wwPDB X-ray Structure Validation Summary Report (i)

Aug 28, 2023 – 09:35 AM EDT

PDB ID	:	3KTV
Title	:	Crystal structure of the human SRP19/S-domain SRP RNA complex
Authors	:	Wild, K.; Bange, G.; Bozkurt, G.; Sinning, I.
Deposited on	:	2009-11-26
Resolution	:	3.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

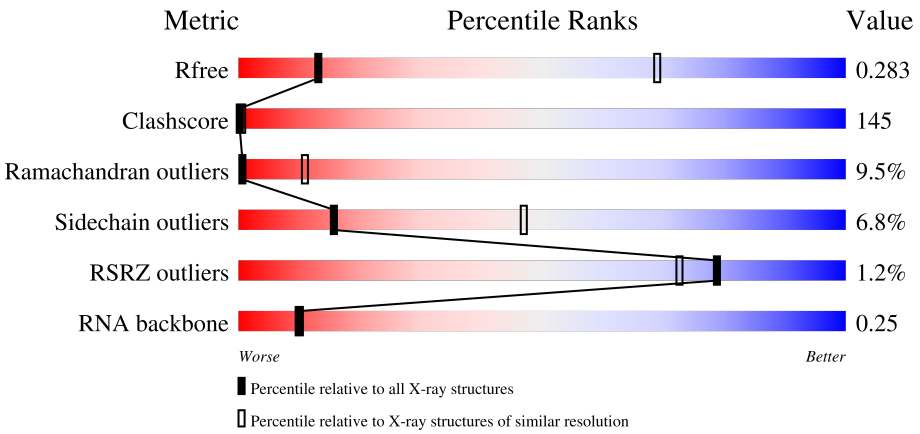
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

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 <=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	108	2%, •, 40%, 52%, 7%
2	B	128	20%, 53%, 9%, •, 17%
2	D	128	16%, 57%, 10%, •, 16%
3	C	108	3%, •, 46%, 48%, •

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
3	GDP	C	122	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6390 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 RNA chain called SRP RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	108	2327	1036	437	746	108	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	122	G	-	insertion	GB NR_002715.1
A	228	U	-	insertion	GB NR_002715.1
A	229	A	-	insertion	GB NR_002715.1

- Molecule 2 is a protein called Signal recognition particle 19 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	106	856	540	154	156	6	0	0	0
2	D	108	869	548	156	159	6	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	121	LEU	-	expression tag	UNP P09132
B	122	GLU	-	expression tag	UNP P09132
B	123	HIS	-	expression tag	UNP P09132
B	124	HIS	-	expression tag	UNP P09132
B	125	HIS	-	expression tag	UNP P09132
B	126	HIS	-	expression tag	UNP P09132
B	127	HIS	-	expression tag	UNP P09132
B	128	HIS	-	expression tag	UNP P09132
D	121	LEU	-	expression tag	UNP P09132
D	122	GLU	-	expression tag	UNP P09132
D	123	HIS	-	expression tag	UNP P09132

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Chain	Residue	Modelled	Actual	Comment	Reference
D	124	HIS	-	expression tag	UNP P09132
D	125	HIS	-	expression tag	UNP P09132
D	126	HIS	-	expression tag	UNP P09132
D	127	HIS	-	expression tag	UNP P09132
D	128	HIS	-	expression tag	UNP P09132

- Molecule 3 is a RNA chain called SRP RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	108	2332	1036	437	750	109	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	122	GDP	-	insertion	GB NR_002715.1
C	228	U	-	insertion	GB NR_002715.1
C	229	A	-	insertion	GB NR_002715.1

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
4	A	1	1	1	0	0
			Total	K		
4	C	1	1	1	0	0
			Total	K		
4	D	1	1	1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

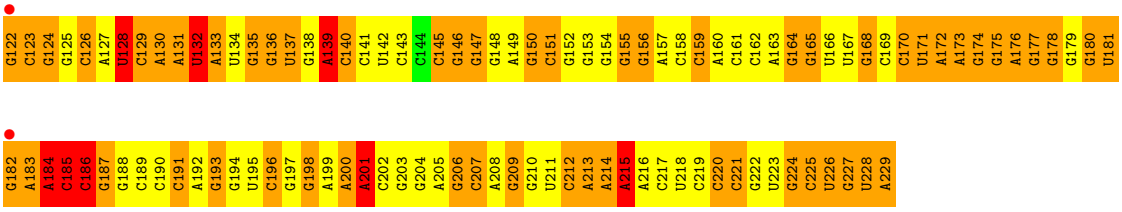
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	1	1	1	0	0
			Total	Mg		
5	C	2	2	2	0	0

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.

