



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 05:31 PM GMT

PDB ID : 3MJZ
Title : The crystal structure of native FG41 MSAD
Authors : Guo, Y.; Serrano, H.; Poelarends, G.J.; Johnson, W.H.Jr.; Hackert, M.L.; Whitman, C.P.
Deposited on : 2010-04-13
Resolution : 2.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

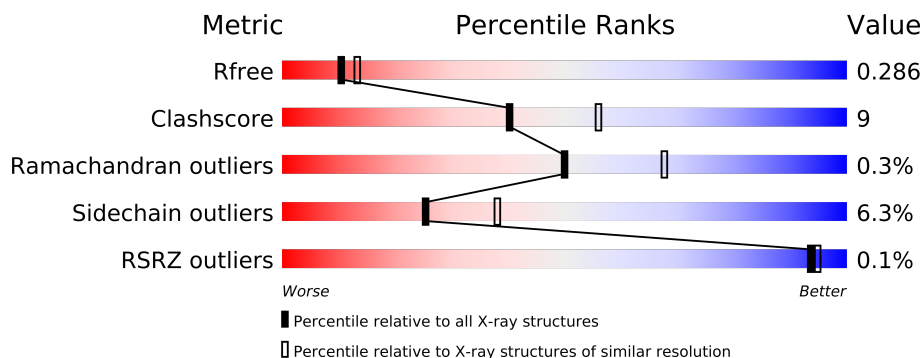
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	136	
1	B	136	
1	C	136	
1	D	136	
1	E	136	
1	F	136	
1	G	136	
1	H	136	
1	I	136	
1	J	136	
1	K	136	
1	L	136	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12993 atoms, of which 0 are hydrogen and 0 are deuterium.

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 FG41 Malonate Semialdehyde Decarboxylase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	131	Total	C	N	O	0	0	0
			1002	634	178	190			
1	B	131	Total	C	N	O	0	0	0
			1002	634	178	190			
1	C	131	Total	C	N	O	0	0	0
			1002	634	178	190			
1	D	131	Total	C	N	O	0	0	0
			996	631	175	190			
1	E	131	Total	C	N	O	0	0	0
			996	631	175	190			
1	F	130	Total	C	N	O	0	0	0
			995	629	177	189			
1	G	131	Total	C	N	O	0	0	0
			1002	634	178	190			
1	H	131	Total	C	N	O	0	0	0
			1002	634	178	190			
1	I	131	Total	C	N	O	0	0	0
			1002	634	178	190			
1	J	131	Total	C	N	O	0	0	0
			1002	634	178	190			
1	K	130	Total	C	N	O	0	0	0
			995	629	177	189			
1	L	131	Total	C	N	O	0	0	0
			1002	634	178	190			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	80	Total	O	0	0
			80	80		
2	B	86	Total	O	0	0
			86	86		

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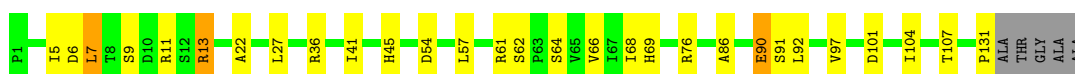
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	92	Total 92	O 92	0	0
2	D	66	Total 66	O 66	0	0
2	E	98	Total 98	O 98	0	0
2	F	106	Total 106	O 106	0	0
2	G	79	Total 79	O 79	0	0
2	H	72	Total 72	O 72	0	0
2	I	85	Total 85	O 85	0	0
2	J	66	Total 66	O 66	0	0
2	K	74	Total 74	O 74	0	0
2	L	91	Total 91	O 91	0	0

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 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.

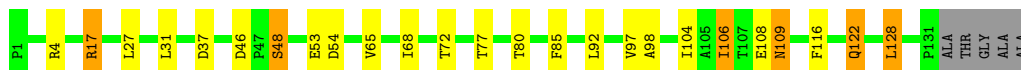
- Molecule 1: FG41 Malonate Semialdehyde Decarboxylase

Chain A: 



- Molecule 1: FG41 Malonate Semialdehyde Decarboxylase

Chain B: 



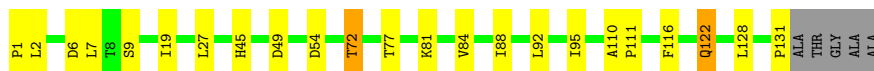
- Molecule 1: FG41 Malonate Semialdehyde Decarboxylase

