Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 09:08 AM BST

PDB ID	:	6SJD
Title	:	ZC3H12B-ribonuclease domain bound to RNA
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Deposited on	:	2019-08-13
Resolution	:	3.29 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 following versions of software and data (see references ⓘ) were used in the production of this report:

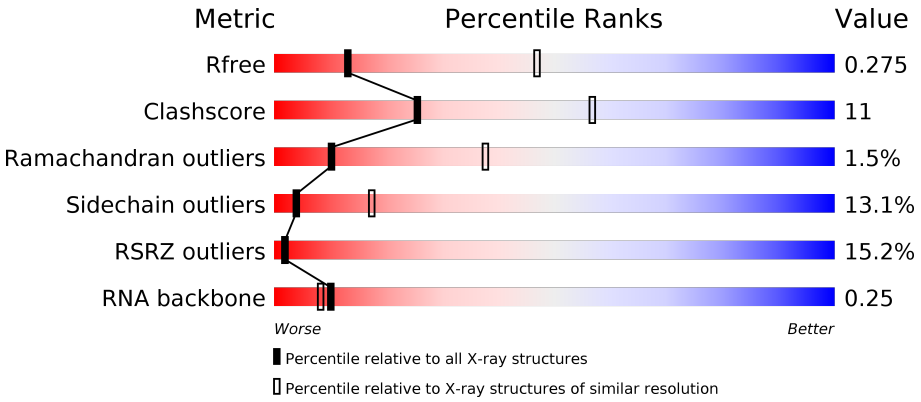
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 3.29 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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 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	178	11% 71% 25%
1	B	178	19% 70% 21% 6%
2	D	21	5% 33% 29% 19% 19%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6263 atoms, of which 3021 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 Probable ribonuclease ZC3H12B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	168	Total	C	H	N	O	S	0	0	0
			2763	879	1380	248	251	5			
1	A	178	Total	C	H	N	O	S	0	0	0
			2921	929	1457	263	266	6			

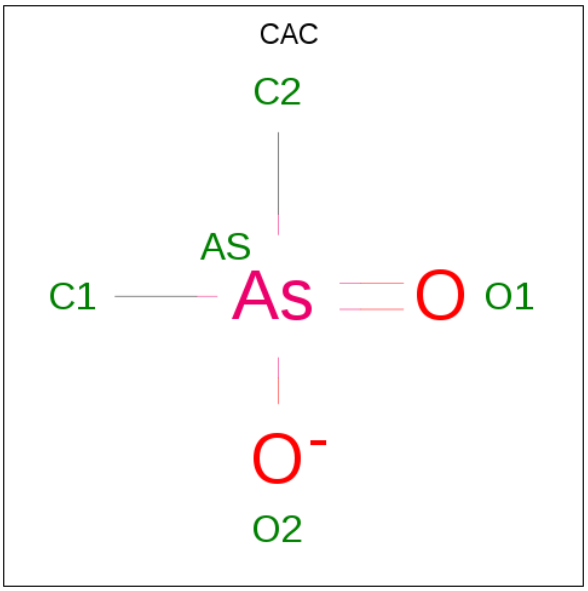
- Molecule 2 is a RNA chain called RNA (5'-R(*UP*GP*CP*GP*AP*CP*AP*GP*UP*CP*GP*GP*UP*AP*GP*CP*A)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	17	Total	C	H	N	O	P	0	0	0
			547	163	184	68	116	16			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	As	C	O		
4	D	1	5	1	2	2	0	0

- Molecule 5 is water.

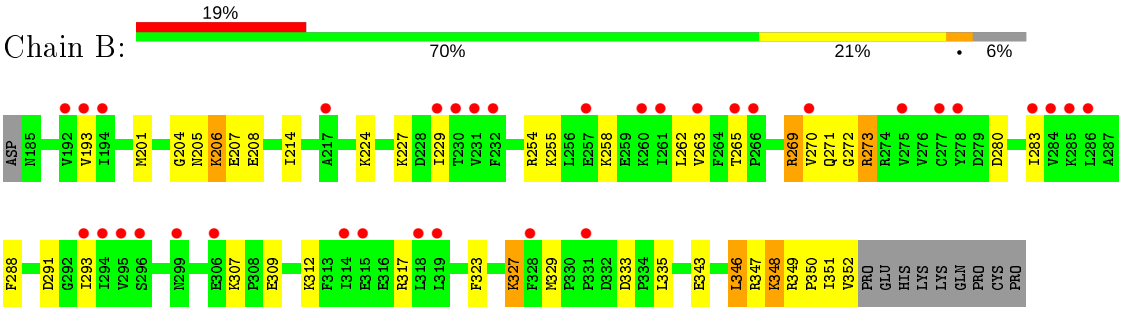
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	7	7	7	0	0
			Total	O		
5	A	7	7	7	0	0
			Total	O		
5	D	11	11	11	0	0

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.

