



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:04 am BST

PDB ID : 5UX0
Title : X-ray crystal structure of Marinitoga piezophila Argonaute in complex with
5' OH guide RNA and target DNA
Authors : Doxzen, K.W.; Doudna, J.A.
Deposited on : 2017-02-21
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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	:	2.11
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

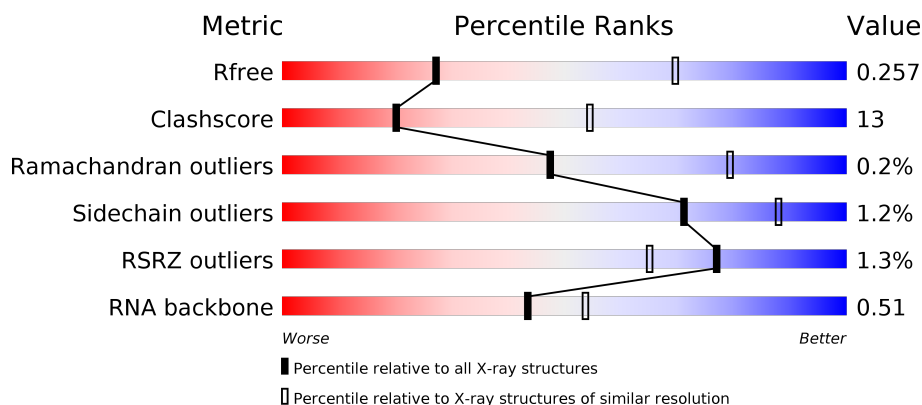
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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	642	<div> <div>2%</div> <div>64%</div> <div>34%</div> <div>.</div> </div>
1	D	642	<div> <div>%</div> <div>71%</div> <div>28%</div> <div>.</div> </div>
2	B	21	<div> <div>10%</div> <div>76%</div> <div>10%</div> <div>5%</div> </div>
2	E	21	<div> <div>24%</div> <div>52%</div> <div>10%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	21	 52% 43% 5%
3	F	21	 43% 33% 24%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12237 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 Argonaute protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	632	Total	C	N	O	S	0	0	0
			5323	3502	840	974	7			
1	D	639	Total	C	N	O	S	0	0	0
			5376	3535	847	987	7			

There are 10 discrepancies between the modelled and reference sequences:

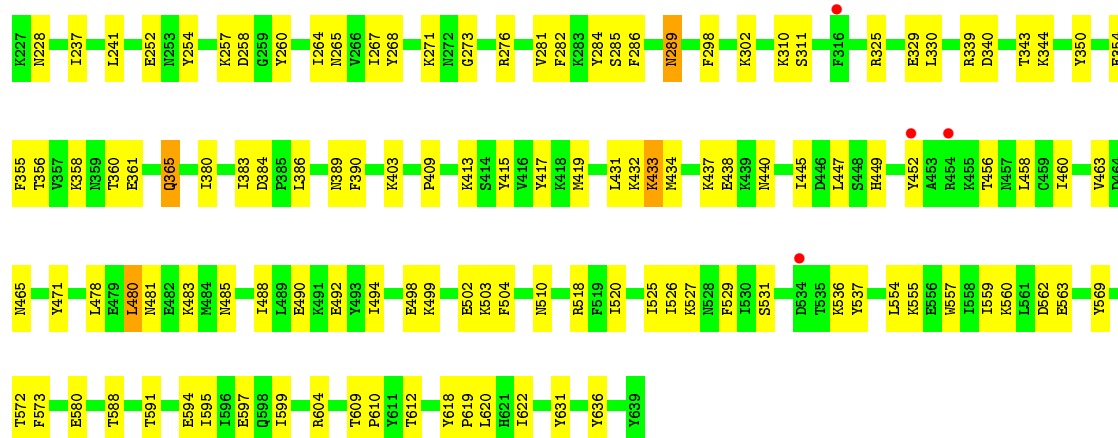
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP H2J4R4
A	-1	ALA	-	expression tag	UNP H2J4R4
A	0	ASN	-	expression tag	UNP H2J4R4
A	1	ALA	-	expression tag	UNP H2J4R4
A	516	ALA	ASP	engineered mutation	UNP H2J4R4
D	-2	GLY	-	expression tag	UNP H2J4R4
D	-1	ALA	-	expression tag	UNP H2J4R4
D	0	ASN	-	expression tag	UNP H2J4R4
D	1	ALA	-	expression tag	UNP H2J4R4
D	516	ALA	ASP	engineered mutation	UNP H2J4R4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	20	Total	C	N	O	P	0	0	0
			415	188	71	137	19			
2	E	18	Total	C	N	O	P	0	0	0
			373	169	64	123	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	20	Total 417	C 198	N 78	O 121	P 20	0	0	0
3	F	16	Total 333	C 158	N 61	O 98	P 16	0	0	0



