



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2021 – 12:40 PM EDT

PDB ID : 7KI3
Title : Human Argonaute2:miR-122 bound to the HCV genotype 1a site-1 RNA
Authors : Gebert, L.F.R.; MacRae, I.J.
Deposited on : 2020-10-22
Resolution : 3.00 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 : 2.23.2
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) : 2.23.2

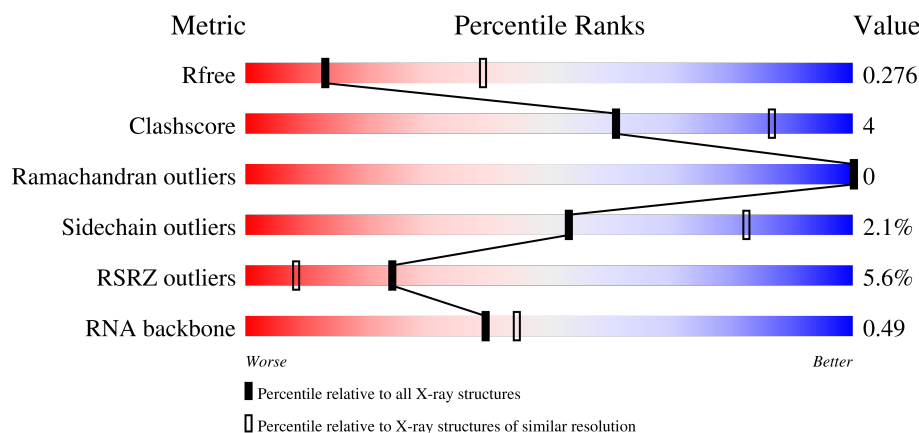
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.




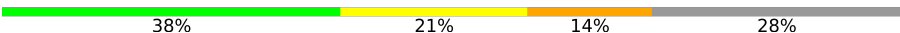
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	859	<div> <div>2%</div> <div>84%</div> <div>9%</div> <div>6%</div> </div>
1	D	859	<div> <div>8%</div> <div>79%</div> <div>12%</div> <div>9%</div> </div>
2	B	23	<div> <div>9%</div> <div>43%</div> <div>26%</div> <div>13%</div> <div>17%</div> </div>
2	E	23	<div> <div>26%</div> <div>17%</div> <div>52%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	29	 48% 41% 10%
3	F	29	 38% 21% 14% 28%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14417 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 Protein argonaute-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	804	Total	C	N	O	S	0	0	0
			6433	4091	1159	1142	41			
1	D	783	Total	C	N	O	S	0	0	0
			6266	3987	1125	1114	40			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	387	ASP	SER	engineered mutation	UNP Q9UKV8
A	824	ALA	SER	engineered mutation	UNP Q9UKV8
A	828	ASP	SER	engineered mutation	UNP Q9UKV8
A	831	ASP	SER	engineered mutation	UNP Q9UKV8
A	834	ALA	SER	engineered mutation	UNP Q9UKV8
D	387	ASP	SER	engineered mutation	UNP Q9UKV8
D	824	ALA	SER	engineered mutation	UNP Q9UKV8
D	828	ASP	SER	engineered mutation	UNP Q9UKV8
D	831	ASP	SER	engineered mutation	UNP Q9UKV8
D	834	ALA	SER	engineered mutation	UNP Q9UKV8

- Molecule 2 is a RNA chain called miR-122.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	19	Total	C	N	O	P	0	0	0
			413	183	75	136	19			
2	E	11	Total	C	N	O	P	0	0	0
			241	106	43	81	11			

- Molecule 3 is a RNA chain called HCV genotype 1a miR-122 site-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	29	Total	C	N	O	P	0	0	0
			614	275	112	199	28			

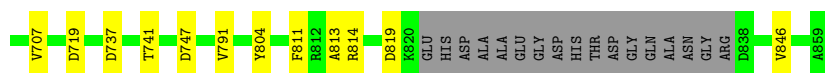
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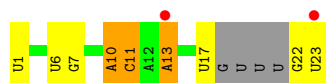
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	21	Total	C	N	O	P	0	0	0
			447	199	82	145	21			

- Molecule 4 is BARIUM ION (three-letter code: BA) (formula: Ba).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ba	0	0
			1	1		
4	C	1	Total	Ba	0	0
			1	1		
4	D	1	Total	Ba	0	0
			1	1		



