Full wwPDB X-ray Structure Validation Report

Feb 19, 2016 – 08:50 PM GMT

PDB ID	:	4Z4D
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

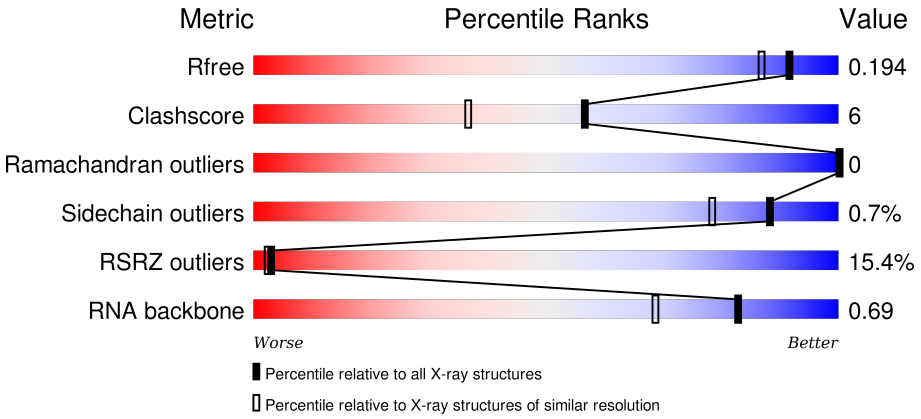
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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}	91344	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)
RNA backbone	2183	1046 (2.70-0.62)

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 <=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	15% 83% 10% 7%
2	B	21	10% 62% 33% 5%
3	D	11	73% 9% 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	906	-	-	-	X
6	IPA	A	907	-	-	-	X
6	IPA	A	908	-	-	X	X
6	IPA	B	102	-	-	-	X
6	IPA	B	103	-	-	-	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			

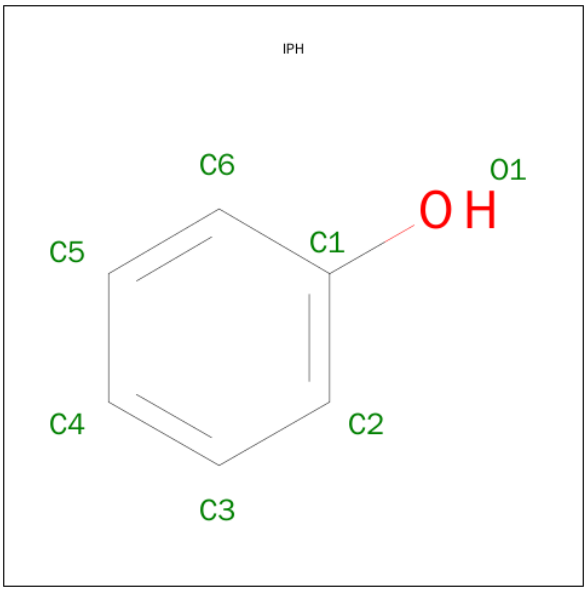
- Molecule 3 is a RNA chain called RNA (5'-R(*CP*AP*AP*UP*GP*UP*GP*AP*G)-3').

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 (three-letter code: MG) (formula: Mg).

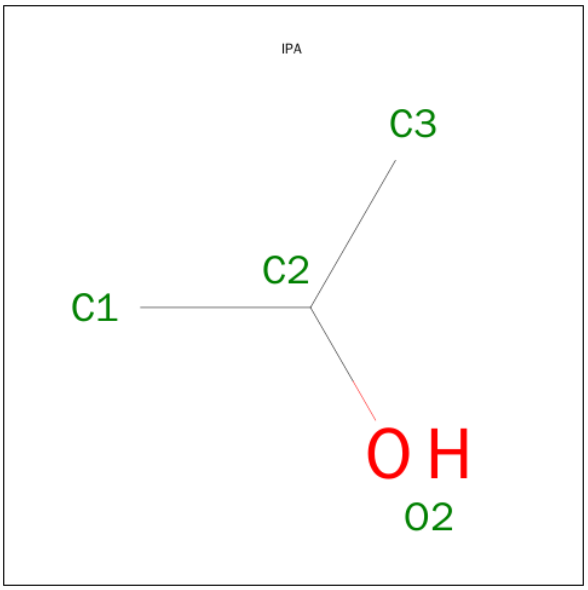
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PHENOL (three-letter code: IPH) (formula: C_6H_6O).



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

- Molecule 6 is ISOPROPYL ALCOHOL (three-letter code: 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.

