



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:29 PM UTC

PDB ID : 1KAF / pdb_00001kaf
Title : DNA Binding Domain Of The Phage T4 Transcription Factor MotA (AA105-211)
Authors : Li, N.; Sickmier, E.A.; Zhang, R.; Joachimiak, A.; White, S.W.
Deposited on : 2001-11-01
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

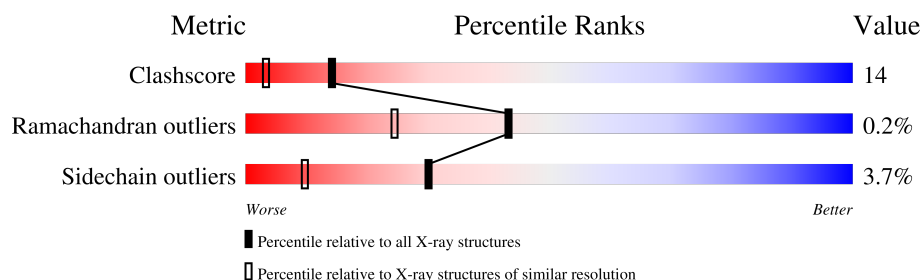
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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))
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	108	83% 13% .
1	B	108	72% 22% 6%
1	C	108	72% 25% .
1	D	108	81% 13% . . .
1	E	108	67% 23% 5% . 5%
1	F	108	62% 29% 6% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5785 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 Transcription regulatory protein MOTA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	S	0	0	0
			874	550	150	166	8			
1	B	108	Total	C	N	O	S	0	0	0
			874	550	150	166	8			
1	C	108	Total	C	N	O	S	0	0	0
			874	550	150	166	8			
1	D	104	Total	C	N	O	S	0	0	0
			842	530	146	159	7			
1	E	103	Total	C	N	O	S	0	0	0
			836	527	145	157	7			
1	F	104	Total	C	N	O	S	0	0	0
			842	530	146	159	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	MET	-	initiating methionine	UNP P22915
B	104	MET	-	initiating methionine	UNP P22915
C	104	MET	-	initiating methionine	UNP P22915
D	104	MET	-	initiating methionine	UNP P22915
E	104	MET	-	initiating methionine	UNP P22915
F	104	MET	-	initiating methionine	UNP P22915

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	100	Total	O	0	0
			100	100		
2	B	119	Total	O	0	0
			119	119		
2	C	142	Total	O	0	0
			142	142		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	105	Total 105	O 105	0	0
2	E	93	Total 93	O 93	0	0
2	F	84	Total 84	O 84	0	0

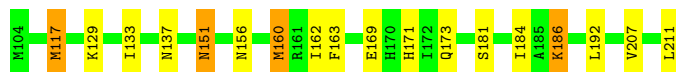
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

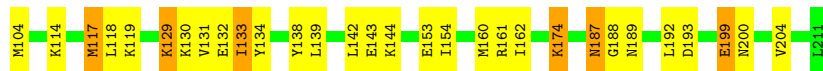
- Molecule 1: Transcription regulatory protein MOTA

Chain A:  83% 13% .



- Molecule 1: Transcription regulatory protein MOTA

Chain B:  72% 22% 6%



- Molecule 1: Transcription regulatory protein MOTA

Chain C:  72% 25% .



- Molecule 1: Transcription regulatory protein MOTA

Chain D:  81% 13% . . .



- Molecule 1: Transcription regulatory protein MOTA

Chain E:  67% 23% 5% 5%



- Molecule 1: Transcription regulatory protein MOTA

Chain F:

62%

29%

6%

MET	GLU	ILE	THR	S108	D109	M110		K114	D115	L116	M117	I118	K119		K129		S136	M137	Y138	L139		E143	K144		M151	F152	E153	I154	I155	M156	M157	G158	M159	M160	R161	I162		M168	E169	H170		Q173	K174		I184	A185	K186	N187	G188	M189		L192		R196		T206		E210	L211
-----	-----	-----	-----	------	------	------	--	------	------	------	------	------	------	--	------	--	------	------	------	------	--	------	------	--	------	------	------	------	------	------	------	------	------	------	------	------	--	------	------	------	--	------	------	--	------	------	------	------	------	------	--	------	--	------	--	------	--	------	------

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	31.28Å 54.73Å 91.44Å 94.77° 91.10° 95.61°	Depositor
Resolution (Å)	30.00 – 1.60	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-1.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5785	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

