



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:51 AM UTC

PDB ID : 5KI6 / pdb_00005ki6
Title : Human Argonaute-2 bound to a guide RNA with a nucleobase modification at position 1
Authors : Schirle, N.T.; MacRae, I.J.
Deposited on : 2016-06-16
Resolution : 2.15 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

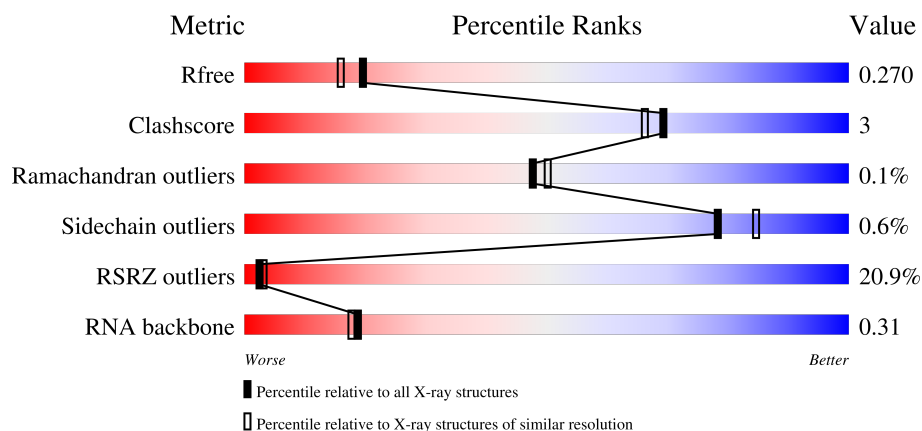
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)
RNA backbone	3983	1112 (2.50-1.82)

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	
2	B	21	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6756 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
			Total	C	N	O	S			
1	A	798	6406	4078	1154	1135	39	0	0	0

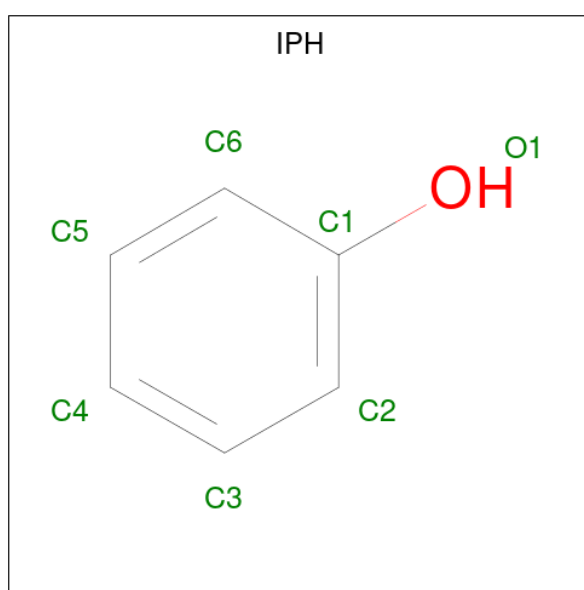
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is a RNA chain called miR-122.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	10	224	103	38	73	10	0	0	0

