Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2019 – 10:02 AM EDT

PDB ID	:	6JP2
Title	:	Crystal structure of pyrrolysyl-tRNA synthetase from Methanomethylophilus alvus
Authors	:	Yanagisawa, T.; Kuratani, M.; Yokoyama, S.
Deposited on	:	2019-03-25
Resolution	:	2.27 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 following versions of software and data (see references ⓘ) were used in the production of this report:

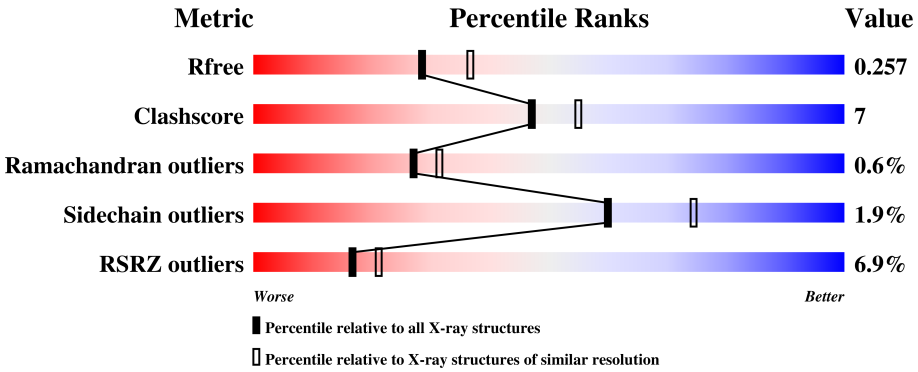
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	rb-20031633
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

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 2.27 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}	111664	6121 (2.30-2.26)
Clashscore	122126	6842 (2.30-2.26)
Ramachandran outliers	120053	6755 (2.30-2.26)
Sidechain outliers	120020	6755 (2.30-2.26)
RSRZ outliers	108989	5992 (2.30-2.26)

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	278	5% 82% 18%
1	B	278	5% 85% 12%
1	C	278	7% 85% 15%
1	D	278	10% 78% 18%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8940 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 Pyrrolysyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2176	1369	373	420	14			
1	B	272	Total	C	N	O	S	0	0	0
			2140	1349	364	413	14			
1	C	276	Total	C	N	O	S	0	0	0
			2170	1366	372	418	14			
1	D	272	Total	C	N	O	S	0	0	0
			2133	1342	368	409	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP M9SC49
A	-1	SER	-	expression tag	UNP M9SC49
A	0	HIS	-	expression tag	UNP M9SC49
B	-2	GLY	-	expression tag	UNP M9SC49
B	-1	SER	-	expression tag	UNP M9SC49
B	0	HIS	-	expression tag	UNP M9SC49
C	-2	GLY	-	expression tag	UNP M9SC49
C	-1	SER	-	expression tag	UNP M9SC49
C	0	HIS	-	expression tag	UNP M9SC49
D	-2	GLY	-	expression tag	UNP M9SC49
D	-1	SER	-	expression tag	UNP M9SC49
D	0	HIS	-	expression tag	UNP M9SC49

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	84	Total	O	0	0
			84	84		
2	B	101	Total	O	0	0
			101	101		

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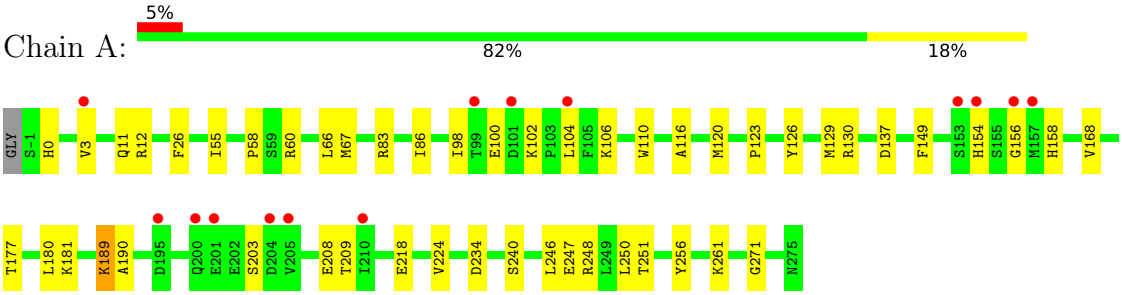
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	72	Total O 72 72	0	0
2	D	64	Total O 64 64	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 geometryand 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.