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	0.44	1/883 (0.1%)	0.88	4/1177 (0.3%)
1	B	0.42	1/883 (0.1%)	0.84	2/1177 (0.2%)
1	C	0.36	0/883	0.88	5/1177 (0.4%)
1	D	0.34	0/851	0.86	3/1134 (0.3%)
1	E	0.34	0/845	0.92	5/1126 (0.4%)
1	F	0.34	0/851	0.86	3/1134 (0.3%)
All	All	0.38	2/5196 (0.0%)	0.87	22/6925 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	MET	SD-CE	-8.28	1.58	1.79
1	B	117	MET	SD-CE	-6.42	1.63	1.79

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	MET	N-CA-C	-7.57	97.40	109.59
1	C	160	MET	N-CA-C	-6.90	98.49	109.59
1	E	129	LYS	N-CA-C	-6.80	103.33	111.69
1	E	160	MET	N-CA-C	-6.73	98.72	109.76
1	F	160	MET	N-CA-C	-6.62	98.93	109.59
1	D	129	LYS	N-CA-C	-6.54	103.64	111.69
1	D	152	PHE	N-CA-C	-6.45	98.38	108.90
1	B	133	ILE	N-CA-C	-6.31	98.65	107.80
1	C	152	PHE	N-CA-C	-6.31	98.61	108.90
1	E	152	PHE	N-CA-C	-6.28	98.66	108.90
1	A	133	ILE	N-CA-C	-6.21	97.42	107.28
1	E	113	ASP	N-CA-C	-6.10	105.10	112.54
1	F	129	LYS	N-CA-C	-6.09	104.72	111.36
1	B	129	LYS	N-CA-C	-5.81	105.03	111.36
1	C	133	ILE	N-CA-C	-5.71	99.52	107.80
1	D	160	MET	N-CA-C	-5.46	100.79	109.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	F	137	ASN	N-CA-C	5.42	116.76	108.52
1	A	129	LYS	N-CA-C	-5.42	105.45	111.36
1	A	181	SER	N-CA-C	-5.24	102.76	110.52
1	E	139	LEU	N-CA-C	5.22	117.02	108.52
1	C	129	LYS	N-CA-C	-5.20	105.29	111.69
1	C	181	SER	N-CA-C	-5.08	102.54	110.42

