



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:26 PM UTC

PDB ID : 6CBD / pdb_00006cbd
Title : Crystal Structure of Human Argonaute2 Bound to Three Tryptophans
Authors : Sheu-Gruttadauria, J.; MacRae, I.J.
Deposited on : 2018-02-02
Resolution : 2.20 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 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

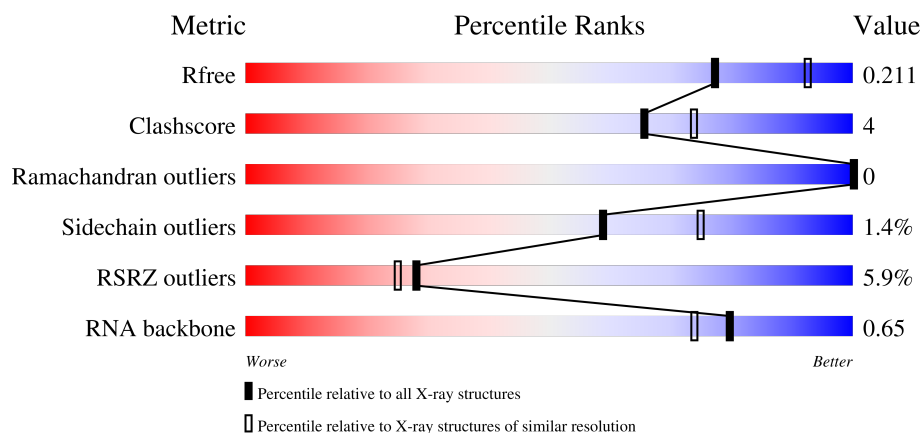
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)
RNA backbone	3983	1052 (2.50-1.90)

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% 83% 8% 8%
2	B	21	67% 19% 5% 10%
3	C	11	9% 82% 9% 9%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7213 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	787	Total	C	N	O	S	0	0	0
			6299	4019	1126	1114	40			

There is a discrepancy between the modelled and reference sequences:

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

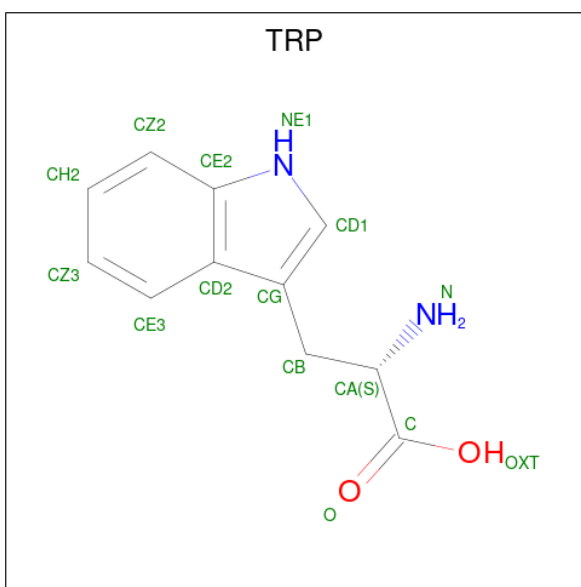
- Molecule 2 is a RNA chain called Guide RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	19	Total	C	N	O	P	0	0	0
			379	168	60	132	19			

- Molecule 3 is a RNA chain called Target RNA.

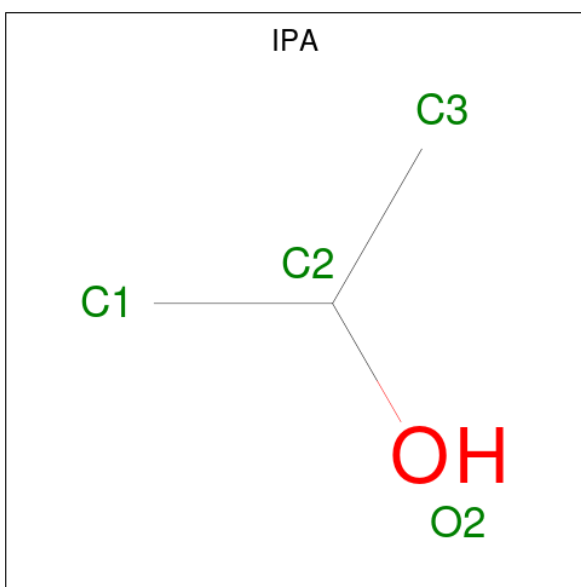
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	P	0	0	0
			196	88	37	62	9			

