



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:55 AM UTC

PDB ID : 4Z4D / pdb_00004z4d
Title : Human Argonaute2 Bound to t1-G Target RNA
Authors : Schirle, N.T.; MacRae, I.J.
Deposited on : 2015-04-02
Resolution : 1.60 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

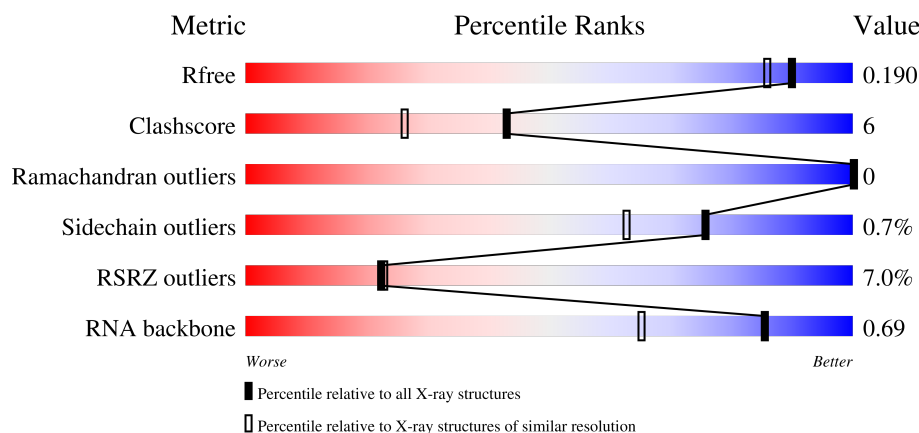
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)
RNA backbone	3983	1010 (2.14-1.06)

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	7% 83% 10% 7%
2	B	21	81% 14% 5%
3	D	11	82% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	IPA	A	908	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7654 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	803	Total	C	N	O	S	0	5	0
			6469	4114	1164	1150	41			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	387	ASP	SER	engineered mutation	UNP Q9UKV8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	20	Total	C	N	O	P	0	0	0
			407	182	62	143	20			

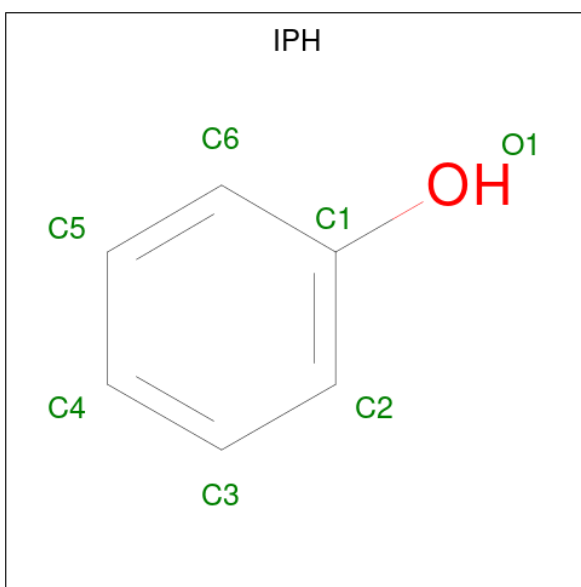
- Molecule 3 is a RNA chain called RNA (5'-R(*CP*AP*AP*UP*GP*UP*GP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	9	Total	C	N	O	P	0	0	0
			173	77	32	56	8			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

