



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:50 AM UTC

PDB ID : 5WEA / pdb_00005wea
Title : Human Argonaute2 Helix-7 Mutant
Authors : Schirle, N.T.; Klum, S.M.; MacRae, I.J.
Deposited on : 2017-07-08
Resolution : 3.12 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

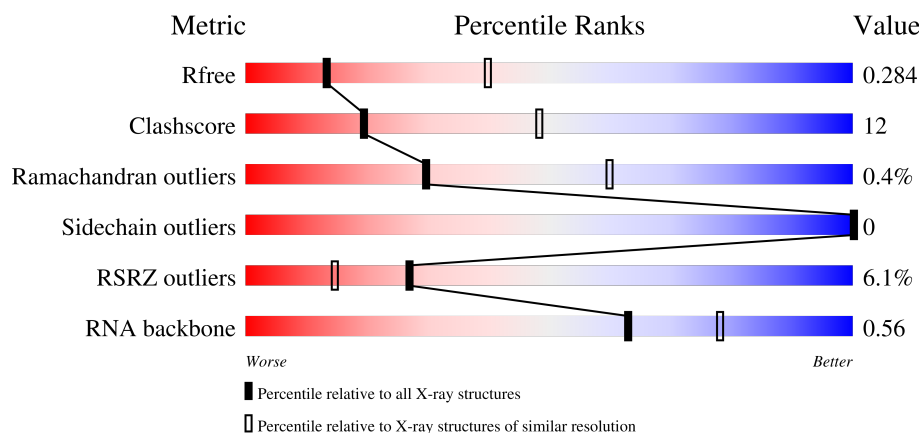
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.12 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	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)
RNA backbone	3983	1017 (3.34-2.90)

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 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% 65% 23% 11%
2	B	8	12% 38% 62%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6340 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	764	Total	C	N	O	S	0	0	0
			6139	3915	1107	1079	38			

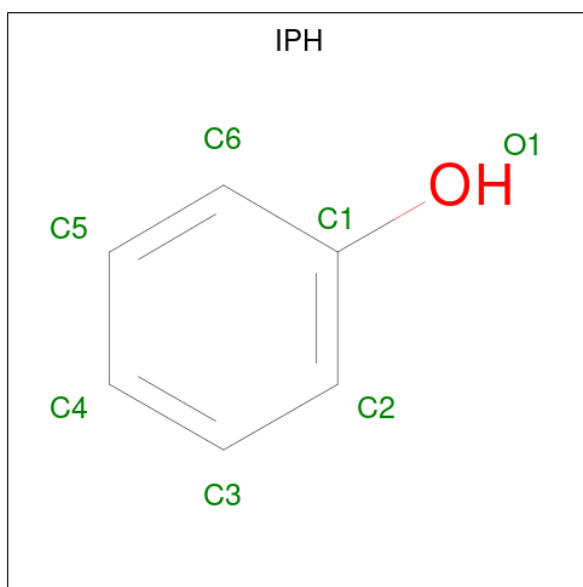
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	364	ALA	MET	engineered mutation	UNP Q9UKV8
A	365	ALA	ILE	engineered mutation	UNP Q9UKV8
A	387	ASP	SER	engineered mutation	UNP Q9UKV8
A	824	ALA	SER	conflict	UNP Q9UKV8
A	828	ASP	SER	conflict	UNP Q9UKV8
A	831	ASP	SER	conflict	UNP Q9UKV8
A	834	ALA	SER	conflict	UNP Q9UKV8

- Molecule 2 is a RNA chain called RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	8	Total	C	N	O	P	0	0	0
			171	76	37	51	7			

- Molecule 3 is PHENOL (CCD ID: IPH) (formula: C₆H₆O).