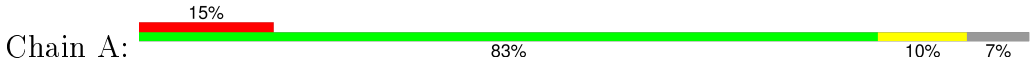
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	470	Total O 470 470	0	0
7	B	47	Total O 47 47	0	0
7	D	37	Total O 37 37	0	0

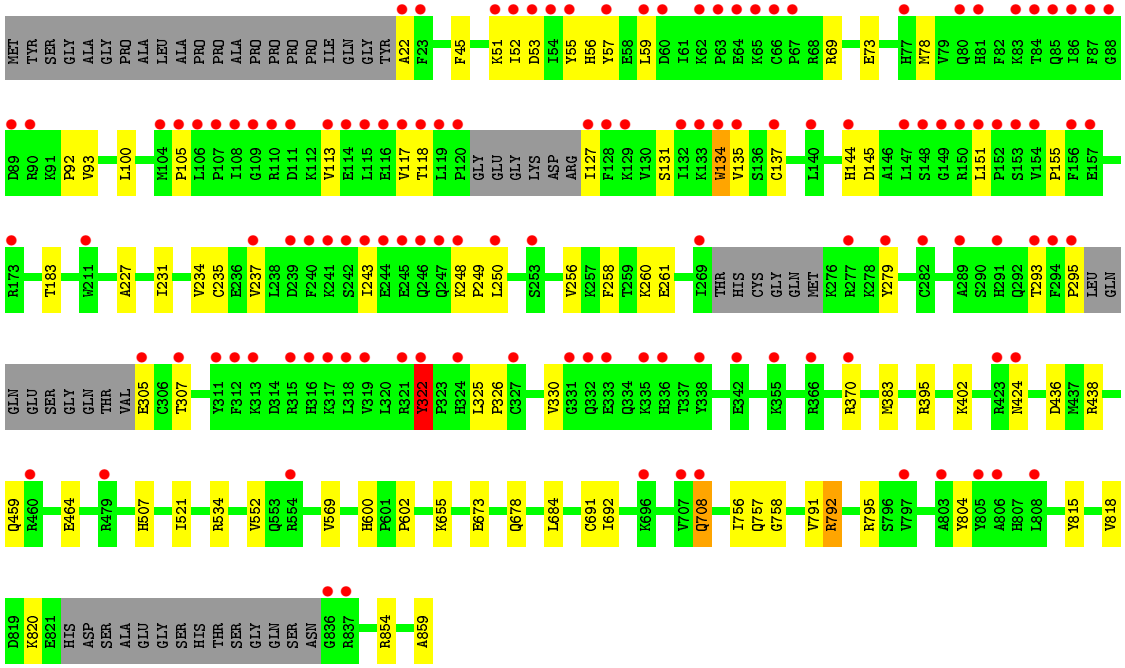
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

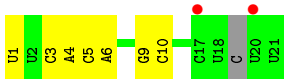
Chain A:





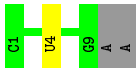
• Molecule 2: RNA (5'-R(P*UP*UP*CP*AP*CP*AP*UP*UP*GP*CP*CP*CP*AP*AP*GP*UP*CP*UP*UP*U)-3')

Chain B:



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

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.78 (at 1.60Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.163 , 0.189 0.174 , 0.194	Depositor DCC
R_{free} test set	5721 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	21.4	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.4	EDS
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 113739 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, 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	0.69	3/6624 (0.0%)	0.72	5/8962 (0.1%)
2	B	1.13	1/450 (0.2%)	1.30	5/692 (0.7%)
3	D	1.19	0/193	1.56	1/300 (0.3%)
All	All	0.74	4/7267 (0.1%)	0.81	11/9954 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	155	PRO	N-CD	12.72	1.65	1.47
2	B	1	U	OP3-P	-9.11	1.50	1.61
1	A	708[A]	GLN	CA-C	5.41	1.67	1.52
1	A	708[B]	GLN	CA-C	5.41	1.67	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	4	U	C5-C6-N1	-6.88	119.26	122.70
2	B	5	C	C6-N1-C2	6.78	123.01	120.30
1	A	708[A]	GLN	CB-CA-C	-5.78	98.84	110.40
1	A	708[B]	GLN	CB-CA-C	-5.78	98.84	110.40
2	B	10	C	O5'-P-OP2	-5.75	100.53	105.70
1	A	322	TYR	C-N-CD	5.73	140.43	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	5	C	C5-C6-N1	-5.63	118.18	121.00
1	A	708[A]	GLN	CA-C-N	-5.28	105.59	117.20
1	A	708[B]	GLN	CA-C-N	-5.28	105.59	117.20
2	B	9	G	C4-C5-N7	-5.21	108.72	110.80
2	B	9	G	C5-N7-C8	5.13	106.86	104.30