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



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

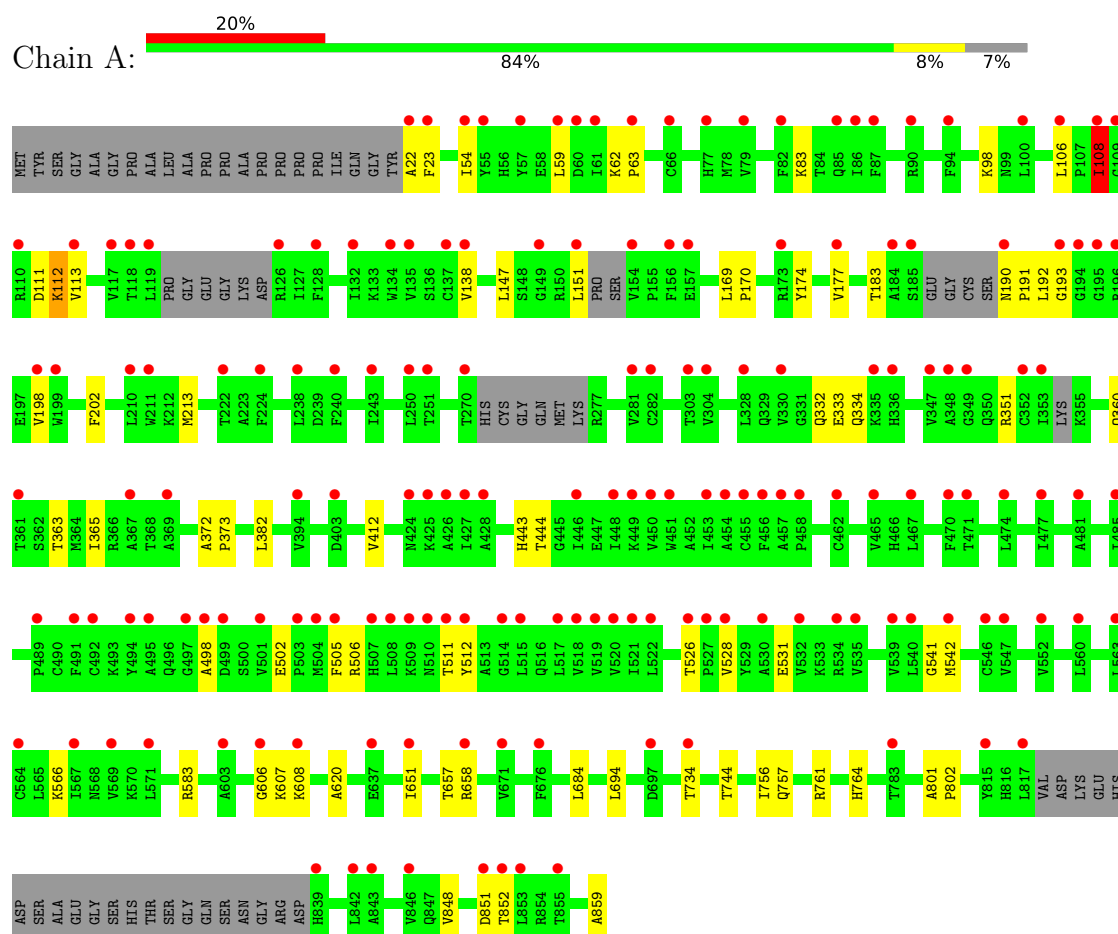
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	100	Total O 100 100	0	0
4	B	5	Total O 5 5	0	0

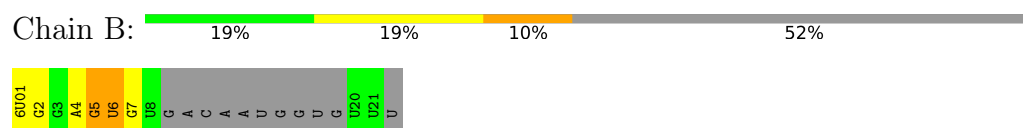
3 Residue-property plots [i](#)

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: miR-122



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.28Å 107.30Å 68.86Å 90.00° 107.44° 90.00°	Depositor
Resolution (Å)	47.57 – 2.15 47.57 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.57-2.15) 99.3 (47.57-2.15)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.16Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.237 , 0.270 0.240 , 0.270	Depositor DCC
R_{free} test set	2382 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.8	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	0.94	EDS
Total number of atoms	6756	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% 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: 6U0, 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	0.41	3/6554 (0.0%)	0.65	7/8867 (0.1%)
2	B	0.98	2/215 (0.9%)	1.51	5/331 (1.5%)
All	All	0.44	5/6769 (0.1%)	0.70	12/9198 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	764	HIS	CG-ND1	-6.15	1.31	1.38
2	B	6	U	O3'-P	-5.52	1.52	1.61
1	A	761	ARG	C-N	5.49	1.40	1.33
1	A	764	HIS	CD2-NE2	-5.25	1.32	1.37
2	B	5	G	O3'-P	-5.22	1.53	1.61