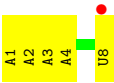
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	6	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		

- Molecule 1: Protein argonaute-2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.26Å 107.88Å 68.72Å 90.00° 107.46° 90.00°	Depositor
Resolution (Å)	65.56 – 3.12 65.56 – 3.12	Depositor EDS
% Data completeness (in resolution range)	94.2 (65.56-3.12) 94.1 (65.56-3.12)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.252 , 0.282 0.254 , 0.284	Depositor DCC
R_{free} test set	739 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	64.4	Xtriage
Anisotropy	0.805	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 72.8	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	0.88	EDS
Total number of atoms	6340	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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: IPH

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	0.11	0/6281	0.34	0/8495
2	B	0.09	0/186	0.22	0/281
All	All	0.11	0/6467	0.34	0/8776

There are no bond length outliers.

There are no bond angle outliers.

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	6139	0	6202	140	0
2	B	171	0	82	10	0
3	A	7	0	6	2	0
4	A	23	0	0	1	0
All	All	6340	0	6290	146	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 12.

All (146) 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:90:ARG:HE	1:A:104:MET:HB2	1.44	0.81
1:A:72:ARG:HB3	1:A:172:MET:HE1	1.62	0.80
2:B:8:U:O4'	2:B:8:U:C3'	2.34	0.75
2:B:8:U:C2'	2:B:8:U:N1	2.52	0.72
2:B:8:U:O4'	2:B:8:U:C2'	2.38	0.72
1:A:549:MET:O	1:A:553:GLN:NE2	2.24	0.71
1:A:325:LEU:HD23	1:A:341:LEU:HD12	1.75	0.69
1:A:478:SER:OG	1:A:483:MET:O	2.11	0.69
1:A:95:ASP:HB2	1:A:99:ASN:HB2	1.76	0.68
1:A:520:VAL:HG11	1:A:532:VAL:HG11	1.80	0.64
1:A:556:THR:HG23	1:A:558:GLN:H	1.63	0.63
1:A:62:LYS:NZ	1:A:114:GLU:OE1	2.32	0.63
1:A:680:LEU:HD22	1:A:768:LEU:HB3	1.80	0.63
1:A:705:ILE:HG12	1:A:767:VAL:HG22	1.82	0.62
1:A:46:GLU:HG2	1:A:214:MET:HE2	1.82	0.62
1:A:72:ARG:NH2	1:A:95:ASP:O	2.33	0.61
1:A:583:ARG:NH1	1:A:621:HIS:O	2.34	0.61
1:A:167:ARG:NH1	1:A:179:ARG:O	2.34	0.60
1:A:222:THR:HG21	1:A:351:ARG:HE	1.67	0.60
2:B:8:U:O4'	2:B:8:U:N1	2.35	0.59
1:A:196:ARG:NE	1:A:352:CYS:SG	2.73	0.59
1:A:608:LYS:O	1:A:634:HIS:ND1	2.32	0.59
1:A:227:ALA:HB2	1:A:348:ALA:HB2	1.84	0.59
1:A:750:LEU:HB3	1:A:765:TYR:HE2	1.67	0.58
1:A:668:ARG:NH1	1:A:669:ASP:O	2.35	0.58
1:A:812:ARG:NH2	4:A:1005:HOH:O	2.36	0.58
1:A:117:VAL:HG22	1:A:128:PHE:H	1.70	0.57
1:A:534:ARG:O	1:A:538:THR:OG1	2.21	0.57
1:A:462:CYS:SG	1:A:463:THR:N	2.78	0.56
