



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 12:25 pm GMT

PDB ID : 3VBA
Title : Crystal structure of methanogen 3-isopropylmalate isomerase small subunit
Authors : Hwang, K.Y.; Lee, E.H.
Deposited on : 2012-01-02
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 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 : trunk31020
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) : trunk31020

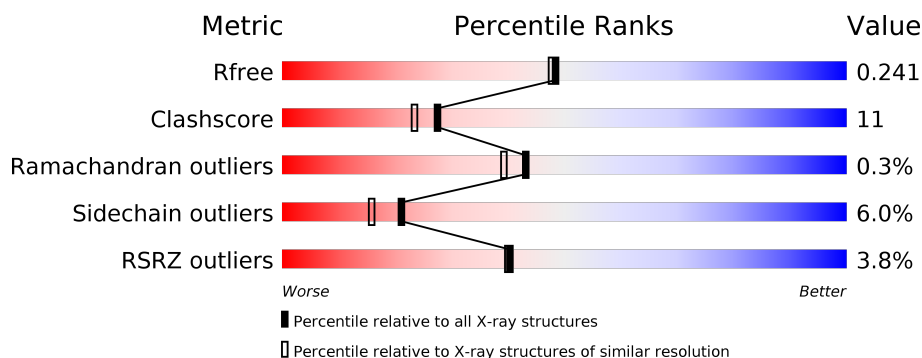
1 Overall quality at a glance

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}	111664	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (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 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 $\leq 5\%$. 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	176	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>• •</div> </div> </div>
1	B	176	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• •</div> </div> </div>
1	C	176	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>23%</div> <div>• 6%</div> </div> </div>
1	D	176	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>15%</div> <div>• 7%</div> </div> </div>
1	E	176	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>• 6%</div> </div> </div>
1	F	176	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>• 6%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8356 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 Isopropylmalate/citramalate isomerase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	0	0
			1295	828	217	241	9			
1	B	169	Total	C	N	O	S	0	0	0
			1295	828	217	241	9			
1	C	166	Total	C	N	O	S	0	0	0
			1269	812	213	236	8			
1	D	163	Total	C	N	O	S	0	0	0
			1250	801	210	231	8			
1	E	165	Total	C	N	O	S	0	0	0
			1263	809	212	233	9			
1	F	165	Total	C	N	O	S	0	0	0
			1263	809	212	233	9			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	LEU	-	EXPRESSION TAG	UNP Q58673
A	170	GLU	-	EXPRESSION TAG	UNP Q58673
A	171	HIS	-	EXPRESSION TAG	UNP Q58673
A	172	HIS	-	EXPRESSION TAG	UNP Q58673
A	173	HIS	-	EXPRESSION TAG	UNP Q58673
A	174	HIS	-	EXPRESSION TAG	UNP Q58673
A	175	HIS	-	EXPRESSION TAG	UNP Q58673
A	176	HIS	-	EXPRESSION TAG	UNP Q58673
B	169	LEU	-	EXPRESSION TAG	UNP Q58673
B	170	GLU	-	EXPRESSION TAG	UNP Q58673
B	171	HIS	-	EXPRESSION TAG	UNP Q58673
B	172	HIS	-	EXPRESSION TAG	UNP Q58673
B	173	HIS	-	EXPRESSION TAG	UNP Q58673
B	174	HIS	-	EXPRESSION TAG	UNP Q58673
B	175	HIS	-	EXPRESSION TAG	UNP Q58673
B	176	HIS	-	EXPRESSION TAG	UNP Q58673
C	169	LEU	-	EXPRESSION TAG	UNP Q58673