Chain C: 



- Molecule 1: FG41 Malonate Semialdehyde Decarboxylase

Chain D: 



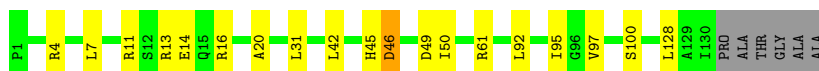
- Molecule 1: FG41 Malonate Semialdehyde Decarboxylase

Chain E: 



- Molecule 1: FG41 Malonate Semialdehyde Decarboxylase

Chain F: 



- Molecule 1: FG41 Malonate Semialdehyde Decarboxylase

Chain G: 



ALA
THR
GLY
ALA
ALA

- Molecule 1: FG41 Malonate Semialdehyde Decarboxylase

Chain H: 



- Molecule 1: FG41 Malonate Semialdehyde Decarboxylase

Chain I: 



E127
I130
P131
ALA
THR
GLY
ALA
ALA

- Molecule 1: FG41 Malonate Semialdehyde Decarboxylase

Chain J: 



Q122
I130
P131
ALA
THR
GLY
ALA
ALA

- Molecule 1: FG41 Malonate Semialdehyde Decarboxylase

Chain K: 



THR
GLY
ALA
ALA

- Molecule 1: FG41 Malonate Semialdehyde Decarboxylase

Chain L: 



