Full wwPDB X-ray Structure Validation Report (i)

Apr 12, 2021 – 12:02 AM EDT

PDB ID	:	4IWM
Title	:	Crystal Structure of the Conserved Hypothetical Protein MJ0927 from Methanocaldococcus jannaschii (in P21 form)
Authors	:	Kuan, S.M.; Chen, S.C.; Yang, C.S.; Chen, Y.R.; Liu, Y.H.; Chen, Y.
Deposited on	:	2013-01-24
Resolution	:	2.70 Å(reported)

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

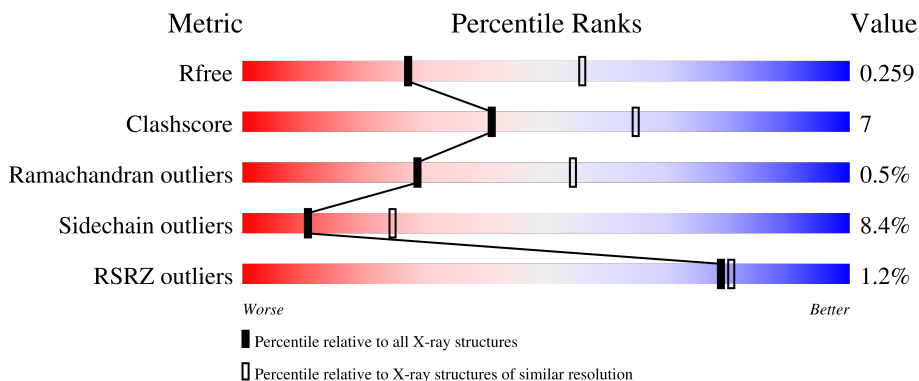|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

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 2.70 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	Percentile Ranks	Value
Rfree		0.259
Clashscore		7
Ramachandran outliers		0.5%
Sidechain outliers		8.4%
RSRZ outliers		1.2%

Worse ← → *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	252	79% 16% · ·
1	B	252	.% 71% 23% · ·
1	C	252	77% 17% · ·
1	D	252	3% 70% 24% · ·
1	E	252	2% 76% 19% · ·

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Mol	Chain	Length	Quality of chain
1	F	252	

2%

68%   25%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 11973 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 UPF0135 protein MJ0927.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	Se	0	0	0
			1932	1255	307	367	1	2			
1	B	244	Total	C	N	O	S	Se	0	0	0
			1932	1255	307	367	1	2			
1	C	244	Total	C	N	O	S	Se	0	0	0
			1932	1255	307	367	1	2			
1	D	244	Total	C	N	O	S	Se	0	0	0
			1932	1255	307	367	1	2			
1	E	244	Total	C	N	O	S	Se	0	0	0
			1932	1255	307	367	1	2			
1	F	244	Total	C	N	O	S	Se	0	0	0
			1932	1255	307	367	1	2			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	250	LEU	-	expression tag	UNP Q58337
A	251	GLU	-	expression tag	UNP Q58337
A	252	HIS	-	expression tag	UNP Q58337
A	253	HIS	-	expression tag	UNP Q58337
A	254	HIS	-	expression tag	UNP Q58337
A	255	HIS	-	expression tag	UNP Q58337
A	256	HIS	-	expression tag	UNP Q58337
A	257	HIS	-	expression tag	UNP Q58337
B	250	LEU	-	expression tag	UNP Q58337
B	251	GLU	-	expression tag	UNP Q58337
B	252	HIS	-	expression tag	UNP Q58337
B	253	HIS	-	expression tag	UNP Q58337
B	254	HIS	-	expression tag	UNP Q58337
B	255	HIS	-	expression tag	UNP Q58337
B	256	HIS	-	expression tag	UNP Q58337
B	257	HIS	-	expression tag	UNP Q58337
C	250	LEU	-	expression tag	UNP Q58337

