Full wwPDB X-ray Structure Validation Report (i)

Jan 23, 2021 – 04:41 PM EST

PDB ID	:	2F4N
Title	:	Crystal structure of protein MJ1651 from Methanococcus jannaschii DSM 2661, Pfam DUF62
Authors	:	Rao, K.N.; Swaminathan, S.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2005-11-23
Resolution	:	2.50 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 (i) symbol.

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

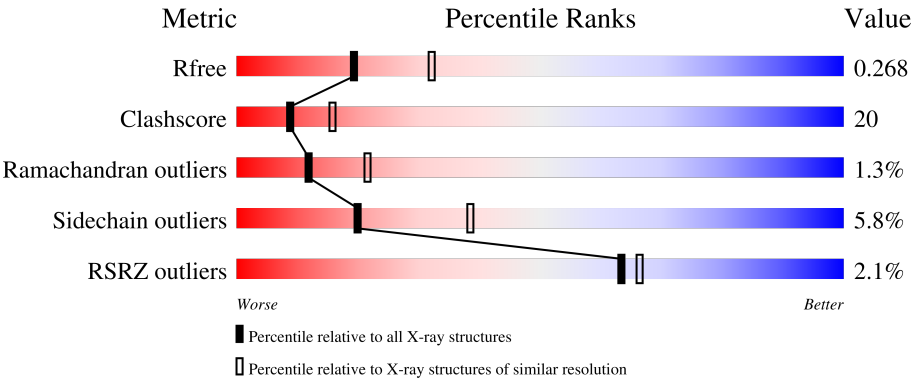
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	273	3% 62% 22% · 13%
1	B	273	2% 52% 32% · 12%
1	C	273	59% 26% · 12%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5570 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 Hypothetical protein MJ1651.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	Se	0	0	0
			1835	1189	291	349	2	4			
1	B	239	Total	C	N	O	S	Se	0	0	0
			1864	1211	303	344	2	4			
1	C	239	Total	C	N	O	S	Se	0	0	0
			1840	1194	293	348	2	3			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	cloning artifact	UNP Q59045
A	2	SER	-	cloning artifact	UNP Q59045
A	3	LEU	-	cloning artifact	UNP Q59045
A	7	MSE	MET	modified residue	UNP Q59045
A	31	MSE	MET	modified residue	UNP Q59045
A	165	MSE	MET	modified residue	UNP Q59045
A	202	MSE	MET	modified residue	UNP Q59045
A	246	MSE	MET	modified residue	UNP Q59045
A	264	GLU	-	cloning artifact	UNP Q59045
A	265	GLY	-	cloning artifact	UNP Q59045
A	266	GLY	-	cloning artifact	UNP Q59045
A	267	SER	-	cloning artifact	UNP Q59045
A	268	HIS	-	expression tag	UNP Q59045
A	269	HIS	-	expression tag	UNP Q59045
A	270	HIS	-	expression tag	UNP Q59045
A	271	HIS	-	expression tag	UNP Q59045
A	272	HIS	-	expression tag	UNP Q59045
A	273	HIS	-	expression tag	UNP Q59045
B	1	MSE	-	cloning artifact	UNP Q59045
B	2	SER	-	cloning artifact	UNP Q59045
B	3	LEU	-	cloning artifact	UNP Q59045
B	7	MSE	MET	modified residue	UNP Q59045
B	31	MSE	MET	modified residue	UNP Q59045

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Chain	Residue	Modelled	Actual	Comment	Reference
B	165	MSE	MET	modified residue	UNP Q59045
B	202	MSE	MET	modified residue	UNP Q59045
B	246	MSE	MET	modified residue	UNP Q59045
B	264	GLU	-	cloning artifact	UNP Q59045
B	265	GLY	-	cloning artifact	UNP Q59045
B	266	GLY	-	cloning artifact	UNP Q59045
B	267	SER	-	cloning artifact	UNP Q59045
B	268	HIS	-	expression tag	UNP Q59045
B	269	HIS	-	expression tag	UNP Q59045
B	270	HIS	-	expression tag	UNP Q59045
B	271	HIS	-	expression tag	UNP Q59045
B	272	HIS	-	expression tag	UNP Q59045
B	273	HIS	-	expression tag	UNP Q59045
C	1	MSE	-	cloning artifact	UNP Q59045
C	2	SER	-	cloning artifact	UNP Q59045
C	3	LEU	-	cloning artifact	UNP Q59045
C	7	MSE	MET	modified residue	UNP Q59045
C	31	MSE	MET	modified residue	UNP Q59045
C	165	MSE	MET	modified residue	UNP Q59045
C	202	MSE	MET	modified residue	UNP Q59045
C	246	MSE	MET	modified residue	UNP Q59045
C	264	GLU	-	cloning artifact	UNP Q59045
C	265	GLY	-	cloning artifact	UNP Q59045
C	266	GLY	-	cloning artifact	UNP Q59045
C	267	SER	-	cloning artifact	UNP Q59045
C	268	HIS	-	expression tag	UNP Q59045
C	269	HIS	-	expression tag	UNP Q59045
C	270	HIS	-	expression tag	UNP Q59045
C	271	HIS	-	expression tag	UNP Q59045
C	272	HIS	-	expression tag	UNP Q59045
C	273	HIS	-	expression tag	UNP Q59045

