



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:40 AM UTC

PDB ID : 6SJD / pdb_00006sjd
Title : ZC3H12B-ribonuclease domain bound to RNA
Authors : Morgunova, E.; Bourenkov, G.; Taipale, J.
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 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

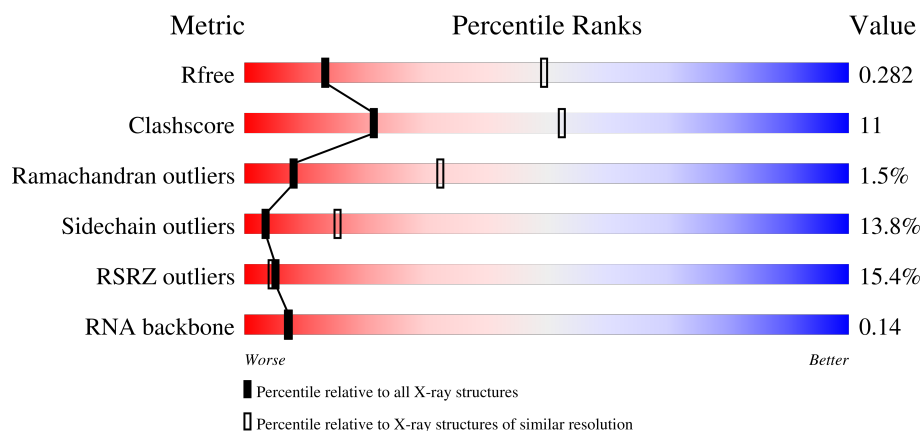
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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 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	178	22% 70% 25% • •
1	B	178	6% 71% 20% • 6%
2	D	21	24% 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			

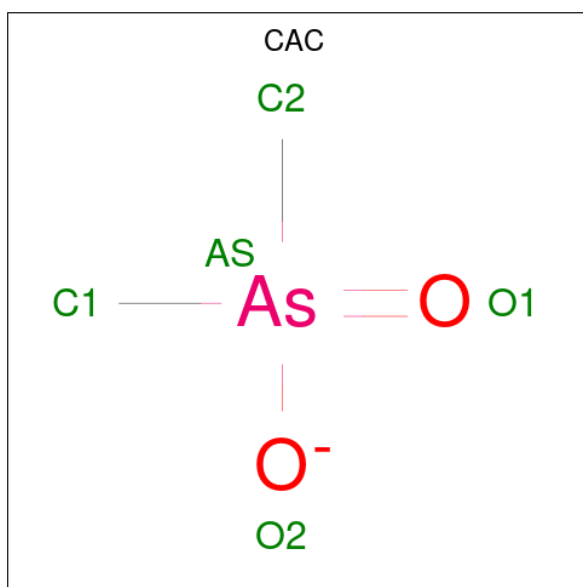
- Molecule 2 is a RNA chain called RNA (5'-R(*UP*GP*CP*GP*AP*CP*AP*GP*UP*CP*GP*GP*UP*AP*GP*CP*A)-3').

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 (CCD ID: 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 (CCD ID: CAC) (formula: C₂H₆AsO₂).



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

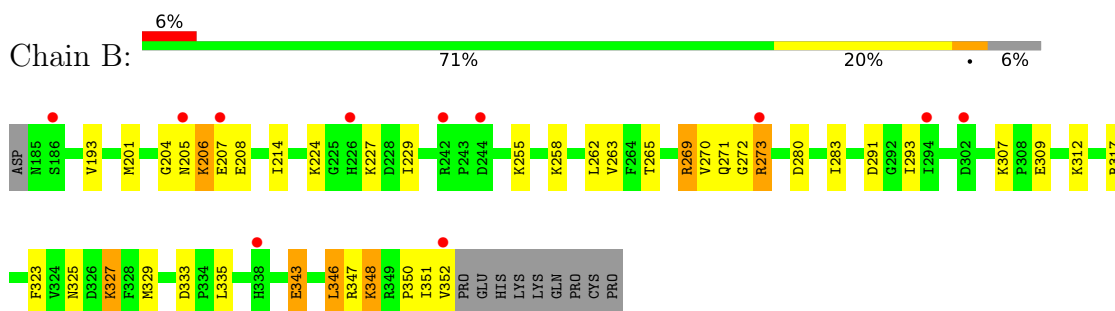
- Molecule 5 is water.