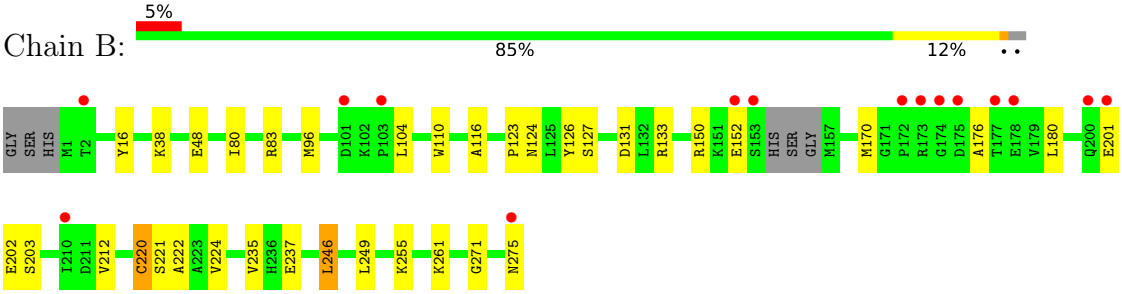
• Molecule 1: Pyrrolysyl-tRNA synthetase

Chain A:



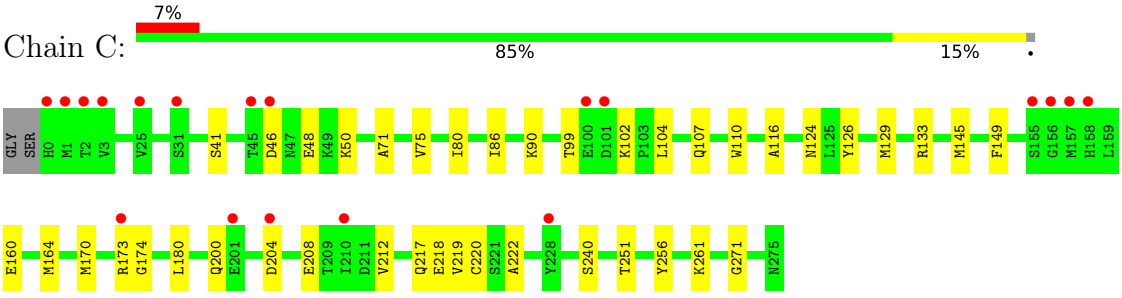
• Molecule 1: Pyrrolysyl-tRNA synthetase

Chain B:



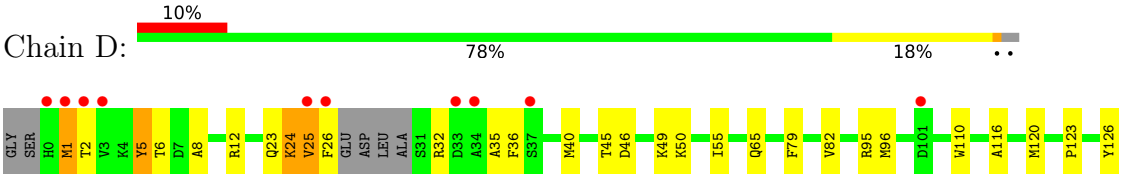
• Molecule 1: Pyrrolysyl-tRNA synthetase

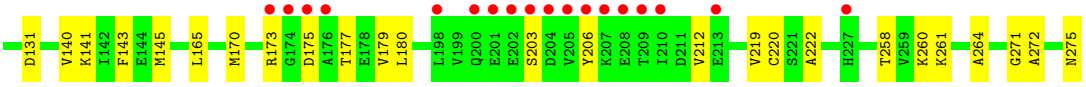
Chain C:



• Molecule 1: Pyrrolysyl-tRNA synthetase

Chain D:




D131
V140
K141
T142
F143
E144
M145
L165
M170
R173
G174
D175
A176
T177
E178
V179
L180
L198
V199
Q200
E201
E202
S203
D204
V205
Y206
K207
E208
T209
I210
D211
V212
E213
V219
C220
S221
A222
H227
T258
V259
K260
K261
A264
G271
A272
N275

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	112.38Å 112.78Å 107.43Å 90.00° 114.21° 90.00°	Depositor
Resolution (Å)	48.99 – 2.27 48.99 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.99-2.27) 99.1 (48.99-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 2.27Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.213 , 0.257 0.213 , 0.257	Depositor DCC
R_{free} test set	2787 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	41.6	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.8	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	0.94	EDS
Total number of atoms	8940	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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	0.25	0/2217	0.42	0/2990
1	B	0.25	0/2178	0.42	0/2936
1	C	0.24	0/2211	0.42	0/2982
1	D	0.25	0/2172	0.44	0/2927
All	All	0.25	0/8778	0.42	0/11835

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	2176	0	2152	29	0
1	B	2140	0	2124	24	0
1	C	2170	0	2147	29	0
1	D	2133	0	2113	43	0
2	A	84	0	0	3	0
2	B	101	0	0	4	0
2	C	72	0	0	4	0
2	D	64	0	0	8	0
All	All	8940	0	8536	115	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 7.

