Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:12 PM GMT

PDB ID	:	1EJ1
Title	:	COCRYSTAL STRUCTURE OF THE MESSENGER RNA 5' CAP-BINDING PROTEIN (EIF4E) BOUND TO 7-METHYL-GDP
Authors	:	Marcotrigiano, J.; Gingras, A.-C.; Sonenberg, N.; Burley, S.K.
Deposited on	:	2000-02-29
Resolution	:	2.20 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

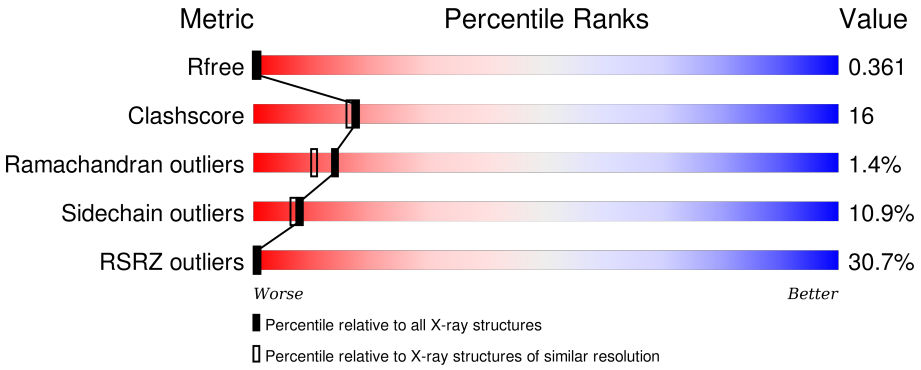
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.20 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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. 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	190	17% 59% 29% 5% • 6%
1	B	190	42% 65% 29% • •

2 Entry composition

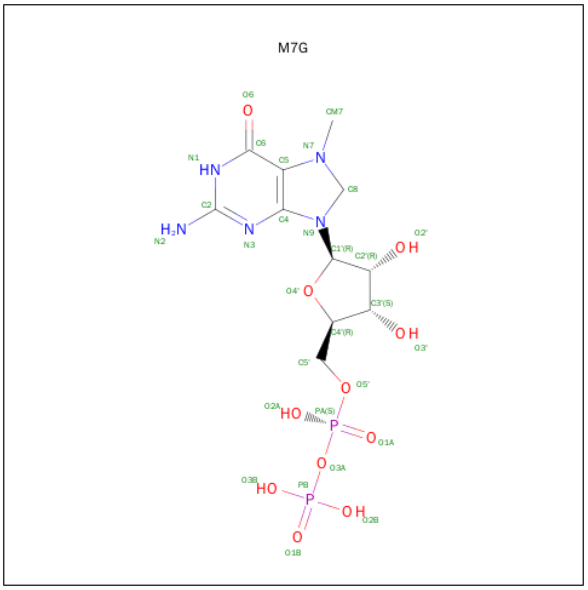
There are 3 unique types of molecules in this entry. The entry contains 3188 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 EUKARYOTIC TRANSLATION INITIATION FACTOR 4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1460	929	258	267	6			
1	B	190	Total	C	N	O	S	0	0	0
			1540	981	270	283	6			

- Molecule 2 is 7N-METHYL-8-HYDROGUANOSINE-5'-DIPHOSPHATE (three-letter code: M7G) (formula: $C_{11}H_{19}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	11	5	11	2		
2	B	1	Total	C	N	O	P	0	0
			29	11	5	11	2		

- Molecule 3 is water.

