	0.40
1:B:18:VAL:HG21	1:B:301:ARG:NH1	2.36	0.40
1:C:213:ILE:O	1:C:255:THR:HA	2.21	0.40
1:B:373:ASP:HA	1:B:376:GLN:HE21	1.86	0.40
1:C:169:TYR:CE2	1:C:301:ARG:NE	2.90	0.40
1:C:339:VAL:HG13	1:C:339:VAL:O	2.21	0.40
1:D:293:VAL:HG12	1:D:326:MET:HE3	2.04	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	401/405 (99%)	390 (97%)	11 (3%)	0	100	100
1	B	402/405 (99%)	394 (98%)	7 (2%)	1 (0%)	47	44
1	C	401/405 (99%)	389 (97%)	12 (3%)	0	100	100
1	D	401/405 (99%)	390 (97%)	11 (3%)	0	100	100
All	All	1605/1620 (99%)	1563 (97%)	41 (3%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	281	ALA

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	339/339 (100%)	313 (92%)	26 (8%)	13	8
1	B	340/339 (100%)	310 (91%)	30 (9%)	10	6
1	C	339/339 (100%)	311 (92%)	28 (8%)	11	7
1	D	339/339 (100%)	309 (91%)	30 (9%)	10	6
All	All	1357/1356 (100%)	1243 (92%)	114 (8%)	11	7

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	16	THR
1	A	31	ILE
1	A	49	LEU
1	A	55	LYS
1	A	91	LEU
1	A	93	SER
1	A	95	ARG
1	A	102	ARG
1	A	142	SER
1	A	143	VAL
1	A	144	ASP
1	A	153	LYS
1	A	154	LYS
1	A	205	MET
1	A	225	GLU
1	A	226	VAL
1	A	227	ASP
1	A	233	MET
1	A	261	THR
1	A	271	TYR
1	A	319	LYS
1	A	345	ARG
1	A	368	LYS
1	A	381	GLU
1	A	395	LYS
1	B	14	VAL
1	B	16	THR
1	B	21[A]	GLN
1	B	21[B]	GLN
1	B	25	LEU
1	B	49	LEU
1	B	91	LEU
1	B	102	ARG
1	B	113	LYS
1	B	121	LYS
1	B	142	SER
1	B	143	VAL
1	B	216	THR
1	B	226	VAL
1	B	228	ASN
1	B	265	PRO
1	B	266	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	271	TYR
1	B	283	ASP
1	B	334	GLU
1	B	335	GLN
1	B	371	SER
1	B	374	VAL
1	B	376	GLN
1	B	381	GLU
1	B	385	GLU
1	B	394	GLN
1	B	395	LYS
1	B	398	LEU
1	B	402	VAL
1	C	4	LYS
1	C	16	THR
1	C	22	LYS
1	C	25	LEU
1	C	31	ILE
1	C	49	LEU
1	C	91	LEU
1	C	103	GLU
1	C	121	LYS
1	C	142	SER
1	C	153	LYS
1	C	167	VAL
1	C	209	LYS
1	C	222	VAL
1	C	225	GLU
1	C	226	VAL
1	C	228	ASN
1	C	246	ILE
1	C	272	ILE
1	C	314	VAL
1	C	325	SER
1	C	352	LYS
1	C	358	LEU
1	C	371	SER
1	C	373	ASP
1	C	376	GLN
1	C	381	GLU
1	C	402	VAL
1	D	14	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	16	THR
1	D	49	LEU
1	D	55	LYS
1	D	78	GLN
1	D	91	LEU
1	D	100	VAL
1	D	104	PHE
1	D	132	VAL
1	D	142	SER
1	D	143	VAL
1	D	153	LYS
1	D	189	ASP
1	D	203	LYS
1	D	209	LYS
1	D	216	THR
1	D	222	VAL
1	D	225	GLU
1	D	226	VAL
1	D	228	ASN
1	D	314	VAL
1	D	319	LYS
1	D	345	ARG
1	D	350	ILE
1	D	371	SER
1	D	381	GLU
1	D	385	GLU
1	D	395	LYS
1	D	398	LEU
1	D	402	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	HIS
1	A	150	ASN
1	A	228	ASN
1	A	316	HIS
1	A	403	ASN
1	B	7	ASN
1	B	125	HIS
1	B	228	ASN
1	B	316	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	376	GLN
1	B	403	ASN
1	C	21	GLN
1	C	125	HIS
1	C	155	ASN
1	C	228	ASN
1	C	316	HIS
1	C	376	GLN
1	C	403	ASN
1	D	78	GLN
1	D	125	HIS
1	D	150	ASN
1	D	228	ASN
1	D	316	HIS
1	D	403	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 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, 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	402/405 (99%)	0.01	14 (3%) 44 43	20, 36, 62, 102	0
1	B	401/405 (99%)	0.05	13 (3%) 47 46	21, 37, 60, 87	0
1	C	402/405 (99%)	0.07	7 (1%) 70 68	25, 43, 67, 89	0
1	D	402/405 (99%)	-0.09	3 (0%) 87 87	23, 38, 62, 92	0
All	All	1607/1620 (99%)	0.01	37 (2%) 60 59	20, 38, 64, 102	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	146	VAL	4.4
1	A	270	TYR	3.8
1	A	268	GLY	3.8
1	B	102	ARG	3.8
1	A	266	LYS	3.7
1	A	102	ARG	3.1
1	A	240	TYR	3.0
1	C	5	VAL	2.9
1	A	230	ASP	2.8
1	D	91	LEU	2.5
1	C	374	VAL	2.5
1	C	266	LYS	2.5
1	C	373	ASP	2.5
1	B	146	VAL	2.5
1	B	266	LYS	2.4
1	C	153	LYS	2.4
1	A	91	LEU	2.4
1	B	307	ALA	2.4
1	B	377	LYS	2.3
1	B	286	SER	2.3
1	B	305	MET	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	232	TYR	2.3
1	A	195	TYR	2.3
1	D	258	TYR	2.3
1	B	150	ASN	2.3
1	B	287	VAL	2.3
1	A	305	MET	2.2
1	A	235	VAL	2.2
1	A	287	VAL	2.2
1	C	378	PRO	2.2
1	B	378	PRO	2.1
1	B	308	ALA	2.1
1	B	68	VAL	2.1
1	B	91	LEU	2.0
1	A	293	VAL	2.0
1	D	256	ASN	2.0
1	A	269	ILE	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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.