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6	U	C1'-C2'-O2'	-13.25	88.53	108.40
2	B	4	A	C1'-C2'-O2'	-11.25	91.53	108.40
2	B	5	G	C1'-C2'-O2'	-9.26	94.51	108.40
1	A	108	ILE	N-CA-C	-8.14	96.40	108.12
1	A	111	ASP	N-CA-C	7.94	121.74	110.23
1	A	756	ILE	N-CA-C	6.88	117.00	110.53
2	B	4	A	C4'-C3'-O3'	6.43	122.64	113.00
1	A	761	ARG	CA-C-N	-6.03	113.57	119.90
1	A	761	ARG	C-N-CA	-6.03	113.57	119.90
2	B	5	G	C4'-C3'-O3'	6.00	122.01	113.00
1	A	111	ASP	CA-C-N	5.27	128.35	120.87
1	A	111	ASP	C-N-CA	5.27	128.35	120.87

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	6406	0	6467	44	0
2	B	224	0	97	4	0
3	A	21	0	18	0	0
4	A	100	0	0	0	0
4	B	5	0	0	0	0
All	All	6756	0	6582	46	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 3.

All (46) 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:190:ASN:HD22	1:A:198:VAL:HB	1.24	0.98
1:A:190:ASN:ND2	1:A:198:VAL:HB	1.82	0.95
1:A:192:LEU:HD11	1:A:198:VAL:CG2	2.21	0.70
1:A:192:LEU:HD11	1:A:198:VAL:HG23	1.74	0.68
1:A:192:LEU:HD22	1:A:360:GLN:O	2.00	0.62
1:A:541:GLY:HA3	1:A:851:ASP:HB2	1.87	0.56
1:A:606:GLY:O	1:A:608:LYS:N	2.40	0.55
1:A:190:ASN:N	1:A:191:PRO:CD	2.68	0.55
1:A:108:ILE:O	1:A:108:ILE:HG12	2.07	0.53
1:A:502:GLU:O	1:A:506:ARG:N	2.40	0.52
1:A:606:GLY:C	1:A:608:LYS:H	2.18	0.51
1:A:566:LYS:NZ	1:A:859:ALA:OXT	2.41	0.50
1:A:59:LEU:N	1:A:98:LYS:O	2.42	0.50
1:A:365:ILE:HD11	2:B:7:G:C5	2.48	0.49
1:A:332:GLN:O	1:A:334:GLN:N	2.43	0.49
1:A:174:TYR:HD1	1:A:183:THR:HG23	1.79	0.48
1:A:192:LEU:HD23	1:A:363:THR:HB	1.96	0.48
1:A:22:ALA:HA	1:A:684:LEU:HD23	1.96	0.47
1:A:526:THR:O	1:A:528:VAL:N	2.42	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLY:O	1:A:360:GLN:NE2	2.45	0.46
1:A:848:VAL:HG22	1:A:852:THR:HB	1.98	0.46
1:A:583:ARG:NH1	1:A:620:ALA:O	2.49	0.46
1:A:651:ILE:HD11	1:A:694:LEU:HD11	1.99	0.45
1:A:606:GLY:C	1:A:608:LYS:N	2.73	0.45
1:A:106:LEU:C	1:A:108:ILE:H	2.25	0.44
1:A:332:GLN:O	1:A:333:GLU:HB2	2.17	0.44
1:A:505:PHE:HB3	1:A:542:MET:HE1	1.98	0.44
1:A:177:VAL:HG11	1:A:351:ARG:HD3	1.99	0.43
1:A:511:THR:HG23	1:A:512:TYR:CD2	2.53	0.43
1:A:657:THR:O	1:A:658:ARG:HG2	2.18	0.43
1:A:169:LEU:HB3	1:A:170:PRO:HD3	1.98	0.43
2:B:1:6U0:O2'	2:B:2:G:OP1	2.35	0.43
1:A:147:LEU:HD21	1:A:213:MET:CE	2.48	0.43
1:A:54:ILE:HB	1:A:138:VAL:HB	2.01	0.42
2:B:5:G:C6	2:B:6:U:O4	2.73	0.42
1:A:112:LYS:HG3	1:A:113:VAL:N	2.34	0.42
1:A:757:GLN:OE1	2:B:5:G:N2	2.50	0.42
1:A:801:ALA:N	1:A:802:PRO:HD2	2.34	0.42
1:A:192:LEU:CD1	1:A:198:VAL:HG23	2.45	0.42
1:A:498:ALA:HB1	1:A:531:GLU:HG3	2.01	0.42
1:A:62:LYS:HA	1:A:63:PRO:C	2.45	0.42
1:A:202:PHE:CB	1:A:382:LEU:HD21	2.50	0.42
1:A:372:ALA:HB3	1:A:373:PRO:HD3	2.03	0.41
1:A:151:LEU:HB3	1:A:744:THR:HG21	2.03	0.40
1:A:443:HIS:ND1	1:A:444:THR:HG23	2.36	0.40
1:A:412:VAL:HG22	1:A:734:THR:HG22	2.03	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	784/859 (91%)	755 (96%)	28 (4%)	1 (0%)	48 50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	607	LYS