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

Chain B: 10% 76% 10% 5%



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

Chain E: 24% 52% 10% 14%



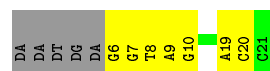
• Molecule 3: DNA (5'-D(P*AP*TP*GP*AP*GP*GP*TP*AP*GP*TP*AP*GP*GP*TP*TP*G P*TP*AP*CP*C)-3')

Chain C: 52% 43% 5%



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

Chain F: 43% 33% 24%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.00Å 130.99Å 171.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.43 – 3.20 47.43 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.43-3.20) 99.7 (47.43-3.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.10 _2155	Depositor
R, R_{free}	0.215 , 0.259 0.215 , 0.257	Depositor DCC
R_{free} test set	1617 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	75.5	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12237	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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](#)

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	0/5451	0.48	2/7347 (0.0%)
1	D	0.27	0/5509	0.47	0/7433
2	B	0.27	0/462	0.90	1/716 (0.1%)
2	E	0.29	0/415	0.89	0/643
3	C	0.56	0/468	1.00	0/722
3	F	0.57	0/373	0.93	0/575
All	All	0.30	0/12678	0.57	3/17436 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	SER	N-CA-CB	8.17	122.76	110.50
2	B	5	C	N1-C2-O2	-5.90	115.36	118.90
1	A	344	LYS	N-CA-C	-5.85	95.20	111.00

There are no chirality outliers.

There are no planarity outliers.

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	5323	0	5361	144	0
1	D	5376	0	5411	122	0
2	B	415	0	215	19	0
2	E	373	0	196	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	417	0	227	10	0
3	F	333	0	182	8	0
All	All	12237	0	11592	295	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 13.