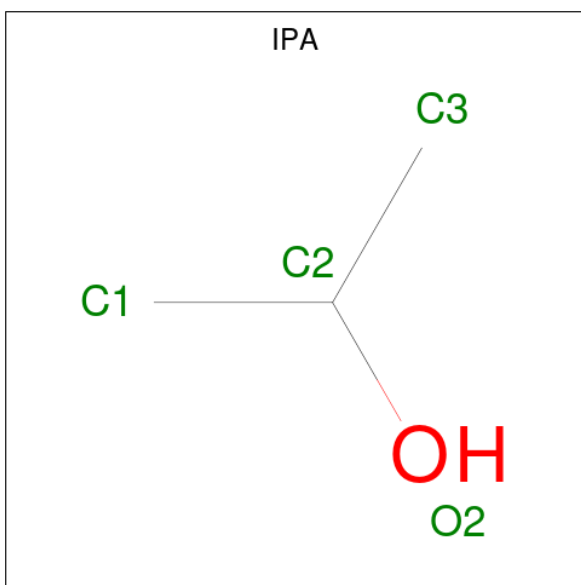
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PHENOL (CCD ID: IPH) (formula: C₆H₆O).



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

- Molecule 6 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 3 1	0	0
6	A	1	Total C O 4 3 1	0	0
6	A	1	Total C O 4 3 1	0	0
6	B	1	Total C O 4 3 1	0	0
6	B	1	Total C O 4 3 1	0	0

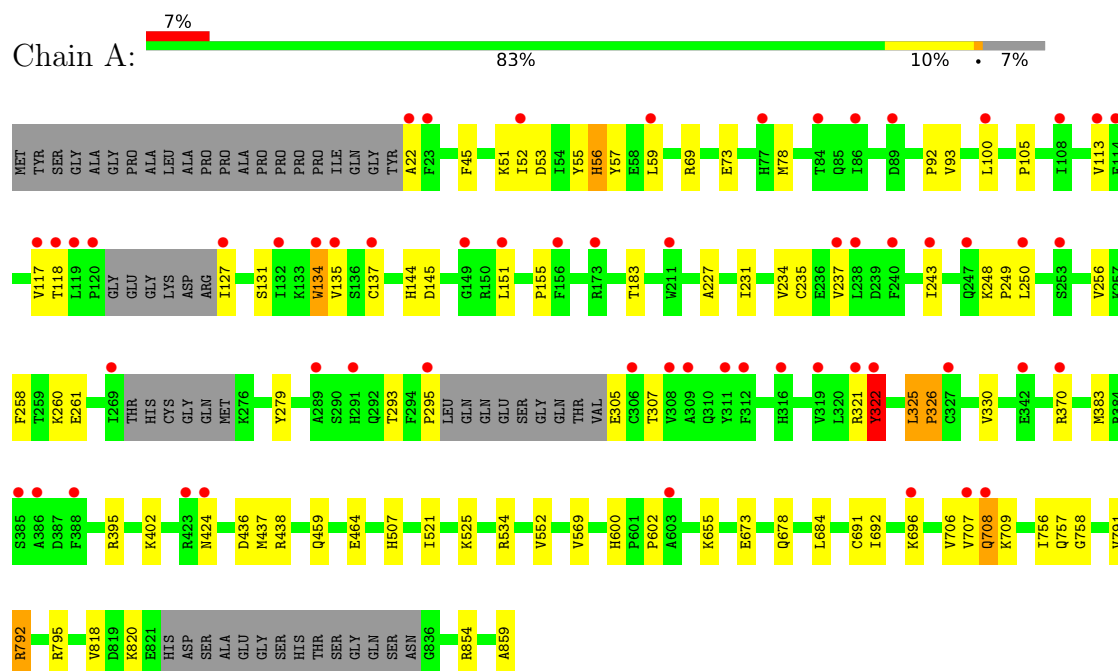
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	470	Total O 470 470	0	0
7	B	47	Total O 47 47	0	0
7	D	37	Total O 37 37	0	0

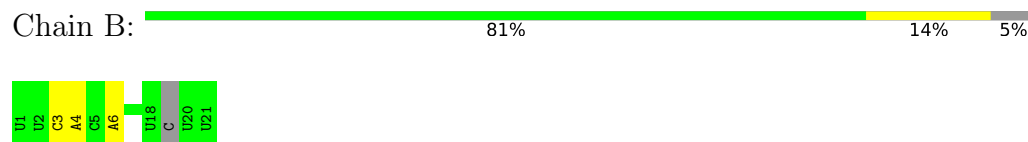
3 Residue-property plots [i](#)

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.

