



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:30 PM UTC

PDB ID : 7KI3 / pdb_00007ki3
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

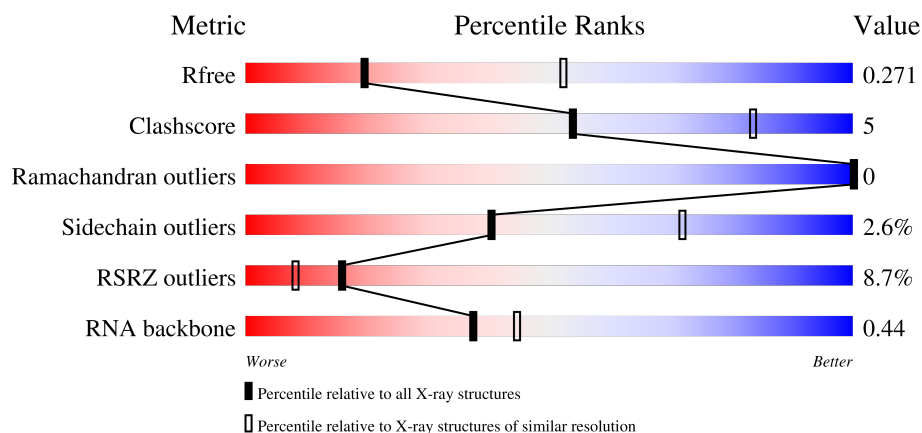
1 Overall quality at a glance

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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	5% 83% 10% 6%
1	D	859	11% 78% 13% 9%
2	B	23	4% 57% 13% 13% 17%
2	E	23	4% 30% 9% 9% 52%

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Mol	Chain	Length	Quality of chain
3	C	29	3% 55% 34% 10%
3	F	29	10% 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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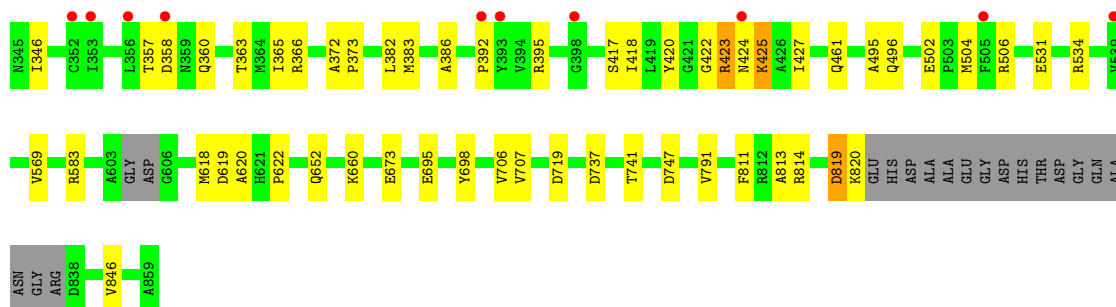
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	21	Total	C	N	O	P	0	0	0
			447	199	82	145	21			

- Molecule 4 is BARIUM ION (CCD ID: BA) (formula: Ba).

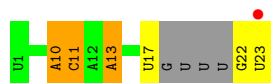
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ba	0	0
			1	1		
4	C	1	Total	Ba	0	0
			1	1		
4	D	1	Total	Ba	0	0
			1	1		

- Molecule 1: Protein argonaute-2

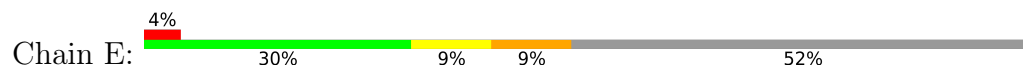




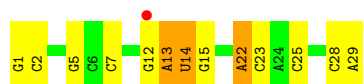
- Molecule 2: miR-122



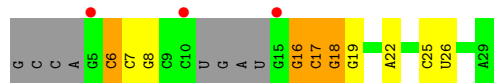
- Molecule 2: miR-122



- 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 99.23 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (99.23-3.00) 94.0 (99.23-3.00)	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 0.231 , 0.271	Depositor DCC
R_{free} test set	2848 reflections (4.83%)	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)	0.29 , 37.6	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 [i](#)

