



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 03:33 PM BST

PDB ID : 6D95
Title : Ternary RsAgo Complex with Guide RNA Paired and Target DNA containing A8-A8' Non-Canonical Pair
Authors : Liu, Y.; Esyunina, D.; Olovnikov, I.; Teplova, M.; Patel, D.J.
Deposited on : 2018-04-27
Resolution : 1.85 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:

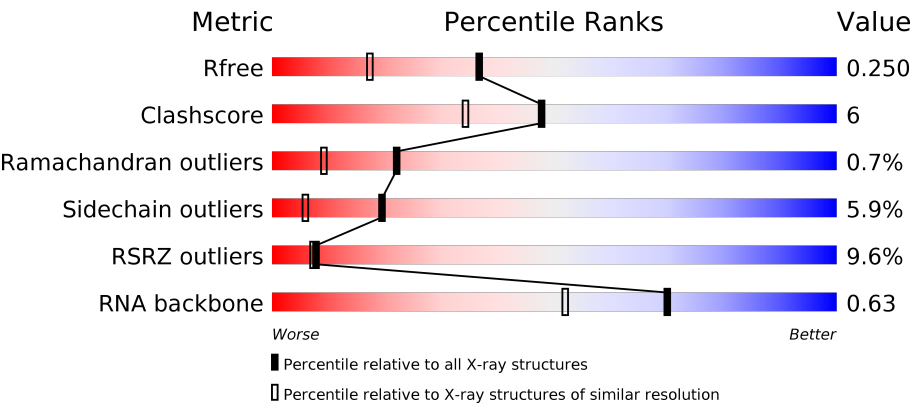
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)
RNA backbone	3102	1026 (2.40-1.32)

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	758	<div><div>7%</div><div><div></div><div>84%</div><div>14%</div><div>..</div></div></div>
1	F	758	<div><div>12%</div><div><div></div><div>87%</div><div>10%</div><div>.</div></div></div>
2	B	18	<div><div></div><div><div>50%</div><div>39%</div><div>11%</div></div></div>
2	H	18	<div><div>6%</div><div><div></div><div>50%</div><div>44%</div><div>6%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	24	<div><div></div><div>4%</div><div>63%</div><div>17%</div><div>21%</div></div>
3	J	24	<div><div></div><div>13%</div><div>63%</div><div>25%</div><div>13%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13786 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
			5761	3673	1023	1049	16			
1	F	755	Total	C	N	O	S	0	0	0
			5725	3649	1013	1047	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	18	Total	C	N	O	P	0	0	0
			386	172	70	126	18			
2	H	18	Total	C	N	O	P	0	2	0
			429	191	78	140	20			

- Molecule 3 is a DNA chain called DNA 24-Mer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	19	Total	C	N	O	P	0	0	0
			387	184	71	113	19			
3	J	21	Total	C	N	O	P	0	0	0
			429	204	78	126	21			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		

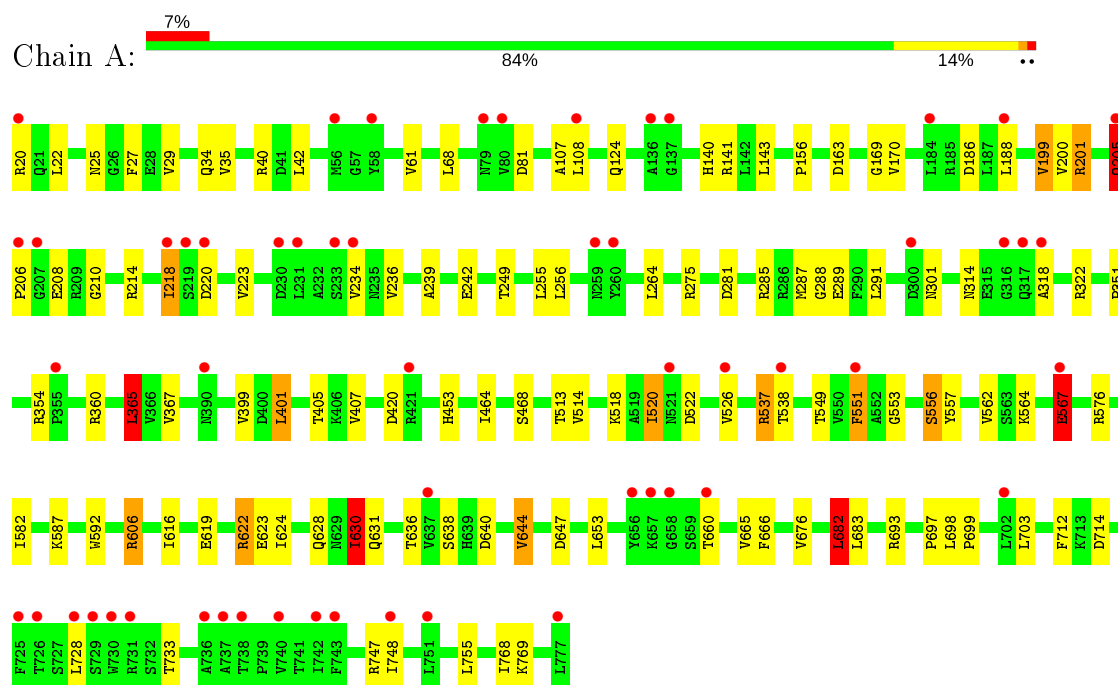
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	277	Total 277	O 277	0	0
5	B	48	Total 48	O 48	0	0
5	F	218	Total 218	O 218	0	0
5	C	43	Total 43	O 43	0	0
5	H	42	Total 42	O 42	0	0
5	J	37	Total 37	O 37	0	0