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Chain	Residue	Modelled	Actual	Comment	Reference
C	251	GLU	-	expression tag	UNP Q58337
C	252	HIS	-	expression tag	UNP Q58337
C	253	HIS	-	expression tag	UNP Q58337
C	254	HIS	-	expression tag	UNP Q58337
C	255	HIS	-	expression tag	UNP Q58337
C	256	HIS	-	expression tag	UNP Q58337
C	257	HIS	-	expression tag	UNP Q58337
D	250	LEU	-	expression tag	UNP Q58337
D	251	GLU	-	expression tag	UNP Q58337
D	252	HIS	-	expression tag	UNP Q58337
D	253	HIS	-	expression tag	UNP Q58337
D	254	HIS	-	expression tag	UNP Q58337
D	255	HIS	-	expression tag	UNP Q58337
D	256	HIS	-	expression tag	UNP Q58337
D	257	HIS	-	expression tag	UNP Q58337
E	250	LEU	-	expression tag	UNP Q58337
E	251	GLU	-	expression tag	UNP Q58337
E	252	HIS	-	expression tag	UNP Q58337
E	253	HIS	-	expression tag	UNP Q58337
E	254	HIS	-	expression tag	UNP Q58337
E	255	HIS	-	expression tag	UNP Q58337
E	256	HIS	-	expression tag	UNP Q58337
E	257	HIS	-	expression tag	UNP Q58337
F	250	LEU	-	expression tag	UNP Q58337
F	251	GLU	-	expression tag	UNP Q58337
F	252	HIS	-	expression tag	UNP Q58337
F	253	HIS	-	expression tag	UNP Q58337
F	254	HIS	-	expression tag	UNP Q58337
F	255	HIS	-	expression tag	UNP Q58337
F	256	HIS	-	expression tag	UNP Q58337
F	257	HIS	-	expression tag	UNP Q58337

- Molecule 2 is water.

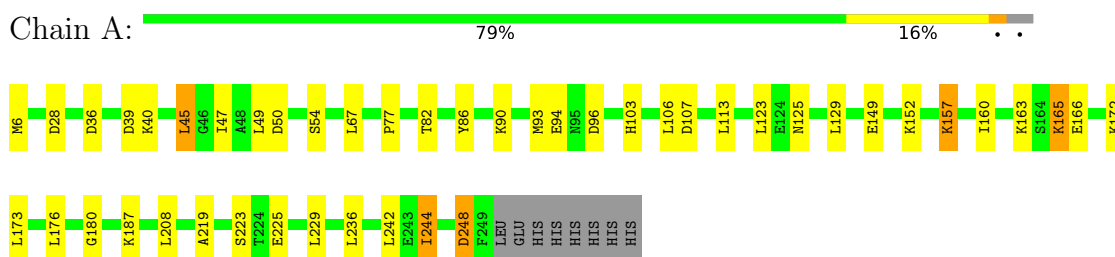| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	80	Total 80	O 80	0	0
2	B	87	Total 87	O 87	0	0
2	C	79	Total 79	O 79	0	0
2	D	50	Total 50	O 50	0	0

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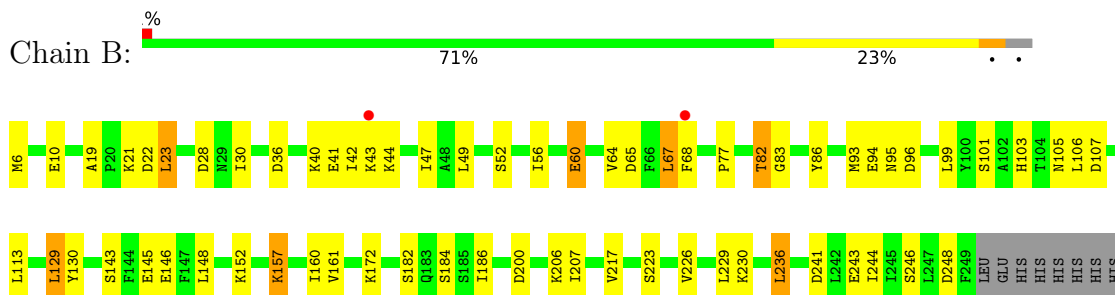| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	49	Total O 49 49		0	0
2	F	36	Total O 36 36		0	0