- Molecule 2 is water.

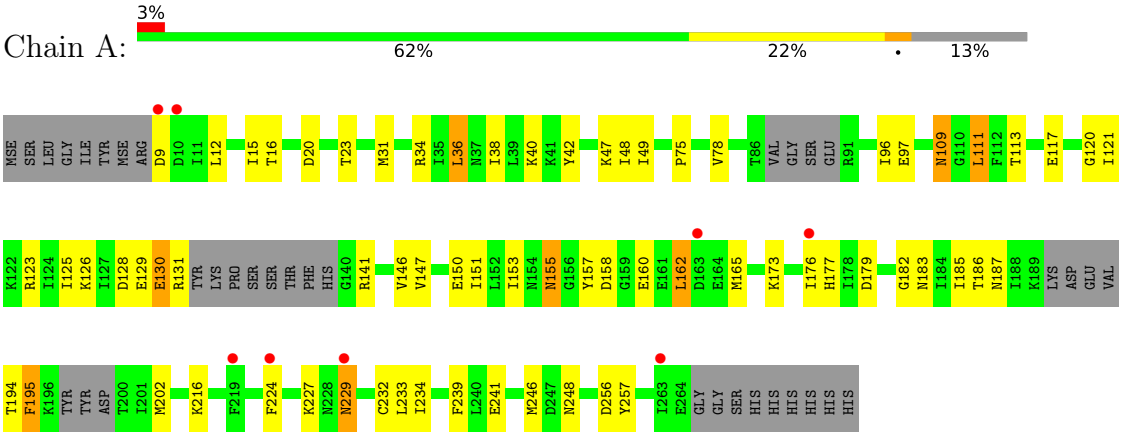
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	12	Total O 12 12	0	0
2	B	7	Total O 7 7	0	0
2	C	12	Total O 12 12	0	0

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.

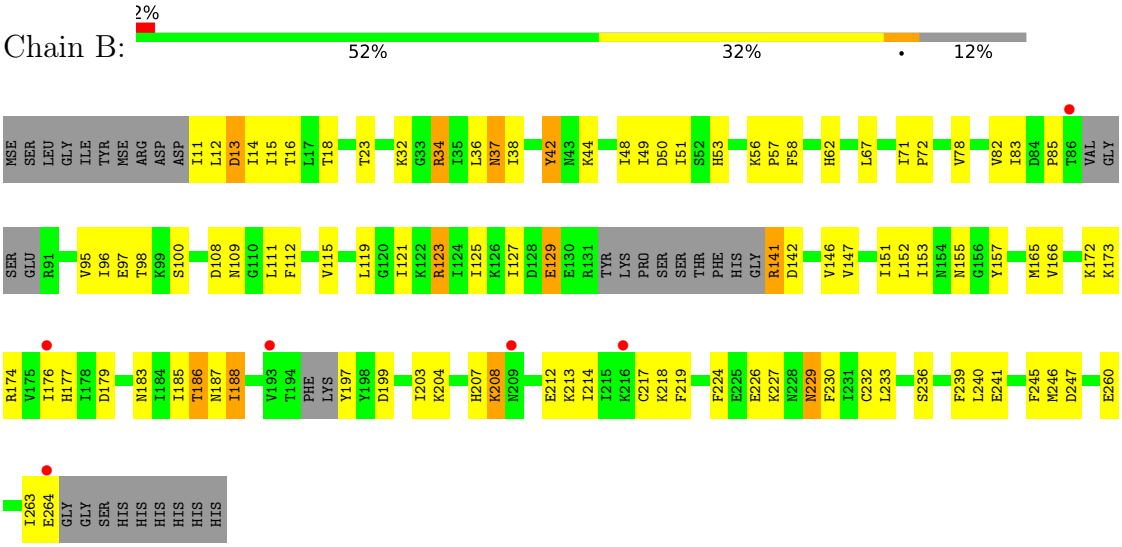
• Molecule 1: Hypothetical protein MJ1651