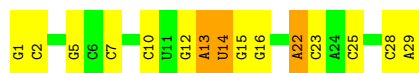
- Molecule 2: miR-122



- Molecule 2: miR-122



- Molecule 3: HCV genotype 1a miR-122 site-1



- Molecule 3: HCV genotype 1a miR-122 site-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.31Å 112.96Å 207.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.23 – 3.00 103.84 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (99.23-3.00) 89.3 (103.84-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.74 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.14rc1_3161	Depositor
R, R_{free}	0.233 , 0.276 0.233 , 0.276	Depositor DCC
R_{free} test set	2847 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	14417	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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

5.1 Standard geometry

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

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	0/6585	0.50	0/8911
1	D	0.32	0/6406	0.50	1/8656 (0.0%)
2	B	0.55	1/461 (0.2%)	0.79	0/714
2	E	0.73	1/268 (0.4%)	0.83	0/413
3	C	0.39	0/685	0.89	2/1066 (0.2%)
3	F	0.25	0/497	0.85	0/770
All	All	0.34	2/14902 (0.0%)	0.57	3/20530 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	U	OP3-P	-10.63	1.48	1.61
2	B	1	U	OP3-P	-10.36	1.48	1.61

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	10	C	C6-N1-C2	7.10	123.14	120.30
1	D	420	TYR	CB-CA-C	-5.27	99.86	110.40
3	C	16	G	C8-N9-C4	5.20	108.48	106.40

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	6433	0	6492	52	2
1	D	6266	0	6310	60	2
2	B	413	0	205	5	0
2	E	241	0	119	3	0
3	C	614	0	318	11	0
3	F	447	0	232	4	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	14417	0	13676	125	2

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 4.