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	874	0	891	15	0
1	B	874	0	891	27	0
1	C	874	0	891	26	0
1	D	842	0	858	17	0
1	E	836	0	853	31	0
1	F	842	0	858	35	0
2	A	100	0	0	1	0
2	B	119	0	0	2	0
2	C	142	0	0	1	0
2	D	105	0	0	1	0
2	E	93	0	0	2	0
2	F	84	0	0	1	0
All	All	5785	0	5242	147	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 (147) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:LYS:HE3	1:D:186:LYS:H	1.27	0.96
1:E:195:LYS:HD3	1:E:195:LYS:H	1.29	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:LYS:HE3	1:C:186:LYS:H	1.28	0.94
1:C:162:ILE:HD13	1:C:180:MET:HE1	1.48	0.92
1:D:186:LYS:H	1:D:186:LYS:CE	1.85	0.89
1:B:104:MET:HE3	1:B:133:ILE:HG22	1.53	0.88
1:F:210:GLU:O	1:F:211:LEU:HB2	1.75	0.85
1:F:139:LEU:HD23	1:F:153:GLU:HB3	1.59	0.84
1:C:104:MET:HE3	1:C:133:ILE:HG22	1.58	0.84
1:B:117:MET:HE2	1:B:160:MET:HE3	1.57	0.84
1:A:186:LYS:HE3	1:A:186:LYS:HA	1.62	0.81
1:F:186:LYS:HD3	1:F:186:LYS:H	1.44	0.81
1:B:129:LYS:HG3	1:B:143:GLU:HA	1.65	0.79
1:C:104:MET:CE	1:C:133:ILE:HG22	2.15	0.77
1:C:186:LYS:H	1:C:186:LYS:CE	1.99	0.75
1:A:151:ASN:HD22	1:A:151:ASN:C	1.99	0.71
1:B:117:MET:CE	1:B:160:MET:HE3	2.20	0.71
1:B:199:GLU:H	1:B:199:GLU:CD	2.00	0.70
1:F:151:ASN:C	1:F:151:ASN:HD22	2.01	0.69
1:E:111:GLU:C	1:E:113:ASP:H	2.01	0.68
1:B:114:LYS:O	1:B:118:LEU:HD23	1.95	0.67
1:D:186:LYS:HE3	1:D:186:LYS:N	2.08	0.66
1:C:186:LYS:HD3	1:F:173:GLN:HE22	1.58	0.66
1:B:129:LYS:CG	1:B:143:GLU:HA	2.25	0.65
1:B:119:LYS:HB3	1:B:119:LYS:NZ	2.12	0.64
1:C:157:ASN:HD22	1:C:157:ASN:C	2.05	0.64
1:C:187:ASN:HD21	1:C:189:ASN:ND2	1.96	0.63
1:C:162:ILE:HD11	1:C:204:VAL:HG11	1.81	0.63
1:A:184:ILE:HD12	1:D:186:LYS:HE2	1.82	0.62
1:A:117:MET:CE	1:A:160:MET:HE3	2.29	0.62
1:C:104:MET:HE1	1:C:135:ARG:N	2.14	0.62
1:C:157:ASN:HD22	1:C:158:GLY:N	1.98	0.62
1:B:187:ASN:ND2	1:B:189:ASN:H	1.96	0.61
1:C:104:MET:CE	1:C:136:SER:H	2.13	0.61
1:B:119:LYS:HD3	2:B:262:HOH:O	2.01	0.60
1:E:187:ASN:ND2	1:E:189:ASN:H	1.99	0.60
1:F:153:GLU:HG3	1:F:161:ARG:HB3	1.83	0.60
1:C:157:ASN:ND2	1:C:159:ASN:H	2.00	0.60
1:E:187:ASN:C	1:E:187:ASN:HD22	2.10	0.60
1:B:139:LEU:HD23	1:B:153:GLU:HB2	1.84	0.59
1:E:137:ASN:ND2	1:E:139:LEU:HD21	2.18	0.59
1:F:117:MET:HE2	1:F:160:MET:HE3	1.85	0.58
1:B:187:ASN:HD22	1:B:188:GLY:N	2.01	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:MET:HE3	1:D:196:ARG:NH2	2.18	0.57
1:C:170:HIS:O	1:C:174:LYS:HG3	2.04	0.57
1:A:151:ASN:ND2	1:A:163:PHE:HB3	2.19	0.57
1:B:130:LYS:HE3	1:B:132:GLU:OE2	2.03	0.57
1:E:113:ASP:HB3	1:E:201:ILE:CD1	2.34	0.57
1:E:195:LYS:HE2	1:E:200:ASN:HD21	1.69	0.56
1:F:186:LYS:H	1:F:186:LYS:CD	2.14	0.56
1:F:187:ASN:C	1:F:187:ASN:HD22	2.10	0.56
1:F:157:ASN:C	1:F:157:ASN:HD22	2.12	0.56
1:D:187:ASN:ND2	1:D:189:ASN:H	2.03	0.55
1:B:187:ASN:HD22	1:B:187:ASN:C	2.14	0.55
1:F:143:GLU:HG3	1:F:144:LYS:HE3	1.87	0.55
1:B:119:LYS:HB3	1:B:119:LYS:HZ3	1.71	0.54
1:F:187:ASN:ND2	1:F:189:ASN:H	2.04	0.54
1:D:187:ASN:HD22	1:D:188:GLY:N	2.05	0.54
1:D:187:ASN:HD22	1:D:187:ASN:C	2.16	0.53
1:F:117:MET:CE	1:F:160:MET:HE3	2.38	0.53
1:E:109:ASP:O	1:E:112:GLU:HG3	2.09	0.53
1:E:178:ILE:HD13	1:E:207:VAL:HG21	1.90	0.53
1:E:187:ASN:HD22	1:E:189:ASN:H	1.57	0.52
1:F:110:MET:HE1	1:F:154:ILE:HG22	1.92	0.52
1:D:110:MET:HG2	1:D:114:LYS:HE3	1.91	0.52
1:A:117:MET:HE2	1:A:160:MET:HE3	1.91	0.52
1:E:187:ASN:HD21	1:E:189:ASN:HB2	1.76	0.51
1:A:207:VAL:O	1:A:211:LEU:HD13	2.11	0.51
1:E:195:LYS:H	1:E:195:LYS:CD	2.05	0.50
1:E:155:ASN:HB2	2:E:252:HOH:O	2.11	0.50
1:F:186:LYS:HD3	1:F:186:LYS:N	2.22	0.50
1:C:137:ASN:ND2	1:C:156:ASN:H	2.10	0.50
1:E:128:LEU:HD22	1:E:128:LEU:N	2.27	0.50
1:E:118:LEU:HD11	1:E:138:TYR:OH	2.12	0.50
