Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 09:48 am BST

PDB ID	:	6D9L
Title	:	Ternary RsAgo Complex with Guide RNA and Target DNA Containing G-A Non-canonical Pair
Authors	:	Liu, Y.; Esyunina, D.; Olovnikov, I.; Teplova, M.; Patel, D.J.
Deposited on	:	2018-04-30
Resolution	:	2.60 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 following versions of software and data (see references ①) were used in the production of this report:

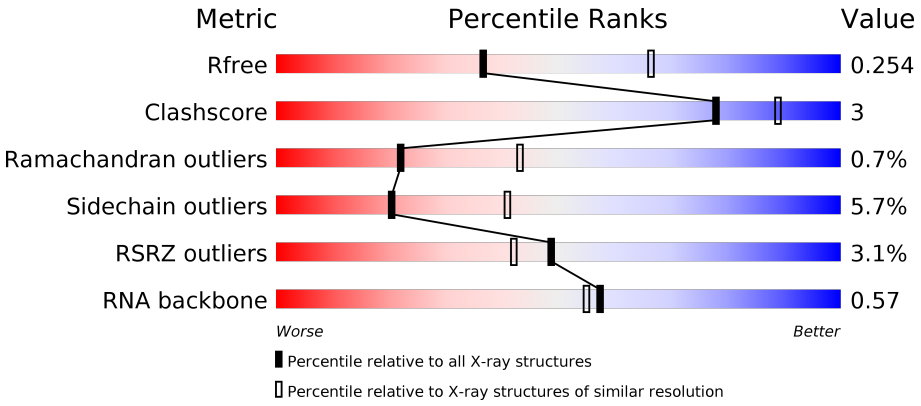
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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 <=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	791	2% 85% 9%
1	F	791	4% 87% 8%
2	C	18	56% 44%
2	H	18	67% 33%

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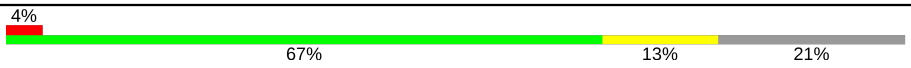
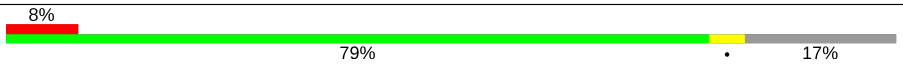
Mol	Chain	Length	Quality of chain
3	G	24	
3	J	24	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13318 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	758	Total	C	N	O	S	0	0	0
			5843	3713	1046	1068	16			
1	F	758	Total	C	N	O	S	0	0	0
			5764	3670	1019	1059	16			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP A4WYU7
A	-12	HIS	-	expression tag	UNP A4WYU7
A	-11	HIS	-	expression tag	UNP A4WYU7
A	-10	HIS	-	expression tag	UNP A4WYU7
A	-9	HIS	-	expression tag	UNP A4WYU7
A	-8	HIS	-	expression tag	UNP A4WYU7
A	-7	HIS	-	expression tag	UNP A4WYU7
A	-6	ASP	-	expression tag	UNP A4WYU7
A	-5	TYR	-	expression tag	UNP A4WYU7
A	-4	LYS	-	expression tag	UNP A4WYU7
A	-3	ASP	-	expression tag	UNP A4WYU7
A	-2	ASP	-	expression tag	UNP A4WYU7
A	-1	ASP	-	expression tag	UNP A4WYU7
A	0	ASP	-	expression tag	UNP A4WYU7
A	1	LYS	-	expression tag	UNP A4WYU7
F	-13	MET	-	initiating methionine	UNP A4WYU7
F	-12	HIS	-	expression tag	UNP A4WYU7
F	-11	HIS	-	expression tag	UNP A4WYU7
F	-10	HIS	-	expression tag	UNP A4WYU7
F	-9	HIS	-	expression tag	UNP A4WYU7
F	-8	HIS	-	expression tag	UNP A4WYU7
F	-7	HIS	-	expression tag	UNP A4WYU7
F	-6	ASP	-	expression tag	UNP A4WYU7
F	-5	TYR	-	expression tag	UNP A4WYU7
F	-4	LYS	-	expression tag	UNP A4WYU7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	ASP	-	expression tag	UNP A4WYU7
F	-2	ASP	-	expression tag	UNP A4WYU7
F	-1	ASP	-	expression tag	UNP A4WYU7
F	0	ASP	-	expression tag	UNP A4WYU7
F	1	LYS	-	expression tag	UNP A4WYU7

- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*UP*AP*CP*UP*GP*CP*GP*CP*AP *GP*GP*UP*GP*AP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	18	Total	C	N	O	P	0	0	0
			387	172	70	127	18			
2	H	18	Total	C	N	O	P	0	0	0
			387	172	70	127	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	19	Total	C	N	O	P	0	0	0
			387	184	71	113	19			
3	J	20	Total	C	N	O	P	0	0	0
			409	194	76	119	20			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	66	Total	O	0	0
			66	66		
5	C	7	Total	O	0	0
			7	7		
5	G	14	Total	O	0	0
			14	14		

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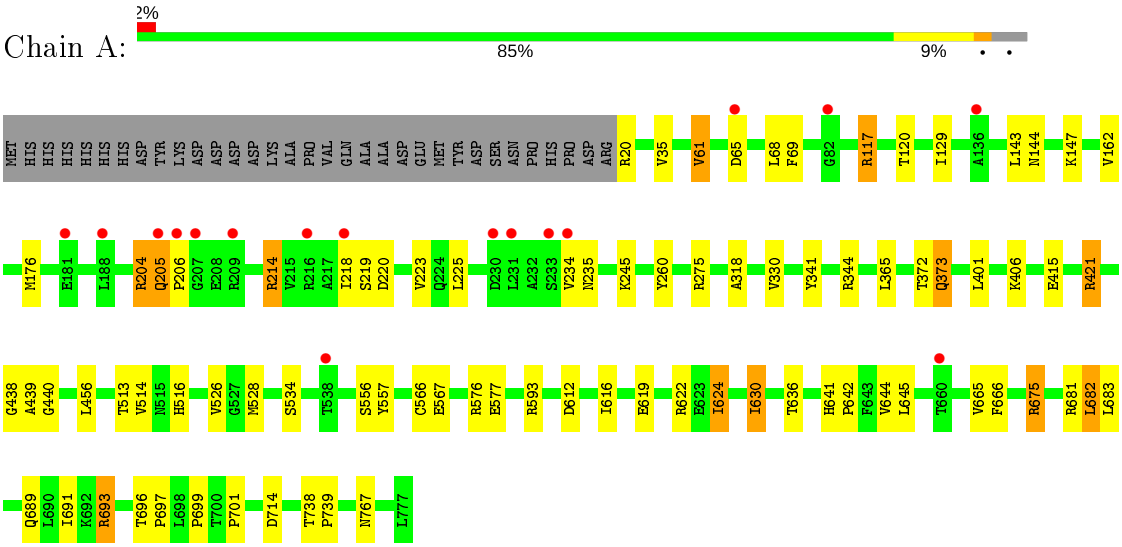
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	43	Total O 43 43	0	0
5	H	1	Total O 1 1	0	0
5	J	8	Total O 8 8	0	0

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 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.