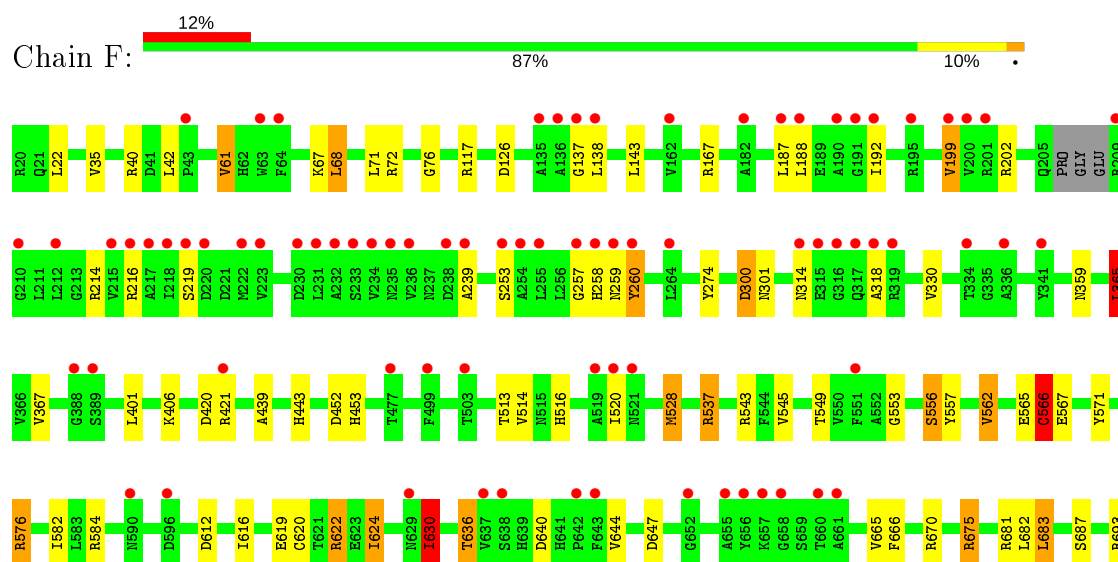
3 Residue-property plots

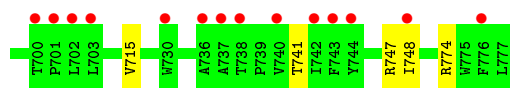
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Uncharacterized protein



• Molecule 1: Uncharacterized protein

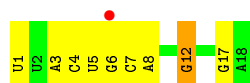




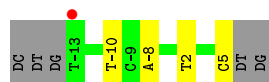
- Molecule 2: RNA (5'-R(P*UP*UP*AP*CP*UP*GP*CP*AP*CP*AP*GP*GP*UP*GP*AP*CP*GP*A)-3')



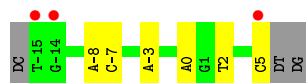
- Molecule 2: RNA (5'-R(P*UP*UP*AP*CP*UP*GP*CP*AP*CP*AP*GP*GP*UP*GP*AP*CP*GP*A)-3')