- Molecule 4 is TRYPTOPHAN (CCD ID: TRP) (formula: C₁₁H₁₂N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	11	2	2		
4	A	1	Total	C	N	O	0	0
			15	11	2	2		
4	A	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 5 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C₃H₈O).



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

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

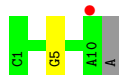
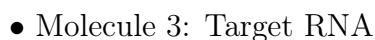
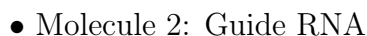
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	229	Total	O	0	0
			229	229		
7	B	31	Total	O	0	0
			31	31		
7	C	19	Total	O	0	0
			19	19		

- 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	55.83Å 117.00Å 70.25Å 90.00° 92.64° 90.00°	Depositor
Resolution (Å)	35.50 – 2.20 35.50 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (35.50-2.20) 98.2 (35.50-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.176 , 0.215 (Not available) , 0.211	Depositor DCC
R_{free} test set	2174 reflections (1.85%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7213	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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: IPA, MG

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	0.32	0/6444	0.71	0/8716
2	B	0.12	0/419	0.29	0/645
3	C	0.18	0/219	0.33	0/340
All	All	0.31	0/7082	0.68	0/9701

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 [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	6299	0	6362	50	0
2	B	379	0	193	4	0
3	C	196	0	98	2	0
4	A	45	0	27	2	0
5	A	8	0	16	0	0
5	B	4	0	8	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	229	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	31	0	0	0	0
7	C	19	0	0	0	0
All	All	7213	0	6704	52	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 4.