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	170	GLU	-	EXPRESSION TAG	UNP Q58673
C	171	HIS	-	EXPRESSION TAG	UNP Q58673
C	172	HIS	-	EXPRESSION TAG	UNP Q58673
C	173	HIS	-	EXPRESSION TAG	UNP Q58673
C	174	HIS	-	EXPRESSION TAG	UNP Q58673
C	175	HIS	-	EXPRESSION TAG	UNP Q58673
C	176	HIS	-	EXPRESSION TAG	UNP Q58673
D	169	LEU	-	EXPRESSION TAG	UNP Q58673
D	170	GLU	-	EXPRESSION TAG	UNP Q58673
D	171	HIS	-	EXPRESSION TAG	UNP Q58673
D	172	HIS	-	EXPRESSION TAG	UNP Q58673
D	173	HIS	-	EXPRESSION TAG	UNP Q58673
D	174	HIS	-	EXPRESSION TAG	UNP Q58673
D	175	HIS	-	EXPRESSION TAG	UNP Q58673
D	176	HIS	-	EXPRESSION TAG	UNP Q58673
E	169	LEU	-	EXPRESSION TAG	UNP Q58673
E	170	GLU	-	EXPRESSION TAG	UNP Q58673
E	171	HIS	-	EXPRESSION TAG	UNP Q58673
E	172	HIS	-	EXPRESSION TAG	UNP Q58673
E	173	HIS	-	EXPRESSION TAG	UNP Q58673
E	174	HIS	-	EXPRESSION TAG	UNP Q58673
E	175	HIS	-	EXPRESSION TAG	UNP Q58673
E	176	HIS	-	EXPRESSION TAG	UNP Q58673
F	169	LEU	-	EXPRESSION TAG	UNP Q58673
F	170	GLU	-	EXPRESSION TAG	UNP Q58673
F	171	HIS	-	EXPRESSION TAG	UNP Q58673
F	172	HIS	-	EXPRESSION TAG	UNP Q58673
F	173	HIS	-	EXPRESSION TAG	UNP Q58673
F	174	HIS	-	EXPRESSION TAG	UNP Q58673
F	175	HIS	-	EXPRESSION TAG	UNP Q58673
F	176	HIS	-	EXPRESSION TAG	UNP Q58673

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	140	Total O 140 140	0	0
2	B	122	Total O 122 122	0	0
2	C	117	Total O 117 117	0	0
2	D	125	Total O 125 125	0	0

Continued on next page...

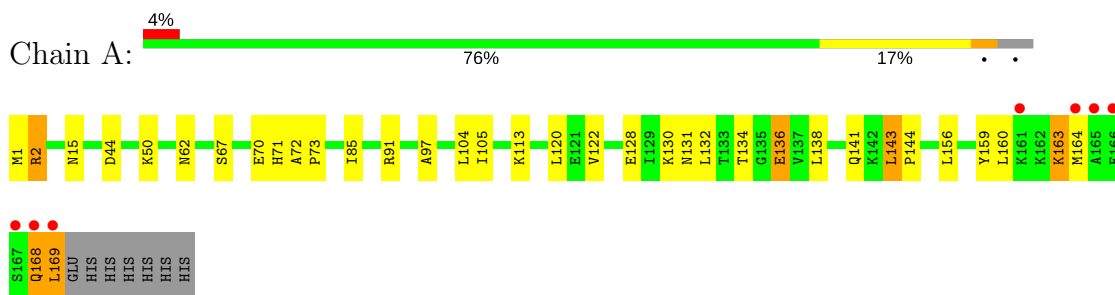
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	105	Total 105	O 105	0	0
2	F	112	Total 112	O 112	0	0

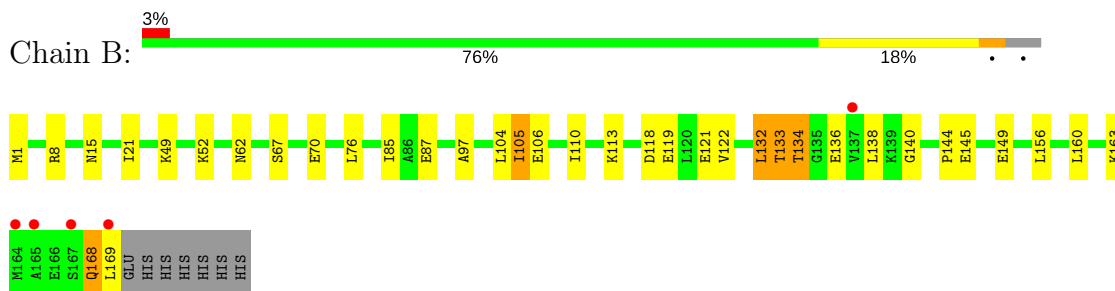
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