Chain A:



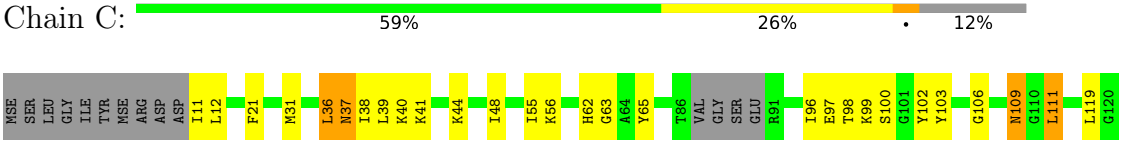
• Molecule 1: Hypothetical protein MJ1651

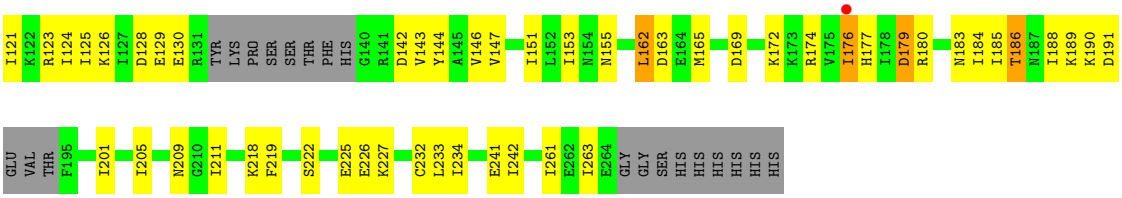
Chain B:



• Molecule 1: Hypothetical protein MJ1651

Chain C:




I121
K122
R123
I124
I125
K126
I127
D128
E129
E130
R131
TYR
LYS
PRO
SER
SER
THR
PHE
HIS
G140
R141
D142
V143
Y144
A145
V146
V147
I151
L152
I153
N154
N155
L162
D163
E164
M165
D169
K172
K173
R174
V175
I176
H177
I178
D179
R180
N183
I184
I185
T186
N187
I188
K189
K190
D191

GLU
VAL
THR
F196
I201
I205
N209
G210
I211
K218
F219
S222
E225
E226
K227
C232
L233
I234
E241
I242
I261
E262
I263
E264
GLY
GLY
SER
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	126.84Å 110.08Å 75.82Å 90.00° 115.39° 90.00°	Depositor
Resolution (Å)	39.86 – 2.50 39.86 – 2.36	Depositor EDS
% Data completeness (in resolution range)	95.4 (39.86-2.50) 95.4 (39.86-2.36)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.37Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.265 0.241 , 0.268	Depositor DCC
R_{free} test set	1800 reflections (2.47%)	wwPDB-VP
Wilson B-factor (Å^2)	40.8	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 65.3	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	0.93	EDS
Total number of atoms	5570	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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	0.39	0/1859	0.63	0/2510
1	B	0.38	0/1890	0.63	0/2547
1	C	0.40	0/1866	0.67	1/2522 (0.0%)
All	All	0.39	0/5615	0.64	1/7579 (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	176	ILE	CB-CA-C	-6.19	99.22	111.60

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	1835	0	1797	61	0
1	B	1864	0	1864	94	0
1	C	1840	0	1793	72	0
2	A	12	0	0	0	0
2	B	7	0	0	1	0
2	C	12	0	0	1	0
All	All	5570	0	5454	224	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 20.

