



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 01:02 am BST

PDB ID : 5JLT
Title : The crystal structure of the bacteriophage T4 MotA C-terminal domain in complex with dsDNA reveals a novel protein-DNA recognition motif
Authors : Cuypers, M.G.; Robertson, R.M.; Knipling, L.; Hinton, D.M.; White, S.W.
Deposited on : 2016-04-27
Resolution : 2.96 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

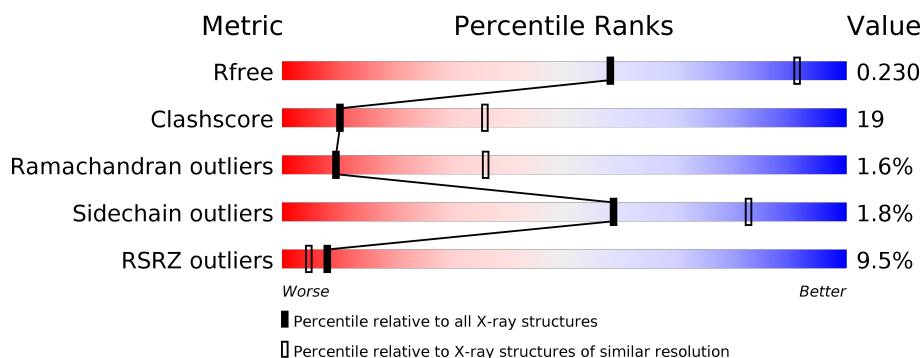
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 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 $\leq 5\%$. 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	125	<div> <div>6%</div> <div> <div></div> <div>57%</div> <div>34%</div> <div>9%</div> </div> </div>
1	B	125	<div> <div>7%</div> <div> <div></div> <div>47%</div> <div>36%</div> <div>14%</div> </div> </div>
1	C	125	<div> <div>17%</div> <div> <div></div> <div>46%</div> <div>36%</div> <div>6%</div> <div>12%</div> </div> </div>
1	D	125	<div> <div>10%</div> <div> <div></div> <div>43%</div> <div>38%</div> <div>15%</div> </div> </div>
2	E	22	<div> <div></div> <div> <div>77%</div> <div>23%</div> </div> </div>
2	H	22	<div> <div>5%</div> <div> <div></div> <div>59%</div> <div>41%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	F	22	 55% 45%
3	G	22	 73% 27%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5739 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 Middle transcription regulatory protein motA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	114	Total	C	N	O	S	0	0	0
			925	579	166	173	7			
1	B	108	Total	C	N	O	S	0	1	0
			885	555	154	169	7			
1	C	110	Total	C	N	O	S	0	0	0
			891	560	156	168	7			
1	D	106	Total	C	N	O	S	0	0	0
			857	540	148	162	7			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	87	GLU	-	expression tag	UNP P22915
A	88	GLY	-	expression tag	UNP P22915
A	89	ASP	-	expression tag	UNP P22915
A	90	ILE	-	expression tag	UNP P22915
A	91	HIS	-	expression tag	UNP P22915
A	92	MET	-	expression tag	UNP P22915
B	87	GLU	-	expression tag	UNP P22915
B	88	GLY	-	expression tag	UNP P22915
B	89	ASP	-	expression tag	UNP P22915
B	90	ILE	-	expression tag	UNP P22915
B	91	HIS	-	expression tag	UNP P22915
B	92	MET	-	expression tag	UNP P22915
C	87	GLU	-	expression tag	UNP P22915
C	88	GLY	-	expression tag	UNP P22915
C	89	ASP	-	expression tag	UNP P22915
C	90	ILE	-	expression tag	UNP P22915
C	91	HIS	-	expression tag	UNP P22915
C	92	MET	-	expression tag	UNP P22915
D	87	GLU	-	expression tag	UNP P22915
D	88	GLY	-	expression tag	UNP P22915
D	89	ASP	-	expression tag	UNP P22915