5.1 Standard geometry [i](#)

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	0.27	0/6585	0.47	4/8911 (0.0%)
1	D	0.31	2/6406 (0.0%)	0.50	4/8656 (0.0%)
2	B	0.15	0/461	0.41	0/714
2	E	0.17	0/268	0.37	0/413
3	C	0.28	0/685	0.40	0/1066
3	F	0.14	0/497	0.31	0/770
All	All	0.28	2/14902 (0.0%)	0.47	8/20530 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	422	GLY	C-N	-6.23	1.24	1.33
1	D	423	ARG	C-N	5.61	1.40	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	420	TYR	CB-CA-C	-8.16	99.86	111.85
1	A	288	PRO	CA-C-O	-6.46	116.53	121.31
1	A	286	ARG	N-CA-C	-6.16	105.08	112.59
1	D	422	GLY	CA-C-O	-6.11	117.70	122.52
1	A	689	GLU	CB-CA-C	-5.75	101.85	110.88
1	D	422	GLY	N-CA-C	-5.50	105.67	112.33
1	A	282	CYS	N-CA-C	5.11	118.97	112.12
1	D	423	ARG	N-CA-C	-5.07	107.10	113.28

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	59	2
1	D	6266	0	6310	64	2
2	B	413	0	205	4	0
2	E	241	0	119	4	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	136	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 5.

All (136) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:607:LYS:O	1:A:608:LYS:C	2.48	0.55
1:A:624:ARG:HA	1:A:856:MET:HE2	1.88	0.54
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:A:495:ALA:HB2	1:A:504:MET:HE1	1.94	0.50
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: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:A:159:ILE:HD12	1:A:213:MET:HE1	1.95	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
1:A:202:PHE:HB3	1:A:382:LEU:CD2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:16:G:O2'	3:F:17:C:P	2.74	0.46
2:E:22:G:O2'	2:E:23:U:O5'	2.34	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:159:ILE:CD1	1:A:213:MET:HE1	2.47	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:A:266:LYS:C	1:A:347:VAL:HG23	2.42	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:608:LYS:O	1:A:609:PRO:C	2.61	0.43
1:A:737:ASP:HA	1:A:741:THR:HG21	1.99	0.43
1:A:457:ALA:HB1	1:A:549:MET:HE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:819:ASP:O	1:D:820:LYS:C	2.63	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:495:ALA:HB2	1:D:504:MET:HE1	2.00	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
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:338:TYR:C	1:D:339:LEU:HD12	2.46	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:D:358:ASP:C	1:D:360:GLN:H	2.29	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 [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	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 [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	709/750 (94%)	695 (98%)	14 (2%)	48	76
1	D	691/750 (92%)	669 (97%)	22 (3%)	34	67
All	All	1400/1500 (93%)	1364 (97%)	36 (3%)	40	72

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	ARG
1	A	127	ILE

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Mol	Chain	Res	Type
1	A	248	LYS
1	A	266	LYS
1	A	272	CYS
1	A	286	ARG
1	A	287	ARG
1	A	290	SER
1	A	316	HIS
1	A	706	VAL
1	A	726	LYS
1	A	727	SER
1	A	818	VAL
1	A	819	ASP
1	D	66	CYS
1	D	114	GLU
1	D	189	SER
1	D	192	LEU
1	D	198	VAL
1	D	214	MET
1	D	274	GLN
1	D	281	VAL
1	D	292	GLN
1	D	325	LEU
1	D	329	GLN
1	D	330	VAL
1	D	365	ILE
1	D	366	ARG
1	D	423	ARG
1	D	424	ASN
1	D	425	LYS
1	D	461	GLN
1	D	496	GLN
1	D	706	VAL
1	D	707	VAL
1	D	819	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	ASN
1	A	376	GLN
1	A	488	GLN
1	A	623	ASN

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Mol	Chain	Res	Type
1	D	168	HIS
1	D	292	GLN
1	D	359	ASN
1	D	376	GLN
1	D	558	GLN
1	D	623	ASN
1	D	839	HIS

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
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