ALA
THR
GLY
ALA
ALA

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.95Å 94.69Å 190.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.02 – 2.40 42.02 – 2.02	Depositor EDS
% Data completeness (in resolution range)	84.8 (42.02-2.40) 85.9 (42.02-2.02)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.279 0.210 , 0.286	Depositor DCC
R_{free} test set	2764 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 24.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	2 of 91145 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12993	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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 53.65 % 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 4.0903e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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	0.56	0/1022	0.73	2/1392 (0.1%)
1	B	0.65	0/1022	0.79	2/1392 (0.1%)
1	C	0.66	0/1022	0.79	1/1392 (0.1%)
1	D	0.55	0/1016	0.71	0/1385
1	E	0.67	0/1016	0.83	3/1385 (0.2%)
1	F	0.66	0/1014	0.78	1/1380 (0.1%)
1	G	0.69	0/1022	0.76	3/1392 (0.2%)
1	H	0.68	0/1022	0.82	3/1392 (0.2%)
1	I	0.69	0/1022	0.79	0/1392
1	J	0.61	0/1022	0.73	0/1392
1	K	0.70	0/1014	0.75	1/1380 (0.1%)
1	L	0.71	0/1022	0.75	1/1392 (0.1%)
All	All	0.65	0/12236	0.77	17/16666 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	61	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	H	61	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	A	61	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	E	61	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	H	60	GLN	N-CA-C	5.96	127.10	111.00
1	A	61	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	E	9	SER	N-CA-C	5.57	126.04	111.00
1	F	11	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	G	61	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	B	37	ASP	CB-CG-OD1	5.39	123.15	118.30
1	G	61	ARG	NE-CZ-NH1	-5.33	117.63	120.30
1	B	37	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	C	7	LEU	CA-CB-CG	5.18	127.22	115.30
1	L	7	LEU	CA-CB-CG	5.11	127.05	115.30
1	E	16	ARG	NE-CZ-NH1	5.10	122.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	27	LEU	CA-CB-CG	5.03	126.87	115.30
1	G	7	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1002	0	998	18	0
1	B	1002	0	998	19	0
1	C	1002	0	998	21	0
1	D	996	0	987	14	0
1	E	996	0	987	18	0
1	F	995	0	991	12	0
1	G	1002	0	998	26	0
1	H	1002	0	998	19	0
1	I	1002	0	998	27	0
1	J	1002	0	998	26	0
1	K	995	0	991	24	0
1	L	1002	0	998	26	0
2	A	80	0	0	2	0
2	B	86	0	0	1	0
2	C	92	0	0	2	0
2	D	66	0	0	1	0
2	E	98	0	0	1	0
2	F	106	0	0	5	0
2	G	79	0	0	2	0
2	H	72	0	0	0	0
2	I	85	0	0	2	0
2	J	66	0	0	1	0
2	K	74	0	0	1	0
2	L	91	0	0	1	0
All	All	12993	0	11940	224	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (224) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:1:PRO:HB3	1:K:72:THR:HG22	1.38	1.05
1:K:1:PRO:HB3	1:K:72:THR:CG2	1.98	0.94
1:K:73:GLN:O	1:K:74:ALA:HB3	1.66	0.92
1:L:116:PHE:H	1:L:122:GLN:NE2	1.77	0.82
1:L:116:PHE:H	1:L:122:GLN:HE22	1.24	0.81
1:A:13:ARG:HD3	1:A:13:ARG:H	1.45	0.81
1:J:4:ARG:HH21	1:L:69:HIS:CD2	1.99	0.79
1:K:73:GLN:O	1:K:74:ALA:CB	2.29	0.79
1:I:46:ASP:HB3	2:I:149:HOH:O	1.83	0.79
1:L:8:THR:HG22	1:L:9:SER:O	1.83	0.78
1:I:116:PHE:H	1:I:122:GLN:HE22	1.32	0.77