All (224) 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:B:141:ARG:HG3	1:B:142:ASP:H	1.22	1.02
1:A:229:ASN:N	1:A:229:ASN:HD22	1.56	1.01
1:B:11:ILE:HA	1:B:155:ASN:HD21	1.26	1.01
1:A:229:ASN:H	1:A:229:ASN:HD22	1.03	0.94
1:C:12:LEU:H	1:C:155:ASN:HD21	0.99	0.91
1:C:12:LEU:H	1:C:155:ASN:ND2	1.70	0.89
1:B:229:ASN:ND2	1:B:230:PHE:H	1.74	0.86
1:A:176:ILE:HG22	1:A:185:ILE:O	1.76	0.85
1:B:34:ARG:HA	1:B:34:ARG:CZ	2.07	0.84
1:C:12:LEU:N	1:C:155:ASN:HD21	1.76	0.84
1:A:202:MSE:HE2	1:A:216:LYS:HE2	1.60	0.83
1:A:194:THR:HG22	1:A:195:PHE:H	1.44	0.82
1:B:141:ARG:HG3	1:B:142:ASP:N	1.94	0.82
1:A:229:ASN:H	1:A:229:ASN:ND2	1.79	0.79
1:C:109:ASN:HD21	1:C:111:LEU:HB2	1.49	0.77
1:B:229:ASN:HD22	1:B:230:PHE:H	1.32	0.76
1:A:229:ASN:N	1:A:229:ASN:ND2	2.30	0.76
1:B:204:LYS:HG3	1:B:214:ILE:HG12	1.71	0.73
1:C:186:THR:HG23	1:C:188:ILE:H	1.51	0.73
1:B:98:THR:HG21	1:B:119:LEU:HB3	1.71	0.73
1:B:208:LYS:H	1:B:208:LYS:HD3	1.52	0.72
1:B:172:LYS:HE2	1:B:260:GLU:HG2	1.72	0.71
1:B:11:ILE:HA	1:B:155:ASN:ND2	2.04	0.71
1:C:56:LYS:HG3	1:C:62:HIS:ND1	2.06	0.70
1:C:11:ILE:HD11	1:C:44:LYS:NZ	2.06	0.70
1:B:204:LYS:HE2	1:B:212:GLU:CD	2.10	0.70
1:B:125:ILE:HD12	1:B:125:ILE:N	2.07	0.69
1:B:13:ASP:HB3	1:B:14:ILE:HD12	1.73	0.69
1:B:176:ILE:HG22	1:B:185:ILE:O	1.91	0.69
1:B:121:ILE:HD13	1:B:165:MSE:HE3	1.75	0.69
1:C:162:LEU:HD23	1:C:163:ASP:H	1.60	0.67
1:A:109:ASN:C	1:A:109:ASN:HD22	1.97	0.67
1:B:218:LYS:HD2	1:B:226:GLU:OE1	1.96	0.65
1:C:11:ILE:HD11	1:C:44:LYS:HZ3	1.62	0.65
1:C:11:ILE:HG13	1:C:155:ASN:ND2	2.12	0.65
1:B:204:LYS:HE2	1:B:212:GLU:OE2	1.98	0.63
1:B:229:ASN:HD22	1:B:230:PHE:N	1.95	0.63
1:B:176:ILE:CG2	1:B:177:HIS:N	2.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:CYS:HA	1:C:241:GLU:O	1.99	0.63
1:B:176:ILE:HG21	1:B:185:ILE:HG22	1.81	0.63
1:A:176:ILE:HG21	1:A:185:ILE:HG22	1.80	0.62
1:A:121:ILE:HD13	1:A:165:MSE:HE3	1.81	0.62
1:C:97:GLU:HG3	1:C:103:TYR:CZ	2.34	0.62
1:A:96:ILE:HD13	1:A:165:MSE:HE1	1.82	0.62
1:A:109:ASN:HD21	1:A:111:LEU:HB2	1.65	0.62
1:C:123:ARG:HG3	1:C:125:ILE:HD11	1.82	0.62
1:A:177:HIS:HA	1:A:257:TYR:CE2	2.35	0.61
1:C:176:ILE:HG22	1:C:177:HIS:HB2	1.83	0.61
1:B:32:LYS:O	1:B:36:LEU:HB2	1.99	0.61
1:A:129:GLU:O	1:A:131:ARG:N	2.33	0.61
1:B:38:ILE:HD11	1:B:146:VAL:HG22	1.83	0.60
1:B:98:THR:HG23	1:B:119:LEU:O	2.01	0.60
1:C:233:LEU:HD23	1:C:233:LEU:N	2.17	0.60
1:C:125:ILE:HD12	1:C:125:ILE:N	2.16	0.60
1:B:179:ASP:OD2	1:B:183:ASN:HB2	2.01	0.59
1:A:128:ASP:OD1	1:A:129:GLU:N	2.30	0.59