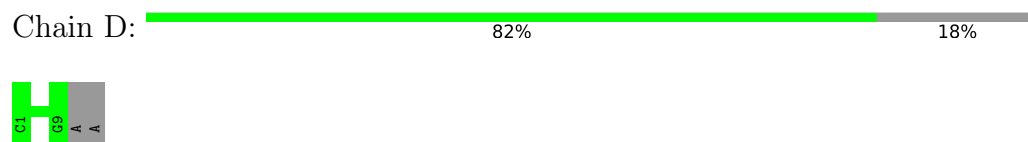
- Molecule 1: Protein argonaute-2



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.74Å 117.02Å 69.87Å 90.00° 92.43° 90.00°	Depositor
Resolution (Å)	35.40 – 1.60 35.40 – 1.60	Depositor EDS
% Data completeness (in resolution range)	96.7 (35.40-1.60) 96.7 (35.40-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.163 , 0.189 0.168 , 0.190	Depositor DCC
R_{free} test set	5721 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7654	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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: IPH, MG, IPA

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	0.86	11/6624 (0.2%)	0.91	6/8962 (0.1%)
2	B	0.61	0/450	0.73	0/692
3	D	0.59	0/193	0.71	0/300
All	All	0.84	11/7267 (0.2%)	0.90	6/9954 (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	A	0	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	155	PRO	N-CD	12.79	1.65	1.47
1	A	708[A]	GLN	CA-C	11.65	1.67	1.53
1	A	708[B]	GLN	CA-C	11.65	1.67	1.53
1	A	708[A]	GLN	C-O	-8.72	1.14	1.23
1	A	708[B]	GLN	C-O	-8.72	1.14	1.23
1	A	325	LEU	C-N	6.82	1.42	1.33
1	A	322	TYR	C-N	6.33	1.41	1.34
1	A	707	VAL	C-O	-5.88	1.17	1.24
1	A	706	VAL	C-O	-5.73	1.17	1.24
1	A	56	HIS	CG-ND1	-5.43	1.32	1.38
1	A	709	LYS	C-O	-5.42	1.17	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	ARG	N-CA-C	-8.61	99.43	110.53
1	A	322	TYR	CA-C-N	-5.37	114.29	119.87
1	A	322	TYR	C-N-CA	-5.37	114.29	119.87
1	A	325	LEU	CA-C-N	-5.04	115.37	120.21
1	A	325	LEU	C-N-CA	-5.04	115.37	120.21
1	A	326	PRO	CA-C-O	-5.03	115.22	122.31

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	708[A]	GLN	Mainchain
1	A	708[B]	GLN	Mainchain