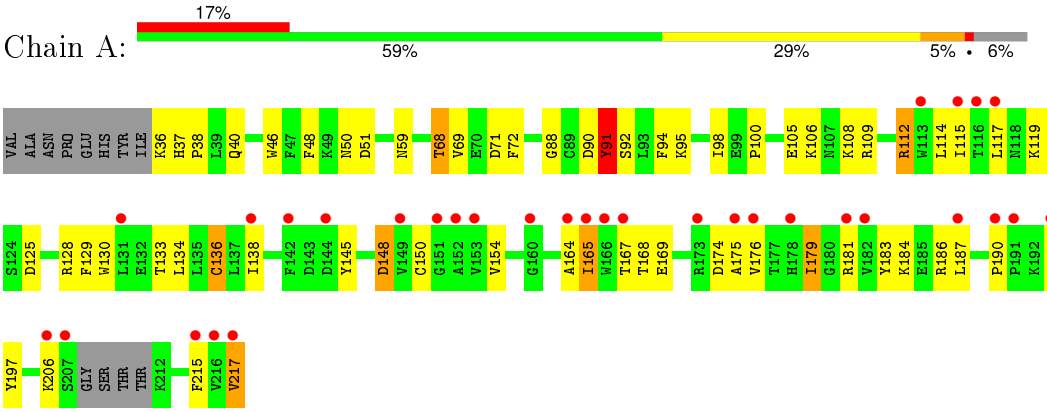
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	79	Total O 79 79	0	0
3	B	51	Total O 51 51	0	0

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 errors 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.

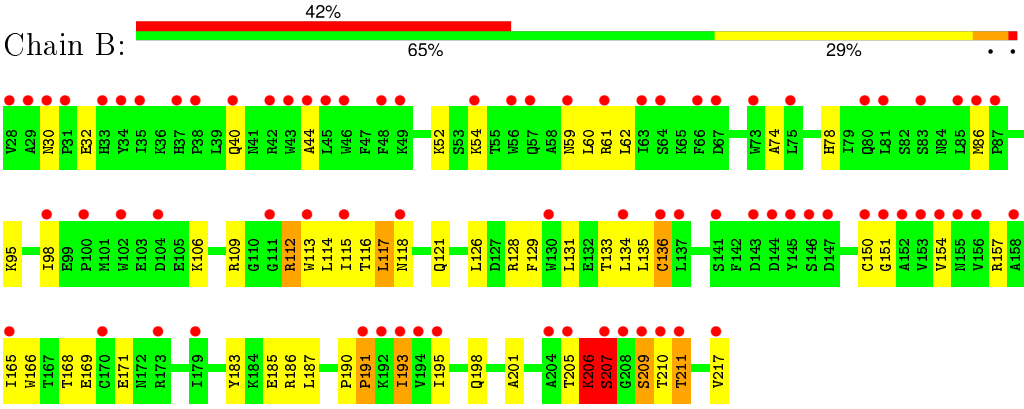
- Molecule 1: EUKARYOTIC TRANSLATION INITIATION FACTOR 4E

Chain A:



- Molecule 1: EUKARYOTIC TRANSLATION INITIATION FACTOR 4E

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.60Å 75.40Å 76.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.20 24.37 – 2.22	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.20) 97.4 (24.37-2.22)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	10.59 (at 2.22Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.209 , 0.235 0.345 , 0.361	Depositor DCC
R_{free} test set	1679 reflections (9.18%)	DCC
Wilson B-factor (Å^2)	19.2	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 57.4	EDS
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 19962 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	3188	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.50% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: M7G

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	0.73	2/1496 (0.1%)	0.89	2/2024 (0.1%)
1	B	0.74	1/1580 (0.1%)	0.93	4/2143 (0.2%)
All	All	0.74	3/3076 (0.1%)	0.91	6/4167 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	CYS	CB-SG	-7.09	1.70	1.82
1	B	136	CYS	CB-SG	-6.05	1.72	1.82
1	A	150	CYS	CB-SG	-5.05	1.73	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	211	THR	N-CA-C	8.12	132.91	111.00
1	A	186	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	B	193	ILE	N-CA-C	-6.39	93.74	111.00
1	A	91	TYR	N-CA-C	-5.39	96.45	111.00
1	B	195	ILE	N-CA-C	-5.19	96.98	111.00
1	B	206	LYS	N-CA-C	-5.09	97.26	111.00

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	1460	0	1411	55	0
1	B	1540	0	1484	41	0
2	A	29	0	16	0	0
2	B	29	0	16	0	0
3	A	79	0	0	1	0
3	B	51	0	0	2	0
All	All	3188	0	2927	96	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 16.