All (295) 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:361:GLU:O	1:D:365:GLN:NE2	2.08	0.86
1:D:339:ARG:NH1	1:D:344:LYS:O	2.11	0.83
2:B:16:C:O2	3:C:6:DG:N2	2.08	0.83
1:D:440:ASN:HD22	1:D:510:ASN:HB2	1.45	0.80
1:A:604:ARG:NH1	1:A:613:ASN:OD1	2.17	0.78
1:A:433:LYS:O	1:A:437:LYS:NZ	2.21	0.73
1:D:562:ASP:OD1	1:D:563:GLU:N	2.22	0.73
1:A:544:LYS:O	1:A:577:LYS:NZ	2.21	0.73
1:D:354:GLU:O	1:D:389:ASN:ND2	2.22	0.72
1:D:257:LYS:H	1:D:257:LYS:HD2	1.54	0.72
1:D:555:LYS:NZ	1:D:572:THR:O	2.21	0.72
1:A:33:LEU:O	1:A:37:ASN:ND2	2.22	0.71
2:B:18:C:H42	3:C:4:DG:H1	1.37	0.71
1:D:449:HIS:HD2	1:D:520:ILE:HD11	1.56	0.71
1:D:28:LEU:O	1:D:32:ASN:ND2	2.24	0.71
1:A:294:LYS:HB3	1:A:338:LEU:HD11	1.73	0.69
2:B:16:C:N3	3:C:6:DG:N1	2.33	0.69
1:A:588:THR:HG23	1:A:590:TYR:H	1.57	0.69
1:A:288:LYS:HD2	1:A:427:LYS:HD3	1.75	0.68
1:A:448:SER:OG	1:A:457:ASN:OD1	2.11	0.68
1:D:433:LYS:O	1:D:437:LYS:NZ	2.27	0.68
1:A:518:ARG:NH2	1:A:580:GLU:OE1	2.27	0.67
1:D:471:TYR:HB2	1:D:499:LYS:HG3	1.75	0.67
2:B:8:C:H2'	2:B:9:C:C6	2.29	0.67
1:A:83:LEU:HA	1:A:86:LYS:HE2	1.75	0.67
1:D:267:ILE:HD11	1:D:432:LYS:HD3	1.74	0.67
1:A:560:LYS:HE3	1:A:563:GLU:HA	1.76	0.66
1:A:443:ILE:HA	1:A:461:ALA:O	1.97	0.65
1:A:396:LEU:HD23	1:A:635:LEU:HD21	1.78	0.65
1:D:33:LEU:O	1:D:37:ASN:ND2	2.28	0.65
1:D:158:LEU:HD12	1:D:158:LEU:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:ASN:ND2	3:C:11:DT:OP2	2.32	0.63
1:D:403:LYS:NZ	2:E:2:G:OP1	2.31	0.63
2:B:17:U:H3	3:C:5:DA:H62	1.46	0.63
1:A:399:ILE:HD12	2:B:2:G:H5'	1.80	0.63
1:D:69:VAL:HG12	1:D:71:LYS:H	1.64	0.63
2:E:11:A:H2'	2:E:12:C:C6	2.34	0.62
1:A:351:ASN:ND2	1:A:356:THR:O	2.32	0.62
1:D:104:LYS:HB3	1:D:108:ASN:HB2	1.81	0.62
1:D:573:PHE:HB3	3:F:19:DA:H4'	1.81	0.62
1:D:265:ASN:OD1	1:D:276:ARG:NH2	2.33	0.62
1:A:224:GLU:O	1:A:228:ASN:HB2	2.00	0.61
1:D:135:HIS:ND1	1:D:144:SER:OG	2.32	0.61
2:B:5:C:H2'	2:B:6:A:C8	2.35	0.61
1:A:282:PHE:CZ	1:A:413:LYS:HB3	2.36	0.61
1:A:8:ILE:HA	1:A:248:THR:HG22	1.81	0.61
1:A:622:ILE:HG23	1:A:637:ILE:HD13	1.84	0.60
1:A:211:ARG:HD2	3:C:15:DT:H4'	1.81	0.60
1:D:438:GLU:HA	1:D:465:ASN:ND2	2.16	0.60
1:A:612:THR:C	1:A:613:ASN:HD22	2.05	0.60
1:D:158:LEU:HD11	1:D:186:LEU:HD23	1.84	0.59
1:D:447:LEU:HD21	1:D:458:LEU:HD12	1.82	0.59
1:A:116:PHE:CE1	1:A:225:ILE:HD11	2.38	0.59
1:A:515:ARG:HH12	1:A:520:ILE:HG12	1.68	0.59
2:B:4:A:H2'	2:B:5:C:O4'	2.03	0.59
3:F:6:DG:H2'	3:F:7:DG:H8	1.67	0.59
1:A:297:PHE:HE2	1:A:312:LEU:HD11	1.68	0.58
1:A:305:PHE:O	1:A:309:GLN:HB2	2.03	0.58
1:D:438:GLU:HA	1:D:465:ASN:HD22	1.67	0.58
1:D:554:LEU:HD22	1:D:559:ILE:HD11	1.86	0.58