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	706/752 (94%)	702 (99%)	4 (1%)	78 84

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	PHE
1	A	83	LYS
1	A	108	ILE
1	A	112	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
1	A	216	ASN
1	A	310	GLN
1	A	316	HIS
1	A	623	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	7/21 (33%)	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](#)

3 ligands are 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	0.71	0	8,8,8	0.29	0
3	IPH	A	903	-	7,7,7	0.74	0	8,8,8	0.28	0
3	IPH	A	902	-	7,7,7	0.72	0	8,8,8	0.28	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
3	IPH	A	903	-	-	-	0/1/1/1
3	IPH	A	902	-	-	-	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.

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	798/859 (92%)	1.15	169 (21%) 2 3	30, 66, 119, 174	0
2	B	9/21 (42%)	0.01	0 100 100	45, 55, 87, 112	0
All	All	807/880 (91%)	1.14	169 (20%) 2 3	30, 66, 119, 174	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	22	ALA	4.8
1	A	194	GLY	4.7
1	A	353	ILE	4.4
1	A	511	THR	4.4
1	A	552	VAL	4.4
1	A	330	VAL	4.4
1	A	519	VAL	4.3
1	A	517	LEU	4.2
1	A	817	LEU	4.2
1	A	497	GLY	4.2
1	A	151	LEU	4.2
1	A	135	VAL	4.2
1	A	119	LEU	4.0
1	A	535	VAL	4.0
1	A	23	PHE	4.0
1	A	540	LEU	3.9
1	A	539	VAL	3.9
1	A	184	ALA	3.9
1	A	498	ALA	3.9
1	A	571	LEU	3.8
1	A	222	THR	3.8
1	A	518	VAL	3.7
1	A	567	ILE	3.7
1	A	530	ALA	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	528	VAL	3.7
1	A	658	ARG	3.7
1	A	485	ILE	3.7
1	A	547	VAL	3.6
1	A	336	HIS	3.6
1	A	465	VAL	3.5
1	A	527	PRO	3.5
1	A	394	VAL	3.5
1	A	450	VAL	3.5
1	A	270	THR	3.4
1	A	456	PHE	3.4
1	A	117	VAL	3.4
1	A	783	THR	3.3
1	A	156	PHE	3.3
1	A	451	TRP	3.3
1	A	86	ILE	3.3
1	A	132	ILE	3.3
1	A	448	ILE	3.3
1	A	515	LEU	3.3
1	A	352	CYS	3.2
1	A	195	GLY	3.2
1	A	520	VAL	3.2
1	A	521	ILE	3.2
1	A	526	THR	3.2
1	A	454	ALA	3.1
1	A	403	ASP	3.1
1	A	839	HIS	3.1
1	A	505	PHE	3.1
1	A	108	ILE	3.1
1	A	59	LEU	3.1
1	A	455	CYS	3.0
1	A	251	THR	3.0
1	A	477	ILE	3.0
1	A	113	VAL	3.0
1	A	210	LEU	2.9
1	A	335	LYS	2.9
1	A	546	CYS	2.9
1	A	304	VAL	2.9
1	A	815	TYR	2.9