All (125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:ALA:HA	1:D:308:VAL:HG23	1.49	0.94
1:A:64:GLU:O	3:C:1:G:C6	2.37	0.76
2:B:11:C:N4	3:C:5:G:O2'	2.22	0.73
1:A:179:ARG:NH1	2:B:13:A:N3	2.39	0.70
1:A:630:ARG:NH1	1:A:641:ASP:OD2	2.25	0.69
1:D:93:VAL:HG21	1:D:165:VAL:HG22	1.76	0.67
1:A:727:SER:HB2	1:A:729:ASN:ND2	2.10	0.67
1:A:230:VAL:O	1:A:234:VAL:HG23	1.95	0.67
1:D:289:ALA:HB1	1:D:309:ALA:HB2	1.78	0.66
1:D:502:GLU:OE2	1:D:506:ARG:NH1	2.28	0.66
1:D:230:VAL:HG11	1:D:341:LEU:HD22	1.79	0.64
1:D:289:ALA:HA	1:D:308:VAL:CG2	2.24	0.64
1:D:290:SER:O	1:D:307:THR:HG21	1.97	0.64
1:D:265:LEU:HD23	1:D:346:ILE:HD12	1.80	0.63
1:A:710:ARG:NE	2:B:10:A:N1	2.43	0.63
1:D:235:CYS:O	1:D:239:ASP:N	2.32	0.61
1:D:660:LYS:NZ	1:D:695:GLU:OE1	2.27	0.61
1:A:287:ARG:HB2	1:A:292:GLN:HB2	1.82	0.61
1:A:234:VAL:HG22	1:A:258:PHE:CE1	2.35	0.61
1:D:262:ILE:HG22	1:D:265:LEU:HD22	1.83	0.60
1:D:262:ILE:HD11	1:D:328:LEU:HD21	1.84	0.58
1:A:93:VAL:HG21	1:A:165:VAL:HG22	1.86	0.58
3:C:13:A:O2'	3:C:14:U:OP2	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:VAL:HG22	1:A:260:LYS:HE3	1.86	0.56
1:D:262:ILE:CD1	1:D:328:LEU:HD21	2.35	0.55
1:D:145:ASP:HB3	1:D:151:LEU:HG	1.89	0.55
1:D:234:VAL:HG22	1:D:258:PHE:CE1	2.42	0.55
1:D:68:ARG:NH2	1:D:95:ASP:O	2.39	0.54
1:A:558:GLN:OE1	3:C:28:C:O2'	2.26	0.53
1:D:308:VAL:HG21	1:D:327:CYS:SG	2.48	0.53
1:A:65:LYS:HG2	3:C:1:G:N2	2.23	0.53
1:A:262:ILE:HA	1:A:265:LEU:HD13	1.90	0.53
1:A:192:LEU:HG	1:A:198:VAL:HG23	1.92	0.52
1:D:234:VAL:HG22	1:D:258:PHE:CD1	2.45	0.52
1:A:671:VAL:HG11	1:A:679:VAL:HG21	1.92	0.51
2:E:3:G:H2'	2:E:4:A:C8	2.45	0.51
1:D:192:LEU:HD23	1:D:198:VAL:HG13	1.92	0.51
1:A:83:LYS:O	1:A:88:GLY:N	2.44	0.51
1:D:813:ALA:HB1	1:D:846:VAL:HG21	1.94	0.50
1:A:211:TRP:O	1:A:212:LYS:HG2	2.12	0.50
1:A:607:LYS:O	1:A:608:LYS:C	2.48	0.50
1:D:282:CYS:HB3	1:D:329:GLN:HB3	1.94	0.50
3:C:1:G:H2'	3:C:2:C:C6	2.47	0.50
1:A:322:TYR:HB3	1:A:325:LEU:HD23	1.93	0.49
1:D:145:ASP:HB2	1:D:151:LEU:HD12	1.94	0.49
3:F:6:C:H42	3:F:19:G:H1	1.59	0.49
1:A:365:ILE:HD13	3:C:25:C:H1'	1.94	0.49
1:D:207:ARG:NH2	1:D:673:GLU:OE2	2.45	0.49
1:D:59:LEU:HD22	1:D:130:VAL:CG1	2.43	0.49
1:A:268:GLU:HG3	1:A:347:VAL:HG22	1.94	0.49
1:D:417:SER:HB3	1:D:427:ILE:HG23	1.94	0.48
1:A:258:PHE:O	1:A:262:ILE:HG22	2.14	0.48
1:D:191:PRO:O	1:D:192:LEU:HD13	2.13	0.48
1:D:339:LEU:HD11	2:E:23:U:H4'	1.96	0.48
1:D:357:THR:HG22	1:D:358:ASP:N	2.29	0.47
2:B:6:U:HO2'	2:B:7:G:H8	1.61	0.47
1:A:202:PHE:HB3	1:A:382:LEU:CD2	2.44	0.46
1:A:169:LEU:HB3	1:A:170:PRO:HD3	1.98	0.46
1:A:354:LYS:HE2	3:C:7:C:H5''	1.96	0.46
1:D:569:VAL:HG11	1:D:791:VAL:HB	1.96	0.46
1:D:143:LEU:HD22	1:D:162:LEU:HD11	1.97	0.46
1:D:169:LEU:HB3	1:D:170:PRO:HD3	1.97	0.46
1:A:478:SER:HB3	1:A:483:MET:O	2.16	0.46
3:F:17:C:O2'	3:F:18:G:P	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:16:G:O2'	3:F:17:C:P	2.74	0.46
1:A:246:GLN:O	1:A:324:HIS:NE2	2.49	0.45
1:D:583:ARG:NH1	1:D:620:ALA:O	2.48	0.45
1:A:322:TYR:CB	1:A:325:LEU:HD23	2.46	0.45
1:D:737:ASP:HA	1:D:741:THR:HG21	1.98	0.45
1:A:727:SER:HB2	1:A:729:ASN:HD22	1.81	0.45
1:D:811:PHE:O	1:D:814:ARG:HG2	2.17	0.45
1:D:145:ASP:HB2	1:D:151:LEU:CD1	2.47	0.45
2:B:17:U:H3	3:C:1:G:H1	1.63	0.45
1:D:382:LEU:O	1:D:386:ALA:N	2.40	0.45
1:A:244:GLU:N	1:A:244:GLU:OE1	2.49	0.45
1:D:87:PHE:O	1:D:90:ARG:HG2	2.17	0.45
1:D:741:THR:HB	1:D:747:ASP:OD1	2.17	0.45
1:D:425:LYS:HD3	1:D:425:LYS:HA	1.71	0.44
1:A:325:LEU:HD22	1:A:325:LEU:N	2.33	0.44
1:D:502:GLU:O	1:D:506:ARG:HG3	2.17	0.44
1:A:115:LEU:N	1:A:115:LEU:HD12	2.33	0.44
1:D:225:TYR:CE2	1:D:265:LEU:HD11	2.53	0.43
1:A:333:GLU:OE1	1:A:333:GLU:N	2.45	0.43
1:A:737:ASP:HA	1:A:741:THR:HG21	1.99	0.43
1:A:87:PHE:O	1:A:90:ARG:NH1	2.50	0.43
1:D:75:VAL:HG21	1:D:94:PHE:CZ	2.53	0.43
1:A:202:PHE:CB	1:A:382:LEU:HD21	2.49	0.43
1:A:85:GLN:OE1	1:A:85:GLN:N	2.48	0.43
1:D:225:TYR:CZ	1:D:265:LEU:HD11	2.54	0.43
1:A:488:GLN:HB3	1:A:489:PRO:HD2	2.00	0.43
1:A:668:ARG:O	1:A:706:VAL:HA	2.19	0.43
1:D:119:LEU:HD22	1:D:128:PHE:CE1	2.54	0.43
1:A:813:ALA:HB1	1:A:846:VAL:CG2	2.49	0.42
1:D:618:MET:SD	1:D:652:GLN:HB3	2.59	0.42
1:A:45:PHE:CZ	1:A:383:MET:HG3	2.54	0.42
1:A:277:ARG:HD2	1:A:279:TYR:OH	2.19	0.42
1:D:531:GLU:OE2	1:D:534:ARG:NH1	2.42	0.42
1:D:619:ASP:OD1	1:D:622:PRO:HA	2.18	0.42
1:D:417:SER:HB3	1:D:427:ILE:CG2	2.48	0.42
1:A:161:ALA:O	1:A:165:VAL:HG23	2.19	0.42
1:D:337:THR:HG22	1:D:339:LEU:HD13	2.02	0.42
1:D:372:ALA:HB3	1:D:373:PRO:HD3	2.01	0.42
1:D:418:ILE:O	1:D:427:ILE:HA	2.19	0.42
1:A:268:GLU:CG	1:A:347:VAL:HG22	2.50	0.42
3:C:22:A:H2'	3:C:23:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:PHE:CZ	1:D:383:MET:HG3	2.54	0.42
1:D:192:LEU:HD11	1:D:363:THR:OG1	2.20	0.42
3:F:25:C:H2'	3:F:26:U:C6	2.54	0.42
1:A:136:SER:OG	1:A:137:CYS:N	2.53	0.41
1:D:39:LYS:NZ	1:D:719:ASP:OD2	2.53	0.41
1:A:202:PHE:HB3	1:A:382:LEU:HD21	2.03	0.41
1:A:202:PHE:CG	1:A:382:LEU:HD21	2.55	0.41
1:D:244:GLU:OE1	1:D:244:GLU:N	2.53	0.41
1:D:392:PRO:HA	1:D:395:ARG:HD3	2.02	0.41
1:A:59:LEU:HD12	1:A:94:PHE:CE1	2.56	0.41
1:A:267:VAL:HG13	1:A:281:VAL:HG21	2.02	0.41
1:D:269:ILE:HA	1:D:344:CYS:HA	2.02	0.40
1:D:695:GLU:HB2	1:D:698:TYR:HB2	2.03	0.40
3:C:15:G:H8	3:C:15:G:OP2	2.03	0.40
1:D:192:LEU:HD12	1:D:360:GLN:HG2	2.03	0.40
1:A:234:VAL:HG21	1:A:341:LEU:HD13	2.02	0.40
1:A:266:LYS:O	1:A:347:VAL:HG23	2.20	0.40
1:A:287:ARG:HA	1:A:288:PRO:HD3	1.91	0.40
1:D:147:LEU:HD13	1:D:212:LYS:HA	2.04	0.40
2:E:3:G:H2'	2:E:4:A:H8	1.86	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:CYS:SG	1:D:188:CYS:SG[2_654]	1.64	0.56
1:A:854:ARG:NE	1:D:148:SER:O[1_455]	2.02	0.18