- Molecule 3: DNA 24-Mer



- Molecule 3: DNA 24-Mer



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.20Å 119.98Å 118.69Å 90.00° 95.51° 90.00°	Depositor
Resolution (Å)	37.44 – 1.85 37.42 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.3 (37.44-1.85) 98.4 (37.42-1.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.210 , 0.250 0.214 , 0.250	Depositor DCC
R_{free} test set	7973 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13786	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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](#)

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	0.62	1/5890 (0.0%)	0.83	12/8016 (0.1%)
1	F	0.56	1/5852 (0.0%)	0.78	6/7966 (0.1%)
2	B	0.82	2/431 (0.5%)	0.97	3/668 (0.4%)
2	H	0.78	1/479 (0.2%)	0.96	2/743 (0.3%)
3	C	0.56	0/433	0.92	2/665 (0.3%)
3	J	0.58	0/480	0.87	1/738 (0.1%)
All	All	0.60	5/13565 (0.0%)	0.82	26/18796 (0.1%)

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	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	U	OP3-P	-12.40	1.46	1.61
2	B	1	U	OP3-P	-9.27	1.50	1.61
1	F	566	CYS	CB-SG	-5.45	1.73	1.81
1	A	206	PRO	N-CD	5.23	1.55	1.47
2	B	7	C	O3'-P	-5.01	1.55	1.61

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	537	ARG	NE-CZ-NH2	-12.24	114.18	120.30
1	A	537	ARG	NE-CZ-NH1	11.08	125.84	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	15	A	O5'-P-OP2	-7.08	99.33	105.70
1	A	630	ILE	CB-CA-C	-6.87	97.86	111.60
1	F	537	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	F	537	ARG	NE-CZ-NH1	6.78	123.69	120.30
2	H	1	U	O5'-P-OP2	-6.71	99.66	105.70
2	H	12	G	O5'-P-OP2	-6.54	99.82	105.70
1	A	606	ARG	NE-CZ-NH1	6.47	123.53	120.30
2	B	6	G	O4'-C1'-N9	6.46	113.37	108.20
1	F	365	LEU	CA-CB-CG	6.43	130.09	115.30
3	C	-8	DA	C1'-O4'-C4'	-6.12	103.97	110.10
1	A	606	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	F	630	ILE	CB-CA-C	-5.78	100.05	111.60
3	J	-8	DA	C1'-O4'-C4'	-5.71	104.39	110.10
1	A	205	GLN	C-N-CD	5.61	140.19	128.40
1	A	281	ASP	CB-CG-OD1	5.55	123.29	118.30
2	B	5	U	O5'-P-OP2	-5.50	100.75	105.70
1	A	365	LEU	CA-CB-CG	5.48	127.90	115.30
1	F	683	LEU	CA-CB-CG	5.41	127.73	115.30
3	C	-10	DT	C1'-O4'-C4'	-5.33	104.77	110.10
1	A	401	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	551	PHE	CB-CA-C	-5.17	100.07	110.40
1	A	714	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	682	LEU	CA-CB-CG	5.12	127.07	115.30
1	F	675	ARG	NE-CZ-NH2	-5.09	117.75	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	565	GLU	Peptide
1	F	566	CYS	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	5761	0	5592	78	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	5725	0	5533	58	0
2	B	386	0	195	3	0
2	H	429	0	217	9	0
3	C	387	0	214	4	0
3	J	429	0	237	7	0
4	B	2	0	0	0	0
4	H	2	0	0	0	0
5	A	277	0	0	5	0
5	B	48	0	0	3	0
5	C	43	0	0	0	0
5	F	218	0	0	9	0
5	H	42	0	0	3	0
5	J	37	0	0	0	0
All	All	13786	0	11988	153	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 6.