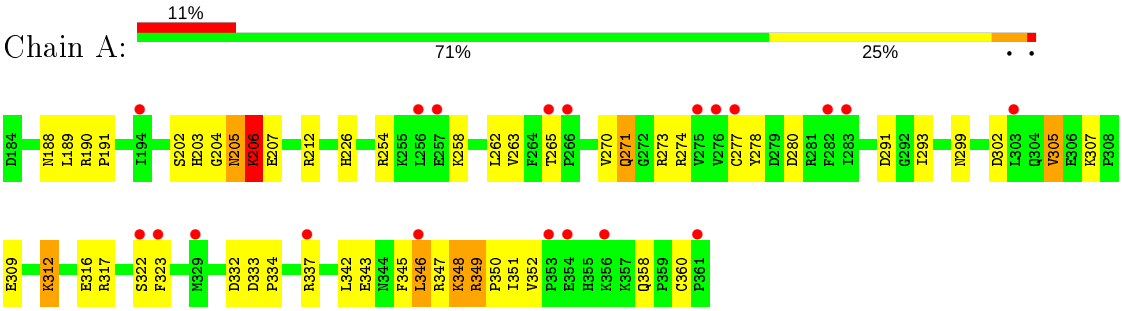
• Molecule 1: Probable ribonuclease ZC3H12B

Chain B:



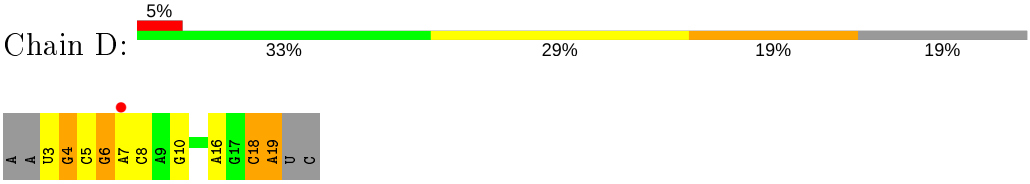
• Molecule 1: Probable ribonuclease ZC3H12B

Chain A:



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

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	114.24Å 114.24Å 165.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.95 – 3.29 93.97 – 3.29	Depositor EDS
% Data completeness (in resolution range)	77.3 (66.95-3.29) 77.4 (93.97-3.29)	Depositor EDS
R_{merge}	0.44	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.235 , 0.279 0.235 , 0.275	Depositor DCC
R_{free} test set	684 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	106.9	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 98.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	6263	wwPDB-VP
Average B, all atoms (Å^2)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.25% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, 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	0.26	0/1500	0.45	0/2026
1	B	0.27	0/1415	0.47	0/1910
2	D	0.33	0/406	1.06	0/632
All	All	0.27	0/3321	0.58	0/4568

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	1464	1457	1457	28	0
1	B	1383	1380	1380	27	0
2	D	363	184	186	11	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	D	5	0	0	0	0
5	A	7	0	0	3	0
5	B	7	0	0	5	0
5	D	11	0	0	3	0
All	All	3242	3021	3023	66	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 11.