5.3 Torsion angles

5.3.1 Protein backbone

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	796/859 (93%)	752 (94%)	44 (6%)	0	100	100
1	D	761/859 (89%)	715 (94%)	46 (6%)	0	100	100
All	All	1557/1718 (91%)	1467 (94%)	90 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	709/750 (94%)	699 (99%)	10 (1%)	67	88
1	D	691/750 (92%)	671 (97%)	20 (3%)	42	76
All	All	1400/1500 (93%)	1370 (98%)	30 (2%)	53	82

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	ARG
1	A	272	CYS
1	A	286	ARG
1	A	287	ARG
1	A	316	HIS
1	A	321	ARG
1	A	726	LYS
1	A	727	SER
1	A	804	TYR
1	A	819	ASP
1	D	66	CYS
1	D	189	SER
1	D	190	ASN
1	D	192	LEU
1	D	274	GLN
1	D	292	GLN
1	D	325	LEU
1	D	329	GLN

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Mol	Chain	Res	Type
1	D	338	TYR
1	D	344	CYS
1	D	365	ILE
1	D	423	ARG
1	D	424	ASN
1	D	461	GLN
1	D	462	CYS
1	D	496	GLN
1	D	506	ARG
1	D	707	VAL
1	D	804	TYR
1	D	819	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	18/23 (78%)	3 (16%)	2 (11%)
2	E	10/23 (43%)	1 (10%)	1 (10%)
3	C	28/29 (96%)	5 (17%)	0
3	F	19/29 (65%)	7 (36%)	2 (10%)
All	All	75/104 (72%)	16 (21%)	5 (6%)