1:C:65:TYR:CD2	1:C:176:ILE:HG21	2.38	0.59
1:C:179:ASP:HB2	1:C:183:ASN:HB2	1.85	0.58
1:C:98:THR:HB	1:C:102:TYR:H	1.69	0.58
1:C:21:PHE:HE2	1:C:31:MSE:HE1	1.68	0.58
1:B:174:ARG:H	1:B:187:ASN:HD22	1.51	0.58
1:B:82:VAL:O	1:B:83:ILE:HG13	2.04	0.58
1:C:98:THR:CG2	1:C:119:LEU:HB3	2.34	0.58
1:A:232:CYS:HA	1:A:241:GLU:O	2.04	0.57
1:B:186:THR:HG22	1:B:240:LEU:O	2.03	0.57
1:A:113:THR:O	1:A:117:GLU:HG3	2.03	0.57
1:B:174:ARG:HG2	1:B:187:ASN:HD21	1.68	0.57
1:A:131:ARG:NH2	1:A:150:GLU:OE1	2.37	0.57
1:B:173:LYS:HA	1:B:187:ASN:HD22	1.70	0.57
1:C:36:LEU:HD13	1:C:48:ILE:HD11	1.84	0.57
1:C:109:ASN:HD22	1:C:109:ASN:C	2.06	0.57
1:C:176:ILE:HG22	1:C:177:HIS:CB	2.35	0.57
1:B:233:LEU:HD23	1:B:233:LEU:H	1.70	0.57
1:B:96:ILE:HD13	1:B:165:MSE:HE1	1.86	0.56
1:B:34:ARG:NE	1:B:34:ARG:HA	2.20	0.56
1:B:174:ARG:HG2	1:B:187:ASN:ND2	2.20	0.56
1:C:38:ILE:HG22	1:C:153:ILE:HD11	1.86	0.56
1:C:218:LYS:HD3	1:C:226:GLU:CB	2.36	0.56
1:B:188:ILE:HD13	1:B:263:ILE:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:THR:HG21	1:C:119:LEU:HB3	1.86	0.56
1:A:75:PRO:HB3	1:B:37:ASN:ND2	2.21	0.55
1:B:50:ASP:OD1	1:B:53:HIS:NE2	2.36	0.55
1:C:142:ASP:O	1:C:146:VAL:HG23	2.06	0.55
1:C:147:VAL:O	1:C:151:ILE:HG13	2.07	0.55
1:B:12:LEU:H	1:B:155:ASN:ND2	2.05	0.55
1:C:176:ILE:HG23	2:C:276:HOH:O	2.07	0.55
1:C:189:LYS:C	1:C:191:ASP:H	2.10	0.55
1:A:176:ILE:HD12	1:A:187:ASN:HA	1.87	0.55
1:C:201:ILE:HD13	1:C:219:PHE:HB2	1.89	0.55
1:C:205:ILE:HG12	1:C:261:ILE:CD1	2.37	0.55
1:A:126:LYS:HB2	1:A:162:LEU:HD23	1.90	0.54
1:B:233:LEU:HD23	1:B:233:LEU:N	2.22	0.54
1:A:125:ILE:N	1:A:125:ILE:HD12	2.22	0.54
1:B:174:ARG:H	1:B:187:ASN:ND2	2.05	0.54
1:C:186:THR:HG23	1:C:188:ILE:N	2.22	0.54
1:C:172:LYS:O	1:C:174:ARG:HG2	2.08	0.54
1:C:185:ILE:N	1:C:185:ILE:HD12	2.24	0.53
1:A:177:HIS:HD2	1:A:185:ILE:HD12	1.74	0.53
1:B:176:ILE:HG23	1:B:177:HIS:N	2.23	0.53
1:C:222:SER:OG	1:C:225:GLU:HG3	2.09	0.52
1:B:207:HIS:HE1	1:B:213:LYS:HG3	1.74	0.52
1:C:109:ASN:ND2	1:C:111:LEU:H	2.07	0.52
1:A:246:MSE:HE2	1:A:246:MSE:HA	1.91	0.52
1:C:37:ASN:C	1:C:37:ASN:HD22	2.13	0.52
1:A:176:ILE:CG2	1:A:185:ILE:HG22	2.40	0.51
1:C:234:ILE:N	1:C:234:ILE:HD12	2.25	0.51
1:B:172:LYS:HE2	1:B:260:GLU:CG	2.39	0.51
1:B:174:ARG:N	1:B:187:ASN:HD22	2.08	0.51
1:B:232:CYS:HA	1:B:241:GLU:O	2.09	0.51
1:A:194:THR:HG22	1:A:195:PHE:N	2.20	0.51
1:C:36:LEU:HD13	1:C:48:ILE:CD1	2.41	0.50
1:B:263:ILE:HG22	1:B:264:GLU:N	2.25	0.50
1:C:41:LYS:HG2	1:C:41:LYS:O	2.11	0.50
1:A:176:ILE:HG22	1:A:185:ILE:C	2.32	0.50
1:B:82:VAL:C	1:B:83:ILE:HG13	2.32	0.50
