Full wwPDB X-ray Structure Validation Report (i)

May 27, 2024 – 09:25 PM EDT

PDB ID	:	6MFN
Title	:	Human Argonaute2-miR-27a bound to HSUR1 target RNA
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Deposited on	:	2018-09-11
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

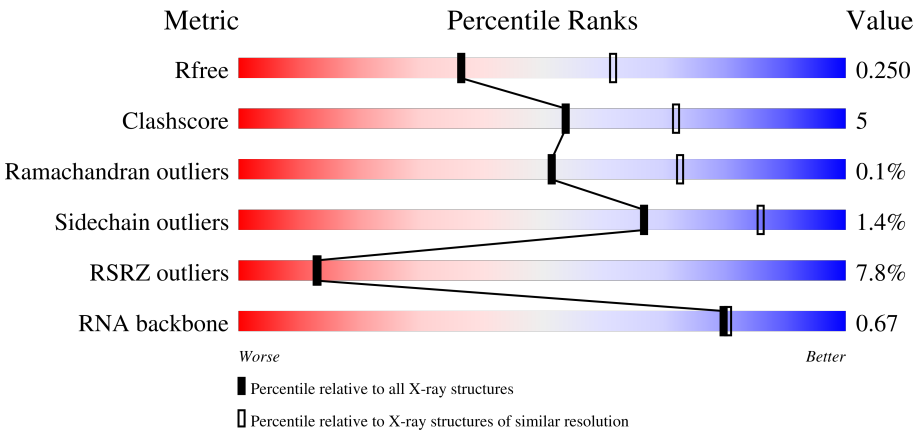
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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 <=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	7%, 80%, 13%, 7%
2	C	21	24%, 5%, 14%, 57%
3	E	22	9%, 32%, 5%, 9%, 55%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6910 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	803	6448	4106	1159	1143	40	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	387	ASP	SER	engineered mutation	UNP Q9UKV8
A	669	ALA	ASP	engineered mutation	UNP Q9UKV8
A	824	ALA	SER	engineered mutation	UNP Q9UKV8
A	828	ASP	SER	engineered mutation	UNP Q9UKV8
A	831	ASP	SER	engineered mutation	UNP Q9UKV8
A	834	ALA	SER	engineered mutation	UNP Q9UKV8

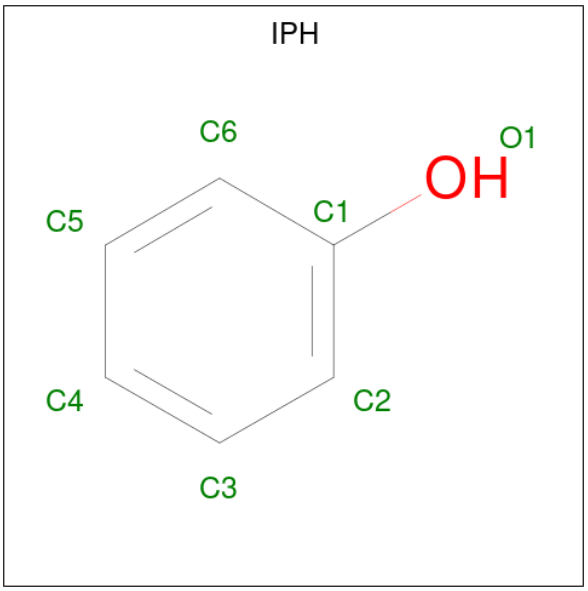
- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*UP*CP*AP*CP*AP*GP*UP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	9	172	75	27	61	9	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	E	10	196	86	34	66	10	0	0	0

- Molecule 4 is PHENOL (three-letter code: IPH) (formula: C_6H_6O).



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

- Molecule 5 is water.