All (96) 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:A:195:ILE:HD11	1:A:217:VAL:HG12	1.11	1.06
1:A:195:ILE:HD11	1:A:217:VAL:CG1	1.98	0.93
1:A:195:ILE:CD1	1:A:217:VAL:HG12	1.98	0.92
1:A:95:LYS:HB2	1:A:98:ILE:HD12	1.53	0.90
1:A:175:ALA:O	1:A:179:ILE:HD13	1.73	0.89
1:B:115:ILE:HD11	1:B:183:TYR:CZ	2.14	0.83
1:A:68:THR:HG22	1:A:71:ASP:H	1.42	0.82
1:B:115:ILE:HD11	1:B:183:TYR:CE2	2.16	0.80
1:B:190:PRO:HD2	1:B:193:ILE:HD11	1.65	0.78
1:B:193:ILE:O	1:B:193:ILE:HG13	1.84	0.78
1:A:190:PRO:HB2	1:A:193:ILE:HD13	1.65	0.76
1:A:184:LYS:HD2	1:A:195:ILE:HD12	1.70	0.72
1:A:195:ILE:H	1:A:195:ILE:HD13	1.55	0.72
1:A:115:ILE:HD11	1:A:183:TYR:CE2	2.28	0.69
1:B:126:LEU:HD12	1:B:163:ILE:HD11	1.75	0.68
1:A:133:THR:HG23	1:A:165:ILE:HD11	1.76	0.65
1:A:184:LYS:HD2	1:A:195:ILE:CD1	2.29	0.62
1:B:112:ARG:O	1:B:112:ARG:HG2	1.98	0.62
1:B:54:LYS:HE3	1:B:59:ASN:OD1	2.02	0.60
1:B:198:GLN:OE1	1:B:211:THR:HG23	2.01	0.60
1:A:115:ILE:HD13	1:A:187:LEU:HD12	1.85	0.59
1:B:95:LYS:HB2	1:B:98:ILE:HD13	1.83	0.59
1:B:98:ILE:HD12	1:B:98:ILE:N	2.18	0.59
1:A:176:VAL:HG11	1:A:215:PHE:CD1	2.38	0.59
1:B:115:ILE:HD13	1:B:187:LEU:CD1	2.33	0.58
1:A:133:THR:CG2	1:A:165:ILE:HD11	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:LEU:HD22	1:B:134:LEU:HD23	1.85	0.58
1:A:94:PHE:CD1	1:A:100:PRO:HB3	2.39	0.58
1:A:190:PRO:CB	1:A:193:ILE:HD13	2.34	0.57
1:B:190:PRO:HB2	1:B:193:ILE:HG12	1.87	0.57
1:A:119:LYS:HE2	1:A:122:ARG:NH2	2.20	0.57
1:B:95:LYS:CB	1:B:98:ILE:HD13	2.35	0.56
1:A:168:THR:HG23	1:A:169:GLU:HG2	1.86	0.56
1:B:106:LYS:O	1:B:168:THR:HG22	2.04	0.56
1:B:157:ARG:HB2	1:B:160:GLY:O	2.06	0.55
1:B:190:PRO:HD2	1:B:193:ILE:CD1	2.36	0.55
1:B:93:LEU:HD22	1:B:134:LEU:CD2	2.37	0.55
1:A:98:ILE:HG12	1:A:106:LYS:HD2	1.88	0.55
1:A:145:TYR:HB3	1:A:179:ILE:HD11	1.91	0.53
1:B:109:ARG:HD2	1:B:169:GLU:OE2	2.09	0.53
1:A:117:LEU:HD11	1:A:129:PHE:CD1	2.43	0.53
1:A:115:ILE:HD11	1:A:183:TYR:CZ	2.45	0.52
1:A:164:ALA:O	1:A:165:ILE:HD12	2.10	0.51
1:B:201:ALA:O	1:B:205:THR:HG23	2.10	0.50
1:A:134:LEU:O	1:A:138:ILE:HB	2.12	0.50
1:A:91:TYR:HB2	1:A:154:VAL:CG1	2.42	0.50
1:A:90:ASP:HA	1:A:154:VAL:O	2.10	0.50
1:A:130:TRP:CZ2	1:A:134:LEU:HD21	2.46	0.50
1:A:112:ARG:O	1:A:112:ARG:HG2	2.13	0.49
1:B:206:LYS:O	1:B:207:SER:HB2	2.12	0.49