All (153) 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:205:GLN:HG2	1:A:208:GLU:CB	2.00	0.91
1:F:67:LYS:CB	5:F:980:HOH:O	2.21	0.88
1:F:513:THR:HG23	1:F:557:TYR:O	1.75	0.87
3:J:5:DC:O2	3:J:5:DC:H2'	1.78	0.83
1:A:576:ARG:HD3	1:A:619:GLU:HG3	1.62	0.81
3:C:5:DC:H2'	3:C:5:DC:O2	1.81	0.81
2:H:6[A]:G:H1'	2:H:7[A]:C:C5	2.18	0.79
2:H:6[A]:G:H1'	2:H:7[A]:C:C6	2.21	0.76
1:A:256:LEU:CB	5:A:1043:HOH:O	2.34	0.76
1:F:72:ARG:NH2	1:F:76:GLY:O	2.20	0.75
1:A:513:THR:HG23	1:A:557:TYR:O	1.87	0.74
1:F:528:MET:HE1	1:F:571:TYR:HB2	1.72	0.72
1:A:61:VAL:HG13	1:A:68:LEU:HD21	1.72	0.71
1:A:549:THR:HG21	1:A:582:ILE:CD1	2.22	0.70
1:A:205:GLN:H	1:A:205:GLN:NE2	1.90	0.69
1:A:205:GLN:H	1:A:205:GLN:CD	1.97	0.67
1:A:20:ARG:N	5:A:802:HOH:O	2.27	0.67
1:F:167:ARG:HD3	5:F:983:HOH:O	1.97	0.65
1:A:537:ARG:CD	5:B:205:HOH:O	2.44	0.64
1:A:513:THR:HG22	1:A:514:VAL:N	2.12	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:ARG:HG3	1:A:623:GLU:N	2.13	0.63
1:F:528:MET:CE	1:F:571:TYR:HB2	2.29	0.63
1:A:354:ARG:O	1:A:360:ARG:NH2	2.32	0.62
3:C:5:DC:C2'	3:C:5:DC:O2	2.47	0.61
1:F:257:GLY:HA2	1:F:258:HIS:C	2.20	0.61
1:F:537:ARG:CD	5:H:201:HOH:O	2.48	0.60
1:F:359:ASN:HD21	1:F:443:HIS:CG	2.20	0.60
1:F:693:ARG:HG2	3:J:2:DT:H5'	1.84	0.59
1:A:537:ARG:HD2	5:B:205:HOH:O	2.03	0.59
1:F:537:ARG:HD2	5:H:201:HOH:O	2.03	0.59
1:F:117:ARG:CB	5:F:1004:HOH:O	2.51	0.59
3:J:5:DC:O2	3:J:5:DC:C2'	2.50	0.58
1:A:549:THR:HG21	1:A:582:ILE:HD11	1.85	0.57
1:A:624:ILE:HD11	1:A:630:ILE:CD1	2.35	0.56
1:F:301:ASN:N	1:F:301:ASN:OD1	2.37	0.56
1:F:619:GLU:OE2	1:F:622:ARG:NH1	2.38	0.56
1:F:624:ILE:HG12	1:F:630:ILE:HD12	1.87	0.56
1:F:576:ARG:HD3	1:F:619:GLU:HG3	1.88	0.56
1:A:537:ARG:HD3	5:B:205:HOH:O	2.03	0.56
1:A:576:ARG:HE	1:A:616:ILE:HD13	1.71	0.55
1:A:275:ARG:HB3	1:A:697:PRO:HB3	1.88	0.55
1:A:513:THR:HG22	1:A:514:VAL:H	1.71	0.55
1:F:647:ASP:O	1:F:666:PHE:HA	2.07	0.55
1:A:107:ALA:O	1:A:108:LEU:HD12	2.06	0.54
2:B:6:G:H1'	2:B:7:C:C5	2.42	0.54
1:F:774:ARG:NH1	5:F:805:HOH:O	2.38	0.54
2:B:6:G:H1'	2:B:7:C:C6	2.42	0.54
1:A:769:LYS:NZ	5:A:807:HOH:O	2.42	0.53
1:F:675:ARG:HG3	1:F:681:ARG:CZ	2.39	0.53
2:H:5:U:H2'	2:H:6[B]:G:C8	2.44	0.53
1:F:612:ASP:O	1:F:616:ILE:HG12	2.09	0.53
1:A:665:VAL:O	1:A:666:PHE:HB2	2.08	0.52
1:A:562:VAL:HG13	1:A:748:ILE:HD13	1.91	0.52