1:B:174:LYS:HB3	1:B:174:LYS:NZ	2.27	0.49
1:E:112:GLU:OE1	1:E:112:GLU:C	2.56	0.49
1:C:128:LEU:HD23	1:C:142:LEU:HD23	1.94	0.49
1:E:110:MET:C	1:E:112:GLU:N	2.71	0.49
1:E:130:LYS:HE2	1:E:132:GLU:OE2	2.13	0.49
1:F:151:ASN:C	1:F:151:ASN:ND2	2.68	0.49
1:F:157:ASN:ND2	1:F:159:ASN:H	2.11	0.49
1:C:137:ASN:HD22	1:C:156:ASN:H	1.60	0.49
1:B:199:GLU:CD	1:B:199:GLU:N	2.68	0.49
1:B:200:ASN:O	1:B:204:VAL:HG23	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:ASN:C	1:C:157:ASN:ND2	2.71	0.49
1:B:119:LYS:HG3	2:B:298:HOH:O	2.11	0.48
1:F:206:THR:O	1:F:210:GLU:HG3	2.12	0.48
1:B:162:ILE:HB	1:B:192:LEU:HB2	1.94	0.48
1:E:161:ARG:NH2	1:E:191:TYR:CD2	2.80	0.48
1:E:195:LYS:HE2	1:E:200:ASN:ND2	2.28	0.48
1:D:129:LYS:HB2	1:D:129:LYS:NZ	2.28	0.48
1:F:136:SER:HB2	1:F:156:ASN:HB2	1.96	0.48
1:B:104:MET:HE1	1:B:134:TYR:HA	1.96	0.48
1:E:111:GLU:C	1:E:113:ASP:N	2.67	0.48
1:F:159:ASN:C	1:F:196:ARG:HG3	2.39	0.47
1:A:137:ASN:ND2	1:A:156:ASN:H	2.12	0.47
1:D:165:TYR:OH	1:D:166:LYS:HE3	2.15	0.47
1:D:171:HIS:HD2	2:D:234:HOH:O	1.98	0.47
1:F:157:ASN:HD22	1:F:158:GLY:N	2.12	0.47
1:C:108:SER:O	1:C:112:GLU:HG3	2.14	0.47
1:A:169:GLU:O	1:A:173:GLN:HG3	2.15	0.46
1:C:186:LYS:HE3	1:C:186:LYS:N	2.13	0.46
1:D:110:MET:HE3	1:D:196:ARG:HH21	1.81	0.46
1:E:110:MET:C	1:E:112:GLU:H	2.23	0.46
1:F:143:GLU:O	1:F:144:LYS:HD3	2.16	0.46
1:C:187:ASN:HD21	1:C:189:ASN:CG	2.23	0.46
1:A:184:ILE:CG2	1:D:186:LYS:HG3	2.46	0.46
1:C:178:ILE:HD13	1:C:207:VAL:HG21	1.97	0.45
1:D:139:LEU:HD12	1:D:139:LEU:N	2.31	0.45
1:F:114:LYS:HG3	1:F:138:TYR:CD2	2.51	0.45
1:E:110:MET:HE2	1:E:113:ASP:OD2	2.16	0.45
1:F:174:LYS:HE3	1:F:211:LEU:HD23	1.99	0.45
1:B:143:GLU:HG2	1:B:144:LYS:HG3	1.98	0.44
1:B:161:ARG:HG2	1:B:193:ASP:OD1	2.18	0.44
1:E:183:LYS:HD2	2:E:233:HOH:O	2.16	0.44
1:F:187:ASN:HD21	1:F:189:ASN:HB2	1.81	0.44
1:A:151:ASN:C	1:A:151:ASN:ND2	2.70	0.44
1:C:104:MET:HE1	1:C:134:TYR:C	2.42	0.44
1:C:165:TYR:OH	1:C:166:LYS:NZ	2.51	0.44
1:F:187:ASN:C	1:F:187:ASN:ND2	2.75	0.44
1:C:104:MET:HG2	2:C:274:HOH:O	2.17	0.44
1:A:137:ASN:HD22	1:A:156:ASN:H	1.66	0.44
1:F:184:ILE:HG23	1:F:184:ILE:O	2.19	0.43
1:B:119:LYS:NZ	1:B:119:LYS:CB	2.81	0.43
1:F:162:ILE:HB	1:F:192:LEU:HB2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:157:ASN:C	1:F:157:ASN:ND2	2.77	0.42
1:E:111:GLU:O	1:E:113:ASP:N	2.52	0.42
1:F:184:ILE:HG22	2:F:281:HOH:O	2.19	0.42
1:D:161:ARG:HB2	1:D:193:ASP:OD1	2.19	0.42
1:F:114:LYS:HD3	1:F:115:ASP:N	2.35	0.42
1:B:118:LEU:HD11	1:B:131:VAL:CG2	2.50	0.42
1:C:104:MET:HE2	1:C:133:ILE:HG22	1.99	0.42
1:F:168:MET:HE3	1:F:170:HIS:CE1	2.55	0.42
1:A:184:ILE:HG21	1:D:186:LYS:HG3	2.01	0.42
1:B:138:TYR:HB2	1:B:154:ILE:HB	2.02	0.42
1:F:211:LEU:HD12	1:F:211:LEU:HA	1.93	0.42
1:A:171:HIS:HD2	2:A:230:HOH:O	2.02	0.41
1:E:126:PHE:O	1:E:128:LEU:HD22	2.19	0.41
1:A:162:ILE:HB	1:A:192:LEU:HB2	2.02	0.41
1:B:129:LYS:HE3	1:B:142:LEU:O	2.21	0.41
1:E:129:LYS:O	1:E:130:LYS:HB3	2.21	0.41
1:E:161:ARG:HD2	1:E:193:ASP:OD2	2.20	0.41
1:E:110:MET:O	1:E:112:GLU:N	2.54	0.41
1:F:168:MET:HE3	1:F:170:HIS:HE1	1.86	0.41
1:E:162:ILE:HB	1:E:192:LEU:HB2	2.03	0.40
1:F:116:LEU:HD12	1:F:119:LYS:HE2	2.03	0.40
1:E:113:ASP:HB3	1:E:201:ILE:HD11	2.04	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	106/108 (98%)	104 (98%)	2 (2%)	0	100	100
1	B	106/108 (98%)	105 (99%)	1 (1%)	0	100	100
1	C	106/108 (98%)	104 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	102/108 (94%)	101 (99%)	1 (1%)	0	100	100
1	E	101/108 (94%)	98 (97%)	2 (2%)	1 (1%)	12	3
1	F	102/108 (94%)	101 (99%)	1 (1%)	0	100	100
All	All	623/648 (96%)	613 (98%)	9 (1%)	1 (0%)	43	24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	112	GLU