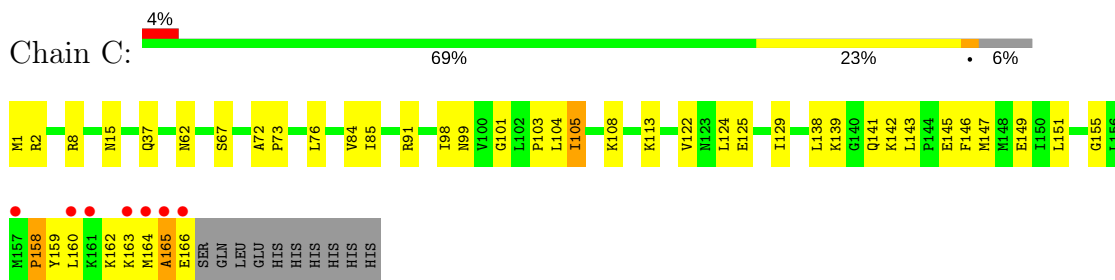
- Molecule 1: Isopropylmalate/citramalate isomerase small subunit



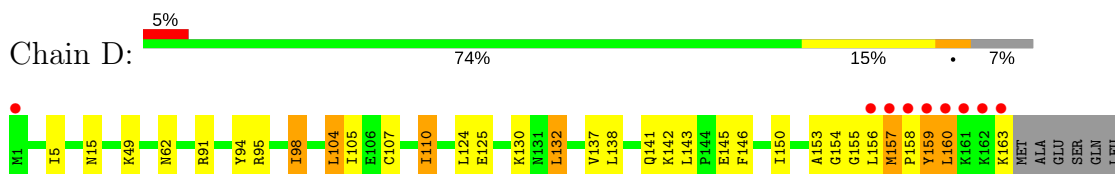
- Molecule 1: Isopropylmalate/citramalate isomerase small subunit



- Molecule 1: Isopropylmalate/citramalate isomerase small subunit

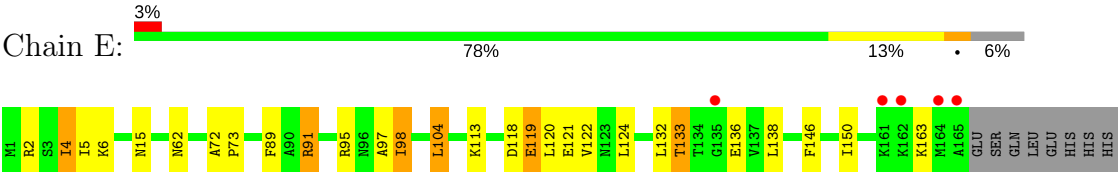


- Molecule 1: Isopropylmalate/citramalate isomerase small subunit



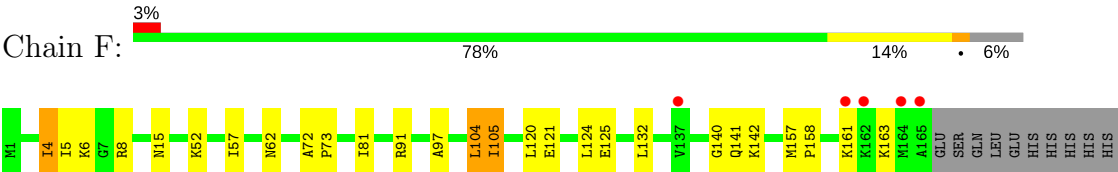
GLU
HIS
HIS
HIS
HIS
HIS
HIS

• Molecule 1: Isopropylmalate/citramalate isomerase small subunit



HIS
HIS
HIS

• Molecule 1: Isopropylmalate/citramalate isomerase small subunit



HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	33.84Å 107.14Å 288.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.90 – 2.00 43.90 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (43.90-2.00) 99.0 (43.90-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 1.81Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.197 , 0.244 0.193 , 0.241	Depositor DCC
R_{free} test set	4877 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8356	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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 56.86 % 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 2.5737e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [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	0.38	0/1317	0.53	0/1770
1	B	0.40	0/1317	0.54	0/1770
1	C	0.37	0/1291	0.55	0/1736
1	D	0.39	0/1272	0.57	0/1710
1	E	0.35	0/1285	0.52	0/1727
1	F	0.36	0/1285	0.50	0/1727
All	All	0.37	0/7767	0.53	0/10440