3 Residue-property plots ⓘ

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.
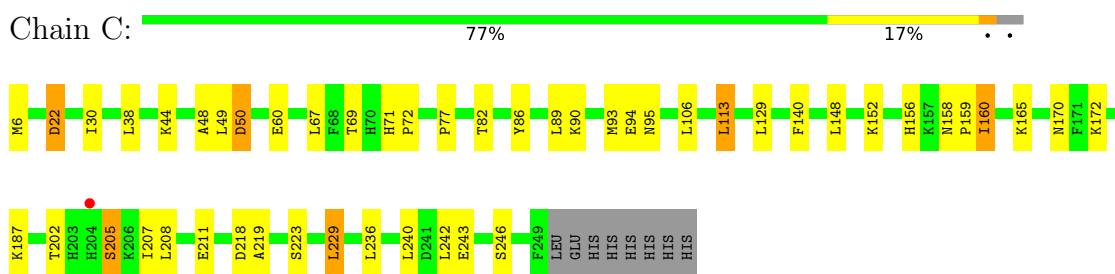
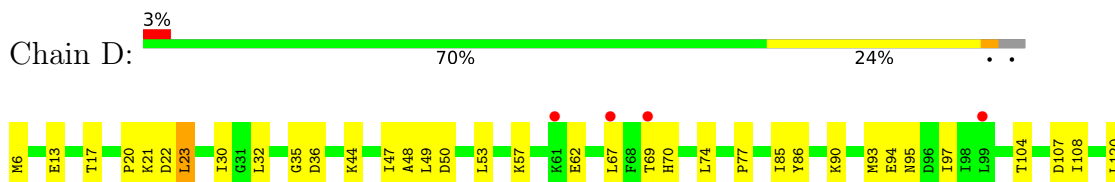- Molecule 1: UPF0135 protein MJ0927
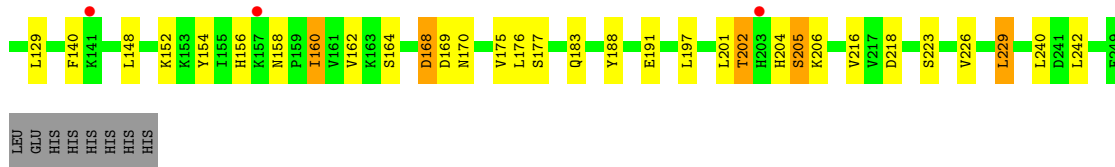
Chain A:

- Molecule 1: UPF0135 protein MJ0927

Chain B:

- Molecule 1: UPF0135 protein MJ0927

Chain C:

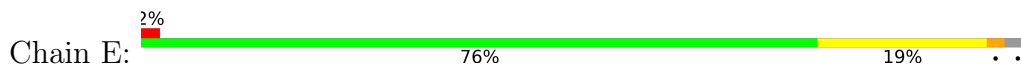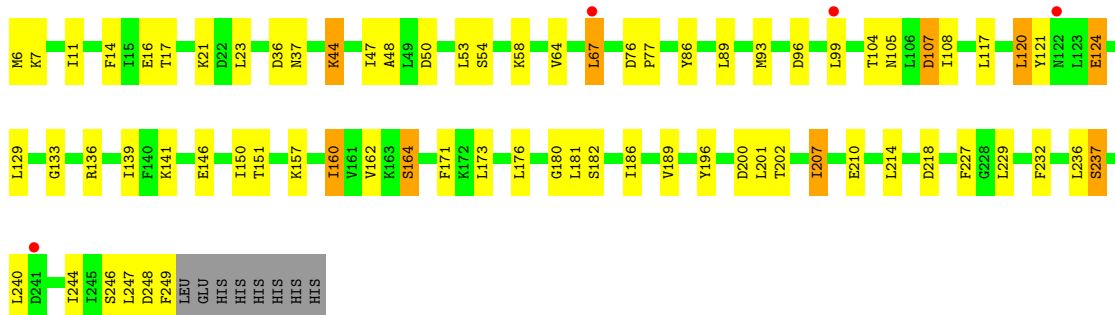- Molecule 1: UPF0135 protein MJ0927

Chain D:

L129 F140 K441 L148 K152 K153 Y154 I155 H156 K157 N158 P159 I160 V161 V162 K163 S164 D168 D169 N170 V175 L176 S177 Q183 Y188 E191 L197 L201 T202 H203 H204 S205 K206 V216 V217 D218 S223 V226 L229 L240 D241 L242 F249

LEU GLU HIS HIS HIS HIS HIS

• Molecule 1: UPF0135 protein MJ0927

Chain E:

2%

76%　　　　19%

M6 P20 K21 D22 L23 A24 I25 D36 I47 A48 L49 D50 S54 E60 L67 H71 D76 P77 Y86 L89 K90 I91 L92 M93 E94 N95 D107 N114 E119 N122 L129 N132 E145 E146 F147 L148 E149 I150 T151 K152 H156 K157

I160 K165 E166 I186 V189 V195 Y196 D200 H204 I207 V215 D218 A219 T220 H221 Y222 S223 V226 L229 L236 L240 D241 L242 E243 I244 I245 S246 F249 LEU GLU HIS HIS HIS HIS HIS

