



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:50 PM GMT

PDB ID : 4Z4H
Title : Human Argonaute2 A481T Mutant Bound to t1-A Target RNA
Authors : Schirle, N.T.; MacRae, I.J.
Deposited on : 2015-04-02
Resolution : 2.50 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

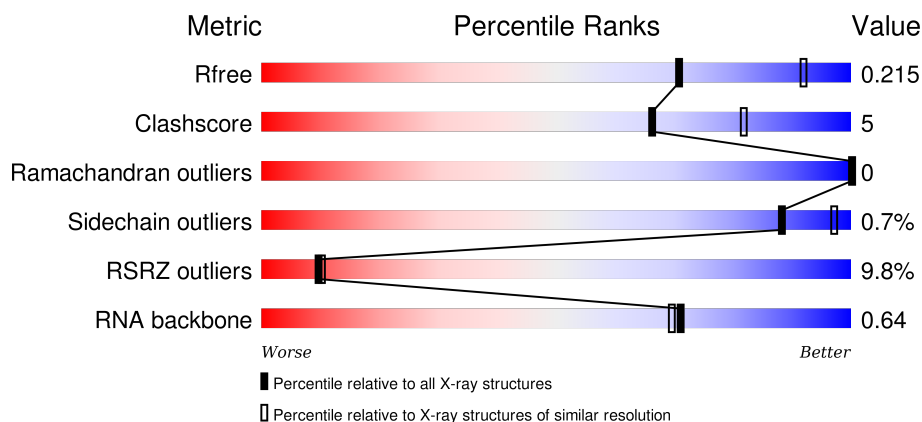
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)
RNA backbone	2183	1172 (3.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>9%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>7%</div> </div> </div>
2	B	21	<div> <div>19%</div> <div> <div></div> <div>67%</div> <div>24%</div> <div>5%</div> <div>5%</div> </div> </div>
3	D	11	<div> <div></div> <div> <div></div> <div>64%</div> <div>9%</div> <div>27%</div> </div> </div>

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
5	IPH	A	902	-	-	-	X
5	IPH	A	903	-	-	-	X
5	IPH	A	904	-	-	-	X
5	IPH	A	905	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7166 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	802	Total	C	N	O	S	0	0	0
			6432	4096	1158	1138	40			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	387	ASP	SER	engineered mutation	UNP Q9UKV8
A	481	THR	ALA	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
			399	177	62	140	20			

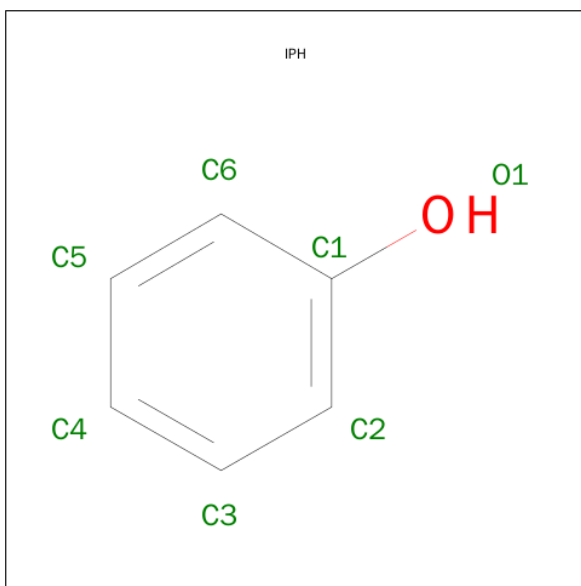
- Molecule 3 is a RNA chain called RNA (5'-R(*CP*AP*AP*UP*GP*UP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	8	Total	C	N	O	P	0	0	0
			169	77	32	53	7			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is PHENOL (three-letter code: 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	110	Total	O	0	0
			110	110		
6	B	12	Total	O	0	0
			12	12		
6	D	13	Total	O	0	0
			13	13		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.70Å 116.60Å 70.10Å 90.00° 92.29° 90.00°	Depositor
Resolution (Å)	44.81 – 2.50 44.81 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (44.81-2.50) 98.6 (44.81-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.172 , 0.211 0.187 , 0.215	Depositor DCC
R_{free} test set	1488 reflections (5.15%)	DCC
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.9	EDS
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 30389 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7166	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, 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	0.48	1/6583 (0.0%)	0.49	3/8906 (0.0%)
2	B	0.57	1/441 (0.2%)	0.77	0/679
3	D	0.59	1/189 (0.5%)	0.62	0/293
All	All	0.49	3/7213 (0.0%)	0.52	3/9878 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	U	OP3-P	-10.82	1.48	1.61
3	D	7	G	O3'-P	-6.24	1.53	1.61
1	A	415	PRO	N-CD	5.16	1.55	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	LYS	C-N-CD	5.87	140.72	128.40
1	A	415	PRO	C-N-CD	5.66	140.29	128.40
1	A	414	GLN	C-N-CD	5.38	139.69	128.40