1:A:491:PHE:CZ	1:A:508:LEU:HD22	2.41	0.56
1:A:578:LEU:HD12	1:A:578:LEU:H	1.68	0.56
1:A:234:VAL:HG21	1:A:341:LEU:HD13	1.88	0.56
1:A:509:LYS:HD3	1:A:540:LEU:HD23	1.88	0.56
1:A:416:PRO:HD2	1:A:788:HIS:CE1	2.41	0.56
1:A:632:GLN:NE2	1:A:638:ILE:O	2.39	0.55
1:A:711:HIS:NE2	1:A:762:PRO:O	2.30	0.55
1:A:469:SER:HA	1:A:472:GLU:HB2	1.90	0.54
1:A:330:VAL:O	1:A:337:THR:OG1	2.26	0.53
1:A:108:ILE:HG21	1:A:132:ILE:HG22	1.91	0.53
1:A:562:ASN:HA	1:A:565:LEU:HD12	1.90	0.53
1:A:441:GLN:HB2	1:A:482:GLY:HA3	1.91	0.53
1:A:455:CYS:HA	1:A:521:ILE:HB	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:PHE:H	1:A:617:SER:HB3	1.74	0.52
1:A:504:MET:HG3	1:A:508:LEU:HD21	1.91	0.52
1:A:417:SER:HB3	1:A:427:ILE:HG23	1.92	0.52
1:A:421:GLY:HA3	1:A:443:HIS:HA	1.92	0.52
1:A:601:PRO:HB3	1:A:814:ARG:HH22	1.74	0.52
1:A:138:VAL:HG13	1:A:158:THR:HG22	1.93	0.51
2:B:8:U:C2'	2:B:8:U:C6	2.94	0.51
1:A:210:LEU:HA	1:A:743:PRO:HB3	1.93	0.50
1:A:159:ILE:HD13	1:A:208:PRO:HG3	1.94	0.50
1:A:237:VAL:HG11	1:A:261:GLU:HG3	1.93	0.50
1:A:560:LEU:HD12	1:A:561:SER:N	2.27	0.50
1:A:117:VAL:HG21	1:A:128:PHE:HD2	1.77	0.50
1:A:50:PRO:HG3	1:A:397:PHE:O	2.12	0.50
1:A:180:SER:HA	1:A:203:HIS:HA	1.94	0.49
1:A:78:MET:HE1	1:A:132:ILE:HD11	1.94	0.49
1:A:40:LEU:HB2	1:A:408:VAL:HG23	1.94	0.49
1:A:68:ARG:HD3	1:A:97:ARG:HE	1.77	0.49
1:A:370:ARG:HE	1:A:375:ARG:HA	1.77	0.49
1:A:75:VAL:HA	1:A:78:MET:HG2	1.95	0.48
1:A:522:LEU:O	1:A:548:GLN:HA	2.13	0.48
1:A:611:ILE:HD12	1:A:814:ARG:HG2	1.94	0.48
1:A:545:GLN:NE2	2:B:1:A:OP3	2.45	0.48
1:A:197:GLU:N	1:A:224:PHE:O	2.47	0.48
1:A:790:TYR:OH	1:A:792:ARG:NH1	2.40	0.48
1:A:69:ARG:O	1:A:73:GLU:HG2	2.12	0.48
1:A:477:ILE:HG13	1:A:560:LEU:HD13	1.96	0.48
1:A:505:PHE:CZ	1:A:536:GLY:HA2	2.49	0.48
1:A:264:GLY:O	1:A:280:ARG:NH1	2.47	0.47
1:A:707:VAL:HG12	1:A:765:TYR:HD1	1.78	0.47
1:A:651:ILE:HA	3:A:901:IPH:H3	1.96	0.47
1:A:737:ASP:OD1	1:A:780:GLN:NE2	2.47	0.47
1:A:506:ARG:HD2	1:A:540:LEU:HD21	1.96	0.47
1:A:478:SER:HA	1:A:481:ALA:HB3	1.96	0.47
1:A:229:PRO:HA	1:A:345:ASN:HA	1.95	0.47
1:A:266:LYS:HE3	1:A:278:LYS:HD2	1.97	0.47
1:A:750:LEU:HB3	1:A:765:TYR:CE2	2.50	0.46
1:A:453:ILE:HD12	1:A:489:PRO:HB3	1.97	0.46
1:A:226:LYS:HD3	1:A:228:GLN:HE21	1.80	0.46
1:A:491:PHE:CD1	1:A:493:LYS:HG2	2.50	0.46
1:A:501:VAL:HG11	1:A:532:VAL:HG22	1.97	0.46
1:A:521:ILE:HD13	1:A:552:VAL:HG11	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ARG:HH21	1:A:354:LYS:HB3	1.81	0.46
1:A:103:ALA:HB2	1:A:396:GLU:HG3	1.98	0.45
1:A:104:MET:HB3	1:A:105:PRO:HD2	1.98	0.45
1:A:167:ARG:HD3	1:A:181:PHE:CZ	2.52	0.45
1:A:658:ARG:O	1:A:658:ARG:HG2	2.15	0.45
1:A:222:THR:HB	1:A:224:PHE:HE1	1.82	0.45
