



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:54 PM UTC

PDB ID : 5GUH / pdb_00005guh
Title : Crystal structure of silkworm PIWI-clade Argonaute Siwi bound to piRNA
Authors : Matsumoto, N.; Nishimasu, H.; Ishitani, R.; Nureki, O.
Deposited on : 2016-08-29
Resolution : 2.40 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

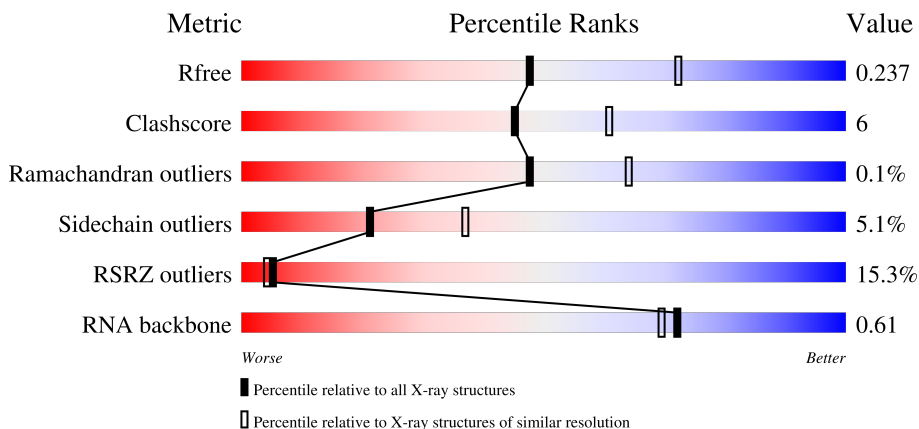
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)
RNA backbone	3983	1155 (2.70-2.10)

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	899	13% 71% 12% • 16%
2	B	28	21% 7% 71%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6078 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 PIWI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	759	Total	C	N	O	S	0	0	0
			5828	3733	993	1074	28			

- Molecule 2 is a RNA chain called RNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	8	Total	C	N	O	P	0	0	0
			164	74	19	63	8			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	83	Total	O	0	0
			83	83		
4	B	1	Total	O	0	0
			1	1		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.90Å 114.62Å 136.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.83 – 2.40 87.83 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (87.83-2.40) 99.5 (87.83-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.40Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.209 , 0.235 0.211 , 0.237	Depositor DCC
R_{free} test set	2001 reflections (4.26%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6078	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: MG, OMU

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	0.12	0/5952	0.30	0/8104
2	B	0.06	0/156	0.16	0/235
All	All	0.12	0/6108	0.29	0/8339