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	97/97 (100%)	95 (98%)	2 (2%)	47	23
1	B	97/97 (100%)	94 (97%)	3 (3%)	35	13
1	C	97/97 (100%)	95 (98%)	2 (2%)	47	23
1	D	93/97 (96%)	89 (96%)	4 (4%)	26	7
1	E	92/97 (95%)	88 (96%)	4 (4%)	26	7
1	F	93/97 (96%)	87 (94%)	6 (6%)	15	3
All	All	569/582 (98%)	548 (96%)	21 (4%)	30	10

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	186	LYS
1	B	174	LYS
1	B	187	ASN
1	B	199	GLU
1	C	157	ASN
1	C	186	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	129	LYS
1	D	137	ASN
1	D	186	LYS
1	D	187	ASN
1	E	112	GLU
1	E	174	LYS
1	E	187	ASN
1	E	195	LYS
1	F	114	LYS
1	F	151	ASN
1	F	157	ASN
1	F	169	GLU
1	F	186	LYS
1	F	187	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	147	ASN
1	A	151	ASN
1	A	171	HIS
1	A	189	ASN
1	B	170	HIS
1	B	187	ASN
1	C	137	ASN
1	C	157	ASN
1	C	187	ASN
1	D	171	HIS
1	D	173	GLN
1	D	187	ASN
1	D	189	ASN
1	E	147	ASN
1	E	151	ASN
1	E	187	ASN
1	E	189	ASN
1	F	124	ASN
1	F	151	ASN
1	F	156	ASN
1	F	157	ASN
1	F	173	GLN
1	F	187	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	189	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.