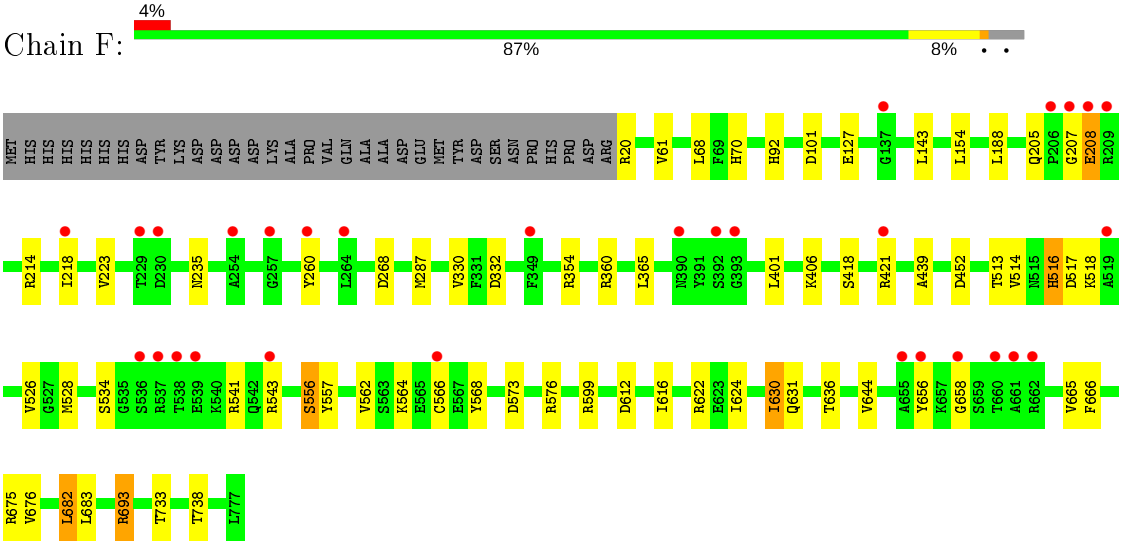
• Molecule 1: Uncharacterized protein

Chain A:



• Molecule 1: Uncharacterized protein

Chain F:

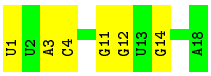


• Molecule 2: RNA (5'-R(P*UP*UP*AP*CP*UP*GP*CP*GP*CP*AP*GP*GP*UP*GP*AP*CP*GP*A)-3')

Chain C:

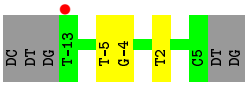
• Molecule 2: RNA (5'-R(P*UP*UP*AP*CP*UP*GP*CP*GP*CP*AP*GP*GP*UP*GP*AP*CP*GP*A)-3')

Chain H:



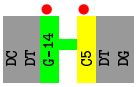
• Molecule 3: DNA (5'-D(P*TP*CP*GP*TP*CP*AP*CP*CP*TP*GP*AP*GP*CP*AP*GP*TP*AP*AP*C)-3')

Chain G:



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

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.05Å 118.25Å 117.83Å 90.00° 95.51° 90.00°	Depositor
Resolution (Å)	41.67 – 2.60 41.64 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (41.67-2.60) 97.6 (41.64-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.212 , 0.253 0.213 , 0.254	Depositor DCC
R_{free} test set	2824 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	45.9	Xtriage
Anisotropy	0.658	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 36.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13318	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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

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

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	0.31	0/5972	0.55	0/8115
1	F	0.30	0/5893	0.52	0/8021
2	C	0.56	1/432 (0.2%)	0.63	0/670
2	H	0.56	1/432 (0.2%)	0.63	0/670
3	G	0.30	0/433	0.77	0/665
3	J	0.26	0/458	0.77	0/704
All	All	0.33	2/13620 (0.0%)	0.56	0/18845

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	F	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	U	OP3-P	-10.34	1.48	1.61
2	H	1	U	OP3-P	-10.31	1.48	1.61

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	566	CYS	Peptide

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	5843	0	5724	35	0
1	F	5764	0	5579	31	0
2	C	387	0	195	5	0
2	H	387	0	195	2	0
3	G	387	0	214	3	0
3	J	409	0	225	1	0
4	C	1	0	0	0	0
4	H	1	0	0	0	0
5	A	66	0	0	0	0
5	C	7	0	0	0	0
5	F	43	0	0	0	0
5	G	14	0	0	0	0
5	H	1	0	0	0	0
5	J	8	0	0	0	0
All	All	13318	0	12132	73	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 3.