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	5828	0	5696	69	0
2	B	164	0	85	1	0
3	A	2	0	0	0	0
4	A	83	0	0	1	0
4	B	1	0	0	0	0
All	All	6078	0	5781	69	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 (69) 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:223:ARG:HD3	1:A:230:MET:HE3	1.55	0.89
1:A:179:GLU:HG2	1:A:223:ARG:HE	1.47	0.80
1:A:136:ARG:NH1	4:A:1001:HOH:O	2.20	0.74
1:A:709:LEU:HB2	1:A:712:HIS:HB2	1.75	0.68
1:A:511:THR:HG22	1:A:513:GLU:H	1.59	0.67
1:A:889:HIS:HD2	1:A:891:SER:H	1.45	0.65
1:A:230:MET:SD	1:A:230:MET:N	2.70	0.65
1:A:380:ILE:HA	1:A:391:ILE:HD13	1.78	0.64
1:A:175:ILE:HG22	1:A:177:PRO:HD2	1.80	0.64
1:A:293:THR:HG23	1:A:304:LEU:HD11	1.82	0.61
1:A:168:LEU:HB3	1:A:240:VAL:HB	1.83	0.60
1:A:223:ARG:H	1:A:230:MET:HE2	1.66	0.60
1:A:510:ASP:HB2	1:A:799:PRO:HD2	1.85	0.58
1:A:228:GLU:HB3	1:A:230:MET:HE1	1.87	0.57
1:A:348:THR:OG1	1:A:351:ASN:ND2	2.26	0.56
1:A:265:GLN:HG2	1:A:267:MET:HE3	1.88	0.56
1:A:441:SER:O	1:A:445:HIS:ND1	2.31	0.56
1:A:710:SER:HA	1:A:754:GLU:HG2	1.89	0.55
1:A:387:TYR:HB2	1:A:389:LEU:HD11	1.89	0.53
1:A:605:ASP:OD1	1:A:606:ARG:N	2.43	0.52
1:A:188:LEU:HD21	1:A:223:ARG:HG3	1.91	0.52
1:A:363:ASN:N	1:A:363:ASN:OD1	2.43	0.52
1:A:298:TYR:CD1	1:A:303:LEU:HB2	2.46	0.51
1:A:223:ARG:CD	1:A:230:MET:HE3	2.36	0.50
1:A:404:LYS:N	1:A:405:PRO:HD2	2.26	0.50
1:A:533:TRP:CE2	1:A:566:PRO:HB3	2.47	0.50
1:A:574:ASP:O	1:A:606:ARG:NH2	2.45	0.50
1:A:176:SER:HB2	1:A:231:ARG:HB3	1.93	0.50
1:A:389:LEU:HD13	1:A:422:LEU:HD21	1.93	0.50
1:A:292:LYS:HG3	1:A:309:ALA:HB2	1.94	0.49
1:A:192:HIS:HE1	1:A:221:SER:HB2	1.78	0.49
1:A:359:ASP:OD1	1:A:360:VAL:N	2.44	0.49
1:A:459:ASN:OD1	1:A:462:ARG:NH1	2.42	0.49
1:A:321:MET:HG2	1:A:337:PHE:HE1	1.78	0.49
1:A:740:ASP:OD1	1:A:741:GLY:N	2.45	0.49
1:A:160:VAL:HB	1:A:302:LEU:HB3	1.94	0.48
1:A:579:TYR:CD2	1:A:606:ARG:HG2	2.50	0.47
1:A:365:SER:OG	1:A:394:PRO:O	2.33	0.46
1:A:629:ASN:HB3	1:A:638:ILE:HD13	1.98	0.46
1:A:223:ARG:HB2	1:A:230:MET:HE3	1.97	0.46
1:A:306:THR:HG21	1:A:460:PHE:CE2	2.51	0.46
1:A:346:VAL:HG21	1:A:423:CYS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:GLU:CD	1:A:229:ARG:H	2.23	0.46
1:A:624:VAL:O	2:B:1:U:H4'	2.16	0.46
1:A:594:LEU:HD13	1:A:646:ILE:HG23	1.98	0.45
1:A:713:MET:HG3	1:A:758:ILE:HD11	1.98	0.45
1:A:821:ASN:HA	1:A:827:ILE:HD11	1.97	0.45
1:A:654:PRO:HB2	1:A:655:TRP:CE3	2.52	0.45
1:A:168:LEU:HD12	1:A:168:LEU:HA	1.83	0.45
1:A:467:THR:HG22	1:A:469:GLU:HG2	1.99	0.45
1:A:154:LEU:HD13	1:A:789:GLN:HB2	1.99	0.44
1:A:393:ASP:OD1	1:A:396:GLN:N	2.49	0.44
1:A:709:LEU:O	1:A:713:MET:N	2.44	0.44
1:A:663:SER:HB3	1:A:733:ALA:H	1.82	0.44
1:A:222:ASP:HA	1:A:230:MET:HG2	1.98	0.44
1:A:584:GLU:HB2	1:A:613:LYS:HD2	2.00	0.43
1:A:501:ALA:HB2	1:A:524:LEU:O	2.19	0.43
1:A:223:ARG:H	1:A:230:MET:CE	2.30	0.42
1:A:419:VAL:HG23	1:A:422:LEU:HB2	2.01	0.42
1:A:351:ASN:ND2	1:A:353:ARG:H	2.18	0.41
1:A:541:GLN:HG2	1:A:627:ALA:HB1	2.03	0.41
1:A:473:GLU:O	1:A:476:THR:HG22	2.21	0.41
1:A:259:PHE:CE1	1:A:293:THR:HG21	2.55	0.41
1:A:311:LYS:HD2	1:A:311:LYS:HA	1.90	0.40
1:A:396:GLN:HE22	1:A:421:GLU:HB2	1.85	0.40
1:A:709:LEU:HD13	1:A:712:HIS:HB2	2.02	0.40
1:A:772:LYS:HB3	1:A:839:THR:HA	2.03	0.40
1:A:530:LEU:HD11	1:A:533:TRP:HB3	2.03	0.40
1:A:480:LYS:HB2	1:A:480:LYS:HE3	1.89	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	751/899 (84%)	718 (96%)	32 (4%)	1 (0%)	48 64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	654	PRO

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	613/783 (78%)	582 (95%)	31 (5%)	21 37

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	LEU
1	A	176	SER
1	A	181	SER
1	A	223	ARG
1	A	230	MET
1	A	262	LEU
1	A	267	MET
1	A	285	LEU
1	A	302	LEU
1	A	313	LEU
1	A	323	SER
1	A	351	ASN
1	A	363	ASN
1	A	364	VAL
1	A	389	LEU
1	A	412	LEU
1	A	424	ARG
1	A	438	LEU
1	A	442	LEU
1	A	469	GLU

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Mol	Chain	Res	Type
1	A	476	THR
1	A	485	LEU
1	A	615	THR
1	A	628	ARG
1	A	709	LEU
1	A	722	LYS
1	A	744	ASP
1	A	792	ARG
1	A	820	GLN
1	A	827	ILE
1	A	861	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	HIS
1	A	213	HIS
1	A	310	HIS
1	A	320	GLN
1	A	351	ASN
1	A	363	ASN
1	A	425	GLN
1	A	602	ASN
1	A	692	GLN
1	A	695	GLN
1	A	701	ASN
1	A	716	ASN
1	A	889	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	6/28 (21%)	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 ⓘ

1 non-standard protein/DNA/RNA residue 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
2	OMU	B	28	2	19,22,23	1.21	2 (10%)	25,31,34	1.83	5 (20%)

