Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 03:12 PM EDT

PDB ID	:	1T98
Title	:	Crystal Structure of MukF(1-287)
Authors	:	Fennell-Fezzie, R.; Berger, J.M.
Deposited on	:	2004-05-14
Resolution	:	2.90 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

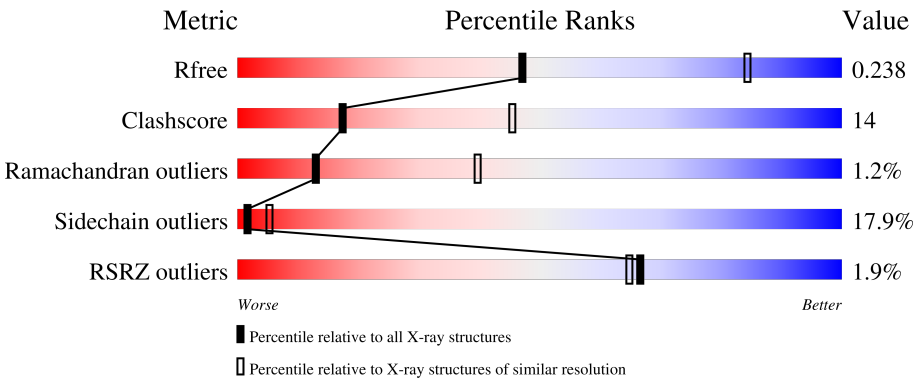
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	287	% 57% 30% 5% • 7%
1	B	287	3% 51% 35% 5% 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4228 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 Chromosome partition protein mukF.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	266	2140	1342	378	414	1	5	0	0	0
1	B	260	2088	1308	368	407	1	4	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

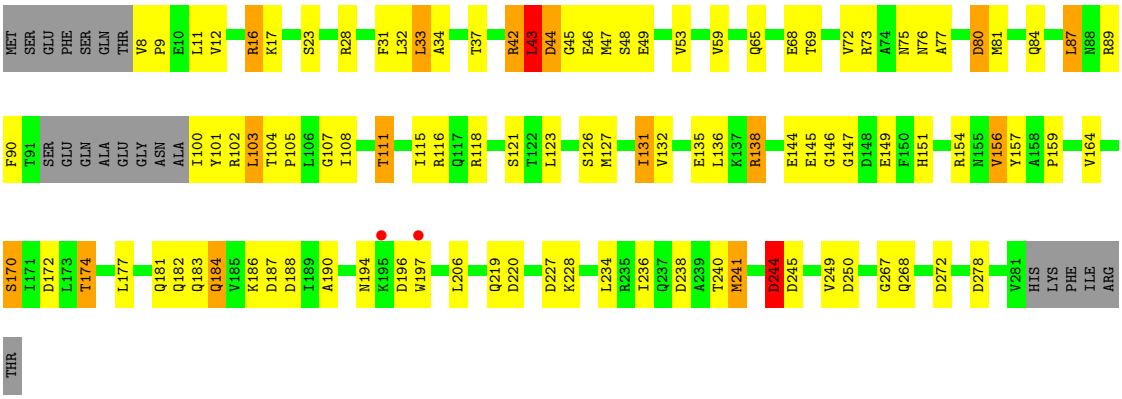
Chain	Residue	Modelled	Actual	Comment	Reference
A	47	MSE	MET	MODIFIED RESIDUE	UNP P60293
A	81	MSE	MET	MODIFIED RESIDUE	UNP P60293
A	127	MSE	MET	MODIFIED RESIDUE	UNP P60293
A	178	MSE	MET	MODIFIED RESIDUE	UNP P60293
A	241	MSE	MET	MODIFIED RESIDUE	UNP P60293
B	47	MSE	MET	MODIFIED RESIDUE	UNP P60293
B	81	MSE	MET	MODIFIED RESIDUE	UNP P60293
B	127	MSE	MET	MODIFIED RESIDUE	UNP P60293
B	178	MSE	MET	MODIFIED RESIDUE	UNP P60293
B	241	MSE	MET	MODIFIED RESIDUE	UNP P60293

3 Residue-property plots (i)

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.