All (16) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	11	C
2	B	13	A
2	B	23	U
3	C	12	G
3	C	13	A
3	C	14	U
3	C	22	A
3	C	29	A
2	E	23	U
3	F	6	C
3	F	7	C
3	F	8	G
3	F	16	G

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Mol	Chain	Res	Type
3	F	17	C
3	F	18	G
3	F	22	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	10	A
2	B	22	G
2	E	22	G
3	F	16	G
3	F	17	C

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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 [i](#)

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	804/859 (93%)	-0.11	19 (2%) 59 30	18, 45, 107, 141	0
1	D	783/859 (91%)	0.17	73 (9%) 8 3	18, 49, 150, 172	0
2	B	19/23 (82%)	0.46	2 (10%) 6 2	31, 72, 153, 155	0
2	E	11/23 (47%)	-0.19	0 100 100	29, 33, 142, 148	0
3	C	29/29 (100%)	0.04	0 100 100	44, 91, 151, 169	0
3	F	21/29 (72%)	0.09	0 100 100	43, 86, 130, 144	0
All	All	1667/1822 (91%)	0.04	94 (5%) 24 8	18, 47, 143, 172	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	240	PHE	7.0
1	D	328	LEU	6.5
1	D	258	PHE	6.4
1	D	130	VAL	6.3
1	D	279	TYR	6.3
1	D	92	PRO	6.2
1	D	93	VAL	6.2
1	D	295	PRO	5.8
1	D	55	TYR	5.6
1	D	252	ASP	5.6
1	D	121	GLY	5.6
1	D	131	SER	5.3
1	D	285	THR	5.2
1	D	133	LYS	5.2
1	D	327	CYS	5.1
1	D	284	VAL	4.9
1	D	247	GLN	4.6
1	D	241	LYS	4.6
1	A	328	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	288	PRO	4.4
1	D	253	SER	4.1
1	D	127	ILE	4.1
1	D	308	VAL	4.1
1	A	312	PHE	4.0
1	D	333	GLU	3.9
1	A	272	CYS	3.9
1	D	114	GLU	3.8
1	A	278	LYS	3.8
1	D	251	THR	3.6
1	D	278	LYS	3.6
1	D	424	ASN	3.6
1	D	86	ILE	3.4
1	A	287	ARG	3.4
1	A	819	ASP	3.4
2	B	13	A	3.4
1	A	273	GLY	3.3
1	A	341	LEU	3.3
1	D	275	MET	3.2
1	D	81	HIS	3.2
1	D	115	LEU	3.1
1	D	132	ILE	3.1
2	B	23	U	3.1
1	D	150	ARG	3.1
1	D	97	ARG	3.1
1	D	94	PHE	3.0
1	D	341	LEU	3.0
1	D	77	HIS	3.0
1	D	151	LEU	3.0
1	D	256	VAL	3.0
1	D	398	GLY	2.9
1	D	48	ASP	2.9
1	D	243	ILE	2.9
1	D	237	VAL	2.8
1	D	192	LEU	2.8
1	D	289	ALA	2.8
1	D	116	GLU	2.8
1	D	194	GLY	2.8
1	D	325	LEU	2.8
1	D	89	ASP	2.8
1	D	290	SER	2.7
1	D	80	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	312	PHE	2.7
1	D	135	VAL	2.6
1	D	246	GLN	2.6
1	A	274	GLN	2.6
1	A	289	ALA	2.6
1	D	317	LYS	2.6
1	A	315	ARG	2.6
1	D	254	GLN	2.5
1	D	90	ARG	2.5
1	D	73	GLU	2.5
1	D	59	LEU	2.5
1	D	293	THR	2.4
1	D	193	GLY	2.4
1	A	292	GLN	2.4
1	A	313	LYS	2.4
1	A	285	THR	2.4
1	A	423	ARG	2.4
1	D	400	MET	2.3
1	D	248	LYS	2.3
1	A	603	ALA	2.3
1	A	320	LEU	2.3
1	D	326	PRO	2.2
1	D	128	PHE	2.2
1	D	236	GLU	2.2
1	D	291	HIS	2.2
1	D	195	GLY	2.2
1	D	337	THR	2.2
1	D	95	ASP	2.2
1	A	293	THR	2.2
1	D	98	LYS	2.2
1	D	242	SER	2.1
1	A	268	GLU	2.1
1	D	310	GLN	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(Å ²)	Q<0.9
4	BA	C	101	1/1	0.89	0.07	128,128,128,128	0
4	BA	A	901	1/1	0.99	0.15	54,54,54,54	0
4	BA	D	901	1/1	0.99	0.14	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.