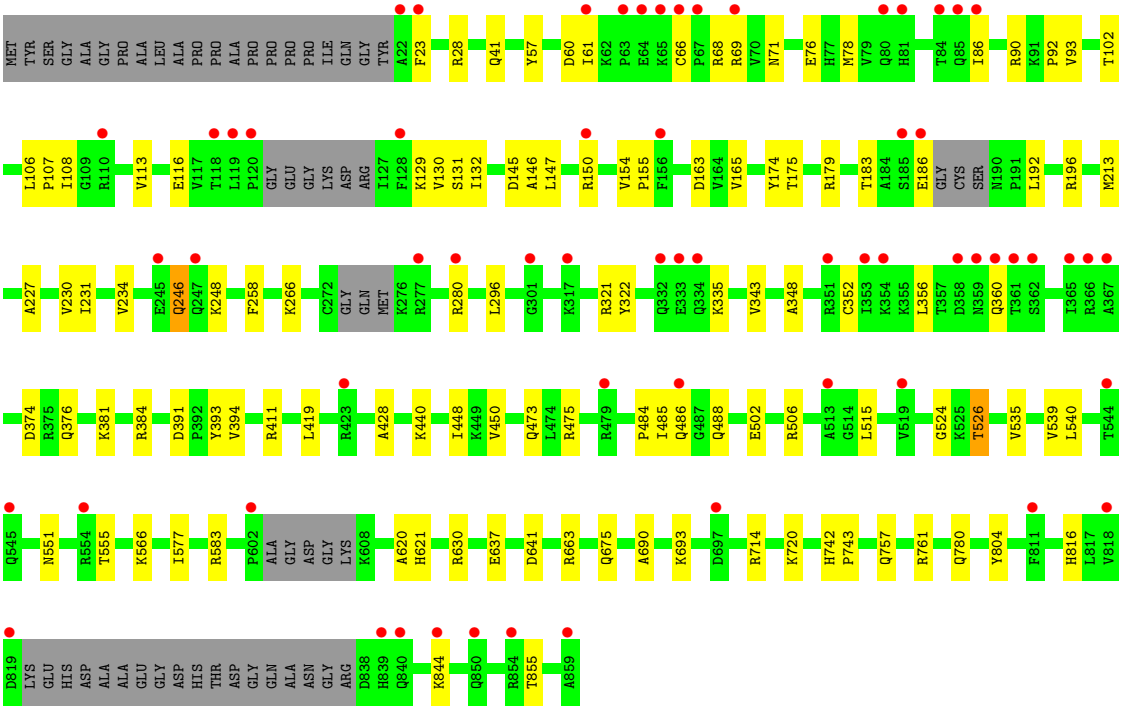
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	85	85	85	0	0
			Total	O		
5	E	2	2	2	0	0

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

Chain A: 7% 80% 13% 7%



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

Chain C: 24% 5% 14% 57%

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

Chain E: 9% 32% 5% 9% 55%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.95Å 104.21Å 152.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.59 – 2.50 28.59 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (28.59-2.50) 99.1 (28.59-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.209 , 0.247 0.212 , 0.250	Depositor DCC
R_{free} test set	1875 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	49.5	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6910	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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, 0.333 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: 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	0.24	0/6600	0.41	0/8934
2	C	0.81	1/190 (0.5%)	0.79	0/292
3	E	0.22	0/217	0.77	0/334
All	All	0.27	1/7007 (0.0%)	0.44	0/9560