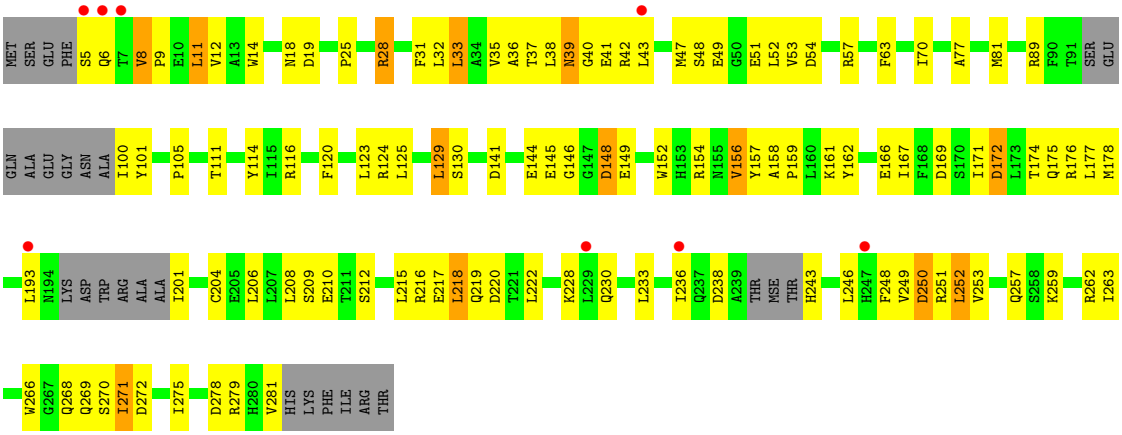
• Molecule 1: Chromosome partition protein mukF

Chain A:



• Molecule 1: Chromosome partition protein mukF

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	58.70Å 58.70Å 307.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90 51.24 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.5 (20.00-2.90) 95.5 (51.24-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.35 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.233 , 0.273 0.202 , 0.238	Depositor DCC
R_{free} test set	625 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	67.4	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 57.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.118 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4228	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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 (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	0.45	0/2169	0.80	11/2926 (0.4%)
1	B	0.44	0/2114	0.79	11/2850 (0.4%)
All	All	0.44	0/4283	0.80	22/5776 (0.4%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	227	ASP	CB-CG-OD2	6.72	124.35	118.30
1	A	172	ASP	CB-CG-OD2	6.15	123.83	118.30
1	B	172	ASP	CB-CG-OD2	6.08	123.78	118.30
1	A	245	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	19	ASP	CB-CG-OD2	5.77	123.50	118.30
1	A	278	ASP	CB-CG-OD2	5.72	123.45	118.30
1	B	250	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	54	ASP	CB-CG-OD2	5.55	123.29	118.30
1	A	80	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	148	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	272	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	220	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	238	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	187	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	272	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	141	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	220	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	278	ASP	CB-CG-OD2	5.12	122.90	118.30
1	A	244	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	169	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	188	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	196	ASP	CB-CG-OD2	5.04	122.83	118.30

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	2140	0	2103	54	0
1	B	2088	0	2048	69	0
All	All	4228	0	4151	116	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 14.