• Molecule 1: UPF0135 protein MJ0927

Chain F:

2%

68%　　　　25%

M6 K7 I11 F14 I15 E16 T17 K21 D22 L23 D36 N37 K44 I47 A48 L49 D50 L53 S54 K58 V64 L67 D76 P77 Y86 L89 M93 D96 L99 T104 N105 L106 D107 I108 L117 L120 Y121 N122 L123 E124

L129 G133 R136 I139 F140 K141 E146 I150 T151 K157 I160 V161 V162 K163 S164 F171 K172 L173 L176 G180 L181 S182 I186 V189 Y196 D200 L201 T202 I207 E210 L214 D218 F227 G228 L229 F232 L236 S237

L240 D241 I244 I245 S246 L247 D248 F249 LEU GLU HIS HIS HIS HIS HIS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.37Å 77.14Å 131.74Å 90.00° 105.36° 90.00°	Depositor
Resolution (Å)	26.90 – 2.70 26.90 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.2 (26.90-2.70) 94.5 (26.90-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.27 (at 2.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.189 , 0.258 0.190 , 0.259	Depositor DCC
R_{free} test set	2606 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	51.2	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 35.0	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11973	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.46	0/1966	0.61	0/2648
1	B	0.45	0/1966	0.58	0/2648
1	C	0.45	0/1966	0.61	1/2648 (0.0%)
1	D	0.38	0/1966	0.55	0/2648
1	E	0.40	0/1966	0.55	0/2648
1	F	0.35	0/1966	0.54	0/2648
All	All	0.42	0/11796	0.57	1/15888 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	242	LEU	CA-CB-CG	5.39	127.69	115.30