All (52) 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:502:GLU:O	1:A:506:ARG:HG3	1.89	0.72
1:A:167:ARG:HG2	1:A:181:PHE:HZ	1.55	0.70
4:A:902:TRP:N	7:A:1003:HOH:O	2.27	0.68
1:A:286:ARG:NH2	1:A:287:ARG:HH12	1.91	0.67
1:A:757:GLN:HG3	3:C:5:G:N2	2.08	0.66
1:A:521:ILE:HD12	1:A:552:VAL:HG21	1.79	0.65
1:A:228:GLN:NE2	1:A:236:GLU:OE2	2.30	0.61
1:A:313:LYS:NZ	7:A:1008:HOH:O	2.33	0.59
1:A:286:ARG:CZ	1:A:287:ARG:HH12	2.17	0.57
1:A:65:LYS:NZ	2:B:16:U:O2'	2.20	0.55
2:B:3:C:H2'	2:B:4:A:C8	2.42	0.54
1:A:148:SER:OG	1:A:150:ARG:NH1	2.39	0.54
1:A:252:ASP:OD1	1:A:255:ARG:NH1	2.31	0.54
1:A:428:ALA:HB2	1:A:440:LYS:HE2	1.89	0.54
1:A:56:HIS:NE2	1:A:99:ASN:OD1	2.37	0.53
1:A:296:LEU:HD12	1:A:296:LEU:H	1.73	0.53
1:A:207:ARG:NH2	1:A:673:GLU:OE1	2.40	0.52
1:A:146:ALA:HA	1:A:151:LEU:HB2	1.92	0.51
1:A:143:LEU:HB2	1:A:158:THR:HG21	1.92	0.51
1:A:50:PRO:HB2	1:A:52:ILE:HG13	1.93	0.51
1:A:148:SER:OG	1:A:149:GLY:N	2.44	0.50
1:A:337:THR:HA	2:B:21:U:H1'	1.94	0.49
1:A:45:PHE:CZ	1:A:383:MET:HG3	2.47	0.49
1:A:757:GLN:HG3	3:C:5:G:H21	1.75	0.49
1:A:251:THR:HG22	1:A:253:SER:H	1.78	0.48
1:A:74:ILE:HG23	1:A:117:VAL:HG21	1.95	0.48
1:A:287:ARG:HG3	1:A:287:ARG:HH11	1.79	0.48
1:A:221:ALA:HB3	1:A:368:THR:HG22	1.95	0.48
1:A:117:VAL:HG23	1:A:128:PHE:HB2	1.95	0.47
1:A:59:LEU:HA	1:A:131:SER:O	2.15	0.47
1:A:167:ARG:HG2	1:A:181:PHE:CZ	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:PRO:HB3	1:A:102:THR:HG22	1.98	0.45
1:A:709:LYS:HG3	7:A:1083:HOH:O	2.17	0.45
1:A:245:GLU:N	1:A:245:GLU:OE1	2.50	0.45
1:A:692:ILE:HD11	4:A:903:TRP:HZ3	1.82	0.45
1:A:60:ASP:HB2	1:A:131:SER:HB2	1.99	0.44
1:A:78:MET:HB2	1:A:117:VAL:HG11	1.99	0.44
1:A:243:ILE:O	1:A:245:GLU:N	2.50	0.44
1:A:419:LEU:HD23	1:A:577:ILE:HD11	2.00	0.44
1:A:634:HIS:CD2	1:A:635:ARG:HG3	2.54	0.43
1:A:447:GLU:OE2	1:A:486:GLN:NE2	2.53	0.42
1:A:669:ASP:OD1	7:A:1001:HOH:O	2.21	0.42
1:A:230:VAL:O	1:A:234:VAL:HG23	2.20	0.42
1:A:151:LEU:HA	1:A:152:PRO:HD3	1.83	0.41
1:A:117:VAL:O	1:A:127:ILE:N	2.54	0.41
1:A:635:ARG:HD3	2:B:11:C:OP1	2.21	0.41
1:A:42:ALA:C	1:A:44:PHE:H	2.29	0.41
1:A:163:ASP:O	1:A:167:ARG:HB2	2.21	0.41
1:A:33:THR:H	1:A:777:ASP:CG	2.29	0.40
1:A:365:ILE:C	1:A:367:ALA:H	2.29	0.40
1:A:425:LYS:HE3	1:A:425:LYS:HB3	1.92	0.40
1:A:694:LEU:HD23	1:A:694:LEU:HA	1.98	0.40

There are no symmetry-related clashes.

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	766/859 (89%)	743 (97%)	23 (3%)	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	696/752 (93%)	686 (99%)	10 (1%)	59 75

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ILE
1	A	65	LYS
1	A	141	GLN
1	A	171	SER
1	A	173	ARG
1	A	207	ARG
1	A	243	ILE
1	A	366	ARG
1	A	459	GLN
1	A	815	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	GLN
1	A	204	GLN
1	A	345	ASN
1	A	488	GLN
1	A	623	ASN
1	A	652	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	16/21 (76%)	1 (6%)	0
3	C	8/11 (72%)	0	0
All	All	24/32 (75%)	1 (4%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	16	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	IPA	A	905	-	3,3,3	0.51	0	3,3,3	0.33	0
4	TRP	A	902	-	15,16,16	0.72	1 (6%)	18,22,22	0.75	1 (5%)
5	IPA	B	101	-	3,3,3	0.55	0	3,3,3	0.31	0
5	IPA	A	904	-	3,3,3	0.52	0	3,3,3	0.33	0
4	TRP	A	901	-	15,16,16	0.71	1 (6%)	18,22,22	0.74	1 (5%)
4	TRP	A	903	-	15,16,16	0.73	1 (6%)	18,22,22	0.77	1 (5%)