1:A:218:ILE:HD12	1:A:223:VAL:HG12	1.91	0.52
1:A:553:GLY:N	1:A:556:SER:O	2.33	0.51
1:F:202:ARG:NE	1:F:239:ALA:O	2.40	0.51
1:F:300:ASP:OD1	1:F:301:ASN:OD1	2.28	0.51
1:F:513:THR:HG22	1:F:514:VAL:N	2.25	0.51
1:A:314:ASN:HA	1:A:318:ALA:O	2.11	0.51
1:A:520:ILE:HD13	1:A:520:ILE:H	1.76	0.51
1:F:187:LEU:O	1:F:192:ILE:CB	2.59	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:LEU:HD21	1:A:287:MET:HE1	1.92	0.51
2:H:17:G:H8	2:H:17:G:H5''	1.76	0.51
1:A:301:ASN:N	1:A:301:ASN:OD1	2.44	0.50
1:A:365:LEU:HD13	1:A:367:VAL:CG2	2.41	0.50
1:F:553:GLY:N	1:F:556:SER:O	2.42	0.50
1:F:167:ARG:CD	5:F:983:HOH:O	2.58	0.50
1:A:549:THR:HG21	1:A:582:ILE:HD13	1.92	0.49
1:A:285:ARG:NH2	1:A:289:GLU:OE2	2.44	0.49
1:F:126:ASP:OD2	1:F:274:TYR:OH	2.20	0.49
1:F:61:VAL:HG13	1:F:68:LEU:HD21	1.95	0.49
1:A:200:VAL:HG23	1:A:210:GLY:C	2.32	0.49
1:F:584:ARG:NH1	5:F:802:HOH:O	2.28	0.49
1:F:640:ASP:O	3:J:-7:DC:H3'	2.13	0.49
1:A:360:ARG:HB3	1:A:405:THR:HG23	1.93	0.49
1:A:587:LYS:HD3	1:A:592:TRP:CE3	2.47	0.49
1:F:537:ARG:HD3	5:H:201:HOH:O	2.10	0.49
2:B:3:A:H2'	2:B:4:C:C6	2.47	0.49
1:A:201:ARG:NH1	1:A:205:GLN:OE1	2.43	0.48
1:F:365:LEU:HD13	1:F:367:VAL:CG2	2.44	0.48
1:F:314:ASN:HA	1:F:318:ALA:O	2.12	0.48
1:A:624:ILE:HD11	1:A:630:ILE:HD12	1.96	0.48
1:A:513:THR:HG21	1:A:556:SER:CB	2.44	0.47
2:H:17:G:H5''	2:H:17:G:C8	2.49	0.47
1:A:468:SER:HB2	1:A:755:LEU:CD2	2.44	0.47
1:A:218:ILE:CD1	1:A:223:VAL:HG12	2.44	0.47
1:A:606:ARG:NE	5:A:801:HOH:O	2.10	0.47
1:F:199:VAL:HG13	1:F:239:ALA:HB1	1.97	0.47
2:H:6[B]:G:C2	3:J:0:DA:C2	3.03	0.47
1:A:199:VAL:HG13	1:A:239:ALA:HB1	1.97	0.47
1:A:205:GLN:CG	1:A:208:GLU:CB	2.86	0.47
1:F:562:VAL:HG21	1:F:748:ILE:HD11	1.96	0.46
1:A:29:VAL:HG21	1:A:170:VAL:HG23	1.97	0.46
1:F:549:THR:HG21	1:F:582:ILE:CD1	2.46	0.46
1:F:665:VAL:O	1:F:666:PHE:HB2	2.15	0.46
1:A:40:ARG:HD2	1:A:81:ASP:O	2.16	0.46
1:A:223:VAL:HG22	1:A:234:VAL:O	2.16	0.46
1:A:287:MET:HE2	1:A:291:LEU:HD11	1.97	0.46
1:A:249:THR:HG22	1:A:264:LEU:HD11	1.98	0.46
1:A:513:THR:HG21	1:A:556:SER:OG	2.15	0.46
1:A:638:SER:HB2	1:A:703:LEU:HB3	1.98	0.46
1:F:566:CYS:N	1:F:567:GLU:HB2	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:61:VAL:HG13	1:F:68:LEU:CD2	2.45	0.46
2:H:7[B]:C:H2'	2:H:8:A:C8	2.51	0.46
1:A:567:GLU:HA	5:A:1020:HOH:O	2.16	0.45