2:K:1271:HOH:O	1:L:36:ARG:HD3	1.85	0.76
1:H:1:PRO:HB3	1:H:72:THR:CG2	2.15	0.76
1:G:1:PRO:HB3	1:G:72:THR:HG23	1.67	0.76
1:B:116:PHE:H	1:B:122:GLN:HE22	1.35	0.75
1:D:84:VAL:O	1:D:88:ILE:HG12	1.88	0.74
1:H:122:GLN:H	1:H:122:GLN:HE21	1.35	0.73
1:J:1:PRO:HD3	1:J:33:ILE:HD13	1.70	0.72
1:J:53:GLU:O	1:J:61:ARG:NH1	2.20	0.72
1:G:6:ASP:OD1	1:G:45:HIS:HE1	1.71	0.72
1:H:122:GLN:NE2	1:H:122:GLN:H	1.88	0.71
1:C:8:THR:HG21	1:C:64:SER:HA	1.73	0.70
1:J:4:ARG:HH21	1:L:69:HIS:HD2	1.38	0.70
1:F:46:ASP:HB3	2:F:1312:HOH:O	1.91	0.69
1:G:4:ARG:HH21	1:I:69:HIS:CD2	2.10	0.69
1:H:23:VAL:O	1:H:27:LEU:HD23	1.93	0.69
1:D:6:ASP:OD2	1:E:4:ARG:NH2	2.26	0.69
1:A:11:ARG:NH1	1:A:64:SER:O	2.23	0.68
1:H:19:ILE:HD12	1:H:92:LEU:HD22	1.76	0.68
1:I:33:ILE:HG23	1:I:37:ASP:HB3	1.74	0.68
1:E:33:ILE:HG13	1:E:34:PRO:HD2	1.76	0.67
1:H:1:PRO:HB3	1:H:72:THR:HG22	1.76	0.67
1:C:73:GLN:HE22	1:C:130:ILE:HG23	1.60	0.66
1:C:69:HIS:HE1	1:C:107:THR:OG1	1.78	0.66
1:L:10:ASP:HB2	2:L:140:HOH:O	1.97	0.65
1:J:16:ARG:HG2	1:J:42:LEU:HD22	1.79	0.65
1:B:53:GLU:HB3	1:C:36:ARG:NH1	2.12	0.64
1:K:22:ALA:HB1	1:K:91:SER:HB3	1.79	0.64
1:A:86:ALA:O	1:A:90:GLU:HG2	1.98	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:1:PRO:HB3	1:H:72:THR:HG23	1.80	0.63
1:A:5:ILE:HG22	1:A:7:LEU:HD22	1.80	0.63
1:L:9:SER:O	1:L:10:ASP:HB2	1.99	0.63
1:F:20:ALA:HB2	1:F:42:LEU:HD21	1.81	0.63
1:G:4:ARG:HH21	1:I:69:HIS:HD2	1.48	0.62
1:B:116:PHE:H	1:B:122:GLN:NE2	1.98	0.62
1:K:95:ILE:HG22	1:K:96:GLY:H	1.64	0.62
1:F:14:GLU:HB2	2:F:287:HOH:O	1.99	0.62
1:G:20:ALA:HB2	1:G:42:LEU:HD21	1.82	0.61
1:I:116:PHE:H	1:I:122:GLN:NE2	1.97	0.60
1:K:27:LEU:O	1:K:31:LEU:HB2	2.00	0.60
1:K:127:GLU:O	1:K:128:LEU:HB2	2.00	0.60
1:A:22:ALA:HB1	1:A:91:SER:HB3	1.84	0.60
1:J:84:VAL:O	1:J:88:ILE:HG12	2.02	0.60
1:H:116:PHE:H	1:H:122:GLN:HE22	1.48	0.60
1:C:92:LEU:HB3	1:C:97:VAL:HB	1.84	0.59
1:E:22:ALA:HB2	1:E:95:ILE:CD1	2.33	0.59
1:G:22:ALA:HB1	1:G:91:SER:HB3	1.85	0.58
1:A:57:LEU:HD21	1:B:122:GLN:HG2	1.87	0.57
1:J:27:LEU:O	1:J:31:LEU:HB2	2.05	0.57
1:E:116:PHE:H	1:E:122:GLN:HE22	1.51	0.57
1:A:54:ASP:O	1:A:57:LEU:HB2	2.04	0.56
1:E:34:PRO:HG2	1:E:37:ASP:HB2	1.87	0.56
1:C:110:ALA:O	1:C:113:ASP:HB2	2.04	0.56
1:E:69:HIS:HE1	1:E:107:THR:OG1	1.89	0.56
1:K:69:HIS:CD2	1:L:4:ARG:HH21	2.24	0.56
1:H:20:ALA:HB2	1:H:42:LEU:HD21	1.87	0.56
1:J:116:PHE:H	1:J:122:GLN:HE22	1.55	0.55
1:H:27:LEU:HD12	1:H:31:LEU:HD22	1.88	0.55
1:A:13:ARG:HH11	1:A:13:ARG:HG2	1.71	0.55
1:B:72:THR:O	1:B:108:GLU:HA	2.06	0.55
1:I:72:THR:O	1:I:108:GLU:HA	2.06	0.55
1:G:13:ARG:HD2	2:G:792:HOH:O	2.06	0.55
1:K:57:LEU:HD21	1:L:128:LEU:HG	1.89	0.55
1:G:8:THR:HA	1:G:45:HIS:O	2.06	0.55
1:J:26:ALA:HB3	1:J:88:ILE:HD13	1.89	0.55
1:G:54:ASP:HB3	1:G:56:GLY:H	1.72	0.54
1:C:16:ARG:NE	2:C:409:HOH:O	2.40	0.54
1:F:13:ARG:HG2	2:F:1395:HOH:O	2.06	0.54
1:A:66:VAL:HG12	1:A:68:ILE:HD11	1.88	0.54
1:K:45:HIS:CD2	1:K:50:ILE:HD11	2.42	0.54
1:K:122:GLN:O	1:K:127:GLU:O	2.26	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:116:PHE:H	1:E:122:GLN:NE2	2.07	0.53
1:I:92:LEU:HB3	1:I:97:VAL:HB	1.91	0.53
1:L:19:ILE:HD12	1:L:97:VAL:HG21	1.90	0.53
1:L:72:THR:O	1:L:108:GLU:HA	2.09	0.53
1:C:110:ALA:HB1	1:C:111:PRO:HD2	1.92	0.52
1:K:92:LEU:HB3	1:K:97:VAL:HB	1.89	0.52
1:C:27:LEU:O	1:C:31:LEU:HB2	2.10	0.52