1:D:103:PHE:O	1:D:168:TYR:OH	2.16	0.58
2:B:12:C:H2'	2:B:13:U:C6	2.39	0.58
1:A:247:ILE:HG13	1:A:248:THR:HG23	1.85	0.58
1:A:441:LEU:HD11	1:A:462:ALA:HB1	1.86	0.58
1:D:282:PHE:CE2	1:D:413:LYS:HB3	2.39	0.58
1:D:16:ARG:NH1	1:D:51:GLU:OE2	2.37	0.57
1:A:471:TYR:OH	1:A:492:GLU:OE1	2.10	0.57
1:D:185:ILE:HG23	1:D:197:GLU:HG3	1.87	0.57
1:D:267:ILE:O	1:D:433:LYS:NZ	2.37	0.57
1:A:224:GLU:O	1:A:228:ASN:CB	2.53	0.57
1:A:271:LYS:HB2	1:A:286:PHE:O	2.05	0.57
1:A:526:ILE:HA	1:A:529:PHE:CE2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LEU:HD22	1:A:204:TYR:HB3	1.87	0.57
1:A:303:LYS:H	1:A:303:LYS:HD2	1.70	0.57
2:B:11:A:H2'	2:B:12:C:C6	2.40	0.57
1:D:526:ILE:HA	1:D:529:PHE:CE2	2.40	0.57
1:A:370:VAL:HG23	1:A:394:LEU:HG	1.84	0.57
1:D:224:GLU:OE2	1:D:228:ASN:ND2	2.38	0.57
1:D:190:ILE:HG22	1:D:191:GLY:H	1.69	0.56
1:D:271:LYS:HB2	1:D:286:PHE:O	2.05	0.56
1:D:14:ILE:HD11	1:D:84:PHE:HB2	1.87	0.56
1:A:13:LYS:NZ	1:A:54:ASP:OD2	2.33	0.56
1:D:254:TYR:OH	1:D:257:LYS:NZ	2.38	0.56
1:D:536:LYS:HB3	1:D:588:THR:HG22	1.87	0.56
1:A:376:LEU:HB2	1:A:400:LEU:HD23	1.87	0.56
1:D:179:ILE:HD12	1:D:195:ILE:HG23	1.88	0.56
1:A:177:PRO:HD2	1:A:189:ASP:O	2.05	0.56
1:A:463:VAL:HG22	1:A:619:PRO:HG3	1.88	0.56
1:D:380:ILE:HD11	1:D:383:ILE:HD12	1.87	0.56
1:A:222:VAL:O	1:A:225:ILE:HG22	2.07	0.55
1:D:456:THR:HG21	1:D:480:LEU:HD13	1.87	0.55
1:A:439:LYS:HD2	1:A:509:GLU:OE1	2.07	0.55
1:D:356:THR:HG22	1:D:389:ASN:HB3	1.87	0.55
2:E:3:U:H2'	2:E:4:A:C8	2.42	0.55
1:A:187:LYS:HE2	1:A:195:ILE:HG22	1.89	0.55
2:E:8:C:H2'	2:E:9:C:C6	2.42	0.55
1:D:121:ASN:HB3	1:D:124:VAL:HG22	1.87	0.55
1:D:289:ASN:ND2	1:D:330:LEU:O	2.38	0.55
1:D:273:GLY:HA3	1:D:284:TYR:CD1	2.42	0.55
1:D:518:ARG:NH2	1:D:580:GLU:OE1	2.33	0.54
1:A:228:ASN:ND2	1:D:252:GLU:OE2	2.36	0.54
1:A:167:LEU:O	1:A:175:SER:HA	2.08	0.54
2:E:12:C:H2'	2:E:13:U:C6	2.43	0.54
1:D:471:TYR:OH	1:D:492:GLU:OE1	2.15	0.54
3:C:3:DT:H2''	3:C:4:DG:C8	2.43	0.54
1:D:167:LEU:O	1:D:175:SER:HA	2.07	0.54
1:D:636:TYR:OH	2:E:1:G:N2	2.39	0.54
1:D:257:LYS:HD3	1:D:260:TYR:CG	2.43	0.54
1:D:16:ARG:NH2	1:D:75:ILE:HD11	2.23	0.54
1:A:256:LEU:HD21	1:A:559:ILE:HG23	1.89	0.53
1:D:463:VAL:HG22	1:D:619:PRO:HG3	1.89	0.53
3:F:9:DA:H1'	3:F:10:DG:H5'	1.89	0.53
3:C:14:DG:H2''	3:C:15:DT:H71	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:GLU:HG3	1:A:571:LYS:HB2	1.91	0.52
1:A:300:SER:HB2	1:A:352:PRO:HG3	1.90	0.52
1:D:325:ARG:O	1:D:329:GLU:HG3	2.09	0.52
1:A:162:ILE:HD12	1:A:216:TYR:CE2	2.44	0.52
1:A:397:GLN:O	1:A:415:TYR:OH	2.27	0.52
1:A:459:CYS:HA	1:A:473:GLY:O	2.08	0.52
3:F:8:DT:H2''	3:F:9:DA:C8	2.45	0.52