All (116) 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:120:PHE:HZ	1:B:218:LEU:HD21	1.17	1.09
1:A:138:ARG:HH11	1:A:138:ARG:HG3	1.13	1.08
1:A:90:PHE:O	1:A:100:ILE:HG13	1.68	0.92
1:B:124:ARG:HD2	1:B:174:THR:HG23	1.51	0.91
1:A:37:THR:HG21	1:B:11:LEU:HD11	1.54	0.89
1:B:120:PHE:CZ	1:B:218:LEU:HD21	2.06	0.89
1:A:48:SER:HA	1:A:100:ILE:HG22	1.54	0.87
1:A:138:ARG:HG3	1:A:138:ARG:NH1	1.86	0.87
1:B:268:GLN:O	1:B:271:ILE:HG22	1.76	0.85
1:A:127:MSE:O	1:A:131:ILE:HG23	1.81	0.80
1:B:201:ILE:N	1:B:204:CYS:HG	1.79	0.80
1:A:23:SER:H	1:A:84:GLN:NE2	1.82	0.77
1:B:28:ARG:HG3	1:B:28:ARG:HH11	1.51	0.75
1:B:31:PHE:CD2	1:B:81:MSE:HE2	2.22	0.74
1:B:216:ARG:HH21	1:B:219:GLN:HG3	1.54	0.71
1:B:125:LEU:HD22	1:B:218:LEU:HD22	1.72	0.71
1:B:32:LEU:HB2	1:B:81:MSE:HE1	1.74	0.69
1:A:104:THR:HB	1:A:105:PRO:HD2	1.74	0.68
1:B:162:TYR:O	1:B:166:GLU:HG3	1.92	0.68
1:A:8:VAL:N	1:A:9:PRO:HD3	2.09	0.67
1:A:184:GLN:HE21	1:A:184:GLN:HA	1.59	0.67
1:B:77:ALA:O	1:B:81:MSE:HG2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:O	1:A:37:THR:HG23	1.96	0.66
1:B:219:GLN:HE22	1:B:271:ILE:HB	1.61	0.66
1:A:8:VAL:N	1:A:9:PRO:CD	2.60	0.65
1:B:233:LEU:O	1:B:236:ILE:HG22	1.98	0.64
1:B:219:GLN:HE22	1:B:271:ILE:CB	2.11	0.63
1:A:219:GLN:NE2	1:A:267:GLY:HA3	2.15	0.62
1:A:23:SER:H	1:A:84:GLN:HE22	1.45	0.61
1:B:204:CYS:O	1:B:208:LEU:HG	2.00	0.61
1:B:39:ASN:HB2	1:B:47:MSE:SE	2.51	0.60
1:A:132:VAL:HG23	1:A:164:VAL:HG22	1.83	0.60
1:B:124:ARG:CD	1:B:174:THR:HG23	2.27	0.60
1:A:48:SER:HA	1:A:100:ILE:CG2	2.30	0.59
1:A:49:GLU:O	1:A:53:VAL:HG23	2.03	0.59
1:B:158:ALA:HB3	1:B:159:PRO:HD3	1.86	0.58
1:A:37:THR:HG21	1:B:11:LEU:CD1	2.32	0.58
1:B:38:LEU:O	1:B:42:ARG:HB2	2.04	0.57
1:B:37:THR:O	1:B:41:GLU:HB3	2.04	0.57
1:A:42:ARG:HD3	1:A:45:GLY:O	2.05	0.57
1:B:124:ARG:HD2	1:B:174:THR:CG2	2.32	0.57
1:A:123:LEU:O	1:A:127:MSE:HG3	2.05	0.56
1:B:14:TRP:O	1:B:18:ASN:ND2	2.29	0.56
1:B:120:PHE:HZ	1:B:218:LEU:CD2	2.04	0.56
1:B:249:VAL:O	1:B:253:VAL:HG23	2.05	0.55
1:B:8:VAL:N	1:B:9:PRO:CD	2.69	0.55
1:B:31:PHE:HD2	1:B:81:MSE:HE2	1.67	0.55
1:A:104:THR:HB	1:A:105:PRO:CD	2.38	0.54
1:A:236:ILE:O	1:A:240:THR:HG23	2.08	0.53
1:B:57:ARG:HG2	1:B:70:ILE:HD13	1.90	0.53
1:B:125:LEU:CD2	1:B:218:LEU:HD22	2.39	0.53
1:A:102:ARG:HD3	1:B:266:TRP:CZ2	2.43	0.53
1:A:190:ALA:O	1:A:194:ASN:ND2	2.42	0.52
1:B:178:MSE:HE2	1:B:215:LEU:CD1	2.40	0.52
1:A:100:ILE:HG23	1:A:101:TYR:CD2	2.45	0.52
1:B:49:GLU:O	1:B:53:VAL:HG23	2.10	0.52
1:B:6:GLN:C	1:B:9:PRO:HD2	2.30	0.52
1:B:28:ARG:HG3	1:B:28:ARG:NH1	2.23	0.52
1:A:183:GLN:NE2	1:B:89:ARG:O	2.43	0.51
1:B:125:LEU:HG	1:B:129:LEU:HD22	1.93	0.51