1:A:69:HIS:HE1	1:A:107:THR:OG1	1.92	0.52
1:I:19:ILE:O	1:I:23:VAL:HG23	2.09	0.52
1:B:27:LEU:O	1:B:31:LEU:HB2	2.10	0.52
1:I:27:LEU:CD1	1:I:88:ILE:HD11	2.39	0.51
1:A:6:ASP:OD1	1:A:45:HIS:HE1	1.93	0.51
1:H:19:ILE:HD13	1:H:95:ILE:HG21	1.92	0.51
1:G:39:PHE:HA	1:I:51:ILE:O	2.11	0.51
1:B:68:ILE:O	1:B:104:ILE:HA	2.10	0.51
1:D:116:PHE:HD2	1:D:122:GLN:HG3	1.76	0.51
1:F:16:ARG:NH2	2:F:595:HOH:O	2.44	0.50
1:F:92:LEU:HB3	1:F:97:VAL:HB	1.92	0.50
1:E:22:ALA:HB2	1:E:95:ILE:HD11	1.94	0.50
1:I:23:VAL:HG13	1:I:88:ILE:HD12	1.94	0.49
1:F:45:HIS:CD2	1:F:50:ILE:HD11	2.47	0.49
1:B:54:ASP:OD1	1:C:36:ARG:NH1	2.45	0.49
1:C:27:LEU:CD1	1:C:88:ILE:HD11	2.41	0.49
1:K:69:HIS:HD2	1:L:4:ARG:HH21	1.59	0.49
1:E:24:HIS:CE1	1:E:38:ARG:HB2	2.47	0.49
1:K:1:PRO:HB3	1:K:72:THR:HG23	1.89	0.49
1:L:1:PRO:HB3	1:L:72:THR:HB	1.94	0.49
1:J:54:ASP:O	1:J:55:ALA:HB3	2.13	0.49
1:A:92:LEU:HB3	1:A:97:VAL:HB	1.94	0.48
1:C:27:LEU:HD12	1:C:88:ILE:HD11	1.95	0.48
1:I:27:LEU:HD12	1:I:88:ILE:HD11	1.95	0.48
1:D:54:ASP:OD1	1:E:36:ARG:HD3	2.13	0.48
1:J:77:THR:HG23	1:J:80:THR:H	1.79	0.48
1:K:95:ILE:HG22	1:K:96:GLY:N	2.28	0.48
1:J:122:GLN:HE21	1:J:122:GLN:H	1.61	0.48
1:I:20:ALA:HB1	1:I:40:GLN:OE1	2.13	0.48
1:D:116:PHE:CD2	1:D:122:GLN:HG3	2.49	0.48
1:L:69:HIS:HE1	1:L:107:THR:OG1	1.96	0.48
1:G:78:ILE:H	1:G:78:ILE:HD12	1.78	0.48
1:K:11:ARG:NH1	1:K:64:SER:HB3	2.28	0.48
1:L:61:ARG:NH1	1:L:100:SER:O	2.46	0.47
1:A:13:ARG:NH1	1:A:13:ARG:HG2	2.29	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:74:ALA:HB2	1:K:108:GLU:HB3	1.96	0.47
1:E:28:VAL:HA	1:E:33:ILE:HG22	1.97	0.47
1:J:33:ILE:HG12	1:J:34:PRO:HD2	1.97	0.47
1:K:57:LEU:HD11	1:L:122:GLN:HG2	1.96	0.47
1:F:49:ASP:OD1	2:F:467:HOH:O	2.21	0.47
1:B:92:LEU:HB3	1:B:97:VAL:HB	1.97	0.47
1:I:26:ALA:HB3	1:I:88:ILE:HD13	1.96	0.47
1:J:54:ASP:OD1	1:K:36:ARG:HD3	2.15	0.46
1:B:98:ALA:HB2	1:I:98:ALA:HB2	1.97	0.46
1:L:15:GLN:O	1:L:19:ILE:HG12	2.14	0.46
1:J:39:PHE:HA	1:L:51:ILE:O	2.15	0.46
1:J:6:ASP:OD1	1:J:45:HIS:HE1	1.98	0.46
1:J:15:GLN:O	1:J:19:ILE:HG12	2.16	0.46
1:B:85:PHE:CE2	1:B:106:ILE:HD11	2.51	0.46
1:C:23:VAL:O	1:C:27:LEU:HD13	2.15	0.46
1:J:91:SER:O	1:J:94:PRO:HD2	2.16	0.46
1:I:116:PHE:HD2	1:I:122:GLN:HE21	1.63	0.46
1:B:122:GLN:HB3	1:B:128:LEU:HB2	1.98	0.46
1:G:69:HIS:HD2	1:H:4:ARG:HH11	1.64	0.46
1:J:62:SER:HB2	1:J:101:ASP:OD2	2.16	0.46
1:L:9:SER:O	1:L:10:ASP:CB	2.55	0.46
1:H:67:ILE:HG23	1:H:103:PHE:HD2	1.80	0.46
1:I:3:ILE:HD13	2:I:140:HOH:O	2.16	0.46
1:L:19:ILE:HD13	1:L:95:ILE:HG21	1.97	0.45
1:J:19:ILE:O	1:J:23:VAL:HG23	2.16	0.45
1:H:13:ARG:CD	1:H:13:ARG:H	2.29	0.45
1:H:27:LEU:O	1:H:31:LEU:HB2	2.17	0.45
1:I:5:ILE:HB	1:I:42:LEU:HD23	1.99	0.45
1:G:42:LEU:HD12	1:I:49:ASP:HA	1.97	0.45
1:D:95:ILE:CG2	1:D:95:ILE:O	2.64	0.45
1:B:77:THR:HG22	1:B:80:THR:OG1	2.15	0.45
1:I:80:THR:O	1:I:84:VAL:HG23	2.16	0.45
1:L:24:HIS:CE1	1:L:38:ARG:HB2	2.52	0.45
1:C:122:GLN:HB3	1:C:128:LEU:HB2	1.99	0.45
1:C:45:HIS:HB3	1:C:49:ASP:HB2	1.97	0.45
1:A:36:ARG:NH2	2:A:755:HOH:O	2.48	0.45
1:C:13:ARG:NH1	2:C:289:HOH:O	2.50	0.45
1:D:131:PRO:HG3	2:D:939:HOH:O	2.15	0.45
1:E:47:PRO:HD3	2:E:839:HOH:O	2.17	0.45
1:L:8:THR:HG23	1:L:47:PRO:HD3	1.98	0.44
1:E:95:ILE:O	1:E:95:ILE:HG22	2.16	0.44
1:J:52:ALA:HB3	1:J:65:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:69:HIS:HE1	1:I:107:THR:OG1	2.00	0.44