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	6469	0	6524	85	0
2	B	407	0	210	2	0
3	D	173	0	87	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	28	0	23	2	0
6	A	12	0	24	8	0
6	B	8	0	16	2	0
7	A	470	0	0	7	0
7	B	47	0	0	0	0
7	D	37	0	0	0	0
All	All	7654	0	6884	87	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 (87) 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:243:ILE:HD11	1:A:322:TYR:CE1	1.97	1.00
1:A:227:ALA:H	6:A:906:IPA:H12	1.25	0.97
1:A:55:TYR:HD2	1:A:134:TRP:HZ3	1.19	0.90
1:A:127:ILE:HG22	1:A:127:ILE:O	1.71	0.90
1:A:134:TRP:HH2	1:A:137:CYS:HG	1.13	0.89
1:A:243:ILE:HD11	1:A:322:TYR:CZ	2.08	0.88
1:A:600:HIS:O	6:B:103:IPA:H13	1.74	0.87
1:A:243:ILE:CD1	1:A:322:TYR:CE1	2.61	0.83
1:A:534:ARG:HD3	6:A:908:IPA:H31	1.67	0.77
1:A:134:TRP:HH2	1:A:137:CYS:SG	2.09	0.75
1:A:459:GLN:NE2	1:A:464:GLU:OE2	2.27	0.68
1:A:93:VAL:O	1:A:100:LEU:HD12	1.95	0.67
6:A:908:IPA:H32	7:A:1211:HOH:O	1.94	0.67
1:A:127:ILE:O	1:A:127:ILE:CG2	2.43	0.66
1:A:231:ILE:HG23	1:A:243:ILE:HG21	1.78	0.65
1:A:52:ILE:HG22	1:A:53:ASP:O	2.01	0.61
1:A:78:MET:HB2	1:A:117:VAL:HG21	1.85	0.59
1:A:92:PRO:CB	1:A:100:LEU:HD11	2.31	0.59
1:A:55:TYR:CZ	1:A:105:PRO:HG3	2.37	0.59
1:A:134:TRP:CH2	1:A:137:CYS:SG	2.84	0.59
1:A:293:THR:HG22	1:A:307:THR:HG22	1.85	0.58
1:A:237:VAL:CG1	1:A:261:GLU:HG3	2.33	0.58
1:A:92:PRO:HB3	1:A:100:LEU:HD11	1.85	0.57
1:A:295:PRO:HA	1:A:305:GLU:HA	1.87	0.57
1:A:55:TYR:HD2	1:A:134:TRP:CZ3	2.11	0.56
1:A:521:ILE:HD12	1:A:552:VAL:HG21	1.87	0.56
1:A:692:ILE:HD11	5:A:902:IPH:H4	1.86	0.56
1:A:243:ILE:CD1	1:A:322:TYR:CZ	2.86	0.56
1:A:57:TYR:CE2	1:A:134:TRP:HB2	2.41	0.56
1:A:243:ILE:HD12	1:A:322:TYR:CD1	2.40	0.56
1:A:237:VAL:HG11	1:A:261:GLU:HG3	1.88	0.55
1:A:134:TRP:C	1:A:134:TRP:CD1	2.85	0.54
1:A:756:ILE:HD11	1:A:795:ARG:NH2	2.23	0.54
1:A:820:LYS:HE3	6:A:908:IPA:H33	1.90	0.53
1:A:602:PRO:HA	6:B:103:IPA:H33	1.92	0.51
1:A:235:CYS:SG	1:A:243:ILE:HG23	2.51	0.51
1:A:250:LEU:HD13	1:A:326:PRO:HD3	1.93	0.51
1:A:51:LYS:HG2	1:A:144:HIS:CE1	2.45	0.51
1:A:424:ASN:HB2	7:A:1154:HOH:O	2.10	0.51
1:A:395:ARG:CZ	1:A:395:ARG:HA	2.42	0.50
1:A:792:ARG:HD2	1:A:859:ALA:OXT	2.11	0.50
1:A:55:TYR:CD2	1:A:134:TRP:HZ3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ARG:NH1	1:A:73:GLU:HG3	2.28	0.49
1:A:45:PHE:CZ	1:A:383:MET:HG3	2.48	0.48
1:A:525:LYS:NZ	7:A:1010:HOH:O	2.47	0.48
1:A:59:LEU:CD1	1:A:100:LEU:CB	2.92	0.48
1:A:402:LYS:NZ	7:A:1008:HOH:O	2.45	0.47
1:A:507:HIS:HE1	7:A:1032:HOH:O	1.97	0.47
1:A:92:PRO:HB2	1:A:100:LEU:HD11	1.96	0.47
1:A:818:VAL:HB	6:A:908:IPA:H11	1.96	0.46
1:A:52:ILE:HG22	1:A:53:ASP:N	2.30	0.46
1:A:145:ASP:HB3	1:A:151:LEU:HD13	1.98	0.46
1:A:691:CYS:HB2	5:A:902:IPH:H3	1.97	0.46
1:A:59:LEU:CD1	1:A:100:LEU:HB2	2.47	0.45
1:A:250:LEU:HD11	1:A:325:LEU:HD22	1.97	0.45
1:A:655:LYS:NZ	1:A:854:ARG:HE	2.13	0.45
1:A:55:TYR:CD1	1:A:55:TYR:N	2.84	0.45
1:A:234:VAL:HG22	1:A:258:PHE:CE1	2.52	0.45
1:A:59:LEU:HD11	1:A:100:LEU:CB	2.47	0.45
1:A:243:ILE:HD12	1:A:322:TYR:CE1	2.46	0.44
1:A:248:LYS:HB3	1:A:249:PRO:HD2	1.99	0.44
1:A:237:VAL:HG13	1:A:261:GLU:HG3	2.00	0.44
1:A:113:VAL:O	1:A:131:SER:HA	2.17	0.44
1:A:256:VAL:O	1:A:260:LYS:HG2	2.18	0.43
1:A:673:GLU:HG3	7:A:1051:HOH:O	2.17	0.43
1:A:227:ALA:N	6:A:906:IPA:H12	2.10	0.43
1:A:818:VAL:O	6:A:908:IPA:H12	2.19	0.43
1:A:57:TYR:CD2	1:A:134:TRP:HB2	2.54	0.43
1:A:231:ILE:CG2	1:A:243:ILE:HG21	2.46	0.43
1:A:235:CYS:SG	1:A:243:ILE:CG2	3.07	0.43
1:A:59:LEU:CD1	1:A:100:LEU:HB3	2.48	0.43
2:B:3:C:H2'	2:B:4:A:C8	2.53	0.43
1:A:757:GLN:OE1	2:B:6:A:H1'	2.19	0.43
1:A:436:ASP:OD2	1:A:438:ARG:NH2	2.48	0.42
1:A:22:ALA:HA	1:A:684:LEU:HD23	2.00	0.42
1:A:52:ILE:CG2	1:A:53:ASP:N	2.83	0.42
1:A:118:THR:HA	1:A:127:ILE:N	2.33	0.42
1:A:370:ARG:O	1:A:758:GLY:HA2	2.20	0.42
1:A:56:HIS:O	1:A:135:VAL:HG12	2.20	0.42
1:A:678:GLN:HG2	7:A:1252:HOH:O	2.20	0.41
1:A:279:TYR:HB3	1:A:330:VAL:HB	2.02	0.41
1:A:569:VAL:HG21	1:A:791:VAL:HB	2.01	0.41
1:A:59:LEU:HD13	1:A:100:LEU:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:HD13	1:A:100:LEU:HB2	2.01	0.41
1:A:756:ILE:HD11	1:A:795:ARG:HH22	1.84	0.41
1:A:45:PHE:CE2	1:A:383:MET:HG3	2.57	0.40
1:A:183:THR:HG22	6:A:907:IPA:O2	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	798/859 (93%)	781 (98%)	17 (2%)	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	715/752 (95%)	710 (99%)	5 (1%)	76	63