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Chain	Residue	Modelled	Actual	Comment	Reference
D	90	ILE	-	expression tag	UNP P22915
D	91	HIS	-	expression tag	UNP P22915
D	92	MET	-	expression tag	UNP P22915

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*AP*AP*GP*CP*TP*TP*TP*GP*CP*TP*TP*AP*AP*TP*AP*AP*TP*CP*CP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	22	Total	C	N	O	P	0	0	0
			445	215	79	130	21			
2	H	22	Total	C	N	O	P	0	0	0
			445	215	79	130	21			

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*TP*GP*GP*AP*TP*TP*AP*TP*TP*AP*AP*GP*CP*AP*AP*AP*GP*CP*TP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	22	Total	C	N	O	P	0	0	0
			451	217	83	130	21			
3	G	22	Total	C	N	O	P	0	0	0
			451	217	83	130	21			

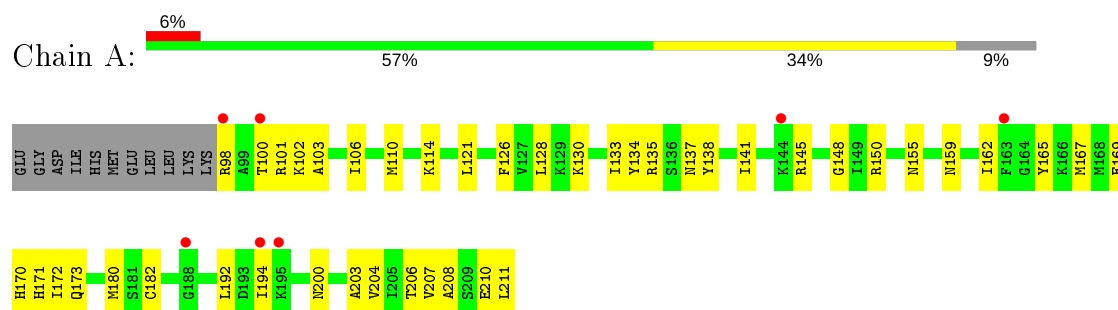
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	58	Total	O	0	0
			58	58		
4	B	46	Total	O	0	2
			46	46		
4	C	67	Total	O	0	5
			68	68		
4	D	75	Total	O	0	1
			76	76		
4	E	29	Total	O	0	0
			29	29		
4	F	37	Total	O	0	0
			37	37		
4	G	35	Total	O	0	2
			35	35		
4	H	40	Total	O	0	0
			40	40		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

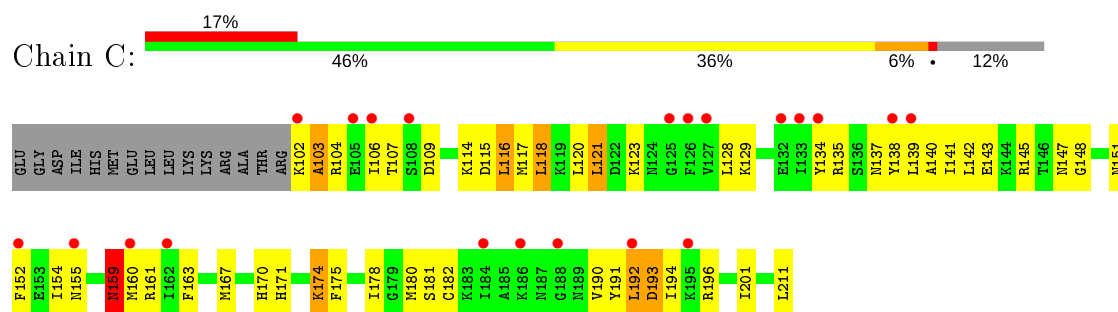
- Molecule 1: Middle transcription regulatory protein motA