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Mol	Chain	Res	Type
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 oligosaccharides 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	804/859 (93%)	0.25	41 (5%) 33 17	18, 45, 107, 141	0
1	D	783/859 (91%)	0.56	98 (12%) 8 5	18, 49, 150, 172	0
2	B	19/23 (82%)	0.55	1 (5%) 32 16	31, 72, 153, 155	0
2	E	11/23 (47%)	-0.04	1 (9%) 15 8	29, 33, 142, 148	0
3	C	29/29 (100%)	0.54	1 (3%) 48 27	44, 91, 151, 169	0
3	F	21/29 (72%)	0.84	3 (14%) 6 3	43, 86, 130, 144	0
All	All	1667/1822 (91%)	0.41	145 (8%) 16 8	18, 47, 143, 172	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	341	LEU	4.9
1	D	92	PRO	4.8
1	D	135	VAL	4.8
1	A	272	CYS	4.7
1	D	130	VAL	4.5
1	D	328	LEU	4.4
1	A	328	LEU	4.4
1	D	278	LYS	4.3
1	D	325	LEU	4.3
3	C	12	G	4.2
1	D	279	TYR	4.2
1	D	240	PHE	4.0
1	A	73	GLU	3.9
1	D	67	PRO	3.9
1	D	61	ILE	3.8
1	D	353	ILE	3.7
1	D	258	PHE	3.7
1	D	256	VAL	3.7
2	B	23	U	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	93	VAL	3.6
1	D	115	LEU	3.6
1	D	124	LYS	3.5
1	D	398	GLY	3.5
1	D	285	THR	3.5
1	D	312	PHE	3.5
1	D	81	HIS	3.5
1	A	315	ARG	3.5
1	D	55	TYR	3.4
1	D	252	ASP	3.4
1	A	312	PHE	3.4
1	D	288	PRO	3.4
1	D	88	GLY	3.2
1	A	252	ASP	3.1
1	D	308	VAL	3.1
1	A	314	ASP	3.1
1	D	132	ILE	3.1
1	A	185	SER	3.0
1	D	86	ILE	3.0
1	A	318	LEU	3.0
3	F	5	G	3.0
1	D	243	ILE	3.0
1	D	290	SER	3.0
1	D	151	LEU	2.9
1	D	150	ARG	2.9
1	D	117	VAL	2.9
1	D	69	ARG	2.9
1	D	341	LEU	2.9
1	D	70	VAL	2.9
1	D	344	CYS	2.8
1	A	122	GLU	2.8
1	A	330	VAL	2.8
1	A	278	LYS	2.8
1	D	133	LYS	2.8
1	A	311	TYR	2.8
1	D	101	TYR	2.8
1	D	295	PRO	2.8
1	A	111	ASP	2.8
2	E	23	U	2.8
1	D	253	SER	2.8
1	A	268	GLU	2.8
1	D	352	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	80	GLN	2.8
1	A	270	THR	2.8
1	D	113	VAL	2.7
1	D	247	GLN	2.7
1	D	274	GLN	2.7
1	D	82	PHE	2.7
1	D	48	ASP	2.7
3	F	10	C	2.7
1	D	292	GLN	2.7
1	D	72	ARG	2.7
1	A	89	ASP	2.7
1	D	161	ALA	2.7
1	D	284	VAL	2.7
1	D	318	LEU	2.7
1	D	339	LEU	2.7
1	D	262	ILE	2.7
1	D	311	TYR	2.7
1	D	327	CYS	2.6
1	D	323	PRO	2.6
1	A	293	THR	2.6
1	A	281	VAL	2.6
1	A	279	TYR	2.6
1	D	326	PRO	2.6
1	D	342	GLU	2.6
1	D	343	VAL	2.6
1	D	275	MET	2.6
1	D	95	ASP	2.6
1	D	313	LYS	2.6
1	D	265	LEU	2.5
1	D	358	ASP	2.5
1	A	513	ALA	2.5
1	A	271	HIS	2.5
3	F	15	G	2.5
1	D	251	THR	2.5
1	A	326	PRO	2.5
1	A	340	PRO	2.5
1	D	291	HIS	2.5
1	D	22	ALA	2.4
1	D	235	CYS	2.4
1	A	84	THR	2.4
1	D	140	LEU	2.4
1	A	289	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	234	VAL	2.3
1	D	393	TYR	2.3
1	A	316	HIS	2.3
1	D	266	LYS	2.3
1	A	295	PRO	2.3
1	A	323	PRO	2.3
1	A	320	LEU	2.3
1	D	337	THR	2.3
1	D	188	CYS	2.3
1	D	241	LYS	2.3
1	A	95	ASP	2.3
1	D	392	PRO	2.2
1	A	267	VAL	2.2
1	D	138	VAL	2.2
1	A	285	THR	2.2
1	D	259	THR	2.2
1	D	307	THR	2.2
1	A	819	ASP	2.2
1	D	319	VAL	2.2
1	D	330	VAL	2.1
1	D	73	GLU	2.1
1	D	264	GLY	2.1
1	D	505	PHE	2.1
1	D	255	ARG	2.1
1	D	114	GLU	2.1
1	D	153	SER	2.1
1	A	344	CYS	2.1
1	D	356	LEU	2.1
1	D	424	ASN	2.1
1	D	539	VAL	2.1
1	A	265	LEU	2.1
1	D	316	HIS	2.1
1	D	254	GLN	2.1
1	A	194	GLY	2.1
1	D	144	HIS	2.1
1	D	211	TRP	2.1
1	D	294	PHE	2.0
1	A	313	LYS	2.0
1	D	89	ASP	2.0
1	D	176	PRO	2.0
1	A	423	ARG	2.0
1	A	269	ILE	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	BA	C	101	1/1	0.94	0.09	128,128,128,128	0
4	BA	A	901	1/1	0.98	0.04	54,54,54,54	0
4	BA	D	901	1/1	0.99	0.02	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.