1:A:380:ILE:O	2:B:1:G:N1	2.27	0.52
1:A:618:TYR:CE2	1:A:622:ILE:HD11	2.45	0.52
1:D:302:LYS:H	1:D:302:LYS:HD2	1.74	0.52
1:A:225:ILE:HG13	1:A:229:LYS:HE3	1.91	0.51
1:A:518:ARG:NH1	1:A:543:ASN:HB2	2.25	0.51
1:D:384:ASP:OD1	1:D:631:TYR:HB2	2.10	0.51
1:A:380:ILE:HG12	2:B:1:G:C2	2.45	0.51
1:A:390:PHE:CD2	1:A:391:PRO:HD2	2.46	0.51
1:D:8:ILE:HG22	1:D:10:ILE:HG12	1.93	0.51
1:A:325:ARG:O	1:A:329:GLU:HG3	2.10	0.51
1:A:431:LEU:HB2	1:A:434:MET:HB2	1.93	0.51
1:A:497:PHE:CE1	1:A:508:PRO:HD2	2.45	0.51
2:E:6:A:H2'	2:E:7:A:C8	2.46	0.51
1:D:118:LEU:HD11	1:D:126:ALA:HB2	1.92	0.51
1:A:12:LYS:O	1:A:77:GLU:HB2	2.11	0.51
1:A:377:ASP:HA	1:A:401:LYS:HE2	1.94	0.50
1:A:116:PHE:CZ	1:A:225:ILE:HD11	2.47	0.50
1:D:498:GLU:O	1:D:502:GLU:HG3	2.10	0.50
1:D:554:LEU:O	1:D:557:TRP:HB2	2.12	0.50
3:F:8:DT:H2''	3:F:9:DA:H8	1.76	0.50
1:A:367:GLU:OE1	1:A:367:GLU:N	2.35	0.50
2:B:6:A:H2'	2:B:7:A:C8	2.47	0.50
1:D:340:ASP:HB3	1:D:343:THR:O	2.12	0.50
3:F:6:DG:H2'	3:F:7:DG:C8	2.46	0.50
2:E:4:A:H2'	2:E:5:C:O4'	2.12	0.50
1:D:209:THR:HG22	2:E:9:C:H1'	1.92	0.50
1:A:21:ASN:OD1	1:A:24:MET:N	2.41	0.49
1:A:232:GLU:O	1:A:236:LYS:HG2	2.12	0.49
1:A:515:ARG:HH22	1:A:521:GLU:HG3	1.78	0.49
2:E:13:U:H2'	2:E:14:A:C8	2.46	0.49
1:A:494:ILE:O	1:A:498:GLU:HG3	2.12	0.49
2:B:13:U:H2'	2:B:14:A:C8	2.48	0.49
1:A:104:LYS:HB3	1:A:108:ASN:HB2	1.94	0.49
1:D:310:LYS:HG3	1:D:311:SER:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ASP:O	1:A:112:ASN:OD1	2.31	0.49
1:A:285:SER:OG	1:A:286:PHE:N	2.45	0.49
1:A:286:PHE:CE1	1:A:330:LEU:HD22	2.48	0.49
1:D:409:PRO:O	1:D:413:LYS:HG3	2.12	0.49
1:D:258:ASP:N	1:D:258:ASP:OD1	2.44	0.49
1:D:591:THR:HG23	1:D:594:GLU:H	1.78	0.49
1:A:523:ILE:O	1:A:527:LYS:HG2	2.12	0.48
1:A:398:PRO:HB2	2:B:1:G:H4'	1.95	0.48
1:A:102:TYR:HB2	1:A:110:ILE:HB	1.94	0.48
1:A:102:TYR:CE1	1:A:170:ILE:HG23	2.49	0.48
1:A:103:PHE:O	1:A:168:TYR:OH	2.27	0.48
1:D:179:ILE:HD11	1:D:195:ILE:HD12	1.96	0.48
1:A:102:TYR:O	1:A:109:PHE:HA	2.14	0.48
1:D:267:ILE:H	1:D:433:LYS:NZ	2.11	0.48
1:D:282:PHE:CZ	1:D:413:LYS:HB3	2.49	0.48
1:D:38:ASN:ND2	1:D:98:ASP:OD1	2.45	0.47
1:D:16:ARG:HH22	1:D:75:ILE:HD11	1.77	0.47
1:A:167:LEU:CD1	1:A:178:TYR:HB2	2.44	0.47
1:A:394:LEU:HD23	1:A:395:ILE:N	2.30	0.47
1:A:403:LYS:HE2	2:B:2:G:N7	2.29	0.47
1:A:455:LYS:HB3	1:A:478:LEU:HA	1.95	0.47
1:D:358:LYS:O	1:D:360:THR:HG23	2.14	0.47
1:D:494:ILE:O	1:D:498:GLU:HG3	2.15	0.47
1:A:294:LYS:NZ	1:A:367:GLU:HG3	2.29	0.47
1:A:444:GLY:O	1:A:460:ILE:HA	2.15	0.47
1:A:41:PHE:CE1	1:A:50:ILE:HD12	2.50	0.47
1:D:237:ILE:HG23	1:D:241:LEU:HD12	1.96	0.47
1:D:339:ARG:HG2	1:D:344:LYS:O	2.14	0.47