- Molecule 1: Middle transcription regulatory protein motA

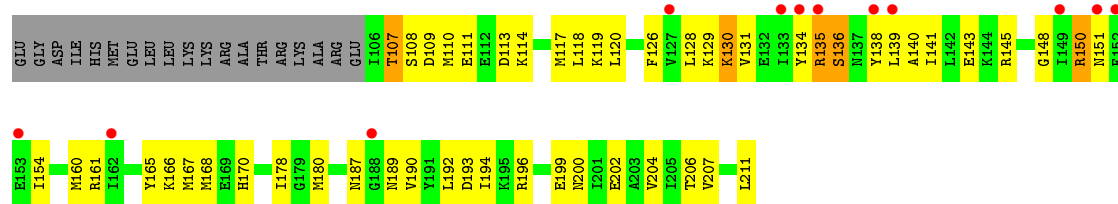


- Molecule 1: Middle transcription regulatory protein motA



- Molecule 1: Middle transcription regulatory protein motA

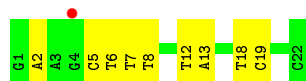




- Molecule 2: DNA (5'-D(*GP*AP*AP*GP*CP*TP*TP*TP*GP*CP*TP*TP*AP*AP*TP*AP*AP*TP*CP*CP*AP*C)-3')



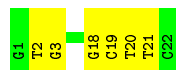
- Molecule 2: DNA (5'-D(*GP*AP*AP*GP*CP*TP*TP*TP*GP*CP*TP*TP*AP*AP*TP*AP*AP*TP*CP*CP*AP*C)-3')



- Molecule 3: DNA (5'-D(*GP*TP*GP*GP*AP*TP*TP*AP*TP*TP*AP*AP*GP*CP*AP*AP*AP*GP*CP*TP*TP*C)-3')



- Molecule 3: DNA (5'-D(*GP*TP*GP*GP*AP*TP*TP*AP*TP*TP*AP*AP*GP*CP*AP*AP*AP*GP*CP*TP*TP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	72.27 Å 72.27 Å 279.37 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	62.59 – 2.96 62.59 – 2.96	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.59-2.96) 100.0 (62.59-2.96)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.96 Å)	Xtriage
Refinement program	PHENIX (dev_2363)	Depositor
R, R_{free}	0.220 , 0.245 0.215 , 0.230	Depositor DCC
R_{free} test set	856 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.910	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.248 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5739	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.32	0/934	0.70	0/1244
1	B	0.34	0/894	0.85	2/1192 (0.2%)
1	C	0.53	0/900	1.21	8/1199 (0.7%)
1	D	0.37	0/866	0.92	5/1155 (0.4%)
2	E	0.52	0/498	0.94	0/766
2	H	0.54	0/498	0.92	0/766
3	F	0.55	0/506	0.92	0/780
3	G	0.51	0/506	0.91	0/780
All	All	0.45	0/5602	0.93	15/7882 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	192	LEU	CB-CG-CD2	-12.04	90.53	111.00
1	C	116	LEU	CA-CB-CG	10.12	138.58	115.30
1	C	159	ASN	CB-CA-C	-9.19	92.03	110.40
1	B	116	LEU	CA-CB-CG	7.96	133.60	115.30
1	C	193	ASP	CB-CA-C	-7.39	95.63	110.40
1	C	174	LYS	CD-CE-NZ	7.34	128.57	111.70
1	C	121	LEU	CA-CB-CG	7.30	132.09	115.30
1	D	130	LYS	CA-CB-CG	7.13	129.09	113.40
1	B	190	VAL	CG1-CB-CG2	-6.53	100.45	110.90
1	D	120	LEU	CA-CB-CG	6.14	129.42	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	150	ARG	CG-CD-NE	-6.13	98.92	111.80
1	D	130	LYS	N-CA-CB	-5.75	100.26	110.60
1	D	119	LYS	CD-CE-NZ	-5.35	99.39	111.70
1	C	159	ASN	N-CA-CB	5.32	120.17	110.60
1	C	118	LEU	CA-CB-CG	5.10	127.02	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	107	THR	Peptide

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	925	0	951	28	0
1	B	885	0	898	47	0
1	C	891	0	913	45	0
1	D	857	0	876	46	0
2	E	445	0	251	5	0
2	H	445	0	251	7	0
3	F	451	0	251	8	0
3	G	451	0	251	5	0
4	A	58	0	0	0	0
4	B	46	0	0	0	0
4	C	68	0	0	0	0
4	D	76	0	0	0	0
4	E	29	0	0	0	0
4	F	37	0	0	1	0
4	G	35	0	0	0	0
4	H	40	0	0	0	0
All	All	5739	0	4642	182	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 19.