2:B:3:A:H2'	2:B:4:A:C8	2.52	0.45
1:A:28:ARG:HA	1:A:746:PHE:HB2	1.99	0.45
1:A:257:LYS:O	1:A:261:GLU:HG2	2.17	0.45
1:A:79:VAL:HA	1:A:87:PHE:CE2	2.52	0.45
1:A:279:TYR:HB3	1:A:330:VAL:HB	1.99	0.45
1:A:375:ARG:HD2	1:A:759:THR:HG21	1.99	0.45
1:A:54:ILE:HB	1:A:138:VAL:HB	1.99	0.45
1:A:473:GLN:O	1:A:477:ILE:HG12	2.17	0.45
1:A:502:GLU:O	1:A:506:ARG:HG2	2.17	0.44
1:A:104:MET:HE3	1:A:105:PRO:HD2	1.98	0.44
1:A:268:GLU:O	1:A:344:CYS:HA	2.18	0.44
1:A:467:LEU:HD23	1:A:492:CYS:SG	2.57	0.44
1:A:541:GLY:HA2	1:A:852:THR:HG23	1.99	0.44
1:A:456:PHE:HA	1:A:495:ALA:O	2.18	0.44
1:A:328:LEU:HD13	1:A:341:LEU:HD22	1.99	0.44
1:A:667:TYR:CE2	1:A:800:PRO:HG2	2.53	0.44
1:A:793:CYS:HB3	2:B:3:A:O2'	2.18	0.44
1:A:458:PRO:O	1:A:462:CYS:N	2.50	0.44
1:A:59:LEU:HB3	1:A:61:ILE:HD11	2.00	0.44
1:A:790:TYR:CZ	1:A:792:ARG:HD3	2.53	0.43
1:A:63:PRO:HD2	1:A:128:PHE:CE1	2.53	0.43
1:A:28:ARG:NH2	1:A:747:ASP:OD1	2.51	0.43
1:A:669:ASP:OD1	1:A:670:GLY:N	2.52	0.43
1:A:707:VAL:HG12	1:A:765:TYR:CD1	2.54	0.43
1:A:92:PRO:HB3	1:A:102:THR:HG22	2.01	0.43
1:A:650:LEU:O	3:A:901:IPH:H4	2.19	0.43
1:A:147:LEU:HD22	1:A:209:SER:O	2.19	0.43
1:A:448:ILE:HB	1:A:485:ILE:HD12	2.00	0.43
1:A:557:PRO:HA	1:A:560:LEU:HD11	2.01	0.43
1:A:737:ASP:CG	1:A:780:GLN:HE22	2.27	0.43
1:A:805:TYR:O	1:A:809:VAL:HG23	2.19	0.42
1:A:177:VAL:HG21	1:A:224:PHE:HZ	1.85	0.42
1:A:441:GLN:HB2	1:A:482:GLY:CA	2.49	0.42
1:A:170:PRO:HB2	1:A:181:PHE:CZ	2.55	0.42
1:A:478:SER:OG	1:A:485:ILE:HG12	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:VAL:HG11	1:A:687:ILE:HG13	2.01	0.42
1:A:790:TYR:CE2	1:A:792:ARG:HB2	2.54	0.42
1:A:469:SER:O	1:A:473:GLN:HG2	2.19	0.42
1:A:466:HIS:O	1:A:470:PHE:N	2.33	0.42
1:A:566:LYS:HE2	1:A:566:LYS:HB3	1.86	0.42
1:A:467:LEU:HA	1:A:470:PHE:HB3	2.00	0.41
1:A:86:ILE:HG13	1:A:87:PHE:N	2.35	0.41
1:A:207:ARG:HA	1:A:208:PRO:HD3	1.95	0.41
1:A:545:GLN:HG2	1:A:567:ILE:HD11	2.02	0.41
1:A:157:GLU:CD	1:A:157:GLU:H	2.27	0.41
1:A:556:THR:HG22	1:A:559:THR:HG23	2.02	0.41
1:A:230:VAL:HA	1:A:233:PHE:HB3	2.02	0.41
1:A:477:ILE:O	1:A:481:ALA:N	2.51	0.41
1:A:559:THR:HG22	2:B:2:A:C6	2.56	0.41
1:A:288:PRO:HB2	1:A:323:PRO:O	2.21	0.40
1:A:464:GLU:O	1:A:468:LYS:N	2.42	0.40
1:A:477:ILE:HG13	1:A:560:LEU:CD1	2.50	0.40
1:A:756:ILE:HD11	1:A:795:ARG:CZ	2.50	0.40
1:A:141:GLN:O	1:A:145:ASP:N	2.52	0.40
1:A:226:LYS:HD3	1:A:228:GLN:NE2	2.36	0.40
1:A:506:ARG:HA	1:A:540:LEU:HD21	2.04	0.40
1:A:559:THR:HG22	2:B:2:A:C5	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	744/859 (87%)	701 (94%)	40 (5%)	3 (0%)	30 60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	370	ARG
1	A	426	ALA
1	A	425	LYS