1:C:128:ASP:O	1:C:130:GLU:N	2.44	0.49
1:C:96:ILE:CD1	1:C:165:MSE:HE1	2.42	0.49
1:C:169:ASP:OD2	1:C:172:LYS:HB2	2.12	0.49
1:B:56:LYS:HG3	1:B:62:HIS:ND1	2.28	0.49
1:C:109:ASN:HD22	1:C:111:LEU:H	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:PHE:HE2	1:C:31:MSE:CE	2.26	0.49
1:B:147:VAL:O	1:B:151:ILE:HG13	2.13	0.49
1:C:96:ILE:HD13	1:C:165:MSE:HE1	1.95	0.49
1:A:97:GLU:OE1	1:A:123:ARG:HD3	2.13	0.49
1:B:176:ILE:HG22	1:B:185:ILE:C	2.33	0.49
1:B:97:GLU:CB	1:B:123:ARG:HG3	2.43	0.48
1:C:162:LEU:HD23	1:C:163:ASP:N	2.25	0.48
1:B:218:LYS:HD2	1:B:226:GLU:CD	2.34	0.48
1:C:12:LEU:HD12	1:C:155:ASN:HA	1.96	0.48
1:A:109:ASN:HD22	1:A:111:LEU:H	1.60	0.48
1:B:58:PHE:HB3	1:B:85:PRO:HB3	1.96	0.48
1:B:98:THR:CG2	1:B:119:LEU:HB3	2.41	0.48
1:A:129:GLU:O	1:A:130:GLU:C	2.52	0.48
1:B:203:ILE:HD12	1:B:217:CYS:SG	2.54	0.48
1:B:38:ILE:HG22	1:B:153:ILE:HD11	1.96	0.48
1:C:124:ILE:C	1:C:125:ILE:HD12	2.35	0.48
1:B:112:PHE:HD1	1:B:115:VAL:HG11	1.80	0.47
1:B:13:ASP:HB2	1:C:40:LYS:NZ	2.29	0.47
1:A:36:LEU:HD13	1:A:48:ILE:HD11	1.97	0.47
1:B:11:ILE:CA	1:B:155:ASN:HD21	2.13	0.47
1:A:194:THR:O	1:A:195:PHE:HB3	2.14	0.47
1:B:18:THR:OG1	1:B:51:ILE:HB	2.14	0.47
1:B:246:MSE:HA	1:B:246:MSE:HE2	1.95	0.47
1:C:121:ILE:HD13	1:C:165:MSE:HE3	1.97	0.47
1:C:143:VAL:O	1:C:147:VAL:HG23	2.14	0.47
1:A:179:ASP:CB	1:A:183:ASN:HB2	2.44	0.46
1:B:179:ASP:HB2	1:B:183:ASN:H	1.80	0.46
1:B:224:PHE:O	1:B:227:LYS:HE3	2.15	0.46
1:A:147:VAL:O	1:A:151:ILE:HG13	2.16	0.46
1:A:195:PHE:O	1:A:195:PHE:CD1	2.69	0.46
1:A:234:ILE:HD12	1:A:234:ILE:N	2.30	0.46
1:C:55:ILE:HD12	1:C:63:GLY:HA2	1.96	0.46
1:A:224:PHE:O	1:A:227:LYS:HG3	2.15	0.46
1:C:186:THR:HG21	1:C:188:ILE:HD12	1.97	0.46
1:B:204:LYS:HE3	1:B:214:ILE:HD11	1.98	0.46
1:B:151:ILE:HG12	1:B:157:TYR:HB2	1.97	0.45
1:B:173:LYS:HD2	1:B:188:ILE:HG13	1.97	0.45
1:A:173:LYS:HD3	1:A:173:LYS:HA	1.74	0.45
1:B:219:PHE:HA	1:B:232:CYS:O	2.17	0.45
1:A:126:LYS:HD3	1:A:160:GLU:CD	2.37	0.45
1:B:177:HIS:HD2	1:B:185:ILE:HD12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:THR:HG22	1:C:99:LYS:N	2.30	0.45
1:A:20:ASP:O	1:C:180:ARG:NH1	2.50	0.45
1:B:42:TYR:CD1	1:B:42:TYR:N	2.85	0.45
1:A:36:LEU:HD13	1:A:48:ILE:CD1	2.47	0.45
1:C:21:PHE:CE2	1:C:31:MSE:HE1	2.51	0.45
1:C:98:THR:HG22	1:C:100:SER:H	1.82	0.45
1:A:109:ASN:ND2	1:A:111:LEU:H	2.15	0.44
1:A:109:ASN:ND2	1:A:109:ASN:C	2.66	0.44
1:B:71:ILE:HD12	1:B:115:VAL:HG21	2.00	0.44
1:C:205:ILE:HG12	1:C:261:ILE:HD13	1.99	0.44
1:A:40:LYS:C	1:A:42:TYR:H	2.20	0.44