1:E:98:ALA:HB2	1:L:98:ALA:HB2	2.00	0.44
1:K:79:GLU:O	1:K:83:ARG:HG3	2.17	0.44
1:B:53:GLU:HB3	1:C:36:ARG:HH12	1.79	0.44
1:J:52:ALA:CB	1:J:65:VAL:HG11	2.48	0.44
1:D:110:ALA:HB1	1:D:111:PRO:HD2	1.99	0.44
1:G:6:ASP:OD1	1:G:45:HIS:CE1	2.62	0.44
1:K:23:VAL:O	1:K:27:LEU:HD22	2.18	0.44
1:D:77:THR:O	1:D:81:LYS:HG3	2.19	0.43
1:F:61:ARG:NH1	1:F:100:SER:O	2.51	0.43
1:G:67:ILE:N	1:G:67:ILE:HD12	2.33	0.43
1:D:1:PRO:HB3	1:D:72:THR:HG23	2.00	0.43
1:G:19:ILE:O	1:G:23:VAL:HG23	2.18	0.43
1:D:6:ASP:OD1	1:D:45:HIS:HE1	2.02	0.43
1:B:109:ASN:C	1:B:109:ASN:HD22	2.21	0.43
1:E:77:THR:HG23	1:E:80:THR:H	1.83	0.43
1:J:68:ILE:HB	1:J:104:ILE:HG23	1.99	0.43
1:G:128:LEU:HD13	1:I:57:LEU:HD13	2.01	0.43
1:D:19:ILE:HD12	1:D:92:LEU:HD22	2.01	0.43
1:G:72:THR:HG22	2:G:143:HOH:O	2.17	0.43
1:F:92:LEU:HD23	1:F:95:ILE:HD11	2.01	0.43
1:G:70:VAL:HB	1:G:106:ILE:HD13	2.00	0.43
1:A:69:HIS:HD2	1:B:4:ARG:HH21	1.67	0.43
1:J:116:PHE:H	1:J:122:GLN:NE2	2.16	0.42
1:G:53:GLU:HB3	1:G:54:ASP:H	1.62	0.42
1:H:54:ASP:OD1	1:I:36:ARG:HD2	2.20	0.42
1:C:110:ALA:HB1	1:C:111:PRO:CD	2.49	0.42
1:A:66:VAL:HG12	1:A:68:ILE:CD1	2.49	0.42
1:H:13:ARG:NE	1:H:13:ARG:H	2.17	0.42
1:B:46:ASP:O	1:B:48:SER:N	2.52	0.42
1:F:92:LEU:CD2	1:F:95:ILE:HD11	2.49	0.42
1:D:95:ILE:O	1:D:95:ILE:HG22	2.19	0.42
1:I:24:HIS:CE1	1:I:38:ARG:HB2	2.54	0.42
1:J:20:ALA:HB2	1:J:42:LEU:HD11	2.02	0.42
1:E:92:LEU:HB3	1:E:97:VAL:HB	2.02	0.42
1:D:45:HIS:HB3	1:D:49:ASP:HB2	2.02	0.42
1:I:57:LEU:HD12	1:I:57:LEU:HA	1.94	0.42
1:C:73:GLN:NE2	1:C:131:PRO:HD2	2.34	0.42
1:E:121:ALA:O	1:E:124:VAL:HG22	2.20	0.42
1:L:31:LEU:HB3	1:L:33:ILE:HG23	2.02	0.41
1:H:57:LEU:HD11	1:I:122:GLN:HG2	2.02	0.41
1:B:17:ARG:NH2	2:B:1218:HOH:O	2.52	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:4:ARG:NH1	2:J:1375:HOH:O	2.52	0.41
1:C:8:THR:HG23	1:C:11:ARG:HG3	2.01	0.41
1:K:93:ALA:N	1:K:94:PRO:HD2	2.36	0.41
1:B:46:ASP:OD2	1:B:48:SER:HB2	2.20	0.41
1:G:27:LEU:O	1:G:31:LEU:HB2	2.19	0.41
1:E:69:HIS:HD2	1:F:4:ARG:HH11	1.69	0.41
1:C:61:ARG:NH1	1:C:100:SER:O	2.53	0.41
1:G:52:ALA:CB	1:G:65:VAL:HG21	2.51	0.41
1:H:60:GLN:O	1:H:61:ARG:CB	2.69	0.41
1:L:68:ILE:HD13	1:L:88:ILE:HG21	2.03	0.41
1:G:69:HIS:HE1	1:G:107:THR:OG1	2.04	0.40
1:A:62:SER:OG	1:A:101:ASP:OD2	2.38	0.40
1:G:2:LEU:HD23	1:G:2:LEU:C	2.42	0.40
1:A:131:PRO:HG3	2:A:421:HOH:O	2.22	0.40
1:G:54:ASP:O	1:G:55:ALA:HB3	2.22	0.40
1:K:3:ILE:O	1:K:40:GLN:HA	2.21	0.40
1:G:61:ARG:NH1	1:G:100:SER:O	2.54	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	129/136 (95%)	126 (98%)	3 (2%)	0	100	100
1	B	129/136 (95%)	125 (97%)	4 (3%)	0	100	100
1	C	129/136 (95%)	126 (98%)	3 (2%)	0	100	100
1	D	129/136 (95%)	124 (96%)	5 (4%)	0	100	100
1	E	129/136 (95%)	126 (98%)	2 (2%)	1 (1%)	27	39
1	F	128/136 (94%)	126 (98%)	2 (2%)	0	100	100
1	G	129/136 (95%)	125 (97%)	4 (3%)	0	100	100
1	H	129/136 (95%)	124 (96%)	4 (3%)	1 (1%)	27	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	129/136 (95%)	126 (98%)	3 (2%)	0	100	100
1	J	129/136 (95%)	126 (98%)	3 (2%)	0	100	100
1	K	128/136 (94%)	122 (95%)	4 (3%)	2 (2%)	14	18
1	L	129/136 (95%)	125 (97%)	3 (2%)	1 (1%)	27	39
All	All	1546/1632 (95%)	1501 (97%)	40 (3%)	5 (0%)	50	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	9	SER
1	L	9	SER
1	H	61	ARG
1	K	74	ALA
1	K	128	LEU