All (115) 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:24:LYS:HG3	1:D:25:VAL:H	1.36	0.90
1:D:25:VAL:HG12	1:D:32:ARG:HG2	1.57	0.86
1:D:258:THR:HG22	1:D:260:LYS:H	1.41	0.85
1:D:219:VAL:O	2:D:301:HOH:O	1.99	0.79
1:D:131:ASP:OD2	2:D:302:HOH:O	2.03	0.77
1:B:104:LEU:HD11	1:B:150:ARG:HE	1.51	0.74
1:D:32:ARG:O	1:D:36:PHE:N	2.20	0.73
1:D:206:TYR:O	2:D:303:HOH:O	2.06	0.72
1:A:180:LEU:HG	1:A:240:SER:HB2	1.70	0.71
1:B:127:SER:OG	2:B:301:HOH:O	2.09	0.69
1:C:90:LYS:NZ	2:C:303:HOH:O	2.25	0.69
1:D:131:ASP:OD1	2:D:304:HOH:O	2.10	0.67
1:D:24:LYS:CG	1:D:25:VAL:H	2.08	0.67
1:C:219:VAL:O	2:C:301:HOH:O	2.15	0.65
1:C:129:MET:HE2	1:C:170:MET:HB2	1.80	0.64
1:D:141:LYS:NZ	2:D:307:HOH:O	2.31	0.64
1:B:124:ASN:HB2	2:B:327:HOH:O	1.98	0.62
1:B:201:GLU:O	1:B:203:SER:N	2.33	0.61
1:C:104:LEU:CD1	1:C:107:GLN:HE21	2.14	0.61
1:B:170:MET:HE1	1:B:235:VAL:HG22	1.84	0.60
1:C:212:VAL:HB	1:C:220:CYS:HB3	1.82	0.59
1:A:203:SER:HB2	1:A:209:THR:HG23	1.85	0.58
1:D:24:LYS:HZ1	1:D:26:PHE:HB2	1.67	0.58
1:A:149:PHE:HZ	1:C:86:ILE:HD12	1.69	0.57
1:C:160:GLU:OE1	2:C:302:HOH:O	2.17	0.56
1:B:180:LEU:HD11	1:B:224:VAL:HG23	1.88	0.56
1:C:173:ARG:N	1:C:174:GLY:HA3	2.21	0.56
1:D:96:MET:HG3	1:D:123:PRO:HG3	1.88	0.56
1:C:71:ALA:HB2	1:C:145:MET:HE2	1.89	0.55
1:C:200:GLN:NE2	1:C:208:GLU:OE1	2.34	0.54
1:D:24:LYS:HG3	1:D:25:VAL:N	2.15	0.54
1:A:55:ILE:HA	1:C:80:ILE:HD11	1.89	0.54
1:D:24:LYS:CG	1:D:25:VAL:N	2.70	0.54
1:D:180:LEU:HD21	1:D:222:ALA:HB1	1.89	0.54
1:D:46:ASP:HA	1:D:49:LYS:HD2	1.90	0.54
1:B:212:VAL:HB	1:B:220:CYS:HB3	1.89	0.54
1:A:180:LEU:HD12	1:A:224:VAL:HG23	1.89	0.54
1:D:261:LYS:HB3	1:D:271:GLY:HA2	1.90	0.54
1:A:58:PRO:HB3	1:C:80:ILE:HG12	1.88	0.54
1:A:12:ARG:HD2	1:B:275:ASN:HD21	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:HB2	1:D:24:LYS:CE	2.39	0.53
1:A:110:TRP:CE3	1:A:116:ALA:HB2	2.44	0.53
1:D:212:VAL:HB	1:D:220:CYS:HB3	1.91	0.53
1:A:251:THR:HG23	1:A:256:TYR:HB2	1.89	0.53
1:A:261:LYS:HB3	1:A:271:GLY:HA2	1.91	0.53
1:D:50:LYS:HD2	1:D:272:ALA:HB2	1.89	0.53
1:B:16:TYR:OH	1:B:275:ASN:ND2	2.40	0.52
1:A:177:THR:OG1	1:A:208:GLU:OE2	2.27	0.52
1:D:6:THR:HG22	1:D:8:ALA:H	1.74	0.52
1:B:38:LYS:NZ	2:B:303:HOH:O	2.28	0.52
1:A:98:ILE:HD12	1:A:104:LEU:HD22	1.92	0.52
1:D:24:LYS:O	1:D:25:VAL:HB	2.10	0.52
1:A:177:THR:HG22	1:A:181:LYS:HE2	1.92	0.51
1:A:100:GLU:N	1:A:100:GLU:OE1	2.43	0.51
1:A:130:ARG:NH1	1:A:234:ASP:OD2	2.44	0.51
1:A:3:VAL:HG13	1:A:26:PHE:HB2	1.92	0.51
1:C:104:LEU:HD12	1:C:107:GLN:HE21	1.75	0.51
1:A:189:LYS:HD2	1:A:190:ALA:N	2.27	0.50
1:A:67:MET:HG2	1:A:246:LEU:HD13	1.94	0.50
1:D:5:TYR:OH	1:D:35:ALA:O	2.30	0.50
1:A:11:GLN:NE2	2:A:307:HOH:O	2.44	0.49
1:C:251:THR:HG23	1:C:256:TYR:HB2	1.95	0.49