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	U	OP3-P	-10.81	1.48	1.61

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	6448	0	6508	68	0
2	C	172	0	85	4	0
3	E	196	0	97	3	0
4	A	7	0	6	0	0
5	A	85	0	0	9	0
5	E	2	0	0	0	0
All	All	6910	0	6696	72	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 (72) 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:196:ARG:HD2	1:A:360:GLN:HE22	1.38	0.87
1:A:266:LYS:HG2	1:A:280:ARG:HG2	1.68	0.73
1:A:374:ASP:OD2	5:A:1001:HOH:O	2.10	0.68
1:A:246:GLN:NE2	1:A:248:LYS:O	2.26	0.68
1:A:502:GLU:OE1	1:A:506:ARG:NH2	2.29	0.65
1:A:76:GLU:OE2	1:A:393:TYR:OH	2.15	0.64
1:A:583:ARG:NH1	1:A:620:ALA:O	2.32	0.63
1:A:720:LYS:NZ	5:A:1008:HOH:O	2.31	0.63
1:A:86:ILE:O	1:A:90:ARG:NH1	2.32	0.63
1:A:57:TYR:HE1	1:A:108:ILE:HG21	1.64	0.61
1:A:539:VAL:HG23	1:A:540:LEU:HG	1.83	0.61
1:A:411:ARG:NH2	1:A:780:GLN:OE1	2.34	0.60
1:A:192:LEU:HD22	1:A:360:GLN:HG3	1.84	0.60
1:A:92:PRO:HB3	1:A:102:THR:HG22	1.84	0.59
1:A:227:ALA:HB2	1:A:348:ALA:HB2	1.85	0.59
1:A:28:ARG:NH1	5:A:1013:HOH:O	2.35	0.58
1:A:714:ARG:HH21	1:A:761:ARG:HD3	1.68	0.58
1:A:855:THR:O	5:A:1002:HOH:O	2.18	0.56
1:A:428:ALA:HB2	1:A:440:LYS:HE2	1.87	0.55
1:A:473:GLN:OE1	1:A:555:THR:OG1	2.24	0.55
1:A:116:GLU:OE2	1:A:129:LYS:HE2	2.08	0.54
1:A:69:ARG:HH22	1:A:175:THR:HG23	1.73	0.54
1:A:663:ARG:NH1	5:A:1010:HOH:O	2.32	0.53
1:A:484:PRO:HB2	1:A:486:GLN:HG3	1.91	0.53
2:C:6:A:O2'	2:C:7:G:OP1	2.26	0.53
1:A:60:ASP:HB2	1:A:131:SER:HB2	1.92	0.52
1:A:450:VAL:HB	1:A:515:LEU:HA	1.93	0.51
1:A:102:THR:HG21	1:A:106:LEU:HD13	1.92	0.50
1:A:147:LEU:HD11	1:A:213:MET:HE2	1.93	0.50
1:A:566:LYS:NZ	2:C:1:U:OP3	2.34	0.49
1:A:41:GLN:OE1	1:A:376:GLN:NE2	2.45	0.48
1:A:488:GLN:NE2	5:A:1018:HOH:O	2.44	0.48
1:A:234:VAL:HG12	1:A:258:PHE:CE1	2.49	0.48
3:E:13:U:O2'	3:E:14:C:OP1	2.29	0.48
1:A:192:LEU:HB3	1:A:360:GLN:HG3	1.95	0.47
1:A:637:GLU:HG3	1:A:675:GLN:HE22	1.79	0.47
1:A:230:VAL:O	1:A:234:VAL:HG13	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:HG22	1:A:130:VAL:HG22	1.96	0.47
1:A:174:TYR:HD2	1:A:183:THR:HB	1.79	0.47
1:A:551:ASN:ND2	2:C:2:U:OP2	2.47	0.46
1:A:196:ARG:HD3	1:A:352:CYS:SG	2.55	0.46
1:A:475:ARG:NE	1:A:485:ILE:O	2.49	0.45
1:A:93:VAL:HG11	1:A:165:VAL:HA	1.98	0.45
3:E:13:U:HO2'	3:E:14:C:P	2.40	0.45
1:A:690:ALA:HA	1:A:693:LYS:HE2	1.98	0.45
1:A:145:ASP:HB3	1:A:150:ARG:HB2	1.98	0.44
1:A:535:VAL:HA	1:A:539:VAL:HG22	1.99	0.43
1:A:757:GLN:NE2	3:E:17:U:O2	2.51	0.43
1:A:231:ILE:O	1:A:234:VAL:HG22	2.18	0.43
1:A:321:ARG:HG3	1:A:322:TYR:CD2	2.54	0.43
1:A:146:ALA:HB1	1:A:154:VAL:HG22	2.01	0.42
1:A:192:LEU:HD13	1:A:360:GLN:HE21	1.84	0.42
1:A:213:MET:HE2	1:A:213:MET:HB2	1.66	0.42
1:A:816:HIS:HD2	5:A:1061:HOH:O	2.02	0.42
1:A:113:VAL:HG23	1:A:132:ILE:HG23	2.01	0.42
2:C:6:A:HO2'	2:C:7:G:P	2.41	0.42
1:A:621:HIS:HD2	5:A:1085:HOH:O	2.01	0.42
1:A:179:ARG:HD3	1:A:179:ARG:HA	1.73	0.41
1:A:335:LYS:HD3	1:A:335:LYS:HA	1.87	0.41
1:A:524:GLY:O	1:A:526:THR:HG22	2.20	0.41
1:A:57:TYR:CE1	1:A:108:ILE:HG21	2.52	0.41
1:A:391:ASP:HB3	1:A:394:VAL:HB	2.03	0.41
1:A:448:ILE:HD12	1:A:485:ILE:HG12	2.02	0.41
1:A:641:ASP:OD1	5:A:1003:HOH:O	2.22	0.41
1:A:844:LYS:HA	1:A:844:LYS:HD3	1.90	0.41
1:A:419:LEU:HD23	1:A:577:ILE:HD11	2.02	0.41
1:A:742:HIS:CG	1:A:743:PRO:HD2	2.55	0.41
1:A:154:VAL:HA	1:A:155:PRO:HD2	1.97	0.40
1:A:78:MET:SD	1:A:130:VAL:HG11	2.62	0.40
1:A:630:ARG:HG3	1:A:641:ASP:HB3	2.04	0.40
1:A:381:LYS:HA	1:A:384:ARG:HG2	2.03	0.40
1:A:68:ARG:O	1:A:71:ASN:HB2	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	791/859 (92%)	756 (96%)	34 (4%)	1 (0%)	51 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	PRO