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	6432	0	6502	67	0
2	B	399	0	203	3	0
3	D	169	0	88	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	0	0
6	A	110	0	0	3	0
6	B	12	0	0	0	0
6	D	13	0	0	0	0
All	All	7166	0	6816	68	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 5.

All (68) 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:O	1:A:244:GLU:HG2	1.31	1.25
1:A:108:ILE:HG22	1:A:109:GLY:O	1.43	1.16
1:A:696:LYS:HB3	1:A:697:ASP:HB2	1.23	1.14
1:A:23:PHE:CD1	1:A:24:LYS:HG2	2.02	0.95
1:A:243:ILE:O	1:A:244:GLU:CG	2.15	0.95
1:A:695:GLU:HG3	1:A:696:LYS:HG3	1.49	0.92
1:A:696:LYS:HB3	1:A:697:ASP:CB	2.02	0.89
1:A:134:TRP:HH2	1:A:137:CYS:HG	0.89	0.85
1:A:23:PHE:HD1	1:A:24:LYS:HG2	1.39	0.84
1:A:134:TRP:HH2	1:A:137:CYS:SG	2.05	0.77
1:A:695:GLU:HG3	1:A:696:LYS:CG	2.16	0.76
1:A:669:ASP:OD1	6:A:1001:HOH:O	2.05	0.73
1:A:108:ILE:CG2	1:A:109:GLY:O	2.33	0.70
1:A:296:LEU:CD1	1:A:306:CYS:HB3	2.22	0.69
1:A:696:LYS:CB	1:A:697:ASP:HB2	2.14	0.69
1:A:57:TYR:CE2	1:A:108:ILE:HD12	2.29	0.68
1:A:296:LEU:HD11	1:A:306:CYS:HB3	1.74	0.67
1:A:696:LYS:HB2	1:A:697:ASP:C	2.16	0.66
1:A:167:ARG:NH2	1:A:204:GLN:O	2.29	0.66
1:A:106:LEU:HD12	1:A:108:ILE:HD11	1.78	0.65
1:A:57:TYR:CE2	1:A:108:ILE:CD1	2.79	0.65
1:A:23:PHE:CE1	1:A:24:LYS:HG2	2.32	0.65
1:A:477:ILE:O	1:A:481:THR:HB	2.02	0.60
1:A:695:GLU:HG2	1:A:698:TYR:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:PHE:CD1	1:A:24:LYS:N	2.73	0.57
1:A:106:LEU:HD12	1:A:108:ILE:CD1	2.36	0.56
1:A:696:LYS:CB	1:A:697:ASP:CA	2.84	0.55
1:A:216:ASN:ND2	6:A:1007:HOH:O	2.41	0.54
1:A:347:VAL:HG12	1:A:350:GLN:NE2	2.23	0.53
1:A:60:ASP:HB3	1:A:131:SER:OG	2.08	0.53
1:A:112:LYS:HG2	1:A:133:LYS:HG2	1.91	0.52
1:A:243:ILE:O	1:A:244:GLU:CB	2.57	0.52
1:A:695:GLU:HG3	1:A:696:LYS:CD	2.43	0.49
1:A:442:PHE:CE2	1:A:481:THR:HG23	2.47	0.49
1:A:58:GLU:C	1:A:59:LEU:HD12	2.33	0.49
1:A:106:LEU:HB2	1:A:108:ILE:CD1	2.42	0.49
1:A:74:ILE:HG23	1:A:117:VAL:HG21	1.93	0.48