All (66) 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:B:327:LYS:O	5:B:1101:HOH:O	1.86	0.93
1:A:349:ARG:O	1:A:349:ARG:NH1	2.02	0.92
1:A:204:GLY:O	1:A:206:LYS:N	2.06	0.88
1:B:329:MET:O	5:B:1102:HOH:O	1.94	0.86
2:D:5:C:O2'	2:D:6:G:OP2	1.94	0.84
1:A:348:LYS:NZ	1:A:348:LYS:O	2.15	0.79
2:D:18:C:O2'	2:D:19:A:O5'	2.02	0.77
1:A:343:GLU:OE1	1:A:347:ARG:NH1	2.19	0.76
2:D:5:C:OP2	5:D:201:HOH:O	2.04	0.75
1:A:277:CYS:O	5:A:1101:HOH:O	2.03	0.74
1:B:205:ASN:O	1:B:207:GLU:N	2.21	0.74
1:B:327:LYS:O	5:B:1103:HOH:O	2.06	0.73
1:B:343:GLU:OE1	1:B:343:GLU:N	2.24	0.70
1:A:205:ASN:O	1:A:207:GLU:N	2.24	0.70
1:A:280:ASP:OD1	5:A:1102:HOH:O	2.08	0.70
1:A:309:GLU:OE1	1:A:309:GLU:N	2.23	0.70
1:A:203:HIS:O	5:A:1103:HOH:O	2.09	0.70
1:B:280:ASP:OD1	5:B:1104:HOH:O	2.11	0.68
1:B:269:ARG:NH1	1:B:272:GLY:O	2.27	0.68
1:B:309:GLU:N	1:B:309:GLU:OE1	2.27	0.67
1:A:291:ASP:OD1	1:A:317:ARG:NH2	2.31	0.62
2:D:18:C:HO2'	2:D:19:A:P	2.22	0.62
2:D:3:U:O5'	5:D:201:HOH:O	2.05	0.62
1:B:262:LEU:HD23	1:B:263:VAL:N	2.14	0.62
1:A:262:LEU:HD23	1:A:263:VAL:N	2.18	0.58
1:A:270:VAL:HG13	1:A:271:GLN:H	1.69	0.56
1:B:270:VAL:HG13	1:B:271:GLN:H	1.70	0.56
2:D:3:U:O2'	2:D:4:G:O5'	2.20	0.56
1:B:205:ASN:O	1:B:208:GLU:N	2.34	0.55
1:A:293:ILE:C	1:A:293:ILE:HD12	2.28	0.53
1:B:329:MET:N	5:B:1103:HOH:O	2.39	0.51
1:B:343:GLU:HA	1:B:346:LEU:HD22	1.91	0.51
1:B:293:ILE:HD12	1:B:293:ILE:O	2.11	0.51
1:A:302:ASP:N	1:A:302:ASP:OD1	2.43	0.50
1:A:293:ILE:O	1:A:293:ILE:HD12	2.10	0.50
1:A:190:ARG:HG3	1:A:191:PRO:HD2	1.93	0.50
2:D:3:U:H3'	2:D:4:G:H5"	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:HIS:CE1	1:A:346:LEU:HD11	2.48	0.48
1:B:347:ARG:NH1	1:B:351:ILE:HG23	2.28	0.48
1:A:333:ASP:N	1:A:333:ASP:OD1	2.47	0.48
2:D:5:C:N4	5:D:205:HOH:O	2.47	0.48
1:A:226:HIS:HE1	1:A:346:LEU:HD11	1.78	0.47
1:B:293:ILE:HD12	1:B:293:ILE:C	2.35	0.47
1:A:188:ASN:HB3	1:A:349:ARG:CG	2.46	0.46
1:B:193:VAL:HG12	1:B:283:ILE:HG23	1.96	0.46
2:D:18:C:H4'	2:D:19:A:OP1	2.15	0.46
1:B:204:GLY:O	1:B:205:ASN:C	2.55	0.46
1:B:348:LYS:O	1:B:350:PRO:HD3	2.16	0.45
1:A:334:PRO:HG3	1:A:342:LEU:HD23	1.99	0.45
1:B:351:ILE:HD12	1:B:351:ILE:C	2.37	0.45
1:B:269:ARG:HA	1:B:273:ARG:O	2.17	0.45
1:A:348:LYS:CE	1:A:348:LYS:O	2.65	0.44
1:B:333:ASP:OD1	1:B:333:ASP:N	2.51	0.44
1:B:351:ILE:HD12	1:B:352:VAL:N	2.33	0.43
1:A:351:ILE:O	1:A:352:VAL:C	2.57	0.43
1:B:270:VAL:HG13	1:B:271:GLN:N	2.34	0.43
2:D:4:G:N3	2:D:4:G:H2'	2.34	0.42
1:A:293:ILE:HG22	1:A:317:ARG:HD2	2.02	0.42
1:A:316:GLU:O	1:A:345:PHE:HE1	2.03	0.42
2:D:4:G:N3	2:D:4:G:C2'	2.83	0.41
1:B:291:ASP:OD1	1:B:317:ARG:NH2	2.53	0.41
1:A:302:ASP:O	1:A:305:VAL:HG12	2.19	0.41
1:B:205:ASN:O	1:B:206:LYS:C	2.58	0.41
1:A:348:LYS:O	1:A:350:PRO:HD3	2.21	0.40
1:B:351:ILE:O	1:B:352:VAL:C	2.60	0.40
1:A:312:LYS:O	1:A:316:GLU:HG2	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	176/178 (99%)	160 (91%)	12 (7%)	4 (2%)	6 29
1	B	166/178 (93%)	153 (92%)	12 (7%)	1 (1%)	25 57
All	All	342/356 (96%)	313 (92%)	24 (7%)	5 (2%)	10 38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	206	LYS
1	A	205	ASN
1	A	206	LYS
1	A	278	TYR
1	A	358	GLN