All (182) 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:196:ARG:CG	1:B:197:SER:H	1.61	1.11
1:B:113:ASP:OD2	1:B:196:ARG:HD2	1.51	1.09
1:D:129:LYS:HB2	1:D:143:GLU:HG2	1.34	1.05
1:B:113:ASP:OD2	1:B:196:ARG:CD	2.05	1.05
1:B:196:ARG:HG2	1:B:197:SER:H	1.16	1.04
1:B:196:ARG:CG	1:B:197:SER:N	2.20	0.96
1:B:196:ARG:HG3	1:B:197:SER:N	1.83	0.90
1:D:129:LYS:CB	1:D:143:GLU:HG2	2.05	0.85
1:D:107:THR:HG23	1:D:108:SER:HB3	1.60	0.82
1:A:100:THR:HG23	2:E:6:DT:H4'	1.61	0.81
1:C:129:LYS:HG3	1:C:143:GLU:HG3	1.60	0.81
1:A:180:MET:HG2	1:A:194:ILE:HB	1.69	0.74
1:C:138:TYR:HB2	1:C:154:ILE:HB	1.69	0.72
1:C:155:ASN:O	1:C:196:ARG:NH1	2.24	0.71
1:B:113:ASP:OD2	1:B:196:ARG:HD3	1.86	0.71
1:B:190:VAL:CG2	1:B:192:LEU:HD11	2.21	0.70
1:B:108:SER:O	1:B:110:MET:N	2.21	0.70
1:B:190:VAL:CG2	1:B:192:LEU:CD1	2.70	0.69
3:G:21:DT:H3	2:H:2:DA:N6	1.92	0.67
1:B:175:PHE:HB3	1:B:180:MET:HE2	1.76	0.67
1:C:135:ARG:HD2	2:H:8:DT:H2'	1.77	0.67
1:A:145:ARG:HH21	1:A:148:GLY:HA2	1.60	0.66
1:C:106:ILE:HG21	1:C:138:TYR:OH	1.94	0.66
1:A:180:MET:HE2	1:A:192:LEU:HB3	1.78	0.66
1:C:161:ARG:CZ	1:C:191:TYR:HB3	2.27	0.64
1:A:133:ILE:HA	1:A:137:ASN:O	1.97	0.64
1:A:162:ILE:HB	1:A:192:LEU:HB2	1.79	0.64
1:C:139:LEU:O	1:C:139:LEU:HD12	1.98	0.64
1:C:107:THR:OG1	1:C:109:ASP:OD1	2.13	0.63
1:B:150:ARG:HD3	1:B:163:PHE:CE2	2.33	0.63
1:B:174:LYS:O	1:B:174:LYS:HD2	1.99	0.62
1:C:161:ARG:HG3	1:C:192:LEU:O	1.98	0.62
1:D:134:TYR:O	1:D:136:SER:N	2.32	0.62
1:D:129:LYS:CA	1:D:143:GLU:HG2	2.29	0.62
1:C:129:LYS:HE3	1:C:143:GLU:HA	1.82	0.62
1:B:150:ARG:HG2	1:B:163:PHE:O	2.00	0.61
1:D:114:LYS:HD3	1:D:138:TYR:CE2	2.35	0.61
1:B:114:LYS:NZ	1:B:115:ASP:OD1	2.33	0.61
1:C:180:MET:HG2	1:C:194:ILE:HB	1.82	0.61
1:D:135:ARG:HD3	3:F:3:DG:OP2	2.00	0.61
1:D:150:ARG:O	1:D:151:ASN:ND2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ARG:O	1:B:197:SER:OG	2.13	0.60
1:D:113:ASP:OD2	1:D:196:ARG:NH1	2.35	0.60
1:A:155:ASN:HB2	1:A:159:ASN:OD1	2.02	0.59
1:B:199:GLU:O	1:B:202:GLU:HG3	2.02	0.59
1:A:98:ARG:HG2	3:F:21:DT:H4'	1.85	0.59