1:B:246:LEU:HD12	1:B:249:LEU:HD12	1.95	0.49
1:C:124:ASN:HB2	2:C:308:HOH:O	2.12	0.49
1:B:110:TRP:CE3	1:B:116:ALA:HB2	2.48	0.48
1:D:175:ASP:O	1:D:177:THR:N	2.39	0.48
1:D:173:ARG:HG2	1:D:179:VAL:HG21	1.94	0.48
1:D:65:GLN:NE2	2:D:318:HOH:O	2.47	0.48
1:C:46:ASP:OD1	1:C:50:LYS:NZ	2.39	0.48
1:C:173:ARG:H	1:C:174:GLY:HA3	1.78	0.47
1:B:255:LYS:HE2	1:B:255:LYS:HA	1.97	0.47
1:C:110:TRP:CE3	1:C:116:ALA:HB2	2.49	0.47
1:A:83:ARG:NH2	2:A:311:HOH:O	2.47	0.47
1:B:261:LYS:HB3	1:B:271:GLY:HA2	1.97	0.47
1:C:71:ALA:HB2	1:C:145:MET:CE	2.43	0.47
1:C:261:LYS:HB3	1:C:271:GLY:HA2	1.96	0.47
1:D:1:MET:HB2	1:D:24:LYS:HE2	1.98	0.46
1:B:180:LEU:HD22	1:B:222:ALA:HB1	1.97	0.45
1:C:217:GLN:HE21	1:C:218:GLU:H	1.63	0.45
1:B:48:GLU:HG2	2:B:377:HOH:O	2.16	0.45
1:D:6:THR:HG22	1:D:8:ALA:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:LEU:HD21	1:C:222:ALA:HB1	1.98	0.45
1:D:24:LYS:NZ	1:D:26:PHE:HB2	2.31	0.45
1:D:145:MET:HG2	1:D:165:LEU:HB2	1.99	0.45
1:D:45:THR:HG22	1:D:49:LYS:HE3	1.99	0.45
1:D:82:VAL:O	2:D:305:HOH:O	2.21	0.45
1:B:133:ARG:NH2	1:B:237:GLU:OE1	2.49	0.45
1:D:110:TRP:CE3	1:D:116:ALA:HB2	2.52	0.45
1:D:140:VAL:HB	1:D:170:MET:HB3	1.98	0.44
1:A:60:ARG:HD2	1:C:75:VAL:HG21	1.99	0.44
1:A:129:MET:SD	1:A:168:VAL:HG11	2.57	0.44
1:A:12:ARG:HD2	1:B:275:ASN:ND2	2.31	0.44
1:D:79:PHE:HB3	1:D:143:PHE:HD1	1.83	0.44
1:C:133:ARG:HB2	1:C:170:MET:HE1	2.00	0.44
1:A:218:GLU:H	1:A:218:GLU:CD	2.19	0.43
1:D:95:ARG:NH1	2:D:319:HOH:O	2.51	0.43
1:D:120:MET:HG3	1:D:123:PRO:HD3	2.01	0.43
1:A:156:GLY:C	1:A:158:HIS:H	2.22	0.43
1:B:83:ARG:HG2	1:D:264:ALA:HB2	2.00	0.43
1:A:86:ILE:HD12	1:C:149:PHE:HZ	1.84	0.42
1:B:176:ALA:HB1	1:B:224:VAL:HG21	2.02	0.42
1:D:145:MET:HB2	1:D:145:MET:HE3	1.95	0.42
1:B:96:MET:HG3	1:B:123:PRO:HG3	2.02	0.42
1:C:217:GLN:HE21	1:C:218:GLU:N	2.17	0.42
1:D:1:MET:HG3	1:D:2:THR:H	1.85	0.41
1:A:247:GLU:OE2	2:A:301:HOH:O	2.21	0.41
1:B:80:ILE:HD11	1:D:55:ILE:HA	2.02	0.41
1:A:100:GLU:C	1:A:102:LYS:H	2.24	0.41
1:A:120:MET:HG3	1:A:123:PRO:HD3	2.03	0.41
1:B:220:CYS:SG	1:B:221:SER:N	2.93	0.41
1:C:145:MET:HA	1:C:164:MET:O	2.20	0.41
1:D:12:ARG:C	1:D:40:MET:HE1	2.42	0.40
1:C:180:LEU:HB2	1:C:240:SER:HB2	2.03	0.40
1:C:99:THR:OG1	1:C:102:LYS:NZ	2.55	0.40
1:B:131:ASP:OD2	1:D:275:ASN:HB3	2.22	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	275/278 (99%)	261 (95%)	12 (4%)	2 (1%)	24 27
1	B	268/278 (96%)	260 (97%)	7 (3%)	1 (0%)	36 43
1	C	274/278 (99%)	270 (98%)	4 (2%)	0	100 100
1	D	268/278 (96%)	250 (93%)	14 (5%)	4 (2%)	11 10
All	All	1085/1112 (98%)	1041 (96%)	37 (3%)	7 (1%)	27 31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	HIS
1	D	1	MET
1	D	25	VAL
1	D	24	LYS
1	D	203	SER
1	A	0	HIS
1	B	202	GLU