1:B:44:LYS:HE2	1:B:152:LEU:O	2.18	0.44
1:C:109:ASN:ND2	1:C:109:ASN:C	2.71	0.44
1:A:15:ILE:HA	1:A:78:VAL:O	2.16	0.44
1:C:162:LEU:CD2	1:C:163:ASP:N	2.81	0.44
1:B:263:ILE:CG2	1:B:264:GLU:N	2.80	0.44
1:A:176:ILE:HG23	1:A:177:HIS:HB3	1.99	0.44
1:B:129:GLU:CD	1:B:129:GLU:O	2.56	0.44
1:B:176:ILE:CG2	1:B:185:ILE:HG22	2.46	0.43
1:A:182:GLY:HA3	1:A:248:ASN:OD1	2.19	0.43
1:B:187:ASN:O	1:B:239:PHE:HD2	2.02	0.43
1:B:245:PHE:CE2	1:B:246:MSE:HG2	2.53	0.43
1:A:47:LYS:HE3	2:B:279:HOH:O	2.18	0.43
1:C:125:ILE:HG22	1:C:126:LYS:O	2.19	0.43
1:A:150:GLU:OE1	1:A:157:TYR:HE1	2.01	0.43
1:B:36:LEU:HD13	1:B:48:ILE:CD1	2.49	0.43
1:A:38:ILE:HG22	1:A:153:ILE:HD11	2.01	0.43
1:B:229:ASN:ND2	1:B:230:PHE:N	2.51	0.43
1:A:31:MSE:HE2	1:A:141:ARG:O	2.19	0.42
1:C:109:ASN:ND2	1:C:111:LEU:HB2	2.25	0.42
1:C:201:ILE:HG23	1:C:263:ILE:HG23	2.01	0.42
1:A:16:THR:HG22	1:A:49:ILE:HB	2.00	0.42
1:C:189:LYS:O	1:C:191:ASP:N	2.50	0.42
1:A:176:ILE:CG2	1:A:177:HIS:N	2.82	0.42
1:B:125:ILE:CD1	1:B:125:ILE:N	2.77	0.42
1:B:186:THR:HG23	1:B:188:ILE:N	2.35	0.42
1:B:95:VAL:HG23	1:B:127:ILE:CG1	2.49	0.42
1:B:15:ILE:HA	1:B:78:VAL:O	2.20	0.42
1:A:186:THR:O	1:A:239:PHE:HB3	2.20	0.42
1:A:34:ARG:HD3	1:A:146:VAL:HG22	2.02	0.42
1:B:176:ILE:HG22	1:B:177:HIS:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:THR:HG22	1:B:100:SER:H	1.84	0.42
1:C:209:ASN:OD1	1:C:211:ILE:N	2.41	0.42
1:A:179:ASP:HB3	1:A:183:ASN:H	1.85	0.41
1:C:184:ILE:HB	1:C:242:ILE:HB	2.00	0.41
1:B:34:ARG:HH21	1:B:37:ASN:CB	2.33	0.41
1:B:186:THR:HG21	1:B:240:LEU:HB3	2.03	0.41
1:C:106:GLY:HA2	1:C:144:TYR:CE1	2.55	0.41
1:B:173:LYS:HA	1:B:173:LYS:HD3	1.80	0.41
1:A:131:ARG:N	1:A:131:ARG:HD2	2.36	0.41
1:B:240:LEU:CD2	1:B:263:ILE:HD11	2.51	0.41
1:B:67:LEU:HD22	1:B:71:ILE:HD11	2.02	0.41
1:C:176:ILE:HG22	1:C:177:HIS:N	2.34	0.41
1:A:12:LEU:HG	1:A:155:ASN:ND2	2.35	0.41
1:A:182:GLY:HA3	1:A:248:ASN:CG	2.42	0.41
1:B:16:THR:HA	1:B:49:ILE:O	2.21	0.41
1:C:125:ILE:CD1	1:C:125:ILE:N	2.83	0.41
1:A:129:GLU:C	1:A:131:ARG:N	2.74	0.40
1:A:256:ASP:CG	1:A:257:TYR:H	2.24	0.40
1:B:108:ASP:OD2	1:B:166:VAL:HG23	2.21	0.40
1:B:58:PHE:CD1	1:B:85:PRO:HA	2.57	0.40
1:B:71:ILE:HB	1:B:72:PRO:HD3	2.03	0.40
1:B:42:TYR:HD1	1:B:42:TYR:N	2.20	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	227/273 (83%)	208 (92%)	16 (7%)	3 (1%)	12	21
1	B	231/273 (85%)	209 (90%)	19 (8%)	3 (1%)	12	21
1	C	231/273 (85%)	214 (93%)	14 (6%)	3 (1%)	12	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	689/819 (84%)	631 (92%)	49 (7%)	9 (1%)	12 21