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 [i](#)

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	1295	0	1335	37	1
1	B	1295	0	1335	40	1
1	C	1269	0	1304	39	0
1	D	1250	0	1291	40	0
1	E	1263	0	1305	21	0
1	F	1263	0	1305	18	0
2	A	140	0	0	1	0
2	B	122	0	0	1	0
2	C	117	0	0	2	0
2	D	125	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	105	0	0	0	0
2	F	112	0	0	2	0
All	All	8356	0	7875	168	1

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 11.

All (168) 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:105:ILE:HG22	1:D:143:LEU:HD11	1.44	1.00
1:B:134:THR:HG22	1:B:136:GLU:H	1.29	0.94
1:A:134:THR:HG21	2:A:245:HOH:O	1.82	0.79
1:C:147:MET:HE3	1:D:146:PHE:HE1	1.44	0.79
1:A:85:ILE:HD11	1:A:122:VAL:HG21	1.67	0.76
1:D:153:ALA:HB3	1:D:159:TYR:HB2	1.67	0.75
1:C:1:MET:HE1	1:C:151:LEU:HB3	1.69	0.74
1:D:91:ARG:NH2	1:D:95:ARG:HH22	1.85	0.74
1:A:134:THR:HG23	1:A:136:GLU:H	1.53	0.74
1:B:119:GLU:H	1:B:133:THR:CG2	2.02	0.72
1:D:107:CYS:O	1:D:110:ILE:HG13	1.90	0.70
1:F:158:PRO:HA	1:F:161:LYS:HE2	1.74	0.69
1:E:91:ARG:HH21	1:E:91:ARG:HG2	1.58	0.69
1:E:91:ARG:NH2	1:E:91:ARG:HG2	2.08	0.69
1:F:15:ASN:HD22	1:F:62:ASN:HD22	1.41	0.69
1:D:159:TYR:C	1:D:159:TYR:CD2	2.67	0.68
1:E:119:GLU:H	1:E:133:THR:CG2	2.08	0.67
1:C:147:MET:HE3	1:D:146:PHE:CE1	2.29	0.66
1:A:15:ASN:HD22	1:A:62:ASN:HD22	1.43	0.66
1:A:163:LYS:HE3	1:B:156:LEU:HD23	1.77	0.66
1:A:144:PRO:HG2	1:B:144:PRO:HG2	1.78	0.66
1:C:105:ILE:HG22	1:C:143:LEU:CD1	2.25	0.66
1:A:168:GLN:HE21	1:B:70:GLU:H	1.45	0.63
1:D:154:GLY:O	1:D:158:PRO:HG2	1.97	0.63
1:A:156:LEU:HD23	1:B:163:LYS:NZ	2.15	0.62
1:E:118:ASP:HA	1:E:133:THR:HG21	1.81	0.61
1:F:15:ASN:ND2	1:F:62:ASN:HD22	1.98	0.60
1:D:159:TYR:C	1:D:159:TYR:HD2	2.05	0.60
1:B:110:ILE:HD12	1:B:138:LEU:HD22	1.83	0.60
1:A:105:ILE:HD13	1:A:143:LEU:HD13	1.83	0.59
1:D:155:GLY:O	1:D:159:TYR:HB3	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:ASN:HD22	1:E:62:ASN:HB3	1.67	0.59
1:D:105:ILE:HG22	1:D:143:LEU:CD1	2.25	0.59