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	1932	0	1978	22	0
1	B	1932	0	1978	36	0
1	C	1932	0	1978	25	0
1	D	1932	0	1978	37	0
1	E	1932	0	1978	26	0
1	F	1932	0	1978	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	80	0	0	2	0
2	B	87	0	0	4	0
2	C	79	0	0	1	0
2	D	50	0	0	1	0
2	E	49	0	0	2	0
2	F	36	0	0	0	0
All	All	11973	0	11868	166	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 (166) 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:F:160:ILE:HG23	1:F:218:ASP:HB3	1.62	0.82
1:A:47:ILE:HD11	1:A:229:LEU:HD22	1.66	0.77
1:D:160:ILE:HG23	1:D:218:ASP:HB3	1.69	0.73
1:A:40:LYS:NZ	1:A:96:ASP:O	2.24	0.70
1:B:94:GLU:OE1	2:B:365:HOH:O	2.09	0.70
1:E:20:PRO:HD2	1:E:23:LEU:HD22	1.73	0.69
1:E:160:ILE:HG23	1:E:218:ASP:HB3	1.74	0.68
1:F:121:TYR:HH	1:F:151:THR:HG1	1.36	0.67
1:A:93:MSE:SE	1:D:93:MSE:HE1	2.46	0.66
1:E:89:LEU:HD22	1:E:93:MSE:HE3	1.80	0.63
1:A:90:LYS:HA	1:D:93:MSE:HE3	1.81	0.62
1:D:202:THR:HG23	1:D:205:SER:HB2	1.82	0.62
1:F:89:LEU:HB3	1:F:93:MSE:HE3	1.83	0.61
1:F:176:LEU:HD12	1:F:180:GLY:HA3	1.83	0.61
1:B:77:PRO:HB2	1:E:77:PRO:HB2	1.83	0.60
1:C:44:LYS:HG3	1:C:243:GLU:HG3	1.82	0.60
1:B:106:LEU:HG	1:B:113:LEU:HD13	1.84	0.59
1:B:145:GLU:HB2	2:B:316:HOH:O	2.02	0.59
1:C:89:LEU:HD22	1:C:93:MSE:HE3	1.85	0.59
1:A:45:LEU:HB3	1:A:244:ILE:HG23	1.85	0.59
1:A:187:LYS:HE3	1:A:208:LEU:HD11	1.84	0.58
1:C:86:TYR:CE1	1:F:36:ASP:HB2	2.39	0.58
1:A:77:PRO:HB2	1:D:77:PRO:HB2	1.85	0.57
1:F:67:LEU:HD13	1:F:99:LEU:HD13	1.85	0.56
1:F:121:TYR:OH	1:F:151:THR:OG1	2.14	0.56
1:A:165:LYS:HE3	1:A:166:GLU:O	2.05	0.56
1:D:20:PRO:HD2	1:D:23:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:LEU:HD13	1:F:201:LEU:HD13	1.87	0.56
1:E:6:MSE:SE	1:E:240:LEU:HD21	2.56	0.56
1:D:183:GLN:NE2	1:D:204:HIS:HB3	2.21	0.56
1:D:188:TYR:O	1:D:191:GLU:HG2	2.06	0.55
1:D:176:LEU:HD13	1:D:177:SER:O	2.07	0.55
1:B:60:GLU:HG3	1:B:95:ASN:ND2	2.21	0.55
1:B:206:LYS:NZ	2:B:334:HOH:O	2.36	0.55
1:D:183:GLN:HE21	1:D:204:HIS:HB3	1.70	0.55
1:A:49:LEU:HD21	1:A:225:GLU:HB3	1.88	0.54
1:E:189:VAL:HG11	1:E:196:TYR:CG	2.42	0.54
1:A:176:LEU:HD12	1:A:180:GLY:HA3	1.89	0.54
1:E:25:ILE:HG22	1:E:132:ASN:HB2	1.90	0.54
1:F:58:LYS:HG2	1:F:247:LEU:HD22	1.89	0.53
1:B:47:ILE:HG13	1:B:68:PHE:HD2	1.74	0.52
1:D:44:LYS:NZ	1:D:62:GLU:O	2.28	0.52
1:B:52:SER:O	1:B:56:ILE:HG13	2.09	0.51
1:F:120:LEU:HD13	1:F:227:PHE:HZ	1.74	0.51
1:B:21:LYS:HD2	1:B:30:ILE:HD12	1.92	0.51
1:F:6:MSE:SE	1:F:240:LEU:HD22	2.61	0.51
1:B:49:LEU:HG	1:B:229:LEU:HD12	1.91	0.51
1:F:171:PHE:HE2	1:F:173:LEU:HB2	1.76	0.50
1:B:143:SER:OG	1:B:146:GLU:HG3	2.11	0.50
1:D:70:HIS:NE2	1:D:107:ASP:OD2	2.42	0.50
1:C:6:MSE:HE1	1:C:240:LEU:HB3	1.93	0.49