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	GLU
1	C	129	GLU
1	C	190	LYS
1	A	195	PHE
1	C	227	LYS
1	A	120	GLY
1	B	236	SER
1	B	188	ILE
1	B	57	PRO

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	194/238 (82%)	184 (95%)	10 (5%)	23 44
1	B	197/238 (83%)	181 (92%)	16 (8%)	11 23
1	C	192/238 (81%)	184 (96%)	8 (4%)	30 54
All	All	583/714 (82%)	549 (94%)	34 (6%)	20 38

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	23	THR
1	A	36	LEU
1	A	109	ASN
1	A	111	LEU
1	A	155	ASN
1	A	158	ASP

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Mol	Chain	Res	Type
1	A	162	LEU
1	A	229	ASN
1	A	233	LEU
1	B	13	ASP
1	B	23	THR
1	B	34	ARG
1	B	37	ASN
1	B	42	TYR
1	B	109	ASN
1	B	111	LEU
1	B	123	ARG
1	B	129	GLU
1	B	141	ARG
1	B	186	THR
1	B	197	TYR
1	B	199	ASP
1	B	208	LYS
1	B	229	ASN
1	B	247	ASP
1	C	36	LEU
1	C	37	ASN
1	C	39	LEU
1	C	109	ASN
1	C	111	LEU
1	C	162	LEU
1	C	179	ASP
1	C	186	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	37	ASN
1	A	109	ASN
1	A	154	ASN
1	A	155	ASN
1	A	229	ASN
1	B	43	ASN
1	B	109	ASN
1	B	154	ASN
1	B	155	ASN
1	B	187	ASN

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Mol	Chain	Res	Type
1	B	229	ASN
1	B	254	ASN
1	C	37	ASN
1	C	109	ASN
1	C	154	ASN
1	C	155	ASN
1	C	254	ASN

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, 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	233/273 (85%)	0.19	8 (3%) 45 48	27, 49, 70, 80	0
1	B	235/273 (86%)	0.10	6 (2%) 56 59	29, 52, 69, 82	0
1	C	235/273 (86%)	-0.07	1 (0%) 92 93	19, 45, 64, 76	0
All	All	703/819 (85%)	0.07	15 (2%) 63 66	19, 49, 68, 82	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	ASP	5.9
1	A	224	PHE	3.8
1	B	193	VAL	3.7
1	A	176	ILE	2.9
1	A	219	PHE	2.7
1	B	264	GLU	2.6
1	A	229	ASN	2.6
1	B	176	ILE	2.4
1	A	163	ASP	2.4
1	B	86	THR	2.4
1	A	10	ASP	2.3
1	B	209	ASN	2.3
1	A	263	ILE	2.0
1	B	216	LYS	2.0
1	C	176	ILE	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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.