1:B:121:GLU:HB2	1:B:132:LEU:HD21	1.85	0.58
1:C:108:LYS:NZ	1:C:141:GLN:OE1	2.36	0.58
1:D:159:TYR:O	1:D:163:LYS:HB3	2.04	0.58
1:A:15:ASN:ND2	1:A:62:ASN:HD22	2.02	0.58
1:D:91:ARG:CZ	1:D:95:ARG:HH22	2.15	0.58
1:D:153:ALA:CB	1:D:159:TYR:HB2	2.34	0.57
1:B:169:LEU:HD12	1:B:169:LEU:N	2.20	0.57
1:A:168:GLN:NE2	1:B:70:GLU:H	2.02	0.57
1:C:164:MET:O	1:C:165:ALA:HB3	2.04	0.57
1:A:131:ASN:CG	1:A:134:THR:HG22	2.25	0.56
1:A:70:GLU:H	1:B:168:GLN:NE2	2.03	0.56
1:A:163:LYS:HG3	1:A:164:MET:N	2.20	0.56
1:C:105:ILE:HG22	1:C:143:LEU:HD13	1.87	0.56
1:B:8:ARG:HH22	1:B:52:LYS:HG2	1.71	0.56
1:E:5:ILE:O	1:E:121:GLU:HA	2.06	0.55
1:C:113:LYS:HG3	1:C:138:LEU:HD11	1.88	0.55
1:C:155:GLY:C	1:C:158:PRO:HD2	2.26	0.55
1:B:105:ILE:HD11	1:B:140:GLY:HA3	1.87	0.55
1:A:70:GLU:H	1:B:168:GLN:HE22	1.55	0.55
1:B:119:GLU:H	1:B:133:THR:HG23	1.69	0.55
1:C:108:LYS:HE3	2:C:248:HOH:O	2.07	0.55
1:A:156:LEU:HD23	1:B:163:LYS:HZ1	1.71	0.55
1:C:105:ILE:HD13	1:C:105:ILE:N	2.22	0.54
1:C:163:LYS:NZ	1:C:163:LYS:HB3	2.22	0.54
1:C:141:GLN:HE22	1:D:142:LYS:NZ	2.04	0.54
1:B:113:LYS:HB2	1:B:138:LEU:HD21	1.89	0.54
1:A:160:LEU:CD2	1:B:160:LEU:HD11	2.38	0.54
1:D:124:LEU:H	1:D:124:LEU:HD22	1.72	0.54
1:C:163:LYS:HD3	1:D:156:LEU:HD13	1.89	0.54
1:E:95:ARG:HA	1:E:98:ILE:HD11	1.88	0.54
1:B:138:LEU:N	1:B:138:LEU:HD12	2.23	0.54
1:C:146:PHE:HE1	1:C:159:TYR:HH	1.55	0.53
1:E:91:ARG:CG	1:E:91:ARG:HH21	2.18	0.53
1:A:169:LEU:N	1:A:169:LEU:HD23	2.23	0.53
1:D:5:ILE:HD12	1:D:124:LEU:HD21	1.91	0.53
1:B:168:GLN:HB2	1:B:169:LEU:HD12	1.91	0.53
1:D:130:LYS:HG2	1:D:132:LEU:HD13	1.91	0.53
1:C:105:ILE:HG22	1:C:143:LEU:HD11	1.91	0.53
1:A:70:GLU:HB2	1:B:169:LEU:HD13	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:ILE:HD11	1:B:122:VAL:HG21	1.91	0.52
1:A:104:LEU:O	1:A:143:LEU:HD11	2.10	0.52
1:A:120:LEU:HD23	1:A:131:ASN:HA	1.92	0.52
1:A:160:LEU:HD11	1:B:160:LEU:CD2	2.39	0.52
1:C:164:MET:O	1:C:165:ALA:CB	2.57	0.52
1:C:147:MET:CE	1:D:146:PHE:HE1	2.18	0.52