1:D:148:LEU:HD21	1:D:152:LYS:HE3	1.94	0.49
1:A:36:ASP:HB3	2:A:322:HOH:O	2.11	0.49
1:A:125:ASN:HB2	2:A:328:HOH:O	2.11	0.49
1:B:86:TYR:CE1	1:E:36:ASP:HB2	2.47	0.49
1:B:6:MSE:N	1:B:41:GLU:OE2	2.45	0.49
1:C:77:PRO:HB2	1:F:77:PRO:HB2	1.93	0.49
1:F:164:SER:OG	1:F:214:LEU:O	2.23	0.49
1:E:22:ASP:OD2	1:E:22:ASP:N	2.37	0.49
1:D:95:ASN:HB2	1:D:97:ILE:HG13	1.94	0.49
1:E:195:VAL:HG22	1:E:215:VAL:HB	1.94	0.48
1:B:19:ALA:O	1:B:105:ASN:ND2	2.41	0.48
1:D:201:LEU:HD13	1:D:216:VAL:HG11	1.95	0.48
1:F:105:ASN:OD1	1:F:105:ASN:N	2.45	0.48
1:C:93:MSE:HG2	1:F:86:TYR:CE2	2.49	0.48
1:B:93:MSE:HG2	1:E:86:TYR:CE2	2.49	0.48
1:E:71:HIS:HB3	2:E:344:HOH:O	2.13	0.47
1:E:236:LEU:HB3	1:E:244:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:146:GLU:O	1:F:150:ILE:HG13	2.14	0.47
1:B:93:MSE:HE1	1:E:93:MSE:SE	2.64	0.47
1:B:129:LEU:HD13	1:B:130:TYR:CE2	2.50	0.47
1:A:152:LYS:HG2	1:A:157:LYS:O	2.14	0.47
1:D:6:MSE:SE	1:D:240:LEU:HD22	2.65	0.47
1:A:28:ASP:OD2	1:A:103:HIS:HB3	2.14	0.47
1:C:158:ASN:ND2	2:C:307:HOH:O	2.48	0.47
1:C:219:ALA:O	1:C:223:SER:HB2	2.14	0.47
1:F:14:PHE:O	1:F:17:THR:HB	2.15	0.47
1:A:219:ALA:O	1:A:223:SER:HB2	2.15	0.47
1:B:30:ILE:HG22	1:B:103:HIS:H	1.79	0.47
1:B:236:LEU:HB3	1:B:244:ILE:HD13	1.97	0.47
1:C:140:PHE:O	1:C:170:ASN:HA	2.15	0.47
1:C:50:ASP:OD1	1:C:71:HIS:ND1	2.47	0.46
1:B:44:LYS:HE3	1:B:243:GLU:CD	2.35	0.46
1:B:93:MSE:HE3	1:E:90:LYS:HA	1.96	0.46
1:C:60:GLU:HG3	1:C:95:ASN:OD1	2.15	0.46
1:D:21:LYS:HB3	1:D:30:ILE:HD12	1.98	0.46
1:C:160:ILE:HG23	1:C:218:ASP:HB3	1.98	0.46
1:B:40:LYS:NZ	1:B:65:ASP:HB2	2.30	0.45
1:D:152:LYS:HA	1:D:156:HIS:O	2.16	0.45
1:B:44:LYS:HB3	1:B:64:VAL:HA	1.98	0.45
1:B:182:SER:O	1:B:186:ILE:HG12	2.16	0.45
1:E:152:LYS:HA	1:E:156:HIS:O	2.17	0.45
1:A:49:LEU:HB2	1:A:248:ASP:OD2	2.17	0.45
1:A:86:TYR:CE2	1:D:93:MSE:HG2	2.52	0.45
1:C:148:LEU:HD23	1:C:148:LEU:HA	1.67	0.45
1:D:48:ALA:O	1:D:69:THR:HA	2.16	0.45
1:F:48:ALA:HB1	1:F:248:ASP:HB2	1.98	0.45
1:C:48:ALA:O	1:C:69:THR:HA	2.17	0.45
1:D:175:VAL:HG12	1:D:197:LEU:HB3	1.99	0.45
1:F:7:LYS:O	1:F:11:ILE:HG13	2.17	0.44
1:B:42:ILE:O	2:B:321:HOH:O	2.21	0.44
1:F:171:PHE:CE2	1:F:173:LEU:HB2	2.52	0.44
1:C:90:LYS:O	1:C:94:GLU:HB2	2.18	0.44
1:B:152:LYS:HG2	1:B:157:LYS:O	2.18	0.44
1:D:93:MSE:HE2	1:D:93:MSE:HB2	1.89	0.44
1:D:168:ASP:HB3	1:D:169:ASP:H	1.59	0.44
1:E:107:ASP:HB3	1:E:114:ASN:ND2	2.33	0.44
1:E:146:GLU:O	1:E:150:ILE:HG13	2.17	0.44
1:D:13:GLU:O	1:D:17:THR:OG1	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:ASP:HA	1:E:77:PRO:HD3	1.83	0.44
1:F:47:ILE:HD11	1:F:249:PHE:HZ	1.83	0.44
1:F:58:LYS:HE3	1:F:58:LYS:HB2	1.70	0.44
1:C:90:LYS:NZ	1:F:93:MSE:O	2.50	0.43
1:C:106:LEU:HG	1:C:113:LEU:HD13	1.99	0.43