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	676/748 (90%)	676 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	HIS
1	A	576	ASN
1	A	621	HIS
1	A	682	HIS
1	A	780	GLN
1	A	807	HIS
1	A	816	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	6/8 (75%)	0	0

There are no RNA backbone outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	IPH	A	901	-	7,7,7	0.34	0	8,8,8	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IPH	A	901	-	-	-	0/1/1/1

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	IPH	2	0

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	764/859 (88%)	0.73	46 (6%) 27 15	29, 72, 129, 161	0
2	B	8/8 (100%)	0.76	1 (12%) 8 5	63, 72, 102, 124	0
All	All	772/867 (89%)	0.73	47 (6%) 27 15	29, 72, 129, 161	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	544	THR	6.8
1	A	756	ILE	3.9
1	A	625	TYR	3.7
1	A	712	HIS	3.6
1	A	859	ALA	3.5
1	A	717	CYS	3.5
1	A	377	GLU	3.4
1	A	370	ARG	3.2
1	A	799	ILE	3.2
1	A	224	PHE	3.1
1	A	305	GLU	3.1
1	A	856	MET	2.9
1	A	449	LYS	2.8
1	A	258	PHE	2.8
1	A	127	ILE	2.8
1	A	104	MET	2.7
1	A	798	SER	2.7
1	A	176	PRO	2.7
1	A	492	CYS	2.7
1	A	637	GLU	2.6
2	B	8	U	2.6
1	A	388	PHE	2.6
1	A	857	TYR	2.5
1	A	450	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	146	ALA	2.4
1	A	501	VAL	2.4
1	A	782	LEU	2.4
1	A	504	MET	2.4
1	A	774	PHE	2.4
1	A	119	LEU	2.3
1	A	626	CYS	2.3
1	A	700	PRO	2.3
1	A	784	TYR	2.3
1	A	772	ASN	2.3
1	A	619	ASP	2.3
1	A	559	THR	2.2
1	A	52	ILE	2.2
1	A	745	GLU	2.2
1	A	410	GLY	2.2
1	A	369	ALA	2.2
1	A	428	ALA	2.2
1	A	484	PRO	2.2
1	A	210	LEU	2.1
1	A	111	ASP	2.1
1	A	556	THR	2.1
1	A	580	PRO	2.1
1	A	615	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 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.

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
-----	------	-------	-----	-------	------	-----	-----------------------------	-------

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	IPH	A	901	7/7	0.84	0.27	125,127,130,132	0

6.5 Other polymers [i](#)

There are no such residues in this entry.