1:A:65:GLN:HB3	1:A:73:ARG:HH22	1.76	0.51
1:A:132:VAL:CG2	1:A:164:VAL:HG13	2.41	0.50
1:A:12:VAL:O	1:A:16:ARG:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:GLN:HE21	1:A:184:GLN:CA	2.24	0.48
1:A:87:LEU:HD12	1:A:103:LEU:HA	1.94	0.48
1:B:8:VAL:O	1:B:12:VAL:HG23	2.14	0.48
1:B:175:GLN:NE2	1:B:263:ILE:HG23	2.29	0.48
1:A:177:LEU:HD23	1:B:105:PRO:HG2	1.95	0.47
1:B:230:GLN:HE22	1:B:257:GLN:HG2	1.78	0.47
1:B:39:ASN:O	1:B:39:ASN:ND2	2.41	0.47
1:A:170:SER:O	1:A:174:THR:HG23	2.15	0.47
1:A:107:GLY:O	1:A:111:THR:HB	2.14	0.47
1:A:16:ARG:HG2	1:B:63:PHE:CZ	2.50	0.46
1:B:152:TRP:CE3	1:B:156:VAL:HG11	2.50	0.46
1:B:275:ILE:O	1:B:279:ARG:HG2	2.16	0.46
1:B:48:SER:OG	1:B:51:GLU:HG3	2.16	0.46
1:B:219:GLN:HE22	1:B:271:ILE:CG1	2.28	0.46
1:B:219:GLN:NE2	1:B:271:ILE:HB	2.30	0.44
1:A:157:TYR:HB2	1:A:249:VAL:HG22	1.99	0.44
1:B:251:ARG:CG	1:B:252:LEU:N	2.81	0.44
1:B:36:ALA:HB2	1:B:111:THR:HG21	2.00	0.44
1:A:43:LEU:HB3	1:A:44:ASP:H	1.58	0.44
1:B:49:GLU:HB2	1:B:101:TYR:HE2	1.83	0.44
1:A:241:MSE:HE2	1:A:241:MSE:HB2	1.98	0.43
1:B:25:PRO:HD2	1:B:28:ARG:HB2	2.00	0.43
1:A:9:PRO:HA	1:A:12:VAL:HG23	2.01	0.43
1:B:32:LEU:HD12	1:B:81:MSE:HE3	2.00	0.43
1:A:127:MSE:HE1	1:B:158:ALA:HB1	2.01	0.42
1:A:89:ARG:NH1	1:A:101:TYR:OH	2.45	0.42
1:B:266:TRP:HA	1:B:269:GLN:HB2	2.01	0.42
1:A:132:VAL:HG23	1:A:164:VAL:HG13	2.01	0.42
1:B:172:ASP:O	1:B:176:ARG:HG3	2.19	0.42
1:B:251:ARG:HG3	1:B:252:LEU:N	2.34	0.42
1:A:73:ARG:HA	1:A:76:ASN:HD22	1.85	0.42
1:B:216:ARG:NH2	1:B:219:GLN:HG3	2.28	0.42
1:B:167:ILE:O	1:B:171:ILE:HD12	2.19	0.42
1:B:123:LEU:HD12	1:B:123:LEU:HA	1.85	0.41
1:B:157:TYR:CZ	1:B:161:LYS:HD2	2.55	0.41
1:B:33:LEU:HD11	1:B:114:TYR:HB2	2.03	0.41
1:B:39:ASN:HD22	1:B:39:ASN:C	2.21	0.41
1:A:75:ASN:HD22	1:A:75:ASN:HA	1.67	0.41
1:A:87:LEU:CD1	1:A:103:LEU:HD13	2.51	0.41
1:A:146:GLY:HA2	1:A:151:HIS:CE1	2.56	0.41
1:A:184:GLN:HA	1:A:184:GLN:NE2	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ARG:HD3	1:B:28:ARG:HA	1.83	0.41
1:B:120:PHE:CD2	1:B:120:PHE:C	2.94	0.41
1:A:31:PHE:O	1:A:34:ALA:HB3	2.21	0.41
1:A:238:ASP:O	1:A:241:MSE:HG3	2.21	0.41
1:A:77:ALA:O	1:A:81:MSE:HG2	2.21	0.41
1:A:138:ARG:NH1	1:A:138:ARG:CG	2.67	0.41
1:A:132:VAL:O	1:A:136:LEU:HB2	2.21	0.41
1:A:72:VAL:HG12	1:A:76:ASN:HD21	1.86	0.40
1:A:156:VAL:C	1:A:159:PRO:HD2	2.41	0.40
1:B:35:VAL:HG13	1:B:47:MSE:HE1	2.04	0.40
1:B:47:MSE:HE2	1:B:52:LEU:HD23	2.03	0.40
1:B:167:ILE:O	1:B:167:ILE:HG22	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	262/287 (91%)	245 (94%)	14 (5%)	3 (1%)	14 42
1	B	252/287 (88%)	234 (93%)	15 (6%)	3 (1%)	13 40
All	All	514/574 (90%)	479 (93%)	29 (6%)	6 (1%)	13 40