1:A:145:TYR:CB	1:A:179:ILE:HD11	2.43	0.49
1:A:165:ILE:N	1:A:165:ILE:CD1	2.76	0.48
1:A:115:ILE:HD13	1:A:187:LEU:CD1	2.44	0.48
1:A:179:ILE:N	1:A:179:ILE:CD1	2.77	0.48
1:B:131:LEU:O	1:B:135:LEU:HG	2.15	0.47
1:A:181:ARG:HG3	1:A:217:VAL:CG2	2.44	0.47
1:A:117:LEU:HD11	1:A:129:PHE:CE1	2.49	0.47
1:A:148:ASP:O	1:A:167:THR:HA	2.15	0.47
1:B:133:THR:HG23	1:B:165:ILE:HD11	1.95	0.47
1:A:112:ARG:O	1:A:197:TYR:HA	2.14	0.47
1:B:117:LEU:N	1:B:117:LEU:HD23	2.29	0.47
1:B:94:PHE:HA	1:B:151:GLY:HA3	1.98	0.45
1:B:117:LEU:HB3	1:B:121:GLN:HB2	1.99	0.45
1:A:105:GLU:OE2	1:A:108:LYS:HE3	2.17	0.45
1:B:112:ARG:NH2	3:B:1007:HOH:O	2.45	0.44
1:B:44:ALA:HB1	1:B:62:LEU:CD1	2.48	0.44
1:B:166:TRP:HB3	3:B:1022:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ALA:O	1:B:78:HIS:CD2	2.71	0.44
1:A:50:ASN:HB2	1:A:88:GLY:HA3	2.00	0.44
1:A:115:ILE:CD1	1:A:187:LEU:HD12	2.47	0.44
1:B:30:ASN:OD1	1:B:32:GLU:HG3	2.17	0.44
1:A:130:TRP:CE3	1:A:154:VAL:HB	2.53	0.43
1:B:74:ALA:O	1:B:78:HIS:HD2	2.02	0.43
1:A:46:TRP:HB2	1:A:92:SER:HB2	2.00	0.43
1:B:115:ILE:CD1	1:B:183:TYR:OH	2.66	0.43
1:B:113:TRP:O	1:B:164:ALA:HA	2.19	0.43
1:A:48:PHE:HB3	1:A:90:ASP:HB2	2.01	0.42
1:A:37:HIS:HA	1:A:38:PRO:HD2	1.83	0.42
1:A:105:GLU:OE1	1:A:109:ARG:NH2	2.52	0.42
1:B:91:TYR:HB2	1:B:154:VAL:CG1	2.50	0.42
1:A:164:ALA:C	1:A:165:ILE:CD1	2.88	0.42
1:A:165:ILE:CD1	1:A:183:TYR:CZ	3.02	0.42
1:A:174:ASP:HB2	3:A:1054:HOH:O	2.18	0.42
1:B:150:CYS:SG	1:B:168:THR:HG23	2.60	0.42
1:A:176:VAL:HG11	1:A:215:PHE:HD1	1.83	0.42
1:A:51:ASP:HB3	1:A:59:ASN:OD1	2.20	0.42
1:A:72:PHE:CD1	1:A:138:ILE:HD13	2.56	0.41
1:A:195:ILE:HD13	1:A:195:ILE:N	2.30	0.41
1:B:198:GLN:OE1	1:B:211:THR:CG2	2.69	0.41
1:B:205:THR:O	1:B:206:LYS:CB	2.69	0.41
1:B:116:THR:C	1:B:117:LEU:HD23	2.42	0.41
1:B:44:ALA:HB1	1:B:62:LEU:HD11	2.03	0.41
1:B:128:ARG:HH12	1:B:129:PHE:HE2	1.69	0.41
1:A:125:ASP:OD1	1:A:128:ARG:NH2	2.53	0.41
1:A:181:ARG:HG3	1:A:217:VAL:HG21	2.03	0.41
1:A:37:HIS:O	1:A:69:VAL:HG23	2.22	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	174/190 (92%)	169 (97%)	5 (3%)	0	100 100
1	B	188/190 (99%)	176 (94%)	7 (4%)	5 (3%)	6 3
All	All	362/380 (95%)	345 (95%)	12 (3%)	5 (1%)	14 10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	207	SER
1	B	206	LYS
1	B	210	THR
1	B	191	PRO
1	B	209	SER