1:F:35:VAL:HG13	1:F:71:LEU:HD13	1.98	0.45
1:A:698:LEU:HD12	1:A:699:PRO:HD2	1.97	0.45
1:A:693:ARG:CG	3:C:2:DT:H5'	2.46	0.45
2:H:3:A:H2'	2:H:4:C:C6	2.52	0.45
1:F:513:THR:HG21	1:F:556:SER:HB3	1.98	0.45
1:A:624:ILE:CD1	1:A:630:ILE:HD12	2.47	0.45
1:A:624:ILE:HD12	1:A:628:GLN:HB2	1.99	0.45
1:A:25:ASN:HB3	1:A:644:VAL:HG13	1.99	0.45
3:J:-3:DA:N3	3:J:-3:DA:H2'	2.31	0.45
1:F:620:CYS:O	1:F:624:ILE:HG23	2.15	0.45
1:F:636:THR:CG2	5:F:955:HOH:O	2.65	0.45
1:F:513:THR:HG22	1:F:514:VAL:H	1.80	0.44
1:A:624:ILE:HG12	1:A:630:ILE:HD12	1.98	0.44
1:F:359:ASN:HD21	1:F:443:HIS:CD2	2.35	0.44
1:F:137:GLY:O	1:F:138:LEU:HD23	2.18	0.44
1:A:624:ILE:HD11	1:A:630:ILE:HD13	1.99	0.44
1:F:681:ARG:CZ	1:F:715:VAL:CG1	2.96	0.44
1:A:156:PRO:HA	1:A:169:GLY:O	2.17	0.43
1:F:543:ARG:NH2	5:F:812:HOH:O	2.51	0.43
1:A:143:LEU:HD23	1:A:143:LEU:HA	1.80	0.43
1:F:624:ILE:CD1	1:F:630:ILE:HD12	2.49	0.43
1:F:260:TYR:OH	3:J:0:DA:OP1	2.30	0.43
1:F:420:ASP:O	1:F:453:HIS:NE2	2.51	0.42
1:F:545:VAL:HG22	1:F:567:GLU:HB3	1.99	0.42
1:A:107:ALA:C	1:A:108:LEU:HD12	2.40	0.42
1:F:670:ARG:H	1:F:687:SER:HB3	1.83	0.42
1:A:647:ASP:O	1:A:666:PHE:HA	2.19	0.42
1:A:676:VAL:CG2	1:A:682:LEU:HD22	2.50	0.42
1:A:399:VAL:HG22	1:A:407:VAL:HG23	2.01	0.42
1:A:631:GLN:HB3	1:A:712:PHE:HB2	2.02	0.42
1:F:675:ARG:HA	1:F:681:ARG:HD3	2.01	0.42
1:A:27:PHE:CZ	1:A:288:GLY:HA3	2.55	0.42
1:F:681:ARG:CZ	1:F:715:VAL:HG13	2.49	0.42
1:A:587:LYS:NZ	1:A:624:ILE:O	2.52	0.41
1:A:464:ILE:HD12	1:A:464:ILE:HA	1.90	0.41
1:A:747:ARG:HA	1:A:747:ARG:NE	2.35	0.41
1:A:351:PRO:O	1:A:354:ARG:HG2	2.21	0.41
1:A:513:THR:CG2	1:A:514:VAL:N	2.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:7[A]:C:H2'	2:H:8:A:C8	2.55	0.41
1:A:420:ASP:O	1:A:453:HIS:NE2	2.54	0.41
1:A:693:ARG:HG2	3:C:2:DT:H5'	2.02	0.41
1:A:29:VAL:CG2	1:A:170:VAL:HG23	2.51	0.41
1:F:513:THR:HG21	1:F:556:SER:CB	2.50	0.41
1:F:253:SER:HB3	1:F:260:TYR:CE2	2.56	0.41
1:A:140:HIS:CE1	1:A:255:LEU:HD22	2.56	0.41
1:A:551:PHE:HE1	1:A:582:ILE:HG23	1.86	0.41
1:A:205:GLN:N	1:A:205:GLN:NE2	2.65	0.40
1:F:584:ARG:HD2	5:F:864:HOH:O	2.21	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	756/758 (100%)	728 (96%)	23 (3%)	5 (1%)	22	9
1	F	751/758 (99%)	715 (95%)	31 (4%)	5 (1%)	22	9
All	All	1507/1516 (99%)	1443 (96%)	54 (4%)	10 (1%)	22	9