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	235/235 (100%)	228 (97%)	7 (3%)	44 58
1	B	231/235 (98%)	227 (98%)	4 (2%)	63 77
1	C	234/235 (100%)	230 (98%)	4 (2%)	63 77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	230/235 (98%)	227 (99%)	3 (1%)	71 83
All	All	930/940 (99%)	912 (98%)	18 (2%)	60 74

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LEU
1	A	106	LYS
1	A	126	TYR
1	A	137	ASP
1	A	189	LYS
1	A	248	ARG
1	A	250	LEU
1	B	126	TYR
1	B	152	GLU
1	B	220	CYS
1	B	246	LEU
1	C	41	SER
1	C	48	GLU
1	C	126	TYR
1	C	204	ASP
1	D	5	TYR
1	D	23	GLN
1	D	126	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	GLN
1	C	107	GLN
1	C	217	GLN
1	D	200	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	277/278 (99%)	0.42	14 (5%)	28	34	33, 44, 68, 81	0
1	B	272/278 (97%)	0.36	15 (5%)	25	30	31, 42, 68, 84	0
1	C	276/278 (99%)	0.44	19 (6%)	17	21	31, 44, 71, 80	0
1	D	272/278 (97%)	0.63	28 (10%)	6	8	31, 48, 84, 101	0
All	All	1097/1112 (98%)	0.47	76 (6%)	17	21	31, 45, 72, 101	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	101	ASP	6.5
1	D	203	SER	6.3
1	D	205	VAL	6.0
1	D	0	HIS	5.7
1	D	26	PHE	5.4
1	A	156	GLY	5.3
1	D	25	VAL	5.0
1	D	175	ASP	4.8
1	D	33	ASP	4.7
1	C	3	VAL	4.5
1	B	101	ASP	4.4
1	B	103	PRO	4.3
1	C	156	GLY	4.3
1	C	0	HIS	4.3
1	A	204	ASP	4.1
1	D	1	MET	4.1
1	D	3	VAL	3.9
1	D	201	GLU	3.9
1	C	101	ASP	3.9
1	C	1	MET	3.8
1	D	101	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	31	SER	3.6
1	B	174	GLY	3.6
1	C	2	THR	3.5
1	D	174	GLY	3.5
1	A	200	GLN	3.5
1	D	202	GLU	3.4
1	B	153	SER	3.4
1	B	175	ASP	3.4
1	D	34	ALA	3.4
1	C	155	SER	3.4
1	C	157	MET	3.4
1	B	178	GLU	3.3
1	A	205	VAL	3.3
1	D	208	GLU	3.3
1	D	173	ARG	3.2
1	B	177	THR	3.2
1	A	99	THR	3.2
1	C	173	ARG	3.1
1	A	154	HIS	3.0
1	C	158	HIS	3.0
1	B	200	GLN	2.9
1	B	172	PRO	2.9
1	B	173	ARG	2.9
1	A	153	SER	2.8
1	C	201	GLU	2.7
1	D	204	ASP	2.7
1	B	2	THR	2.7
1	A	157	MET	2.6
1	A	195	ASP	2.5
1	C	204	ASP	2.5
1	D	206	TYR	2.4
1	B	275	ASN	2.4
1	D	176	ALA	2.4
1	B	201	GLU	2.4
1	D	37	SER	2.4
1	A	201	GLU	2.4
1	C	210	ILE	2.3
1	B	210	ILE	2.2
1	A	210	ILE	2.2
1	C	228	TYR	2.2
1	C	25	VAL	2.2
1	C	46	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	200	GLN	2.1
1	C	45	THR	2.1
1	B	152	GLU	2.1
1	D	209	THR	2.1
1	A	3	VAL	2.1
1	D	210	ILE	2.1
1	D	227	HIS	2.1
1	A	104	LEU	2.0
1	D	198	LEU	2.0
1	C	100	GLU	2.0
1	D	2	THR	2.0
1	D	207	LYS	2.0
1	D	213	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.