2:E:6:DT:H2'	2:E:7:DT:C6	2.39	0.58
1:D:167:MET:SD	1:D:190:VAL:HG21	2.44	0.57
1:D:207:VAL:O	1:D:211:LEU:HD13	2.04	0.57
1:D:165:TYR:CE1	1:D:166:LYS:HG3	2.40	0.57
3:F:12:DA:N7	4:F:101:HOH:O	2.33	0.57
1:B:190:VAL:HG23	1:B:192:LEU:HD11	1.87	0.56
1:C:118:LEU:HA	1:C:121:LEU:HG	1.88	0.56
1:B:190:VAL:HG22	1:B:192:LEU:CD1	2.35	0.56
1:B:180:MET:HE3	1:B:192:LEU:HB3	1.88	0.56
1:B:139:LEU:HD23	1:B:153:GLU:OE1	2.05	0.56
1:C:180:MET:HE2	1:C:192:LEU:HB3	1.88	0.56
1:A:203:ALA:O	1:A:206:THR:HG22	2.06	0.55
1:D:165:TYR:HE2	2:E:13:DA:H2'	1.69	0.55
1:A:145:ARG:NH2	1:A:148:GLY:HA2	2.22	0.55
1:D:161:ARG:NH1	3:F:5:DA:OP2	2.38	0.55
1:C:145:ARG:HH11	1:C:148:GLY:HA2	1.72	0.54
1:D:129:LYS:HB2	1:D:143:GLU:CG	2.23	0.54
3:G:2:DT:H2''	3:G:3:DG:C8	2.43	0.54
1:A:102:LYS:N	1:A:103:ALA:HA	2.24	0.53
1:B:198:ALA:O	1:B:200:ASN:N	2.33	0.53
1:D:128:LEU:HD22	1:D:140:ALA:HB1	1.90	0.53
1:A:130:LYS:HE3	1:A:141:ILE:HD12	1.90	0.53
1:C:167:MET:SD	1:C:190:VAL:HG21	2.49	0.53
1:C:134:TYR:O	1:C:137:ASN:HB2	2.09	0.53
3:G:18:DG:H2''	3:G:19:DC:H5''	1.91	0.52
1:B:190:VAL:HG23	1:B:192:LEU:CD1	2.38	0.52
1:D:129:LYS:O	1:D:130:LYS:HB2	2.08	0.52
1:B:118:LEU:HD21	1:B:131:VAL:HG11	1.92	0.52
1:C:116:LEU:HD22	1:C:201:ILE:HD11	1.92	0.52
1:C:103:ALA:O	1:C:104:ARG:HB2	2.09	0.52
1:D:148:GLY:HA3	1:D:167:MET:HG2	1.92	0.51
1:C:182:CYS:HA	1:C:191:TYR:O	2.11	0.51
3:F:2:DT:H2''	3:F:3:DG:C8	2.46	0.51
1:C:129:LYS:CG	1:C:143:GLU:HG3	2.36	0.51
1:D:141:ILE:HA	1:D:151:ASN:ND2	2.26	0.50
1:B:197:SER:OG	1:B:198:ALA:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:ILE:HD11	1:C:180:MET:SD	2.51	0.50
1:C:147:ASN:HD22	1:C:171:HIS:HE1	1.58	0.50
1:D:114:LYS:HD3	1:D:138:TYR:CD2	2.47	0.50
1:D:168:MET:SD	1:D:170:HIS:HE1	2.35	0.50
1:A:200:ASN:O	1:A:204:VAL:HG23	2.12	0.50
1:C:151:ASN:OD1	1:C:163:PHE:HB3	2.11	0.49
1:D:180:MET:HG2	1:D:194:ILE:HB	1.94	0.49
1:A:100:THR:CG2	2:E:6:DT:H4'	2.39	0.49
1:B:142:LEU:HB2	1:B:150:ARG:O	2.12	0.49
1:A:167:MET:HG2	1:A:172:ILE:HG13	1.94	0.49
1:A:169:GLU:O	1:A:173:GLN:HG3	2.12	0.49
1:C:141:ILE:CD1	1:C:151:ASN:HB3	2.42	0.49