1:A:56:HIS:NE2	1:A:99:ASN:OD1	2.43	0.48
1:A:68:ARG:CZ	1:A:97:ARG:NH1	2.77	0.48
1:A:68:ARG:NH1	2:B:14:A:OP1	2.42	0.48
1:A:347:VAL:CG1	1:A:350:GLN:NE2	2.77	0.48
1:A:68:ARG:CZ	1:A:97:ARG:HH12	2.27	0.47
1:A:106:LEU:CD1	1:A:108:ILE:HD11	2.46	0.46
1:A:57:TYR:CE2	1:A:108:ILE:HD13	2.49	0.46
1:A:279:TYR:HB3	1:A:330:VAL:HB	1.98	0.45
1:A:256:VAL:HG13	1:A:257:LYS:N	2.31	0.45
1:A:243:ILE:HG12	1:A:244:GLU:H	1.82	0.45
1:A:57:TYR:CZ	1:A:108:ILE:HD12	2.52	0.45
1:A:106:LEU:HB2	1:A:108:ILE:HD12	1.99	0.45
1:A:696:LYS:HB2	1:A:698:TYR:N	2.31	0.45
1:A:134:TRP:CH2	1:A:137:CYS:SG	2.93	0.45
1:A:389:ASN:O	1:A:395:ARG:NH2	2.50	0.45
1:A:243:ILE:HG12	1:A:244:GLU:N	2.32	0.44
1:A:92:PRO:HB3	1:A:102:THR:HG22	2.00	0.44
1:A:234:VAL:HG22	1:A:258:PHE:CE1	2.53	0.44
1:A:696:LYS:CB	1:A:697:ASP:C	2.85	0.43
1:A:714:ARG:NE	6:A:1012:HOH:O	2.50	0.43
1:A:583:ARG:NH1	1:A:620:ALA:O	2.51	0.43
1:A:372:ALA:HB3	1:A:373:PRO:HD3	2.01	0.43
2:B:3:C:H2'	2:B:4:A:C8	2.54	0.43
1:A:694:LEU:HA	1:A:694:LEU:HD23	1.82	0.43
1:A:801:ALA:N	1:A:802:PRO:HD2	2.33	0.43
1:A:45:PHE:CZ	1:A:383:MET:HG3	2.55	0.42
1:A:58:GLU:O	1:A:59:LEU:HD12	2.20	0.41
1:A:336:HIS:ND1	2:B:21:U:O2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:GLU:N	1:A:503:PRO:HD2	2.36	0.41
1:A:253:SER:O	1:A:256:VAL:HG12	2.22	0.40
1:A:84:THR:O	1:A:85:GLN:HB3	2.22	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	790/859 (92%)	764 (97%)	26 (3%)	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	710/753 (94%)	705 (99%)	5 (1%)	88	97

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

Mol	Chain	Res	Type
1	A	387	ASP
1	A	481	THR
1	A	695	GLU

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Mol	Chain	Res	Type
1	A	804	TYR
1	A	815	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	17/21 (80%)	2 (11%)	0
3	D	7/11 (63%)	0	0
All	All	24/32 (75%)	2 (8%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	17	C
2	B	21	U