1:D:96:PHE:O	1:D:101:PHE:HB2	2.15	0.47
1:A:135:HIS:CD2	1:A:144:SER:HB3	2.49	0.46
2:B:5:C:H2'	2:B:6:A:H8	1.76	0.46
1:D:153:SER:HB3	1:D:206:PHE:HB2	1.97	0.46
2:E:7:A:H2'	2:E:8:C:C6	2.50	0.46
1:A:500:TYR:CD2	1:A:508:PRO:HD3	2.50	0.46
1:D:298:PHE:HB3	1:D:350:TYR:CD2	2.50	0.46
1:D:102:TYR:CZ	1:D:112:ASN:HB3	2.50	0.46
1:A:338:LEU:HB3	1:A:362:PHE:HZ	1.81	0.46
1:A:16:ARG:NH2	1:A:51:GLU:OE2	2.34	0.46
1:A:15:LYS:HE2	1:A:17:LEU:HD21	1.97	0.46
1:A:409:PRO:O	1:A:413:LYS:HG3	2.16	0.46
1:A:86:LYS:O	1:A:90:LYS:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:GLU:O	1:A:318:ASN:ND2	2.48	0.46
1:D:285:SER:OG	1:D:286:PHE:N	2.47	0.46
1:A:586:ASN:OD1	1:A:588:THR:HG22	2.15	0.45
1:A:309:GLN:HA	1:A:312:LEU:HB3	1.99	0.45
1:D:595:ILE:O	1:D:599:ILE:HG12	2.16	0.45
1:A:14:ILE:HG23	1:A:84:PHE:HD1	1.81	0.45
1:D:618:TYR:O	1:D:622:ILE:HG13	2.15	0.45
1:D:281:VAL:HG13	1:D:282:PHE:HD1	1.82	0.45
1:A:169:ASN:HB3	1:A:172:SER:HB3	1.99	0.45
1:D:298:PHE:HB3	1:D:350:TYR:HD2	1.82	0.45
1:A:116:PHE:HE1	1:A:225:ILE:HD11	1.82	0.45
1:D:108:ASN:HD22	1:D:148:LYS:HE2	1.80	0.45
1:D:94:LYS:NZ	1:D:98:ASP:OD2	2.37	0.45
1:A:18:TYR:CD2	1:A:49:TRP:HB3	2.53	0.44
1:A:378:LYS:HE3	1:A:378:LYS:HB2	1.82	0.44
1:A:63:ASN:O	1:A:66:GLN:HG2	2.17	0.44
1:D:452:TYR:HB2	2:E:13:U:O3'	2.16	0.44
1:A:465:ASN:N	1:A:465:ASN:OD1	2.50	0.44
1:D:554:LEU:O	1:D:569:TYR:HB2	2.17	0.44
1:D:179:ILE:CD1	1:D:195:ILE:HD12	2.47	0.44
1:A:440:ASN:HA	1:A:510:ASN:O	2.17	0.44
1:A:110:ILE:HG23	1:A:127:HIS:HB3	2.00	0.44
1:A:443:ILE:HG12	1:A:513:ILE:HD13	2.00	0.44
1:A:444:GLY:HA2	1:A:514:LEU:O	2.18	0.44
1:A:618:TYR:O	1:A:622:ILE:HG13	2.18	0.44
1:A:614:TYR:HE2	1:A:618:TYR:HE1	1.66	0.43
1:A:486:LEU:HD11	1:A:522:ASP:HB3	2.00	0.43
1:D:267:ILE:H	1:D:433:LYS:HZ1	1.66	0.43
1:D:503:LYS:HE2	1:D:504:PHE:CZ	2.53	0.43
1:D:573:PHE:HZ	3:F:20:DC:H4'	1.32	0.43
1:A:536:LYS:HB3	1:A:588:THR:HA	1.99	0.43
1:A:595:ILE:O	1:A:599:ILE:HD13	2.18	0.43
1:A:614:TYR:HE2	1:A:618:TYR:CE1	2.36	0.43
1:A:286:PHE:HE1	1:A:330:LEU:HD22	1.84	0.43
1:A:124:VAL:HG21	1:A:218:PHE:CE2	2.53	0.43
1:A:297:PHE:HE1	1:A:337:PHE:CD1	2.37	0.43
1:D:478:LEU:HD13	1:D:488:ILE:HG13	2.00	0.43
1:D:618:TYR:CE2	1:D:622:ILE:HD11	2.52	0.43
1:A:498:GLU:HA	1:A:501:ILE:HG12	2.00	0.43
1:D:437:LYS:HB3	1:D:440:ASN:OD1	2.19	0.43
1:D:264:ILE:HD12	1:D:597:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:PHE:CE1	1:A:357:VAL:HG11	2.53	0.43
2:B:18:C:N4	3:C:4:DG:H22	2.16	0.43
1:D:169:ASN:HB3	1:D:172:SER:HB2	2.01	0.43
1:D:620:LEU:HD23	1:D:620:LEU:HA	1.84	0.43
1:A:77:GLU:OE2	1:A:81:LYS:HE2	2.19	0.43