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	TRP
1	A	322	TYR

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Mol	Chain	Res	Type
1	A	437	MET
1	A	696	LYS
1	A	792	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	376	GLN
1	A	488	GLN
1	A	507	HIS
1	A	548	GLN
1	A	558	GLN
1	A	636	GLN
1	A	681	HIS
1	A	712	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	18/21 (85%)	0	0
3	D	7/11 (63%)	0	0
All	All	25/32 (78%)	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](#)

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 for Mogul analysis.

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	$\# Z > 2$
5	IPH	A	902	-	7,7,7	0.60	0	8,8,8	0.52	0
6	IPA	B	103	-	3,3,3	0.51	0	3,3,3	0.46	0
6	IPA	A	907	-	3,3,3	0.56	0	3,3,3	0.13	0
6	IPA	A	908	-	3,3,3	0.63	0	3,3,3	1.08	0
6	IPA	B	102	-	3,3,3	0.61	0	3,3,3	0.33	0
5	IPH	A	905	-	7,7,7	0.57	0	8,8,8	0.75	0
5	IPH	A	903	-	7,7,7	0.37	0	8,8,8	1.06	0
6	IPA	A	906	-	3,3,3	0.58	0	3,3,3	0.38	0
5	IPH	A	904	-	7,7,7	0.73	0	8,8,8	0.87	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
5	IPH	A	905	-	-	-	0/1/1/1
5	IPH	A	902	-	-	-	0/1/1/1
5	IPH	A	904	-	-	-	0/1/1/1
5	IPH	A	903	-	-	-	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.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	902	IPH	2	0
6	B	103	IPA	2	0
6	A	907	IPA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	908	IPA	5	0
6	A	906	IPA	2	0