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

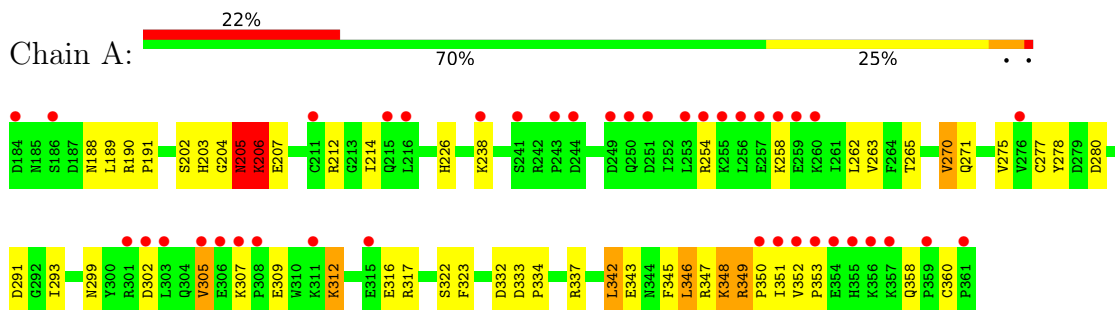
3 Residue-property plots

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.

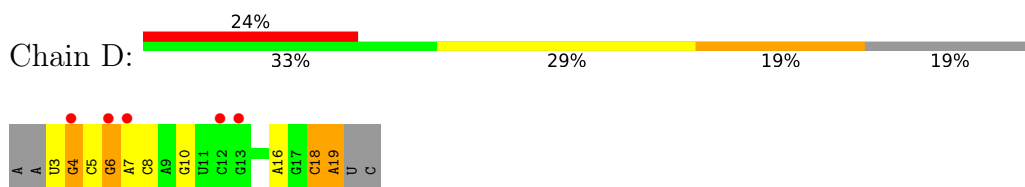
• Molecule 1: Probable ribonuclease ZC3H12B



• Molecule 1: Probable ribonuclease ZC3H12B



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



4 Data and refinement statistics

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 66.95 – 3.29	Depositor EDS
% Data completeness (in resolution range)	77.3 (66.95-3.29) 77.4 (66.95-3.29)	Depositor EDS
R_{merge}	0.44	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.235 , 0.279 0.237 , 0.282	Depositor DCC
R_{free} test set	684 reflections (3.97%)	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)	0.35 , 130.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	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.*

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: 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	0.16	0/1500	0.39	0/2026
1	B	0.16	0/1415	0.40	0/1910
2	D	0.18	0/406	0.45	0/632
All	All	0.16	0/3321	0.40	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	31	0
1	B	1383	1380	1380	27	0
2	D	363	184	186	10	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	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 11.

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:B:327:LYS:O	5:B:1101:HOH:O	1.86	0.93
1:A:349:ARG:NH1	1:A:349:ARG:O	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:N	1:B:343:GLU:OE1	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: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:293:ILE:C	1:A:293:ILE:HD12	2.28	0.57
1:B:270:VAL:HG13	1:B:271:GLN:H	1.70	0.56
1:A:270:VAL:HG13	1:A:271:GLN:H	1.69	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:B:293:ILE:HD12	1:B:293:ILE:C	2.35	0.52
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:B:351:ILE:C	1:B:351:ILE:HD12	2.37	0.50
1:A:302:ASP:N	1:A:302:ASP:OD1	2.43	0.50
1:B:204:GLY:O	1:B:205:ASN:C	2.55	0.50
1:A:293:ILE:HD12	1:A:293:ILE:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:347:ARG:NH1	1:B:351:ILE:HG23	2.28	0.48
1:A:226:HIS:CE1	1:A:346:LEU:HD11	2.48	0.48
1:A:333:ASP:OD1	1:A:333:ASP:N	2.47	0.48
1:A:351:ILE:O	1:A:352:VAL:C	2.57	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: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:205:ASN:O	1:B:206:LYS:C	2.58	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:O	1:B:352:VAL:C	2.60	0.45
1:B:269:ARG:HA	1:B:273:ARG:O	2.17	0.45
1:B:333:ASP:OD1	1:B:333:ASP:N	2.51	0.44
1:A:348:LYS:O	1:A:348:LYS:CE	2.65	0.44
1:A:204:GLY:O	1:A:205:ASN:C	2.60	0.43
1:B:351:ILE:HD12	1:B:352:VAL:N	2.33	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:352:VAL:O	1:A:353:PRO:C	2.63	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:A:262:LEU:HD23	1:A:262:LEU:C	2.46	0.41
1:A:348:LYS:O	1:A:350:PRO:HD3	2.21	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%)	5	25
1	B	166/178 (93%)	153 (92%)	12 (7%)	1 (1%)	21	52
All	All	342/356 (96%)	313 (92%)	24 (7%)	5 (2%)	8	32