1:F:164:SER:HB3	1:F:210:GLU:HA	2.00	0.43
1:F:182:SER:O	1:F:186:ILE:HG12	2.18	0.43
1:A:106:LEU:HG	1:A:113:LEU:HD13	2.00	0.43
1:B:28:ASP:OD2	1:B:103:HIS:HB3	2.17	0.43
1:D:47:ILE:HD11	1:D:229:LEU:HD22	2.01	0.43
1:D:74:LEU:HD21	1:D:85:ILE:HD13	2.01	0.43
1:C:187:LYS:HE3	1:C:208:LEU:HD21	2.00	0.43
1:F:108:ILE:O	1:F:136:ARG:NH2	2.52	0.43
1:D:90:LYS:NZ	1:D:94:GLU:OE2	2.51	0.43
1:F:237:SER:HA	1:F:244:ILE:HD12	2.00	0.42
1:A:94:GLU:HG2	1:D:94:GLU:HG2	2.01	0.42
1:B:157:LYS:HB3	1:B:157:LYS:HE2	1.89	0.42
1:B:67:LEU:HD13	1:B:99:LEU:HD13	2.02	0.42
1:B:107:ASP:HA	1:B:113:LEU:HB2	2.01	0.42
1:F:124:GLU:OE1	1:F:141:LYS:HE2	2.19	0.42
1:B:82:THR:OG1	1:B:83:GLY:N	2.52	0.42
1:E:223:SER:HA	1:E:226:VAL:HG12	2.02	0.42
1:D:36:ASP:HB3	2:D:316:HOH:O	2.19	0.42
1:E:165:LYS:HE3	1:E:166:GLU:O	2.20	0.42
1:F:108:ILE:HG12	1:F:133:GLY:O	2.19	0.42
1:F:124:GLU:HB3	1:F:139:ILE:HB	2.02	0.42
1:A:123:LEU:HD21	1:A:173:LEU:HD23	2.01	0.42
1:A:107:ASP:HA	1:A:113:LEU:HB2	2.01	0.42
1:D:140:PHE:O	1:D:170:ASN:HA	2.19	0.42
1:B:161:VAL:HG22	1:B:217:VAL:HG22	2.02	0.42
1:D:53:LEU:HG	1:D:57:LYS:HE3	2.01	0.42
1:B:23:LEU:HD21	1:C:211:GLU:HG3	2.01	0.42
1:F:207:ILE:HD13	1:F:207:ILE:HA	1.77	0.41
1:B:226:VAL:HG22	1:B:230:LYS:HE3	2.00	0.41
1:F:44:LYS:HB3	1:F:64:VAL:HA	2.02	0.41
1:C:202:THR:OG1	1:C:205:SER:HB2	2.20	0.41
1:D:32:LEU:HD11	1:D:35:GLY:HA3	2.03	0.41
1:E:189:VAL:HG21	1:E:196:TYR:CZ	2.55	0.41
1:C:22:ASP:OD2	1:C:22:ASP:N	2.45	0.41
1:F:16:GLU:HG2	1:F:21:LYS:HG3	2.02	0.41
1:D:120:LEU:HD11	1:D:154:TYR:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:189:VAL:HG11	1:F:196:TYR:CG	2.54	0.41
1:C:229:LEU:HD23	1:C:229:LEU:HA	1.79	0.41
1:A:36:ASP:HB2	1:D:86:TYR:CD1	2.56	0.41
1:F:232:PHE:O	1:F:236:LEU:HB2	2.20	0.41
1:C:71:HIS:HA	1:C:72:PRO:HD3	1.93	0.41
1:F:104:THR:HA	1:F:107:ASP:HB2	2.03	0.41
1:E:91:ILE:O	1:E:95:ASN:ND2	2.49	0.41
1:B:36:ASP:HB3	1:E:86:TYR:CD1	2.56	0.40
1:B:207:ILE:HD13	1:B:207:ILE:HA	1.94	0.40
1:C:158:ASN:HA	1:C:159:PRO:HD3	1.88	0.40
1:E:145:GLU:HB2	2:E:317:HOH:O	2.22	0.40
1:E:89:LEU:HD23	1:E:89:LEU:HA	1.74	0.40
1:C:152:LYS:HA	1:C:156:HIS:O	2.21	0.40
1:D:104:THR:O	1:D:108:ILE:HG13	2.21	0.40
1:D:223:SER:HA	1:D:226:VAL:HG12	2.03	0.40
1:D:162:VAL:HG21	1:D:206:LYS:HG3	2.03	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	242/252 (96%)	231 (96%)	11 (4%)	0	100	100
1	B	242/252 (96%)	230 (95%)	11 (4%)	1 (0%)	34	60
1	C	242/252 (96%)	229 (95%)	13 (5%)	0	100	100
1	D	242/252 (96%)	229 (95%)	12 (5%)	1 (0%)	34	60
1	E	242/252 (96%)	224 (93%)	15 (6%)	3 (1%)	13	32
1	F	242/252 (96%)	223 (92%)	17 (7%)	2 (1%)	19	43
All	All	1452/1512 (96%)	1366 (94%)	79 (5%)	7 (0%)	29	54