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	713/749 (95%)	703 (99%)	10 (1%)	67 86

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

Mol	Chain	Res	Type
1	A	23	PHE
1	A	66	CYS
1	A	163	ASP
1	A	186	GLU
1	A	246	GLN
1	A	296	LEU
1	A	343	VAL
1	A	356	LEU
1	A	526	THR
1	A	804	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	GLN
1	A	360	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	7/21 (33%)	1 (14%)	1 (14%)
3	E	8/22 (36%)	1 (12%)	1 (12%)
All	All	15/43 (34%)	2 (13%)	2 (13%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	7	G
3	E	14	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	6	A
3	E	13	U

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand 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	$\#\|Z\| > 2$
4	IPH	A	901	-	7,7,7	0.39	0	8,8,8	0.24	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
4	IPH	A	901	-	-	-	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	803/859 (93%)	0.38	62 (7%) 13 13	30, 57, 99, 124	0
2	C	9/21 (42%)	-0.05	0 100 100	40, 49, 111, 136	0
3	E	10/22 (45%)	0.75	2 (20%) 1 0	51, 67, 110, 136	0
All	All	822/902 (91%)	0.38	64 (7%) 13 13	30, 58, 99, 136	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	66	CYS	6.7
1	A	353	ILE	6.0
1	A	360	GLN	6.0
1	A	602	PRO	5.3
1	A	65	LYS	5.1
1	A	84	THR	4.9
3	E	13	U	4.8
1	A	64	GLU	4.6
1	A	118	THR	4.4
1	A	819	ASP	4.3
1	A	67	PRO	4.2
1	A	119	LEU	4.0
3	E	14	C	3.9
1	A	359	ASN	3.8
1	A	332	GLN	3.8
1	A	333	GLU	3.7
1	A	367	ALA	3.7
1	A	120	PRO	3.7
1	A	351	ARG	3.6
1	A	22	ALA	3.5
1	A	844	LYS	3.5
1	A	839	HIS	3.5
1	A	156	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	554	ARG	3.5
1	A	354	LYS	3.3
1	A	365	ILE	3.1
1	A	358	ASP	3.1
1	A	86	ILE	3.0
1	A	81	HIS	2.9
1	A	277	ARG	2.9
1	A	185	SER	2.9
1	A	317	LYS	2.9
1	A	366	ARG	2.9
1	A	69	ARG	2.8
1	A	334	GLN	2.8
1	A	247	GLN	2.7
1	A	545	GLN	2.7
1	A	362	SER	2.7
1	A	63	PRO	2.7
1	A	280	ARG	2.6
1	A	519	VAL	2.6
1	A	110	ARG	2.6
1	A	186	GLU	2.5
1	A	423	ARG	2.4
1	A	61	ILE	2.4
1	A	811	PHE	2.4
1	A	697	ASP	2.4
1	A	859	ALA	2.3
1	A	840	GLN	2.3
1	A	486	GLN	2.3
1	A	361	THR	2.3
1	A	818	VAL	2.3
1	A	85	GLN	2.2
1	A	80	GLN	2.2
1	A	850	GLN	2.2
1	A	544	THR	2.2
1	A	23	PHE	2.2
1	A	128	PHE	2.2
1	A	479	ARG	2.1
1	A	854	ARG	2.1
1	A	245	GLU	2.1
1	A	150	ARG	2.1
1	A	513	ALA	2.0
1	A	301	GLY	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 monosaccharides 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
4	IPH	A	901	7/7	0.90	0.20	59,60,64,68	0

6.5 Other polymers (i)

There are no such residues in this entry.