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 ⓘ

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%)	140 (85%)	25 (15%)	3	13
1	B	155/165 (94%)	136 (88%)	19 (12%)	4	19
All	All	320/330 (97%)	276 (86%)	44 (14%)	3	15

All (44) 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	255	LYS
1	B	258	LYS
1	B	265	THR

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Mol	Chain	Res	Type
1	B	269	ARG
1	B	273	ARG
1	B	307	LYS
1	B	312	LYS
1	B	323	PHE
1	B	325	ASN
1	B	327	LYS
1	B	335	LEU
1	B	343	GLU
1	B	346	LEU
1	B	348	LYS
1	A	189	LEU
1	A	202	SER
1	A	205	ASN
1	A	206	LYS
1	A	212	ARG
1	A	214	ILE
1	A	238	LYS
1	A	254	ARG
1	A	258	LYS
1	A	265	THR
1	A	270	VAL
1	A	275	VAL
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	342	LEU
1	A	346	LEU
1	A	348	LYS
1	A	349	ARG
1	A	360	CYS

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

Mol	Chain	Res	Type
1	B	205	ASN
1	A	338	HIS

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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	-	2,4,4	2.67	2 (100%)	4,6,6	1.55	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	101	CAC	AS-C2	2.69	1.96	1.90
4	D	101	CAC	AS-C1	2.64	1.96	1.90

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	178/178 (100%)	1.08	40 (22%) 2 2	51, 120, 316, 391	0
1	B	168/178 (94%)	0.58	11 (6%) 25 17	47, 113, 206, 249	0
2	D	17/21 (80%)	1.34	5 (29%) 1 1	113, 160, 287, 307	0
All	All	363/377 (96%)	0.86	56 (15%) 5 4	47, 119, 273, 391	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	251	ASP	6.3
1	A	254	ARG	5.6
1	A	257	GLU	5.2
1	A	350	PRO	5.0
1	B	244	ASP	4.9
1	A	255	LYS	4.4
1	B	242	ARG	4.2
1	A	249	ASP	4.1
1	A	258	LYS	4.0
1	A	355	HIS	3.8
1	A	241	SER	3.6
1	A	352	VAL	3.6
1	A	306	GLU	3.5
1	A	243	PRO	3.5
1	A	357	LYS	3.4
1	B	273	ARG	3.3
1	A	359	PRO	3.3
1	B	205	ASN	3.2
2	D	6	G	3.1
1	A	351	ILE	3.1
1	A	244	ASP	3.1
1	A	256	LEU	3.1
1	A	215	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	250	GLN	3.0
1	A	303	LEU	3.0
1	B	207	GLU	3.0
1	A	260	LYS	2.9
2	D	7	A	2.9
1	B	186	SER	2.8
1	A	356	LYS	2.8
1	A	238	LYS	2.8
1	A	308	PRO	2.7
1	A	302	ASP	2.7
1	A	186	SER	2.7
1	A	361	PRO	2.7
1	A	305	VAL	2.6
2	D	13	G	2.6
1	A	253	LEU	2.5
1	B	302	ASP	2.5
1	A	184	ASP	2.5
1	B	352	VAL	2.5
1	A	211	CYS	2.4
1	A	259	GLU	2.4
1	B	226	HIS	2.4
1	A	354	GLU	2.4
1	B	338	HIS	2.3
1	A	315	GLU	2.3
1	A	216	LEU	2.2
1	A	276	VAL	2.2
1	B	294	ILE	2.2
1	A	307	LYS	2.2
1	A	301	ARG	2.2
2	D	4	G	2.2
1	A	353	PRO	2.1
2	D	12	C	2.0
1	A	311	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

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($\text{\AA}^2$)	Q<0.9
4	CAC	D	101	5/5	0.81	0.14	226,226,227,228	0
3	MG	A	1001	1/1	0.82	0.36	102,102,102,102	0
3	MG	B	1001	1/1	0.95	0.14	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.