All (73) 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:204:ARG:HA	1:A:205:GLN:HB2	1.55	0.88
1:A:204:ARG:HA	1:A:205:GLN:CB	2.07	0.84
1:F:421:ARG:HG3	1:F:421:ARG:HH11	1.43	0.82
1:F:418:SER:O	1:F:421:ARG:NH1	2.17	0.77
1:F:61:VAL:HG13	1:F:68:LEU:HD21	1.73	0.69
1:F:624:ILE:HD11	1:F:630:ILE:HD12	1.75	0.68
1:A:218:ILE:HD12	1:A:223:VAL:HG12	1.78	0.66
1:A:513:THR:HG23	1:A:557:TYR:O	1.97	0.65
1:A:61:VAL:HG13	1:A:68:LEU:HD21	1.82	0.61
1:F:513:THR:HG21	1:F:556:SER:HB3	1.83	0.60
1:A:438:GLY:O	1:A:440:GLY:N	2.35	0.59
1:F:513:THR:HG23	1:F:557:TYR:O	2.02	0.58
1:F:624:ILE:HD11	1:F:630:ILE:CD1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:ASP:O	1:A:616:ILE:HG12	2.04	0.57
1:F:421:ARG:HH11	1:F:421:ARG:CG	2.13	0.57
1:F:513:THR:HG21	1:F:556:SER:CB	2.39	0.53
1:A:513:THR:CG2	1:A:557:TYR:O	2.57	0.52
1:F:421:ARG:NH1	1:F:421:ARG:CG	2.73	0.52
1:A:275:ARG:HD3	1:A:697:PRO:HG3	1.92	0.51
1:A:576:ARG:HD3	1:A:619:GLU:HG3	1.92	0.51
1:A:513:THR:HG21	1:A:556:SER:HB3	1.93	0.51
1:F:656:TYR:O	1:F:658:GLY:HA2	2.11	0.50
1:A:117:ARG:HH21	1:A:117:ARG:CG	2.24	0.50
2:C:3:A:H2'	2:C:4:C:C6	2.46	0.50
1:A:421:ARG:HG2	1:A:456:LEU:HD21	1.93	0.50
1:A:738:THR:OG1	1:A:739:PRO:HD2	2.12	0.49
3:G:-5:DT:H2"	3:G:-4:DG:O5'	2.13	0.49
1:F:543:ARG:NH2	2:H:14:G:OP1	2.46	0.49
1:A:162:VAL:HG12	1:A:318:ALA:HA	1.94	0.48
1:F:218:ILE:HD12	1:F:223:VAL:HG12	1.94	0.48
1:F:624:ILE:CD1	1:F:630:ILE:HD12	2.43	0.48
1:F:612:ASP:O	1:F:616:ILE:HG12	2.14	0.47
1:A:204:ARG:CA	1:A:205:GLN:CB	2.89	0.47
1:F:207:GLY:HA2	1:F:208:GLU:CB	2.45	0.47
1:F:68:LEU:HD22	1:F:70:HIS:CE1	2.49	0.47
1:A:341:TYR:OH	1:A:689:GLN:NE2	2.48	0.47
1:F:188:LEU:HD11	1:F:218:ILE:HG13	1.96	0.47
2:C:7:C:H2'	2:C:8:G:C8	2.50	0.46