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	165/165 (100%)	143 (87%)	22 (13%)	4 17
1	B	155/165 (94%)	135 (87%)	20 (13%)	4 18
All	All	320/330 (97%)	278 (87%)	42 (13%)	4 17

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	201	MET
1	B	214	ILE
1	B	224	LYS
1	B	227	LYS
1	B	229	ILE
1	B	254	ARG
1	B	255	LYS
1	B	258	LYS
1	B	265	THR
1	B	269	ARG
1	B	273	ARG

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Mol	Chain	Res	Type
1	B	288	PHE
1	B	307	LYS
1	B	312	LYS
1	B	323	PHE
1	B	327	LYS
1	B	335	LEU
1	B	346	LEU
1	B	348	LYS
1	B	349	ARG
1	A	189	LEU
1	A	202	SER
1	A	206	LYS
1	A	212	ARG
1	A	254	ARG
1	A	258	LYS
1	A	265	THR
1	A	271	GLN
1	A	273	ARG
1	A	274	ARG
1	A	299	ASN
1	A	305	VAL
1	A	307	LYS
1	A	312	LYS
1	A	322	SER
1	A	323	PHE
1	A	332	ASP
1	A	337	ARG
1	A	346	LEU
1	A	348	LYS
1	A	349	ARG
1	A	360	CYS

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	D	16/21 (76%)	8 (50%)	1 (6%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	D	4	G
2	D	6	G
2	D	7	A
2	D	8	C
2	D	10	G
2	D	16	A
2	D	18	C
2	D	19	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	18	C

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)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
4	CAC	D	101	-	0,4,4	0.00	-	0,6,6	0.00	-

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

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	178/178 (100%)	1.01	20 (11%) 5 5	45, 108, 288, 367	0
1	B	168/178 (94%)	1.21	34 (20%) 1 1	47, 101, 186, 231	0
2	D	17/21 (80%)	0.58	1 (5%) 22 22	105, 150, 266, 289	0
All	All	363/377 (96%)	1.08	55 (15%) 2 2	45, 108, 240, 367	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	356	LYS	6.8
1	B	293	ILE	4.7
1	B	294	ILE	4.0
1	B	270	VAL	3.8
1	B	277	CYS	3.7
1	A	275	VAL	3.2
1	B	232	PHE	3.2
1	B	328	PHE	3.2
2	D	7	A	3.1
1	B	318	LEU	3.0
1	B	299	ASN	3.0
1	B	229	ILE	2.9
1	B	265	THR	2.9
1	B	194	ILE	2.9
1	A	282	PHE	2.8
1	B	231	VAL	2.8
1	B	192	VAL	2.7
1	B	278	TYR	2.7
1	A	277	CYS	2.7
1	B	331	PRO	2.7
1	B	260	LYS	2.7
1	B	295	VAL	2.7
1	A	322	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	193	VAL	2.6
1	B	266	PRO	2.6
1	A	257	GLU	2.6
1	B	283	ILE	2.5
1	B	217	ALA	2.5
1	B	314	ILE	2.5
1	B	284	VAL	2.5
1	A	361	PRO	2.5
1	A	276	VAL	2.5
1	B	306	GLU	2.5
1	B	230	THR	2.4
1	A	194	ILE	2.4
1	B	275	VAL	2.4
1	B	263	VAL	2.4
1	B	319	LEU	2.4
1	B	296	SER	2.3
1	A	265	THR	2.3
1	A	303	LEU	2.3
1	A	353	PRO	2.3
1	B	315	GLU	2.3
1	A	329	MET	2.3
1	B	286	LEU	2.3
1	A	323	PHE	2.2
1	A	283	ILE	2.2
1	B	261	ILE	2.1
1	A	256	LEU	2.1
1	B	285	LYS	2.1
1	A	266	PRO	2.1
1	A	337	ARG	2.1
1	B	257	GLU	2.0
1	A	346	LEU	2.0
1	A	354	GLU	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

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, 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	B-factors(Å^2)	Q<0.9
4	CAC	D	101	5/5	0.93	0.16	226,226,227,228	0
3	MG	B	1001	1/1	0.94	0.16	52,52,52,52	0
3	MG	A	1001	1/1	0.96	0.22	102,102,102,102	0

6.5 Other polymers

There are no such residues in this entry.