1:B:49:LYS:HE2	2:B:256:HOH:O	2.09	0.52
1:F:125:GLU:O	1:F:142:LYS:HB2	2.10	0.52
1:D:124:LEU:HD22	1:D:124:LEU:N	2.24	0.52
1:B:134:THR:HG22	1:B:136:GLU:N	2.12	0.51
1:C:1:MET:HE1	1:C:151:LEU:CB	2.39	0.51
1:A:97:ALA:HB3	1:A:104:LEU:HD11	1.93	0.51
1:A:134:THR:HG23	1:A:136:GLU:HB2	1.92	0.51
1:C:146:PHE:HB2	1:D:94:TYR:CE2	2.46	0.50
1:E:97:ALA:HB3	1:E:104:LEU:HD22	1.93	0.50
1:D:49:LYS:N	1:D:49:LYS:HD2	2.26	0.50
1:E:95:ARG:HD2	1:E:98:ILE:CD1	2.41	0.50
1:E:95:ARG:HD2	1:E:98:ILE:HD12	1.92	0.50
1:A:156:LEU:O	1:A:159:TYR:HB3	2.11	0.50
1:A:160:LEU:HD22	1:B:160:LEU:HD11	1.94	0.50
1:B:21:ILE:HG23	1:B:76:LEU:HD11	1.95	0.49
1:E:4:ILE:HA	1:E:122:VAL:O	2.13	0.49
1:E:89:PHE:CZ	1:E:104:LEU:HG	2.47	0.49
1:B:145:GLU:O	1:B:149:GLU:HG3	2.13	0.49
1:B:105:ILE:HD12	1:B:106:GLU:O	2.13	0.49
1:D:157:MET:HA	1:D:160:LEU:HB2	1.95	0.48
1:C:85:ILE:HD11	1:C:122:VAL:HG21	1.96	0.48
1:D:94:TYR:O	1:D:98:ILE:HG22	2.13	0.48
1:B:134:THR:CG2	1:B:136:GLU:H	2.14	0.48
1:F:8:ARG:HH22	1:F:52:LYS:HG2	1.77	0.48
1:B:113:LYS:HD3	1:B:136:GLU:OE1	2.14	0.48
1:E:6:LYS:HA	1:E:120:LEU:O	2.13	0.48
1:D:49:LYS:N	1:D:49:LYS:CD	2.77	0.48
1:A:113:LYS:HD2	1:A:138:LEU:HD11	1.96	0.47
1:C:160:LEU:HD13	1:D:160:LEU:HD21	1.97	0.47
1:C:129:ILE:HB	1:C:138:LEU:HB2	1.97	0.47
1:C:91:ARG:NE	1:D:145:GLU:OE2	2.45	0.47
1:D:124:LEU:CD2	1:D:124:LEU:H	2.27	0.46
1:C:162:LYS:O	1:C:166:GLU:HB2	2.15	0.46
1:F:4:ILE:HG12	1:F:5:ILE:N	2.30	0.46
1:B:134:THR:CG2	1:B:136:GLU:HB2	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ASN:HD22	1:B:62:ASN:HD22	1.64	0.46
1:C:145:GLU:O	1:C:149:GLU:HG3	2.16	0.46
1:B:15:ASN:HD22	1:B:62:ASN:HB3	1.80	0.46
1:A:70:GLU:HB2	1:B:169:LEU:CD1	2.46	0.46
1:A:91:ARG:NH2	1:B:145:GLU:OE2	2.49	0.45
1:F:105:ILE:HD11	1:F:140:GLY:HA3	1.98	0.45
1:F:4:ILE:HD11	1:F:121:GLU:HG3	1.98	0.45
1:B:15:ASN:ND2	1:B:62:ASN:HD22	2.14	0.45
1:E:119:GLU:H	1:E:133:THR:HG22	1.80	0.45
1:A:105:ILE:CD1	1:A:143:LEU:HD13	2.47	0.45
1:F:91:ARG:HG2	2:F:287:HOH:O	2.17	0.45