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	GLY
1	A	244	ASP
1	B	146	GLY
1	B	43	LEU
1	A	43	LEU
1	B	40	GLY

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	231/244 (95%)	185 (80%)	46 (20%)	1 4
1	B	227/244 (93%)	191 (84%)	36 (16%)	2 7
All	All	458/488 (94%)	376 (82%)	82 (18%)	2 5

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	16	ARG
1	A	17	LYS
1	A	28	ARG
1	A	32	LEU
1	A	33	LEU
1	A	42	ARG
1	A	43	LEU
1	A	44	ASP
1	A	46	GLU
1	A	47	MSE
1	A	59	VAL
1	A	68	GLU
1	A	69	THR
1	A	80	ASP
1	A	87	LEU
1	A	103	LEU
1	A	108	ILE
1	A	111	THR
1	A	115	ILE
1	A	116	ARG
1	A	118	ARG
1	A	121	SER
1	A	126	SER
1	A	131	ILE
1	A	135	GLU
1	A	138	ARG

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Mol	Chain	Res	Type
1	A	144	GLU
1	A	145	GLU
1	A	149	GLU
1	A	154	ARG
1	A	156	VAL
1	A	170	SER
1	A	174	THR
1	A	181	GLN
1	A	182	GLN
1	A	184	GLN
1	A	186	LYS
1	A	197	TRP
1	A	206	LEU
1	A	228	LYS
1	A	234	LEU
1	A	241	MSE
1	A	244	ASP
1	A	250	ASP
1	A	268	GLN
1	B	5	SER
1	B	8	VAL
1	B	11	LEU
1	B	28	ARG
1	B	33	LEU
1	B	39	ASN
1	B	100	ILE
1	B	116	ARG
1	B	129	LEU
1	B	130	SER
1	B	144	GLU
1	B	145	GLU
1	B	148	ASP
1	B	149	GLU
1	B	154	ARG
1	B	156	VAL
1	B	177	LEU
1	B	193	LEU
1	B	206	LEU
1	B	209	SER
1	B	210	GLU
1	B	212	SER
1	B	217	GLU

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Mol	Chain	Res	Type
1	B	218	LEU
1	B	222	LEU
1	B	228	LYS
1	B	243	HIS
1	B	246	LEU
1	B	248	PHE
1	B	250	ASP
1	B	252	LEU
1	B	259	LYS
1	B	262	ARG
1	B	270	SER
1	B	271	ILE
1	B	281	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	76	ASN
1	A	84	GLN
1	A	88	ASN
1	A	128	GLN
1	A	151	HIS
1	A	155	ASN
1	A	182	GLN
1	A	184	GLN
1	A	194	ASN
1	A	219	GLN
1	B	39	ASN
1	B	151	HIS
1	B	219	GLN
1	B	230	GLN
1	B	257	GLN
1	B	268	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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	261/287 (90%)	0.06	2 (0%)	86	86	15, 32, 53, 65	0
1	B	256/287 (89%)	0.16	8 (3%)	49	44	13, 32, 54, 65	0
All	All	517/574 (90%)	0.11	10 (1%)	66	65	13, 32, 54, 65	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	GLN	3.7
1	B	5	SER	3.0
1	A	195	LYS	2.7
1	B	236	ILE	2.7
1	B	247	HIS	2.5
1	A	197	TRP	2.3
1	B	193	LEU	2.3
1	B	7	THR	2.2
1	B	43	LEU	2.2
1	B	229	LEU	2.1

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 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.