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
2	OMU	B	28	2	-	0/9/27/28	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	28	OMU	C4-N3	-2.56	1.34	1.38
2	B	28	OMU	C2-N3	-2.14	1.34	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	28	OMU	C4-N3-C2	-4.86	120.57	126.61
2	B	28	OMU	N3-C2-N1	4.36	120.56	114.89
2	B	28	OMU	C5-C4-N3	3.76	120.07	114.80
2	B	28	OMU	O4-C4-C5	-2.99	120.01	125.16
2	B	28	OMU	O2-C2-N1	-2.55	119.47	122.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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	759/899 (84%)	0.83	117 (15%) 5 4	30, 63, 116, 149	0
2	B	7/28 (25%)	0.79	0 100 100	63, 66, 114, 175	0
All	All	766/927 (82%)	0.83	117 (15%) 5 4	30, 63, 116, 175	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	ILE	5.4
1	A	329	LYS	5.3
1	A	223	ARG	5.1
1	A	140	VAL	5.0
1	A	709	LEU	5.0
1	A	408	ILE	4.8
1	A	141	THR	4.7
1	A	406	ARG	4.5
1	A	328	THR	4.4
1	A	430	ASP	4.4
1	A	336	ILE	4.3
1	A	135	THR	4.2
1	A	326	ALA	4.0
1	A	433	ARG	3.9
1	A	428	LEU	3.8
1	A	431	GLU	3.8
1	A	215	ASP	3.8
1	A	225	THR	3.7
1	A	130	ILE	3.7
1	A	233	LEU	3.7
1	A	229	ARG	3.7
1	A	710	SER	3.6
1	A	139	ALA	3.6
1	A	324	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	133	LEU	3.5
1	A	338	LEU	3.5
1	A	436	PHE	3.5
1	A	678	LYS	3.4
1	A	411	GLY	3.4
1	A	242	PRO	3.2
1	A	134	ARG	3.2
1	A	177	PRO	3.2
1	A	673	HIS	3.2
1	A	230	MET	3.2
1	A	222	ASP	3.2
1	A	410	ALA	3.1
1	A	327	ALA	3.1
1	A	138	GLU	3.0
1	A	226	ASP	3.0
1	A	388	ASN	3.0
1	A	703	HIS	2.9
1	A	227	ASN	2.9
1	A	216	PRO	2.9
1	A	711	SER	2.9
1	A	429	SER	2.9
1	A	335	LYS	2.9
1	A	294	THR	2.8
1	A	131	SER	2.8
1	A	228	GLU	2.8
1	A	337	PHE	2.8
1	A	169	TYR	2.8
1	A	572	ARG	2.8
1	A	260	ASN	2.8
1	A	437	LYS	2.8
1	A	247	TYR	2.7
1	A	422	LEU	2.7
1	A	573	HIS	2.7
1	A	248	ILE	2.7
1	A	340	ASP	2.7
1	A	236	LEU	2.6
1	A	634	SER	2.6
1	A	377	ILE	2.6
1	A	171	TYR	2.6
1	A	214	PRO	2.6
1	A	391	ILE	2.5
1	A	389	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	235	LYS	2.5
1	A	627	ALA	2.5
1	A	176	SER	2.5
1	A	137	PRO	2.5
1	A	218	GLU	2.5
1	A	266	LEU	2.5
1	A	239	GLU	2.4
1	A	220	TYR	2.4
1	A	447	LYS	2.4
1	A	212	LEU	2.4
1	A	695	GLN	2.4
1	A	238	CYS	2.4
1	A	663	SER	2.3
1	A	322	LEU	2.3
1	A	385	LYS	2.3
1	A	495	PRO	2.3
1	A	237	THR	2.3
1	A	271	TYR	2.3
1	A	602	ASN	2.2
1	A	323	SER	2.2
1	A	325	TYR	2.2
1	A	672	CYS	2.2
1	A	404	LYS	2.2
1	A	432	MET	2.2
1	A	677	SER	2.2
1	A	374	ASP	2.2
1	A	440	ARG	2.2
1	A	520	ARG	2.2
1	A	412	LEU	2.2
1	A	415	LEU	2.2
1	A	427	GLY	2.2
1	A	221	SER	2.2
1	A	434	ALA	2.2
1	A	243	GLY	2.2
1	A	725	ARG	2.2
1	A	184	VAL	2.1
1	A	626	CYS	2.1
1	A	356	ARG	2.1
1	A	745	GLY	2.1
1	A	213	HIS	2.1
1	A	339	GLU	2.1
1	A	380	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	360	VAL	2.1
1	A	364	VAL	2.1
1	A	539	GLU	2.1
1	A	278	ILE	2.1
1	A	603	TYR	2.1
1	A	543	ARG	2.0
1	A	472	GLU	2.0
1	A	679	GLU	2.0
1	A	675	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	OMU	B	28	21/22	0.94	0.11	68,82,92,97	0

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(Å ²)	Q<0.9
3	MG	A	902	1/1	0.90	0.25	60,60,60,60	0
3	MG	A	901	1/1	1.00	0.04	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.