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 (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	6469	0	6524	83	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	6	0
7	B	47	0	0	0	0
7	D	37	0	0	0	0
All	All	7654	0	6884	85	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 (85) 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: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:134:TRP:CH2	1:A:137:CYS:SG	2.84	0.70
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:CG2	1:A:127:ILE:O	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: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:243:ILE:HD12	1:A:322:TYR:CD1	2.40	0.56
1:A:57:TYR:CE2	1:A:134:TRP:HB2	2.41	0.56
1:A:237:VAL:HG11	1:A:261:GLU:HG3	1.88	0.55
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:424:ASN:HB2	7:A:1154:HOH:O	2.10	0.51
1:A:51:LYS:HG2	1:A:144:HIS:CE1	2.45	0.51
1:A:792:ARG:HD2	1:A:859:ALA:OXT	2.11	0.50
1:A:395:ARG:CZ	1:A:395:ARG:HA	2.42	0.50
1:A:134:TRP:C	1:A:134:TRP:CD1	2.85	0.49
1:A:55:TYR:CD2	1:A:134:TRP:HZ3	2.11	0.49
1:A:69:ARG:NH1	1:A:73:GLU:HG3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:PHE:CZ	1:A:383:MET:HG3	2.48	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:N	1:A:55:TYR:CD1	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:235:CYS:SG	1:A:243:ILE:CG2	3.07	0.43
1:A:231:ILE:CG2	1:A:243:ILE:HG21	2.46	0.43
1:A:57:TYR:CD2	1:A:134:TRP:HB2	2.54	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:118:THR:HA	1:A:127:ILE:N	2.33	0.42
1:A:52:ILE:CG2	1:A:53:ASP:N	2.83	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	88 78

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

Mol	Chain	Res	Type
1	A	134	TRP
1	A	322	TYR
1	A	792	ARG
1	A	804	TYR

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Mol	Chain	Res	Type
1	A	815	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	459	GLN
1	A	507	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 carbohydrates 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	0.58	0	8,8,8	0.46	0
5	IPH	A	903	-	7,7,7	0.36	0	8,8,8	1.03	0
5	IPH	A	904	-	7,7,7	0.68	0	8,8,8	0.76	0
5	IPH	A	905	-	7,7,7	0.55	0	8,8,8	0.71	0
6	IPA	A	906	-	3,3,3	0.58	0	3,3,3	0.36	0
6	IPA	A	907	-	3,3,3	0.57	0	3,3,3	0.14	0
6	IPA	A	908	-	3,3,3	0.63	0	3,3,3	1.00	0
6	IPA	B	102	-	3,3,3	0.61	0	3,3,3	0.32	0
6	IPA	B	103	-	3,3,3	0.52	0	3,3,3	0.42	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
6	IPA	A	906	-	-	0/0/0/0	0/0/0/0
6	IPA	A	907	-	-	0/0/0/0	0/0/0/0
6	IPA	A	908	-	-	0/0/0/0	0/0/0/0
6	IPA	B	102	-	-	0/0/0/0	0/0/0/0
6	IPA	B	103	-	-	0/0/0/0	0/0/0/0