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	ASP
1	A	567	GLU
1	F	219	SER
1	F	259	ASN
1	F	300	ASP
1	A	518	LYS
1	F	143	LEU
1	F	439	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	236	VAL
1	A	768	ILE

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	580/642 (90%)	544 (94%)	36 (6%)	18	5
1	F	575/642 (90%)	543 (94%)	32 (6%)	21	7
All	All	1155/1284 (90%)	1087 (94%)	68 (6%)	19	6

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

Mol	Chain	Res	Type
1	A	22	LEU
1	A	34	GLN
1	A	35	VAL
1	A	42	LEU
1	A	124	GLN
1	A	141	ARG
1	A	163	ASP
1	A	186	ASP
1	A	188	LEU
1	A	199	VAL
1	A	201	ARG
1	A	205	GLN
1	A	214	ARG
1	A	218	ILE
1	A	242	GLU
1	A	322	ARG
1	A	365	LEU
1	A	401	LEU
1	A	520	ILE
1	A	522	ASP
1	A	526	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	538	THR
1	A	556	SER
1	A	564	LYS
1	A	567	GLU
1	A	622	ARG
1	A	630	ILE
1	A	636	THR
1	A	640	ASP
1	A	644	VAL
1	A	653	LEU
1	A	660	THR
1	A	682	LEU
1	A	683	LEU
1	A	728	LEU
1	A	733	THR
1	F	22	LEU
1	F	40	ARG
1	F	42	LEU
1	F	61	VAL
1	F	68	LEU
1	F	188	LEU
1	F	199	VAL
1	F	214	ARG
1	F	216	ARG
1	F	260	TYR
1	F	330	VAL
1	F	365	LEU
1	F	401	LEU
1	F	406	LYS
1	F	421	ARG
1	F	452	ASP
1	F	516	HIS
1	F	520	ILE
1	F	528	MET
1	F	556	SER
1	F	562	VAL
1	F	566	CYS
1	F	576	ARG
1	F	622	ARG
1	F	624	ILE
1	F	630	ILE
1	F	636	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	644	VAL
1	F	682	LEU
1	F	683	LEU
1	F	741	THR
1	F	747	ARG

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	30	ASN
1	A	516	HIS
1	A	591	ASN
1	F	84	HIS
1	F	359	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	17/18 (94%)	2 (11%)	0
2	H	15/18 (83%)	1 (6%)	0
All	All	32/36 (88%)	3 (9%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	12	G
2	B	18	A
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 monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 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, 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	758/758 (100%)	0.38	55 (7%) 15 14	23, 45, 74, 120	2 (0%)
1	F	755/758 (99%)	0.66	93 (12%) 4 4	27, 47, 84, 108	1 (0%)
2	B	18/18 (100%)	-0.18	0 100 100	30, 33, 56, 86	0
2	H	18/18 (100%)	-0.04	1 (5%) 24 23	30, 36, 51, 57	0
3	C	19/24 (79%)	-0.01	1 (5%) 26 25	28, 38, 101, 117	0
3	J	21/24 (87%)	0.22	3 (14%) 2 2	30, 45, 91, 106	0
All	All	1589/1600 (99%)	0.50	153 (9%) 8 7	23, 45, 79, 120	3 (0%)