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	156/169 (92%)	140 (90%)	16 (10%)	9 8
1	B	164/169 (97%)	145 (88%)	19 (12%)	7 6
All	All	320/338 (95%)	285 (89%)	35 (11%)	8 7

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	40	GLN
1	A	68	THR
1	A	91	TYR
1	A	112	ARG
1	A	114	LEU
1	A	120	GLN
1	A	122	ARG
1	A	123	ARG
1	A	136	CYS
1	A	148	ASP

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Mol	Chain	Res	Type
1	A	165	ILE
1	A	179	ILE
1	A	195	ILE
1	A	206	LYS
1	A	217	VAL
1	B	40	GLN
1	B	52	LYS
1	B	60	LEU
1	B	61	ARG
1	B	86	MET
1	B	90	ASP
1	B	91	TYR
1	B	112	ARG
1	B	114	LEU
1	B	117	LEU
1	B	118	ASN
1	B	136	CYS
1	B	171	GLU
1	B	185	GLU
1	B	186	ARG
1	B	191	PRO
1	B	207	SER
1	B	209	SER
1	B	217	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	80	GLN
1	B	41	ASN
1	B	77	ASN
1	B	78	HIS

5.3.3 RNA

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)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	M7G	A	1000	-	26,31,31	2.15	6 (23%)	35,49,49	2.50	10 (28%)
2	M7G	B	1001	-	26,31,31	2.16	6 (23%)	35,49,49	2.44	8 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	M7G	A	1000	-	-	0/16/44/44	0/3/3/3
2	M7G	B	1001	-	-	0/16/44/44	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	M7G	C8-N9	-7.70	1.34	1.45
2	A	1000	M7G	C8-N9	-7.69	1.34	1.45
2	A	1000	M7G	C8-N7	-2.77	1.30	1.43
2	B	1001	M7G	C8-N7	-2.65	1.31	1.43
2	B	1001	M7G	PB-O2B	-2.10	1.47	1.54
2	A	1000	M7G	C2-N3	-2.09	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	M7G	O6-C6	2.04	1.29	1.24
2	B	1001	M7G	O2'-C2'	2.60	1.49	1.43
2	B	1001	M7G	C4-N3	2.81	1.38	1.34
2	A	1000	M7G	C1'-N9	2.86	1.50	1.44
2	A	1000	M7G	C6-N1	3.41	1.39	1.33
2	B	1001	M7G	C6-N1	3.60	1.39	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1000	M7G	C5-C6-N1	-8.36	110.61	123.46
2	B	1001	M7G	C5-C6-N1	-7.81	111.45	123.46
2	B	1001	M7G	C4-N9-C1'	-4.61	115.60	126.70
2	A	1000	M7G	C4-N9-C1'	-4.50	115.86	126.70
2	B	1001	M7G	PA-O3A-PB	-3.97	119.35	132.67
2	B	1001	M7G	C5-C4-N3	-3.30	123.61	126.82
2	A	1000	M7G	C5-C4-N3	-3.11	123.79	126.82
2	A	1000	M7G	O4'-C4'-C3'	-3.10	98.90	105.15
2	B	1001	M7G	O4'-C4'-C3'	-2.16	100.79	105.15
2	A	1000	M7G	PA-O3A-PB	-2.09	125.67	132.67
2	A	1000	M7G	C3'-C2'-C1'	-2.07	97.24	101.40
2	A	1000	M7G	CM7-N7-C8	2.06	126.37	120.52
2	B	1001	M7G	O3A-PA-O5'	2.29	109.01	102.94
2	A	1000	M7G	O3A-PA-O5'	3.01	110.93	102.94
2	B	1001	M7G	C5-C4-N9	3.15	110.82	106.18
2	A	1000	M7G	C5-C4-N9	3.69	111.61	106.18
2	B	1001	M7G	C6-N1-C2	7.28	126.05	115.94