1:A:693:ARG:HG2	3:G:2:DT:H5'	1.97	0.46
1:F:513:THR:HG22	1:F:514:VAL:N	2.30	0.46
1:A:645:LEU:HD21	1:A:682:LEU:HD23	1.98	0.46
2:H:3:A:H2'	2:H:4:C:C6	2.51	0.46
1:F:573:ASP:OD1	1:F:576:ARG:NH1	2.50	0.45
1:F:268:ASP:OD2	1:F:693:ARG:NH2	2.50	0.45
1:A:513:THR:HG22	1:A:514:VAL:N	2.32	0.45
1:A:691:ILE:HG23	1:A:696:THR:HG21	1.99	0.44
1:A:117:ARG:HH21	1:A:117:ARG:HG3	1.83	0.44
1:A:117:ARG:NH2	1:A:117:ARG:CG	2.79	0.44
1:A:675:ARG:HG3	1:A:681:ARG:CZ	2.48	0.43
1:F:543:ARG:NH2	1:F:568:TYR:OH	2.51	0.43
1:F:421:ARG:HH22	1:F:452:ASP:HB3	1.83	0.43
1:F:599:ARG:NH1	1:F:631:GLN:OE1	2.52	0.43
2:C:10:A:C2	3:G:-4:DG:C2	3.06	0.43
1:A:214:ARG:O	1:A:225:LEU:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:THR:O	1:A:373:GLN:C	2.56	0.42
1:A:641:HIS:NE2	1:A:701:PRO:O	2.49	0.42
1:A:176:MET:O	2:C:8:G:H5"	2.20	0.42
1:F:676:VAL:HG21	1:F:682:LEU:HD13	2.02	0.42
1:F:154:LEU:HD11	1:F:287:MET:HE2	2.02	0.42
3:J:5:DC:C2'	3:J:5:DC:O2	2.67	0.41
1:A:234:VAL:HG12	1:A:235:ASN:N	2.36	0.41
1:A:665:VAL:O	1:A:666:PHE:HB2	2.21	0.41
1:F:516:HIS:CE1	1:F:518:LYS:HG3	2.55	0.41
1:A:691:ILE:HD11	1:A:699:PRO:CG	2.50	0.41
1:A:513:THR:HG22	1:A:514:VAL:H	1.86	0.41
1:F:421:ARG:HG3	1:F:421:ARG:NH1	2.19	0.41
1:F:665:VAL:O	1:F:666:PHE:HB2	2.21	0.41
2:C:5:U:H2'	2:C:6:G:O4'	2.21	0.40
1:F:534:SER:HB2	1:F:541:ARG:HG2	2.03	0.40
1:A:641:HIS:HB2	1:A:642:PRO:HD2	2.02	0.40
1:A:624:ILE:HD11	1:A:630:ILE:CD1	2.52	0.40
1:A:68:LEU:HD23	1:A:69:PHE:N	2.37	0.40
1:F:354:ARG:O	1:F:360:ARG:NH2	2.53	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	756/791 (96%)	726 (96%)	23 (3%)	7 (1%)	17	35
1	F	756/791 (96%)	718 (95%)	34 (4%)	4 (0%)	29	52
All	All	1512/1582 (96%)	1444 (96%)	57 (4%)	11 (1%)	22	43