3:G:21:DT:H3	2:H:2:DA:H61	1.58	0.49
1:B:120:LEU:HD12	1:B:201:ILE:HG22	1.95	0.49
1:C:114:LYS:CG	1:C:115:ASP:N	2.75	0.49
1:C:128:LEU:HD13	1:C:140:ALA:HB1	1.95	0.48
1:D:110:MET:HG3	1:D:111:GLU:H	1.78	0.48
1:D:113:ASP:OD2	1:D:196:ARG:HD2	2.14	0.48
1:B:208:ALA:HA	1:B:211:LEU:CD1	2.44	0.47
1:C:147:ASN:HD22	1:C:171:HIS:CE1	2.32	0.47
1:C:175:PHE:O	1:C:178:ILE:HG12	2.13	0.47
1:B:178:ILE:CD1	1:B:207:VAL:HG21	2.44	0.47
1:C:102:LYS:HE2	1:C:104:ARG:HA	1.97	0.47
1:C:128:LEU:HD23	1:C:142:LEU:HD23	1.97	0.47
1:D:145:ARG:NH1	1:D:148:GLY:HA2	2.30	0.47
1:D:160:MET:SD	1:D:204:VAL:HG21	2.54	0.47
1:B:159:ASN:HA	1:B:195:LYS:HA	1.95	0.47
1:B:120:LEU:HD13	1:B:202:GLU:HA	1.95	0.47
1:B:208:ALA:HA	1:B:211:LEU:HD11	1.95	0.47
1:A:208:ALA:HA	1:A:211:LEU:HD12	1.97	0.47
1:A:106:ILE:HG23	1:A:110:MET:SD	2.55	0.47
1:A:137:ASN:ND2	1:A:155:ASN:OD1	2.35	0.47
1:B:180:MET:HG2	1:B:194:ILE:HB	1.97	0.47
1:B:196:ARG:HG2	1:B:197:SER:N	1.99	0.46
1:C:178:ILE:HG13	1:C:180:MET:HG3	1.97	0.46
1:A:121:LEU:HD13	1:A:128:LEU:HD11	1.96	0.46
1:D:110:MET:HG3	1:D:111:GLU:N	2.31	0.46
1:A:207:VAL:HA	1:A:210:GLU:HG2	1.97	0.46
1:C:161:ARG:HE	1:C:192:LEU:C	2.18	0.46
1:D:199:GLU:O	1:D:202:GLU:HG2	2.16	0.46
3:F:18:DG:H2"	3:F:19:DC:H5"	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:GLN:HA	1:B:176:THR:HG22	1.97	0.46
1:D:187:ASN:HD21	1:D:189:ASN:ND2	2.13	0.46
1:C:171:HIS:O	1:C:174:LYS:HB2	2.16	0.46
1:C:180:MET:HA	1:C:193:ASP:O	2.16	0.45
1:C:147:ASN:CG	1:C:211:LEU:HB3	2.37	0.45
1:D:161:ARG:HA	1:D:192:LEU:O	2.16	0.45
1:B:165:TYR:CD1	1:B:189:ASN:OD1	2.70	0.45
1:D:202:GLU:O	1:D:206:THR:HG23	2.16	0.45
1:C:141:ILE:HD13	1:C:151:ASN:HB3	1.97	0.45
1:D:131:VAL:HA	1:D:139:LEU:O	2.17	0.45
1:D:145:ARG:HH11	1:D:148:GLY:HA2	1.81	0.45
1:C:170:HIS:O	1:C:174:LYS:HG2	2.17	0.45
1:C:104:ARG:HB2	1:C:104:ARG:NH1	2.32	0.44
1:C:117:MET:SD	1:C:152:PHE:HB3	2.57	0.44
1:A:150:ARG:HE	1:A:165:TYR:HB2	1.83	0.44
1:A:102:LYS:HB2	1:A:103:ALA:C	2.38	0.44
1:C:160:MET:HB2	1:C:196:ARG:HG2	1.99	0.44
1:D:178:ILE:O	1:D:178:ILE:HG22	2.17	0.44