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	0.33	0	8,8,8	0.25	0
5	IPH	A	903	-	7,7,7	0.27	0	8,8,8	0.25	0
5	IPH	A	904	-	7,7,7	0.36	0	8,8,8	0.29	0
5	IPH	A	905	-	7,7,7	0.44	0	8,8,8	0.23	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	902	-	-	0/0/0/0	0/1/1/1
5	IPH	A	903	-	-	0/0/0/0	0/1/1/1
5	IPH	A	904	-	-	0/0/0/0	0/1/1/1
5	IPH	A	905	-	-	0/0/0/0	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	802/859 (93%)	0.24	77 (9%) 10 11	19, 44, 109, 152	0
2	B	20/21 (95%)	-0.01	4 (20%) 1 1	26, 57, 143, 177	0
3	D	8/11 (72%)	-0.98	0 100 100	34, 39, 44, 51	0
All	All	830/891 (93%)	0.23	81 (9%) 10 10	19, 44, 112, 177	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	GLN	7.3
1	A	331	GLY	6.7
1	A	334	GLN	6.6
1	A	119	LEU	5.3
1	A	90	ARG	5.2
1	A	332	GLN	5.0
1	A	423	ARG	5.0
1	A	110	ARG	4.7
1	A	108	ILE	4.6
1	A	115	LEU	4.6
1	A	279	TYR	4.5
1	A	333	GLU	4.3
1	A	296	LEU	4.2
1	A	294	PHE	4.1
1	A	151	LEU	4.0
1	A	142	ALA	3.8
1	A	243	ILE	3.8
1	A	117	VAL	3.7
1	A	366	ARG	3.7
1	A	312	PHE	3.7
1	A	311	TYR	3.6
1	A	116	GLU	3.5
1	A	276	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	20	U	3.4
1	A	277	ARG	3.4
2	B	21	U	3.3
1	A	85	GLN	3.3
1	A	149	GLY	3.2
1	A	64	GLU	3.2
2	B	17	C	3.2
1	A	336	HIS	3.1
1	A	295	PRO	3.1
1	A	319	VAL	3.1
1	A	268	GLU	3.0
1	A	61	ILE	3.0
1	A	316	HIS	2.9
1	A	52	ILE	2.9
1	A	79	VAL	2.9
1	A	133	LYS	2.8
1	A	114	GLU	2.8
1	A	51	LYS	2.7
1	A	128	PHE	2.7
1	A	109	GLY	2.7
1	A	65	LYS	2.7
1	A	154	VAL	2.6
1	A	554	ARG	2.6
1	A	23	PHE	2.5
1	A	318	LEU	2.5
1	A	328	LEU	2.5
1	A	113	VAL	2.4
1	A	317	LYS	2.4
1	A	156	PHE	2.4
1	A	313	LYS	2.4
1	A	134	TRP	2.4
1	A	81	HIS	2.4
1	A	103	ALA	2.3
1	A	59	LEU	2.3
1	A	95	ASP	2.3
1	A	141	GLN	2.3
1	A	88	GLY	2.3
1	A	262	ILE	2.3
1	A	321	ARG	2.2
1	A	130	VAL	2.2
1	A	118	THR	2.2
1	A	479	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	247	GLN	2.2
1	A	250	LEU	2.2
1	A	152	PRO	2.2
2	B	18	U	2.2
1	A	62	LYS	2.2
1	A	267	VAL	2.2
1	A	424	ASN	2.2
1	A	111	ASP	2.1
1	A	335	LYS	2.1
1	A	55	TYR	2.1
1	A	422	GLY	2.1
1	A	104	MET	2.0
1	A	330	VAL	2.0
1	A	74	ILE	2.0
1	A	248	LYS	2.0
1	A	132	ILE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	IPH	A	905	7/7	0.83	0.29	9.90	59,63,65,66	0
5	IPH	A	902	7/7	0.92	0.25	5.40	49,52,53,60	0
5	IPH	A	903	7/7	0.95	0.18	5.33	42,43,46,51	0
5	IPH	A	904	7/7	0.83	0.21	2.34	67,71,73,74	0
4	MG	A	901	1/1	0.97	0.18	1.27	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MG	B	101	1/1	0.90	0.05	-	73,73,73,73	0
4	MG	D	101	1/1	0.96	0.03	-	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.