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	105/106 (99%)	97 (92%)	8 (8%)	19	28
1	B	105/106 (99%)	98 (93%)	7 (7%)	23	35
1	C	105/106 (99%)	98 (93%)	7 (7%)	23	35
1	D	104/106 (98%)	97 (93%)	7 (7%)	23	35
1	E	104/106 (98%)	99 (95%)	5 (5%)	35	53
1	F	104/106 (98%)	100 (96%)	4 (4%)	44	65
1	G	105/106 (99%)	97 (92%)	8 (8%)	19	28
1	H	105/106 (99%)	98 (93%)	7 (7%)	23	35
1	I	105/106 (99%)	97 (92%)	8 (8%)	19	28
1	J	105/106 (99%)	100 (95%)	5 (5%)	35	53
1	K	104/106 (98%)	99 (95%)	5 (5%)	35	53
1	L	105/106 (99%)	97 (92%)	8 (8%)	19	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1256/1272 (99%)	1177 (94%)	79 (6%)	25	38

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	9	SER
1	A	13	ARG
1	A	27	LEU
1	A	41	ILE
1	A	76	ARG
1	A	90	GLU
1	A	104	ILE
1	B	17	ARG
1	B	48	SER
1	B	65	VAL
1	B	106	ILE
1	B	109	ASN
1	B	122	GLN
1	B	128	LEU
1	C	7	LEU
1	C	8	THR
1	C	13	ARG
1	C	31	LEU
1	C	33	ILE
1	C	88	ILE
1	C	128	LEU
1	D	2	LEU
1	D	7	LEU
1	D	9	SER
1	D	27	LEU
1	D	72	THR
1	D	122	GLN
1	D	128	LEU
1	E	7	LEU
1	E	9	SER
1	E	46	ASP
1	E	109	ASN
1	E	122	GLN
1	F	7	LEU
1	F	31	LEU
1	F	46	ASP