1:D:200:ASN:O	1:D:204:VAL:HG13	2.18	0.44
3:G:20:DT:H2"	3:G:21:DT:C6	2.52	0.44
1:A:150:ARG:NE	1:A:165:TYR:HB2	2.32	0.43
1:D:128:LEU:HD12	1:D:128:LEU:N	2.33	0.43
1:A:133:ILE:HD11	1:A:138:TYR:CZ	2.52	0.43
1:B:181:SER:O	1:B:192:LEU:HA	2.17	0.43
1:D:204:VAL:O	1:D:207:VAL:HG12	2.18	0.43
1:C:120:LEU:O	1:C:123:LYS:HB3	2.18	0.43
1:D:180:MET:HA	1:D:193:ASP:O	2.19	0.43
1:C:145:ARG:NH1	1:C:148:GLY:HA2	2.33	0.43
1:B:159:ASN:HB2	1:B:194:ILE:O	2.18	0.43
1:D:129:LYS:N	1:D:141:ILE:O	2.52	0.43
1:B:114:LYS:HD3	1:B:138:TYR:CD2	2.53	0.42
1:D:207:VAL:HG22	1:D:211:LEU:CD1	2.49	0.42
1:C:121:LEU:HD11	1:C:128:LEU:HD11	2.01	0.42
1:B:120:LEU:CD1	1:B:201:ILE:HG22	2.49	0.42
1:B:145:ARG:HB2	1:B:149:ILE:O	2.19	0.42
2:H:5:DC:H2'	2:H:6:DT:C6	2.55	0.42
1:B:173:GLN:O	1:B:176:THR:HG22	2.20	0.42
1:A:170:HIS:CE1	1:A:171:HIS:CE1	3.08	0.42
1:B:114:LYS:HB3	1:B:114:LYS:HE3	1.85	0.42
1:D:154:ILE:HD13	1:D:154:ILE:HA	1.94	0.42
1:D:117:MET:HG2	1:D:118:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:SER:O	1:C:192:LEU:HA	2.20	0.41
3:F:14:DC:H2''	3:F:15:DA:C8	2.55	0.41
1:A:134:TYR:CD2	1:A:135:ARG:HD3	2.56	0.41
1:D:114:LYS:HB2	1:D:138:TYR:HD2	1.86	0.41
2:E:18:DT:H2''	2:E:19:DC:H5''	2.02	0.41
1:B:161:ARG:HG3	1:B:193:ASP:OD2	2.21	0.41
1:B:160:MET:SD	1:B:204:VAL:HG11	2.61	0.41
1:C:155:ASN:ND2	1:C:159:ASN:OD1	2.54	0.41
2:H:18:DT:H2''	2:H:19:DC:H5''	2.03	0.41
1:B:106:ILE:HG22	1:B:108:SER:H	1.86	0.41
1:D:134:TYR:CD1	1:D:135:ARG:HG3	2.56	0.40
2:H:6:DT:H2'	2:H:7:DT:C6	2.55	0.40
1:A:121:LEU:HB3	1:A:126:PHE:HB2	2.03	0.40
1:D:143:GLU:H	1:D:143:GLU:HG3	1.79	0.40
1:D:126:PHE:HB3	1:D:128:LEU:HD11	2.03	0.40
2:H:12:DT:H2''	2:H:13:DA:C8	2.57	0.40
3:F:5:DA:H2'	3:F:6:DT:C6	2.56	0.40
1:B:160:MET:N	1:B:194:ILE:O	2.46	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	112/125 (90%)	110 (98%)	2 (2%)	0	100	100
1	B	107/125 (86%)	99 (92%)	5 (5%)	3 (3%)	5	22
1	C	108/125 (86%)	104 (96%)	3 (3%)	1 (1%)	17	51
1	D	104/125 (83%)	101 (97%)	0	3 (3%)	4	21
All	All	431/500 (86%)	414 (96%)	10 (2%)	7 (2%)	9	36