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	803/859 (93%)	0.26	58 (7%) 21 22	7, 29, 70, 87	5 (0%)
2	B	20/21 (95%)	-0.10	0 100 100	15, 30, 106, 116	0
3	D	9/11 (81%)	-0.49	0 100 100	22, 25, 33, 36	1 (11%)
All	All	832/891 (93%)	0.24	58 (6%) 22 23	7, 29, 71, 116	6 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	PHE	4.6
1	A	127	ILE	4.6
1	A	342	GLU	4.2
1	A	211	TRP	3.8
1	A	295	PRO	3.7
1	A	108	ILE	3.7
1	A	707	VAL	3.5
1	A	22	ALA	3.3
1	A	156	PHE	3.3
1	A	134	TRP	3.2
1	A	84	THR	3.0
1	A	132	ILE	3.0
1	A	306	CYS	3.0
1	A	52	ILE	3.0
1	A	118	THR	2.9
1	A	59	LEU	2.9
1	A	291	HIS	2.9
1	A	386	ALA	2.9
1	A	269	ILE	2.9
1	A	135	VAL	2.8
1	A	117	VAL	2.8
1	A	327	CYS	2.7
1	A	240	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	119	LEU	2.7
1	A	289	ALA	2.6
1	A	321	ARG	2.6
1	A	86	ILE	2.6
1	A	424	ASN	2.6
1	A	250	LEU	2.5
1	A	237	VAL	2.5
1	A	120	PRO	2.4
1	A	708[A]	GLN	2.4
1	A	308	VAL	2.4
1	A	696	LYS	2.4
1	A	151	LEU	2.4
1	A	89	ASP	2.4
1	A	149	GLY	2.3
1	A	311	TYR	2.3
1	A	253	SER	2.3
1	A	114	GLU	2.3
1	A	113	VAL	2.3
1	A	385	SER	2.2
1	A	77	HIS	2.2
1	A	316	HIS	2.2
1	A	388	PHE	2.2
1	A	312	PHE	2.2
1	A	238	LEU	2.1
1	A	370	ARG	2.1
1	A	173	ARG	2.1
1	A	423	ARG	2.1
1	A	322	TYR	2.1
1	A	309	ALA	2.1
1	A	603	ALA	2.1
1	A	100	LEU	2.1
1	A	243	ILE	2.1
1	A	247	GLN	2.0
1	A	319	VAL	2.0
1	A	137	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
6	IPA	A	907	4/4	0.69	0.26	55,56,57,59	0
6	IPA	A	906	4/4	0.78	0.20	29,37,42,52	0
6	IPA	B	103	4/4	0.82	0.19	32,39,45,53	0
6	IPA	B	102	4/4	0.83	0.17	37,43,46,47	0
5	IPH	A	902	7/7	0.85	0.11	33,34,40,46	0
5	IPH	A	905	7/7	0.85	0.11	30,32,34,36	0
6	IPA	A	908	4/4	0.90	0.13	19,27,35,42	0
5	IPH	A	904	7/7	0.91	0.09	17,23,24,36	0
5	IPH	A	903	7/7	0.96	0.05	20,23,26,35	0
4	MG	B	101	1/1	0.98	0.07	29,29,29,29	0
4	MG	D	101	1/1	0.99	0.05	19,19,19,19	0
4	MG	A	901	1/1	0.99	0.03	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.