1:D:3:LEU:HD23	1:D:5:LEU:HD12	2.01	0.43
1:D:355:PHE:HB3	1:D:386:LEU:HA	2.00	0.43
1:A:308:VAL:O	1:A:312:LEU:HB2	2.18	0.43
1:A:554:LEU:O	1:A:557:TRP:HB2	2.19	0.43
1:D:138:SER:OG	1:D:138:SER:O	2.30	0.43
1:D:4:ASN:ND2	1:D:145:ILE:O	2.43	0.42
1:D:609:THR:HG23	1:D:612:THR:H	1.83	0.42
1:D:483:LYS:HD3	1:D:525:ILE:HD11	2.01	0.42
1:A:310:LYS:O	1:A:314:GLU:HG2	2.19	0.42
1:A:475:HIS:NE2	1:A:492:GLU:OE2	2.49	0.42
1:A:94:LYS:HE2	1:A:98:ASP:OD2	2.19	0.42
1:D:121:ASN:HD22	1:D:216:TYR:HB3	1.84	0.42
1:D:148:LYS:HB2	1:D:226:TYR:OH	2.19	0.42
1:D:573:PHE:CB	3:F:19:DA:H4'	2.48	0.42
1:A:157:ALA:HB2	1:A:167:LEU:HD21	2.01	0.42
1:D:527:LYS:HD2	1:D:537:TYR:OH	2.19	0.42
1:A:7:LYS:NZ	1:A:140:GLU:OE1	2.52	0.42
1:D:20:TYR:CE2	1:D:22:PRO:HG3	2.55	0.42
1:D:560:LYS:HE3	1:D:563:GLU:HA	2.02	0.42
2:B:18:C:H2'	2:B:19:A:O4'	2.20	0.42
1:D:431:LEU:HB2	1:D:434:MET:HB2	2.01	0.42
1:A:351:ASN:OD1	1:A:354:GLU:HB2	2.19	0.42
1:A:527:LYS:O	1:A:531:SER:CB	2.68	0.42
1:D:415:TYR:O	1:D:419:MET:HG3	2.20	0.42
1:A:407:ILE:HD12	1:A:408:LYS:H	1.84	0.41
1:A:407:ILE:HD11	1:A:412:ILE:HG12	2.00	0.41
3:C:16:DT:H2''	3:C:17:DG:H8	1.85	0.41
1:A:501:ILE:HG22	1:A:507:SER:HA	2.02	0.41
1:A:344:LYS:HB3	1:A:344:LYS:HE3	1.88	0.41
1:D:490:GLU:HG3	1:D:529:PHE:CD1	2.55	0.41
1:A:584:LEU:HA	1:A:584:LEU:HD12	1.90	0.41
1:A:602:LEU:O	1:A:605:VAL:HG22	2.19	0.41
1:A:123:ASN:HB3	1:A:162:ILE:HG12	2.02	0.41
1:D:18:TYR:CD2	1:D:49:TRP:HB3	2.55	0.41
1:A:439:LYS:HG2	1:A:439:LYS:H	1.41	0.41
1:A:471:TYR:CE1	1:A:495:LYS:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:TYR:CG	1:D:610:PRO:HD3	2.56	0.41
1:A:386:LEU:O	1:A:390:PHE:HB2	2.20	0.41
1:A:626:VAL:HG22	1:A:633:TRP:CD2	2.55	0.41
1:D:268:TYR:OH	1:D:604:ARG:HD2	2.20	0.41
1:D:310:LYS:HG3	1:D:311:SER:N	2.35	0.41
1:A:301:SER:OG	1:A:304:GLN:HG2	2.21	0.41
1:A:105:LYS:O	1:A:108:ASN:ND2	2.53	0.41
1:D:481:ASN:HB2	1:D:485:ASN:OD1	2.20	0.41
1:D:13:LYS:HB3	1:D:13:LYS:HE3	1.81	0.40
1:D:151:PHE:CE1	1:D:222:VAL:HG13	2.56	0.40
1:A:257:LYS:HB2	1:A:260:TYR:CD1	2.56	0.40
1:A:231:PHE:HD1	1:A:551:TYR:HB2	1.86	0.40
1:D:445:ILE:HG23	1:D:460:ILE:HG22	2.02	0.40
1:A:3:LEU:HA	1:A:3:LEU:HD12	1.91	0.40
1:A:533:ASN:O	1:A:535:THR:HG23	2.21	0.40
1:D:102:TYR:CE1	1:D:170:ILE:HB	2.56	0.40
1:A:613:ASN:N	1:A:613:ASN:HD22	2.18	0.40
1:D:41:PHE:CE1	1:D:50:ILE:HD12	2.56	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	622/642 (97%)	608 (98%)	13 (2%)	1 (0%)	47	79
1	D	637/642 (99%)	619 (97%)	17 (3%)	1 (0%)	47	79
All	All	1259/1284 (98%)	1227 (98%)	30 (2%)	2 (0%)	47	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	ASN
1	D	289	ASN