1:C:108:LYS:HG2	2:C:302:HOH:O	2.16	0.45
1:C:72:ALA:HB3	1:C:73:PRO:CD	2.47	0.45
1:D:146:PHE:O	1:D:150:ILE:HG13	2.17	0.45
1:A:156:LEU:O	1:A:160:LEU:HG	2.17	0.44
1:A:160:LEU:HD11	1:B:160:LEU:HD21	1.99	0.44
1:C:15:ASN:HD22	1:C:62:ASN:HD22	1.64	0.44
1:E:15:ASN:ND2	1:E:62:ASN:HD22	2.14	0.44
1:F:15:ASN:HD22	1:F:62:ASN:HB3	1.83	0.44
1:A:2:ARG:HD3	1:A:2:ARG:HA	1.65	0.44
1:D:94:TYR:CD1	1:D:104:LEU:HD23	2.53	0.44
1:F:72:ALA:HB3	1:F:73:PRO:HD3	1.99	0.44
1:F:6:LYS:HA	1:F:120:LEU:O	2.18	0.43
1:C:125:GLU:O	1:C:142:LYS:HE3	2.19	0.43
1:A:128:GLU:OE2	1:A:130:LYS:HE3	2.19	0.43
1:C:98:ILE:HD12	1:C:99:ASN:N	2.34	0.43
1:D:15:ASN:HD22	1:D:62:ASN:HD22	1.65	0.43
1:C:141:GLN:HE22	1:D:142:LYS:HZ1	1.65	0.43
1:F:15:ASN:ND2	1:F:62:ASN:HB3	2.34	0.43
1:F:57:ILE:HG13	1:F:81:ILE:HD12	2.01	0.43
1:A:72:ALA:HB3	1:A:73:PRO:CD	2.49	0.43
1:E:146:PHE:CE2	1:E:150:ILE:HD11	2.53	0.43
1:B:97:ALA:HB3	1:B:104:LEU:HD11	2.01	0.43
1:C:164:MET:SD	1:D:157:MET:HE3	2.60	0.42
1:B:118:ASP:HA	1:B:133:THR:HG21	2.02	0.42
1:C:163:LYS:HD3	1:D:156:LEU:CD1	2.49	0.42
1:D:5:ILE:CD1	1:D:124:LEU:HD21	2.49	0.42
1:D:125:GLU:HG3	2:D:254:HOH:O	2.20	0.42
1:C:84:VAL:HB	1:C:104:LEU:HD22	2.02	0.42
1:D:15:ASN:HD22	1:D:62:ASN:HB3	1.85	0.42
1:E:98:ILE:HG13	1:E:98:ILE:H	1.58	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:MET:N	1:D:158:PRO:CD	2.83	0.41
1:A:71:HIS:HE1	1:C:37:GLN:HE22	1.67	0.41
1:F:15:ASN:HD22	1:F:62:ASN:ND2	2.15	0.41
1:F:72:ALA:HB3	1:F:73:PRO:CD	2.49	0.41
1:C:101:GLY:O	1:C:103:PRO:HD3	2.20	0.41
1:A:44:ASP:OD2	1:A:50:LYS:HE3	2.20	0.41
1:F:8:ARG:HD2	2:F:274:HOH:O	2.21	0.41
1:E:72:ALA:HB3	1:E:73:PRO:CD	2.51	0.41
1:E:121:GLU:HB2	1:E:132:LEU:HD11	2.02	0.41
1:C:72:ALA:HB3	1:C:73:PRO:HD3	2.02	0.40
1:D:143:LEU:N	1:D:143:LEU:HD12	2.36	0.40
1:C:76:LEU:HD23	1:C:76:LEU:HA	1.90	0.40
1:F:97:ALA:HB3	1:F:104:LEU:HD22	2.03	0.40
1:E:113:LYS:HE2	1:E:136:GLU:OE1	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:O	1:B:1:MET:O[1_455]	1.93	0.27