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	219	SER	7.6
1	F	519	ALA	6.1
1	F	135	ALA	5.7
1	F	656	TYR	5.7
1	F	215	VAL	5.4
1	F	188	LEU	5.0
1	A	205	GLN	4.7
1	F	660	THR	4.5
1	F	239	ALA	4.4
1	F	234	VAL	4.3
1	F	258	HIS	4.3
1	F	195	ARG	4.2
1	A	260	TYR	4.2
1	F	136	ALA	4.2
1	F	238	ASP	4.2
1	F	218	ILE	4.1
1	F	260	TYR	4.0
1	F	661	ALA	4.0
1	F	264	LEU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	191	GLY	3.9
1	F	317	GLN	3.9
1	A	207	GLY	3.7
1	A	551	PHE	3.6
1	A	742	ILE	3.6
1	A	234	VAL	3.6
1	A	656	TYR	3.5
1	F	389	SER	3.5
1	A	58	TYR	3.5
3	J	-15	DT	3.4
1	A	740	VAL	3.4
1	A	219	SER	3.3
1	F	700	THR	3.3
1	F	257	GLY	3.3
1	F	63	TRP	3.3
1	F	138	LEU	3.3
1	A	188	LEU	3.2
1	F	703	LEU	3.2
1	F	737	ALA	3.1
1	F	222	MET	3.1
1	F	187	LEU	3.1
1	A	737	ALA	3.1
1	A	736	ALA	3.1
1	F	253	SER	3.1
1	A	660	THR	3.0
1	F	190	ALA	3.0
1	A	777	LEU	3.0
1	F	336	ALA	3.0
1	F	223	VAL	3.0
1	F	259	ASN	2.9
1	A	231	LEU	2.9
1	F	388	GLY	2.9
1	F	702	LEU	2.9
1	A	748	ILE	2.9
1	F	520	ILE	2.9
1	F	318	ALA	2.8
1	F	216	ARG	2.8
3	J	-14	DG	2.8
1	A	316	GLY	2.8
1	F	637	VAL	2.8
1	F	201	ARG	2.8
1	F	319	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	182	ALA	2.8
1	F	738	THR	2.8
1	A	726	THR	2.8
1	A	729	SER	2.8
1	F	551	PHE	2.8
1	F	776	PHE	2.8
1	F	64	PHE	2.7
1	F	316	GLY	2.7
1	F	220	ASP	2.7
1	F	217	ALA	2.7
1	A	137	GLY	2.7
1	A	731	ARG	2.7
1	F	315	GLU	2.7
1	A	108	LEU	2.7
3	C	-13	DT	2.6
1	F	421	ARG	2.6
1	F	236	VAL	2.6
1	F	743	PHE	2.6
1	A	728	LEU	2.6
1	A	538	THR	2.6
1	F	742	ILE	2.5
1	F	199	VAL	2.5
1	A	233	SER	2.5
1	F	736	ALA	2.5
1	A	743	PHE	2.5
3	J	5	DC	2.5
1	F	740	VAL	2.5
1	F	730	TRP	2.5
1	F	235	ASN	2.5
1	F	233	SER	2.5
1	A	20	ARG	2.5
1	F	212	LEU	2.4
1	A	521	ASN	2.4
1	F	162	VAL	2.4
1	A	206	PRO	2.4
1	A	300	ASP	2.4
1	A	751	LEU	2.4
1	A	56	MET	2.4
1	F	230	ASP	2.3
1	A	184	LEU	2.3
1	F	231	LEU	2.3
1	A	259	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	730	TRP	2.3
1	F	658	GLY	2.3
1	A	421	ARG	2.3
1	A	318	ALA	2.3
1	F	642	PRO	2.3
1	A	657	LYS	2.3
1	F	314	ASN	2.3
1	F	341	TYR	2.3
1	F	499	PHE	2.3
1	A	355	PRO	2.3
1	F	503	THR	2.3
2	H	6[A]	G	2.2
1	F	43	PRO	2.2
1	A	218	ILE	2.2
1	F	744	TYR	2.2
1	F	209	ARG	2.2
1	F	655	ALA	2.2
1	A	390	ASN	2.2
1	F	643	PHE	2.2
1	A	526	VAL	2.2
1	A	136	ALA	2.2
1	A	658	GLY	2.2
1	A	79	ASN	2.2
1	F	200	VAL	2.2
1	F	192	ILE	2.2
1	F	701	PRO	2.2
1	A	738	THR	2.2
1	F	334	THR	2.2
1	F	232	ALA	2.1
1	A	317	GLN	2.1
1	A	567	GLU	2.1
1	F	521	ASN	2.1
1	F	748	ILE	2.1
1	A	725	PHE	2.1
1	A	637	VAL	2.1
1	F	629	ASN	2.1
1	F	590	ASN	2.1
1	F	210	GLY	2.1
1	F	477	THR	2.1
1	F	638	SER	2.1
1	A	230	ASP	2.1
1	F	596	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	254	ALA	2.1
1	A	702	LEU	2.1
1	F	657	LYS	2.1
1	A	220	ASP	2.0
1	F	137	GLY	2.0
1	F	652	GLY	2.0
1	F	255	LEU	2.0
1	A	80	VAL	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 monosaccharides 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. The B-factors column lists the minimum, median, 95th 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(\AA^2)	Q<0.9
4	MG	H	102	1/1	0.97	0.06	48,48,48,48	0
4	MG	B	102	1/1	0.97	0.04	39,39,39,39	0
4	MG	B	101	1/1	0.99	0.18	27,27,27,27	0
4	MG	H	101	1/1	0.99	0.14	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.