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	168	ASP
1	E	241	ASP
1	E	242	LEU
1	B	200	ASP
1	F	96	ASP
1	F	200	ASP
1	E	220	THR

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	215/221 (97%)	197 (92%)	18 (8%)	11	25
1	B	215/221 (97%)	195 (91%)	20 (9%)	9	21
1	C	215/221 (97%)	198 (92%)	17 (8%)	12	28
1	D	215/221 (97%)	202 (94%)	13 (6%)	19	42
1	E	215/221 (97%)	196 (91%)	19 (9%)	10	23
1	F	215/221 (97%)	193 (90%)	22 (10%)	7	17
All	All	1290/1326 (97%)	1181 (92%)	109 (8%)	11	25

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	MSE
1	A	39	ASP
1	A	45	LEU
1	A	50	ASP
1	A	54	SER
1	A	67	LEU
1	A	82	THR
1	A	129	LEU
1	A	149	GLU
1	A	157	LYS

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Mol	Chain	Res	Type
1	A	160	ILE
1	A	163	LYS
1	A	165	LYS
1	A	172	LYS
1	A	236	LEU
1	A	242	LEU
1	A	244	ILE
1	A	248	ASP
1	B	10	GLU
1	B	22	ASP
1	B	23	LEU
1	B	43	LYS
1	B	60	GLU
1	B	67	LEU
1	B	82	THR
1	B	96	ASP
1	B	101	SER
1	B	129	LEU
1	B	148	LEU
1	B	157	LYS
1	B	160	ILE
1	B	172	LYS
1	B	184	SER
1	B	223	SER
1	B	236	LEU
1	B	241	ASP
1	B	246	SER
1	B	248	ASP
1	C	22	ASP
1	C	30	ILE
1	C	38	LEU
1	C	49	LEU
1	C	50	ASP
1	C	67	LEU
1	C	82	THR
1	C	113	LEU
1	C	129	LEU
1	C	160	ILE
1	C	165	LYS
1	C	172	LYS
1	C	205	SER
1	C	207	ILE

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Mol	Chain	Res	Type
1	C	229	LEU
1	C	236	LEU
1	C	246	SER
1	D	22	ASP
1	D	23	LEU
1	D	49	LEU
1	D	50	ASP
1	D	67	LEU
1	D	129	LEU
1	D	158	ASN
1	D	160	ILE
1	D	164	SER
1	D	202	THR
1	D	205	SER
1	D	229	LEU
1	D	242	LEU
1	E	22	ASP
1	E	23	LEU
1	E	47	ILE
1	E	49	LEU
1	E	50	ASP
1	E	54	SER
1	E	60	GLU
1	E	67	LEU
1	E	107	ASP
1	E	119	GLU
1	E	122	ASN
1	E	129	LEU
1	E	148	LEU
1	E	165	LYS
1	E	186	ILE
1	E	207	ILE
1	E	229	LEU
1	E	240	LEU
1	E	246	SER
1	F	23	LEU
1	F	37	ASN
1	F	44	LYS
1	F	50	ASP
1	F	53	LEU
1	F	54	SER
1	F	67	LEU

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Mol	Chain	Res	Type
1	F	76	ASP
1	F	107	ASP
1	F	117	LEU
1	F	120	LEU
1	F	124	GLU
1	F	129	LEU
1	F	157	LYS
1	F	160	ILE
1	F	162	VAL
1	F	164	SER
1	F	202	THR
1	F	207	ILE
1	F	229	LEU
1	F	237	SER
1	F	246	SER

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

Mol	Chain	Res	Type
1	C	95	ASN
1	D	183	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 monosaccharides 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	242/252 (96%)	-0.34	0	100	100	33, 45, 63, 75	0
1	B	242/252 (96%)	-0.29	2 (0%)	86	87	34, 48, 65, 73	0
1	C	242/252 (96%)	-0.28	1 (0%)	92	93	33, 51, 66, 76	0
1	D	242/252 (96%)	0.04	7 (2%)	51	52	47, 62, 80, 88	0
1	E	242/252 (96%)	-0.16	4 (1%)	70	72	41, 61, 74, 89	0
1	F	242/252 (96%)	0.08	4 (1%)	70	72	47, 73, 93, 109	0
All	All	1452/1512 (96%)	-0.16	18 (1%)	79	80	33, 56, 84, 109	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	204	HIS	3.3
1	D	99	LEU	2.9
1	D	67	LEU	2.7
1	D	157	LYS	2.6
1	D	141	LYS	2.5
1	D	69	THR	2.5
1	F	241	ASP	2.3
1	F	99	LEU	2.3
1	E	204	HIS	2.2
1	E	157	LYS	2.2
1	D	203	HIS	2.2
1	B	68	PHE	2.1
1	E	200	ASP	2.1
1	D	61	LYS	2.1
1	F	67	LEU	2.1
1	F	122	ASN	2.1
1	B	43	LYS	2.1
1	E	222	TYR	2.0

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 monosaccharides 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.