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	167/176 (95%)	164 (98%)	2 (1%)	1 (1%)	27	21
1	B	167/176 (95%)	167 (100%)	0	0	100	100
1	C	164/176 (93%)	158 (96%)	4 (2%)	2 (1%)	14	7
1	D	161/176 (92%)	157 (98%)	4 (2%)	0	100	100
1	E	163/176 (93%)	160 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	163/176 (93%)	161 (99%)	2 (1%)	0	100	100
All	All	985/1056 (93%)	967 (98%)	15 (2%)	3 (0%)	43	39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	165	ALA
1	A	168	GLN
1	C	158	PRO

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	139/146 (95%)	131 (94%)	8 (6%)	22	17
1	B	139/146 (95%)	132 (95%)	7 (5%)	27	22
1	C	135/146 (92%)	129 (96%)	6 (4%)	31	27
1	D	134/146 (92%)	124 (92%)	10 (8%)	15	9
1	E	135/146 (92%)	125 (93%)	10 (7%)	15	10
1	F	135/146 (92%)	127 (94%)	8 (6%)	21	16
All	All	817/876 (93%)	768 (94%)	49 (6%)	21	16

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	67	SER
1	A	132	LEU
1	A	136	GLU
1	A	141	GLN
1	A	143	LEU
1	A	163	LYS
1	A	169	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	67	SER
1	B	87	GLU
1	B	105	ILE
1	B	132	LEU
1	B	133	THR
1	B	134	THR
1	B	168	GLN
1	C	2	ARG
1	C	8	ARG
1	C	67	SER
1	C	105	ILE
1	C	124	LEU
1	C	139	LYS
1	D	98	ILE
1	D	104	LEU
1	D	110	ILE
1	D	132	LEU
1	D	137	VAL
1	D	138	LEU
1	D	141	GLN
1	D	157	MET
1	D	159	TYR
1	D	160	LEU
1	E	2	ARG
1	E	4	ILE
1	E	91	ARG
1	E	98	ILE
1	E	104	LEU
1	E	119	GLU
1	E	124	LEU
1	E	133	THR
1	E	138	LEU
1	E	163	LYS
1	F	4	ILE
1	F	104	LEU
1	F	105	ILE
1	F	124	LEU
1	F	132	LEU
1	F	141	GLN
1	F	157	MET
1	F	163	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	96	ASN
1	A	168	GLN
1	B	15	ASN
1	B	141	GLN
1	B	168	GLN
1	C	15	ASN
1	C	37	GLN
1	D	15	ASN
1	E	15	ASN
1	F	15	ASN
1	F	99	ASN
1	F	141	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 carbohydrates 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	169/176 (96%)	-0.40	7 (4%)	37 37	10, 17, 38, 59	0
1	B	169/176 (96%)	-0.26	5 (2%)	50 49	9, 19, 40, 56	0
1	C	166/176 (94%)	-0.18	7 (4%)	36 35	10, 19, 51, 75	0
1	D	163/176 (92%)	-0.12	9 (5%)	25 25	9, 19, 46, 70	0
1	E	165/176 (93%)	-0.24	5 (3%)	50 49	13, 22, 45, 69	0
1	F	165/176 (93%)	-0.19	5 (3%)	50 49	11, 21, 44, 73	0
All	All	997/1056 (94%)	-0.23	38 (3%)	40 40	9, 19, 46, 75	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	165	ALA	10.3
1	F	164	MET	8.2
1	D	158	PRO	6.9
1	C	165	ALA	6.5
1	D	162	LYS	6.5
1	E	165	ALA	6.5
1	A	169	LEU	5.6
1	D	160	LEU	5.6
1	C	160	LEU	5.1
1	E	164	MET	4.9
1	D	161	LYS	4.8
1	C	164	MET	4.6
1	B	164	MET	4.5
1	F	161	LYS	4.4
1	A	167	SER	4.3
1	D	159	TYR	4.2
1	C	166	GLU	3.7
1	D	157	MET	3.6
1	E	161	LYS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	157	MET	3.2
1	B	167	SER	3.2
1	C	161	LYS	3.2
1	B	169	LEU	3.2
1	E	162	LYS	2.7
1	B	165	ALA	2.6
1	D	1	MET	2.6
1	D	156	LEU	2.6
1	A	165	ALA	2.5
1	C	163	LYS	2.5
1	F	162	LYS	2.4
1	A	164	MET	2.3
1	F	137	VAL	2.3
1	B	137	VAL	2.2
1	E	135	GLY	2.2
1	D	163	LYS	2.2
1	A	166	GLU	2.1
1	A	161	LYS	2.1
1	A	168	GLN	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.