1	A	211	TRP	2.9
1	A	449	LYS	2.9
1	A	349	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	504	MET	2.9
1	A	185	SER	2.8
1	A	491	PHE	2.8
1	A	361	THR	2.8
1	A	193	GLY	2.8
1	A	603	ALA	2.8
1	A	250	LEU	2.8
1	A	154	VAL	2.8
1	A	281	VAL	2.8
1	A	425	LYS	2.7
1	A	57	TYR	2.7
1	A	134	TRP	2.7
1	A	106	LEU	2.7
1	A	79	VAL	2.7
1	A	149	GLY	2.7
1	A	467	LEU	2.7
1	A	494	TYR	2.7
1	A	458	PRO	2.6
1	A	347	VAL	2.6
1	A	471	THR	2.6
1	A	60	ASP	2.6
1	A	110	ARG	2.6
1	A	126	ARG	2.6
1	A	462	CYS	2.6
1	A	457	ALA	2.6
1	A	509	LYS	2.6
1	A	82	PHE	2.6
1	A	474	LEU	2.6
1	A	243	ILE	2.5
1	A	852	THR	2.5
1	A	453	ILE	2.5
1	A	508	LEU	2.5
1	A	560	LEU	2.5
1	A	651	ILE	2.5
1	A	137	CYS	2.5
1	A	512	TYR	2.4
1	A	564	CYS	2.4
1	A	100	LEU	2.4
1	A	492	CYS	2.4
1	A	542	MET	2.4
1	A	676	PHE	2.4
1	A	54	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	90	ARG	2.4
1	A	426	ALA	2.4
1	A	853	LEU	2.4
1	A	157	GLU	2.4
1	A	606	GLY	2.4
1	A	851	ASP	2.4
1	A	446	ILE	2.4
1	A	173	ARG	2.3
1	A	77	HIS	2.3
1	A	569	VAL	2.3
1	A	199	TRP	2.3
1	A	87	PHE	2.3
1	A	224	PHE	2.3
1	A	855	THR	2.3
1	A	534	ARG	2.3
1	A	697	ASP	2.3
1	A	238	LEU	2.3
1	A	55	TYR	2.3
1	A	507	HIS	2.2
1	A	128	PHE	2.2
1	A	503	PRO	2.2
1	A	734	THR	2.2
1	A	846	VAL	2.2
1	A	563	LEU	2.2
1	A	138	VAL	2.2
1	A	532	VAL	2.2
1	A	608	LYS	2.2
1	A	495	ALA	2.2
1	A	843	ALA	2.2
1	A	66	CYS	2.2
1	A	489	PRO	2.2
1	A	196	ARG	2.2
1	A	63	PRO	2.1
1	A	177	VAL	2.1
1	A	85	GLN	2.1
1	A	510	ASN	2.1
1	A	61	ILE	2.1
1	A	427	ILE	2.1
1	A	198	VAL	2.1
1	A	671	VAL	2.1
1	A	481	ALA	2.1
1	A	94	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	240	PHE	2.1
1	A	470	PHE	2.1
1	A	367	ALA	2.1
1	A	282	CYS	2.1
1	A	424	ASN	2.1
1	A	118	THR	2.1
1	A	303	THR	2.1
1	A	109	GLY	2.1
1	A	501	VAL	2.1
1	A	348	ALA	2.1
1	A	328	LEU	2.0
1	A	514	GLY	2.0
1	A	637	GLU	2.0
1	A	369	ALA	2.0
1	A	428	ALA	2.0
1	A	190	ASN	2.0
1	A	522	LEU	2.0
1	A	842	LEU	2.0
1	A	499	ASP	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
3	IPH	A	903	7/7	0.78	0.15	57,59,63,72	0
3	IPH	A	901	7/7	0.87	0.12	46,54,60,62	0
3	IPH	A	902	7/7	0.91	0.13	66,66,69,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.