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Mol	Chain	Res	Type
1	F	128	LEU
1	G	7	LEU
1	G	13	ARG
1	G	29	GLU
1	G	60	GLN
1	G	65	VAL
1	G	68	ILE
1	G	72	THR
1	G	130	ILE
1	H	7	LEU
1	H	13	ARG
1	H	36	ARG
1	H	51	ILE
1	H	60	GLN
1	H	76	ARG
1	H	122	GLN
1	I	7	LEU
1	I	14	GLU
1	I	33	ILE
1	I	57	LEU
1	I	104	ILE
1	I	122	GLN
1	I	127	GLU
1	I	130	ILE
1	J	7	LEU
1	J	27	LEU
1	J	57	LEU
1	J	104	ILE
1	J	122	GLN
1	K	7	LEU
1	K	9	SER
1	K	13	ARG
1	K	27	LEU
1	K	109	ASN
1	L	7	LEU
1	L	13	ARG
1	L	31	LEU
1	L	76	ARG
1	L	88	ILE
1	L	92	LEU
1	L	122	GLN
1	L	127	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	60	GLN
1	A	69	HIS
1	B	73	GLN
1	B	82	GLN
1	B	109	ASN
1	B	122	GLN
1	C	60	GLN
1	C	69	HIS
1	C	73	GLN
1	C	112	HIS
1	D	45	HIS
1	D	82	GLN
1	D	122	GLN
1	E	69	HIS
1	E	73	GLN
1	E	109	ASN
1	E	122	GLN
1	G	45	HIS
1	G	60	GLN
1	G	69	HIS
1	H	122	GLN
1	I	69	HIS
1	I	73	GLN
1	I	122	GLN
1	J	45	HIS
1	J	112	HIS
1	J	122	GLN
1	K	15	GLN
1	K	40	GLN
1	K	69	HIS
1	K	73	GLN
1	K	109	ASN
1	K	112	HIS
1	L	60	GLN
1	L	69	HIS
1	L	122	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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, 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(Å²)	Q<0.9	
1	A	131/136 (96%)	-0.55	0	100	100	8, 18, 28, 37	0
1	B	131/136 (96%)	-0.63	0	100	100	5, 12, 24, 35	0
1	C	131/136 (96%)	-0.61	0	100	100	5, 11, 19, 27	0
1	D	131/136 (96%)	-0.56	0	100	100	6, 17, 25, 35	0
1	E	131/136 (96%)	-0.60	0	100	100	5, 12, 21, 36	0
1	F	130/136 (95%)	-0.69	0	100	100	5, 12, 19, 30	0
1	G	131/136 (96%)	-0.48	0	100	100	6, 15, 28, 36	0
1	H	131/136 (96%)	-0.46	0	100	100	6, 17, 28, 38	0
1	I	131/136 (96%)	-0.60	0	100	100	5, 13, 23, 36	0
1	J	131/136 (96%)	-0.42	1 (0%)	83	82	8, 17, 29, 37	0
1	K	130/136 (95%)	-0.33	0	100	100	10, 18, 28, 37	0
1	L	131/136 (96%)	-0.61	0	100	100	5, 14, 24, 37	0
All	All	1570/1632 (96%)	-0.55	1 (0%)	93	95	5, 15, 27, 38	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	130	ILE	2.8

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.