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	GLN
1	A	206	PRO
1	A	439	ALA
1	F	208	GLU
1	F	439	ALA
1	A	220	ASP
1	A	373	GLN
1	A	714	ASP
1	A	219	SER
1	F	205	GLN
1	F	260	TYR

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	600/672 (89%)	561 (94%)	39 (6%)	17 34
1	F	583/672 (87%)	554 (95%)	29 (5%)	24 47
All	All	1183/1344 (88%)	1115 (94%)	68 (6%)	20 41

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	35	VAL
1	A	61	VAL
1	A	65	ASP
1	A	117	ARG
1	A	120	THR
1	A	129	ILE
1	A	143	LEU
1	A	144	ASN
1	A	147	LYS
1	A	204	ARG
1	A	214	ARG
1	A	245	LYS

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Mol	Chain	Res	Type
1	A	260	TYR
1	A	330	VAL
1	A	344	ARG
1	A	365	LEU
1	A	401	LEU
1	A	406	LYS
1	A	415	GLU
1	A	421	ARG
1	A	516	HIS
1	A	526	VAL
1	A	528	MET
1	A	534	SER
1	A	566	CYS
1	A	567	GLU
1	A	577	GLU
1	A	593	ARG
1	A	622	ARG
1	A	624	ILE
1	A	630	ILE
1	A	636	THR
1	A	644	VAL
1	A	675	ARG
1	A	682	LEU
1	A	683	LEU
1	A	693	ARG
1	A	767	ASN
1	F	20	ARG
1	F	92	HIS
1	F	101	ASP
1	F	127	GLU
1	F	143	LEU
1	F	214	ARG
1	F	235	ASN
1	F	330	VAL
1	F	332	ASP
1	F	365	LEU
1	F	401	LEU
1	F	406	LYS
1	F	516	HIS
1	F	517	ASP
1	F	526	VAL
1	F	528	MET

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Mol	Chain	Res	Type
1	F	556	SER
1	F	562	VAL
1	F	564	LYS
1	F	622	ARG
1	F	630	ILE
1	F	636	THR
1	F	644	VAL
1	F	675	ARG
1	F	682	LEU
1	F	683	LEU
1	F	693	ARG
1	F	733	THR
1	F	738	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	465	HIS
1	A	591	ASN
1	A	689	GLN
1	F	140	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	17/18 (94%)	0	0
2	H	17/18 (94%)	2 (11%)	0
All	All	34/36 (94%)	2 (5%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	H	11	G
2	H	12	G

There are no RNA pucker outliers to report.

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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	758/791 (95%)	-0.07	17 (2%) 62 56	24, 46, 86, 120	3 (0%)
1	F	758/791 (95%)	0.10	30 (3%) 38 31	27, 56, 91, 135	3 (0%)
2	C	18/18 (100%)	-0.65	0 100 100	27, 37, 68, 87	0
2	H	18/18 (100%)	-0.38	0 100 100	35, 44, 60, 60	0
3	G	19/24 (79%)	-0.37	1 (5%) 26 20	35, 41, 96, 128	0
3	J	20/24 (83%)	-0.28	2 (10%) 7 4	35, 57, 102, 106	0
All	All	1591/1666 (95%)	-0.01	50 (3%) 49 42	24, 51, 87, 135	6 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	660	THR	5.2
1	F	519	ALA	4.7
3	G	-13	DT	4.3
1	A	230	ASP	4.3
1	F	207	GLY	4.3
1	A	206	PRO	4.0
1	F	538	THR	4.0
1	F	661	ALA	3.8
1	A	207	GLY	3.7
1	F	218	ILE	3.6
1	F	206	PRO	3.4
1	F	536	SER	3.3
1	A	233	SER	3.3
1	A	209	ARG	3.2
1	F	662	ARG	3.1
1	F	566	CYS	3.0
1	A	660	THR	3.0
1	F	656	TYR	2.9
1	F	137	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	208	GLU	2.9
1	A	231	LEU	2.8
1	A	234	VAL	2.8
1	A	218	ILE	2.7
1	F	655	ALA	2.7
1	A	188	LEU	2.6
1	F	393	GLY	2.6
1	F	537	ARG	2.6
3	J	-14	DG	2.6
1	F	421	ARG	2.5
1	A	136	ALA	2.5
1	F	264	LEU	2.5
1	A	82	GLY	2.5
1	F	209	ARG	2.5
1	F	543	ARG	2.5
1	F	392	SER	2.4
1	F	390	ASN	2.4
1	F	230	ASP	2.4
1	A	65	ASP	2.3
1	A	181	GLU	2.2
1	F	260	TYR	2.2
1	A	205	GLN	2.2
1	F	658	GLY	2.1
1	F	229	THR	2.1
1	A	538	THR	2.1
1	F	254	ALA	2.1
1	F	349	PHE	2.1
3	J	5	DC	2.1
1	F	539	GLU	2.0
1	F	257	GLY	2.0
1	A	216	ARG	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

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. 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	B-factors(Å^2)	Q<0.9
4	MG	H	101	1/1	0.86	0.30	38,38,38,38	0
4	MG	C	101	1/1	0.95	0.14	35,35,35,35	0

6.5 Other polymers

There are no such residues in this entry.