2	A	1000	M7G	C6-N1-C2	7.39	126.19	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	178/190 (93%)	1.28	33 (18%)	2 1	3, 11, 21, 41	0
1	B	190/190 (100%)	2.09	80 (42%)	0 0	3, 14, 32, 52	0
All	All	368/380 (96%)	1.69	113 (30%)	1 0	3, 13, 28, 52	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	208	GLY	10.1
1	B	207	SER	8.9
1	B	211	THR	8.3
1	A	207	SER	7.9
1	B	191	PRO	7.8
1	B	61	ARG	5.7
1	B	217	VAL	5.6
1	A	117	LEU	5.0
1	B	209	SER	4.9
1	A	217	VAL	4.9
1	B	29	ALA	4.8
1	B	210	THR	4.5
1	B	193	ILE	4.4
1	B	28	VAL	4.1
1	A	175	ALA	4.0
1	B	63	ILE	3.9
1	A	193	ILE	3.8
1	B	145	TYR	3.8
1	B	35	ILE	3.7
1	B	34	TYR	3.7
1	B	64	SER	3.7
1	B	153	VAL	3.5
1	A	165	ILE	3.4
1	B	137	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	194	VAL	3.4
1	A	115	ILE	3.2
1	A	187	LEU	3.2
1	B	146	SER	3.2
1	B	205	THR	3.2
1	B	204	ALA	3.2
1	B	85	LEU	3.2
1	B	66	PHE	3.1
1	B	165	ILE	3.1
1	A	206	LYS	3.1
1	A	151	GLY	3.1
1	A	191	PRO	3.1
1	A	116	THR	3.0
1	A	123	ARG	3.0
1	B	156	VAL	3.0
1	B	30	ASN	3.0
1	B	98	ILE	3.0
1	A	215	PHE	2.9
1	B	56	TRP	2.9
1	B	44	ALA	2.9
1	A	176	VAL	2.9
1	A	113	TRP	2.9
1	B	102	TRP	2.8
1	B	38	PRO	2.8
1	B	83	SER	2.8
1	B	150	CYS	2.8
1	B	163	ILE	2.7
1	B	164	ALA	2.7
1	A	190	PRO	2.7
1	B	57	GLN	2.7
1	B	115	ILE	2.6
1	B	118	ASN	2.6
1	B	43	TRP	2.6
1	B	80	GLN	2.6
1	B	40	GLN	2.6
1	B	87	PRO	2.5
1	B	158	ALA	2.5
1	B	147	ASP	2.5
1	B	94	PHE	2.5
1	B	37	HIS	2.5
1	B	111	GLY	2.5
1	B	173	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	152	ALA	2.5
1	B	54	LYS	2.4
1	B	46	TRP	2.4
1	B	48	PHE	2.4
1	A	216	VAL	2.4
1	B	136	CYS	2.4
1	B	42	ARG	2.4
1	B	192	LYS	2.4
1	B	33	HIS	2.3
1	A	144	ASP	2.3
1	B	195	ILE	2.3
1	B	100	PRO	2.3
1	B	104	ASP	2.3
1	B	59	ASN	2.3
1	B	113	TRP	2.3
1	B	141	SER	2.3
1	B	144	ASP	2.3
1	A	182	VAL	2.3
1	A	178	HIS	2.3
1	A	166	TRP	2.3
1	B	45	LEU	2.3
1	B	130	TRP	2.3
1	A	142	PHE	2.2
1	A	167	THR	2.2
1	B	155	ASN	2.2
1	B	151	GLY	2.2
1	B	170	CYS	2.2
1	A	164	ALA	2.2
1	B	154	VAL	2.2
1	B	49	LYS	2.1
1	B	143	ASP	2.1
1	A	160	GLY	2.1
1	B	81	LEU	2.1
1	A	138	ILE	2.1
1	B	73	TRP	2.1
1	B	134	LEU	2.1
1	B	179	ILE	2.1
1	B	75	LEU	2.1
1	B	67	ASP	2.1
1	A	173	ARG	2.1
1	A	181	ARG	2.1
1	A	153	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	131	LEU	2.0
1	B	86	MET	2.0
1	A	149	VAL	2.0
1	A	152	ALA	2.0
1	B	31	PRO	2.0

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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	M7G	A	1000	29/29	0.87	0.17	-0.74	9,17,25,27	0
2	M7G	B	1001	29/29	0.82	0.20	-1.40	11,22,25,27	0

6.5 Other polymers (i)

There are no such residues in this entry.