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
4	TRP	A	901	-	-	0/8/8/8	0/2/2/2
4	TRP	A	903	-	-	7/8/8/8	0/2/2/2
4	TRP	A	902	-	-	3/8/8/8	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	903	TRP	OXT-C	-2.24	1.23	1.30
4	A	901	TRP	OXT-C	-2.17	1.23	1.30
4	A	902	TRP	OXT-C	-2.17	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	TRP	OXT-C-O	-2.68	117.99	124.08
4	A	902	TRP	OXT-C-O	-2.63	118.11	124.08
4	A	903	TRP	OXT-C-O	-2.59	118.21	124.08

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	903	TRP	OXT-C-CA-CB
4	A	902	TRP	OXT-C-CA-N
4	A	903	TRP	OXT-C-CA-N
4	A	903	TRP	O-C-CA-CB
4	A	903	TRP	N-CA-CB-CG
4	A	903	TRP	O-C-CA-N
4	A	902	TRP	N-CA-CB-CG
4	A	903	TRP	CA-CB-CG-CD2
4	A	903	TRP	CA-CB-CG-CD1
4	A	902	TRP	O-C-CA-N

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	902	TRP	1	0
4	A	903	TRP	1	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	787/859 (91%)	0.19	47 (5%) 27 24	19, 39, 90, 112	0
2	B	19/21 (90%)	-0.38	0 100 100	24, 42, 107, 120	0
3	C	10/11 (90%)	-0.28	1 (10%) 12 10	37, 40, 55, 82	0
All	All	816/891 (91%)	0.17	48 (5%) 28 25	19, 39, 91, 120	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	LEU	5.2
1	A	243	ILE	4.6
1	A	127	ILE	4.2
1	A	108	ILE	3.9
1	A	88	GLY	3.9
1	A	319	VAL	3.6
1	A	119	LEU	3.5
1	A	22	ALA	3.4
1	A	152	PRO	3.4
1	A	77	HIS	3.3
1	A	269	ILE	3.2
1	A	59	LEU	3.2
1	A	23	PHE	3.1
1	A	87	PHE	3.0
1	A	836	GLY	3.0
1	A	327	CYS	3.0
1	A	84	THR	2.9
1	A	118	THR	2.9
1	A	151	LEU	2.9
1	A	368	THR	2.7
1	A	757	GLN	2.7
1	A	308	VAL	2.6
1	A	312	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	82	PHE	2.5
1	A	120	PRO	2.5
1	A	156	PHE	2.4
1	A	134	TRP	2.4
1	A	262	ILE	2.4
1	A	342	GLU	2.4
1	A	306	CYS	2.4
1	A	607	LYS	2.3
1	A	318	LEU	2.3
1	A	339	LEU	2.2
1	A	290	SER	2.2
1	A	66	CYS	2.2
1	A	250	LEU	2.2
1	A	309	ALA	2.2
1	A	386	ALA	2.2
1	A	79	VAL	2.1
1	A	113	VAL	2.1
1	A	242	SER	2.1
3	C	10	A	2.1
1	A	330	VAL	2.1
1	A	132	ILE	2.0
1	A	279	TYR	2.0
1	A	149	GLY	2.0
1	A	83	LYS	2.0
1	A	107	PRO	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
5	IPA	B	101	4/4	0.76	0.18	35,44,48,51	0
4	TRP	A	903	15/15	0.80	0.13	39,45,62,67	15
5	IPA	A	904	4/4	0.81	0.18	48,56,62,67	0
4	TRP	A	901	15/15	0.82	0.12	36,47,73,77	0
4	TRP	A	902	15/15	0.83	0.11	35,41,73,79	0
6	MG	B	102	1/1	0.84	0.12	60,60,60,60	0
5	IPA	A	905	4/4	0.87	0.16	38,42,44,51	0
6	MG	C	101	1/1	0.97	0.03	38,38,38,38	0
6	MG	A	906	1/1	1.00	0.02	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.