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	109	ASP
1	D	136	SER
1	B	108	SER
1	B	196	ARG
1	D	135	ARG
1	D	109	ASP
1	C	103	ALA

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	101/111 (91%)	98 (97%)	3 (3%)	41	72
1	B	98/111 (88%)	95 (97%)	3 (3%)	40	71
1	C	98/111 (88%)	97 (99%)	1 (1%)	76	90
1	D	95/111 (86%)	95 (100%)	0	100	100
All	All	392/444 (88%)	385 (98%)	7 (2%)	59	82

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	ARG
1	A	114	LYS
1	A	182	CYS
1	B	104	ARG
1	B	145	ARG
1	B	182	CYS
1	C	159	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	HIS
1	C	155	ASN
1	C	159	ASN

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Mol	Chain	Res	Type
1	C	171	HIS
1	D	151	ASN
1	D	170	HIS
1	D	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 carbohydrates 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

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	114/125 (91%)	0.34	7 (6%) 21 12	56, 79, 116, 132	0
1	B	108/125 (86%)	0.48	9 (8%) 11 6	64, 89, 135, 254	0
1	C	110/125 (88%)	0.91	21 (19%) 1 0	76, 128, 181, 199	0
1	D	106/125 (84%)	0.45	12 (11%) 5 3	60, 98, 155, 181	0
2	E	22/22 (100%)	-0.66	0 100 100	53, 64, 74, 78	0
2	H	22/22 (100%)	-0.12	1 (4%) 33 21	54, 72, 97, 115	0
3	F	22/22 (100%)	-0.57	0 100 100	51, 62, 77, 91	0
3	G	22/22 (100%)	-0.44	0 100 100	51, 66, 75, 78	0
All	All	526/588 (89%)	0.38	50 (9%) 8 5	51, 89, 160, 254	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	106	ILE	5.6
1	C	188	GLY	4.9
1	A	195	LYS	4.9
1	A	98	ARG	4.3
1	B	107	THR	3.7
1	C	133	ILE	3.6
1	C	138	TYR	3.6
1	C	106	ILE	3.4
1	D	152	PHE	3.4
1	D	151	ASN	3.3
1	C	105	GLU	3.2
1	C	160	MET	3.1
1	D	138	TYR	3.1
1	A	188	GLY	3.1
1	C	192	LEU	3.0
1	C	134	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	105	GLU	3.0
1	D	134	TYR	3.0
1	B	186	LYS	3.0
1	D	127	VAL	2.9
1	C	125	GLY	2.9
1	C	184	ILE	2.9
1	A	163	PHE	2.9
1	B	195	LYS	2.9
1	D	188	GLY	2.9
1	C	155	ASN	2.8
1	C	108	SER	2.8
1	B	144	LYS	2.8
1	D	133	ILE	2.7
1	B	158	GLY	2.6
1	C	152	PHE	2.5
1	A	100	THR	2.5
1	C	186	LYS	2.5
1	D	139	LEU	2.4
1	C	132	GLU	2.3
1	C	102	LYS	2.3
1	A	144	LYS	2.3
1	C	195	LYS	2.2
1	C	127	VAL	2.2
1	B	182	CYS	2.1
2	H	4	DG	2.1
1	D	153	GLU	2.1
1	D	149	ILE	2.1
1	C	139	LEU	2.1
1	D	162	ILE	2.1
1	D	135	ARG	2.0
1	C	162	ILE	2.0
1	C	126	PHE	2.0
1	A	194	ILE	2.0
1	B	165	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 [i](#)

There are no carbohydrates 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.