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	A	906	IPA	2	0
6	A	907	IPA	1	0
6	A	908	IPA	5	0
6	B	103	IPA	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	0.68	126 (15%) 3 2	13, 29, 70, 87	0
2	B	20/21 (95%)	0.16	2 (10%) 9 8	15, 30, 106, 116	0
3	D	9/11 (81%)	-0.37	0 100 100	22, 25, 33, 50	1 (11%)
All	All	832/891 (93%)	0.66	128 (15%) 3 2	13, 29, 71, 116	1 (0%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	ILE	9.4
1	A	84	THR	8.7
1	A	52	ILE	8.2
1	A	23	PHE	7.9
1	A	89	ASP	7.6
1	A	151	LEU	7.4
1	A	86	ILE	6.9
1	A	423	ARG	6.3
1	A	247	GLN	6.2
1	A	88	GLY	6.1
1	A	134	TRP	6.0
1	A	311	TYR	6.0
1	A	707	VAL	6.0
1	A	321	ARG	5.7
1	A	315	ARG	5.7
1	A	107	PRO	5.3
1	A	149	GLY	5.2
1	A	211	TRP	5.1
1	A	152	PRO	5.0
1	A	708[A]	GLN	5.0
1	A	342	GLU	4.9
1	A	248	LYS	4.8
1	A	120	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	85	GLN	4.7
1	A	241	LYS	4.7
1	A	424	ASN	4.7
1	A	150	ARG	4.6
1	A	319	VAL	4.5
1	A	322	TYR	4.4
1	A	65	LYS	4.3
1	A	243	ILE	4.3
1	A	119	LEU	4.3
1	A	80	GLN	4.2
1	A	114	GLU	4.1
1	A	156	PHE	4.1
1	A	316	HIS	4.1
1	A	55	TYR	4.1
1	A	133	LYS	4.1
1	A	113	VAL	4.0
1	A	109	GLY	3.9
1	A	331	GLY	3.9
1	A	318	LEU	3.8
1	A	87	PHE	3.7
1	A	115	LEU	3.7
1	A	295	PRO	3.6
1	A	66	CYS	3.6
1	A	279	TYR	3.6
1	A	104	MET	3.6
1	A	117	VAL	3.6
1	A	317	LYS	3.5
1	A	51	LYS	3.5
1	A	64	GLU	3.5
1	A	106	LEU	3.5
1	A	111	ASP	3.5
1	A	148	SER	3.5
1	A	127	ILE	3.5
1	A	63	PRO	3.5
1	A	332	GLN	3.4
1	A	244	GLU	3.4
1	A	90	ARG	3.4
1	A	355	LYS	3.3
1	A	132	ILE	3.3
1	A	60	ASP	3.3
1	A	116	GLU	3.3
1	A	239	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	336	HIS	3.2
1	A	246	GLN	3.2
1	A	277	ARG	3.1
1	A	81	HIS	3.1
1	A	59	LEU	3.1
1	A	313	LYS	3.1
1	A	696	LYS	3.1
1	A	53	ASP	3.0
1	A	324	HIS	3.0
1	A	83	LYS	3.0
1	A	54	ILE	3.0
1	A	147	LEU	3.0
1	A	312	PHE	3.0
1	A	808	LEU	3.0
1	A	140	LEU	2.9
1	A	118	THR	2.9
1	A	135	VAL	2.8
1	A	77	HIS	2.8
1	A	837	ARG	2.8
2	B	20	U	2.7
1	A	460	ARG	2.7
1	A	338	TYR	2.7
1	A	333	GLU	2.7
1	A	554	ARG	2.6
1	A	291	HIS	2.6
1	A	154	VAL	2.6
1	A	22	ALA	2.6
1	A	62	LYS	2.6
1	A	157	GLU	2.6
1	A	57	TYR	2.5
1	A	153	SER	2.5
1	A	366	ARG	2.5
1	A	253	SER	2.5
1	A	240	PHE	2.5
1	A	294	PHE	2.5
1	A	269	ILE	2.5
1	A	245	GLU	2.4
1	A	305	GLU	2.4
1	A	129	LYS	2.4
1	A	335	LYS	2.4
1	A	293	THR	2.3
1	A	250	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	144	HIS	2.3
1	A	803	ALA	2.3
1	A	128	PHE	2.3
1	A	242	SER	2.3
1	A	370	ARG	2.3
1	A	137	CYS	2.2
1	A	105	PRO	2.2
1	A	110	ARG	2.2
1	A	289	ALA	2.2
1	A	67	PRO	2.1
1	A	479	ARG	2.1
1	A	797	VAL	2.1
1	A	806	ALA	2.1
1	A	173	ARG	2.1
1	A	805	TYR	2.1
1	A	237	VAL	2.1
1	A	282	CYS	2.1
1	A	327	CYS	2.1
2	B	17	C	2.1
1	A	836	GLY	2.0
1	A	307	THR	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, 95^{th} 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
6	IPA	B	102	4/4	0.92	0.18	12.76	37,43,46,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	IPA	A	908	4/4	0.88	0.16	9.26	19,27,35,42	0
6	IPA	A	907	4/4	0.81	0.19	6.88	55,56,57,59	0
6	IPA	A	906	4/4	0.74	0.17	2.58	29,37,42,52	0
6	IPA	B	103	4/4	0.75	0.15	2.30	32,39,45,53	0
5	IPH	A	902	7/7	0.86	0.09	0.29	33,34,40,46	0
5	IPH	A	905	7/7	0.91	0.10	-0.29	30,32,34,36	0
5	IPH	A	904	7/7	0.94	0.09	-0.35	17,23,24,36	0
5	IPH	A	903	7/7	0.97	0.06	-2.43	20,23,26,35	0
4	MG	A	901	1/1	1.00	0.06	-2.51	16,16,16,16	0
4	MG	D	101	1/1	0.98	0.03	-	19,19,19,19	0
4	MG	B	101	1/1	0.99	0.15	-	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.