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	593/599 (99%)	587 (99%)	6 (1%)	76	90
1	D	598/599 (100%)	590 (99%)	8 (1%)	69	87
All	All	1191/1198 (99%)	1177 (99%)	14 (1%)	71	88

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	226	TYR
1	A	369	ASN
1	A	384	ASP
1	A	518	ARG
1	A	585	GLU
1	A	589	ASP
1	D	13	LYS
1	D	140	GLU
1	D	182	LEU
1	D	365	GLN
1	D	390	PHE
1	D	433	LYS
1	D	480	LEU
1	D	531	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	HIS
1	A	369	ASN
1	D	440	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	19/21 (90%)	3 (15%)	0
2	E	17/21 (80%)	2 (11%)	0
All	All	36/42 (85%)	5 (13%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	3	U
2	B	19	A
2	B	20	U
2	E	3	U
2	E	13	U

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	632/642 (98%)	-0.18	13 (2%) 63 49	33, 78, 126, 175	0
1	D	639/642 (99%)	-0.25	4 (0%) 89 83	34, 71, 113, 150	0
2	B	20/21 (95%)	-0.04	0 100 100	61, 99, 173, 182	0
2	E	18/21 (85%)	-0.19	0 100 100	53, 70, 162, 168	0
3	C	20/21 (95%)	-0.19	0 100 100	72, 110, 148, 161	0
3	F	16/21 (76%)	-0.28	0 100 100	79, 103, 162, 181	0
All	All	1345/1368 (98%)	-0.21	17 (1%) 77 65	33, 75, 126, 182	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	484	MET	3.3
1	A	196	VAL	3.1
1	A	198	VAL	3.1
1	A	353	GLU	3.0
1	A	482	GLU	3.0
1	A	179	ILE	2.9
1	A	355	PHE	2.6
1	A	197	GLU	2.5
1	D	454	ARG	2.3
1	A	199	ALA	2.3
1	D	452	TYR	2.3
1	D	534	ASP	2.2
1	A	188	ILE	2.2
1	D	316	PHE	2.1
1	A	358	LYS	2.1
1	A	295	ALA	2.0
1	A	186	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.