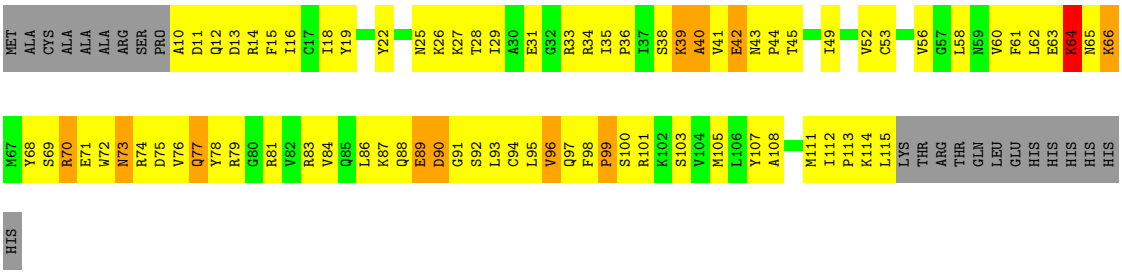
• Molecule 1: SRP RNA

Chain A: 2% • 40% 52% 7%



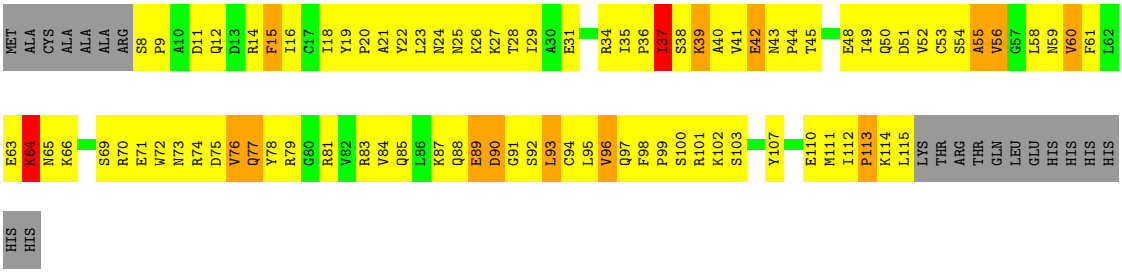
• Molecule 2: Signal recognition particle 19 kDa protein

Chain B: 20% 53% 9% • 17%



• Molecule 2: Signal recognition particle 19 kDa protein

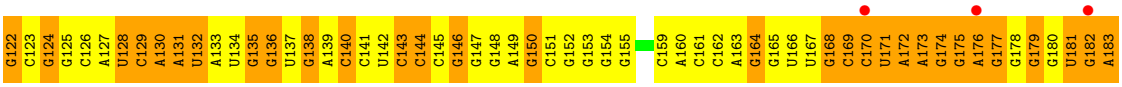
Chain D: 16% 57% 10% • 16%



• Molecule 3: SRP RNA

Chain C:

3%
46%
48%


G122 C123 G124 G125 C126 A127 U128 C129 A130 A131 U132 A133 U134 G135 G136 U137 G138 A139 C140 C141 U142 C143 C144 C145 G146 G147 G148 A149 G150 C151 G152 G153 G154 G155 C159 A160 C161 C162 A163 G164 G165 U166 U167 G168 C169 C170 U171 A172 A173 G174 G175 A176 G177 G178 G179 G180 U181 G182 A183

A184 C185 C186 G187 G188 C189 C190 C191 A192 G193 G194 U195 C196 G197 G198 A199 A200 A201 C202 G203 G204 A205 G206 C207 A208 G209 G210 U211 C212 A213 A214 A215 A216 C217 U218 C219 C220 C221 G222 U223 G224 C225 U226 G227 U228 A229

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	100.12Å 100.12Å 293.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.01 – 3.80 69.95 – 3.79	Depositor EDS
% Data completeness (in resolution range)	94.3 (70.01-3.80) 94.0 (69.95-3.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.291 , 0.329 0.253 , 0.283	Depositor DCC
R_{free} test set	711 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	160.9	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 99.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6390	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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: GDP, K, 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	0.68	0/2606	1.26	19/4066 (0.5%)
2	B	0.45	0/870	0.60	0/1172
2	D	0.45	0/884	0.61	0/1192
3	C	0.64	0/2580	1.26	13/4025 (0.3%)
All	All	0.61	0/6940	1.15	32/10455 (0.3%)

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	185	C	P-O3'-C3'	-7.71	110.44	119.70
3	C	185	C	C3'-C2'-C1'	-7.14	95.79	101.50
3	C	198	G	C4'-C3'-C2'	-6.93	95.67	102.60
1	A	201	A	P-O3'-C3'	-6.67	111.70	119.70
1	A	215	A	P-O3'-C3'	-6.38	112.05	119.70

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	2327	0	1172	639	4
2	B	856	0	874	209	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	869	0	884	178	0
3	C	2332	0	1171	511	2
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	C	2	0	0	0	0
All	All	6390	0	4101	1499	5

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 145.

The worst 5 of 1499 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:127:A:C2	1:A:173:A:H2	1.14	1.64
1:A:171:U:C2	1:A:173:A:H5"	1.20	1.64
1:A:226:U:H2'	1:A:227:G:C5'	1.26	1.62
1:A:226:U:C2'	1:A:227:G:H5"	1.21	1.60
1:A:177:G:N2	1:A:178:G:C4	1.76	1.53

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:C:N3	1:A:185:C:N3[7_555]	1.65	0.55
1:A:185:C:N4	1:A:185:C:N4[7_555]	1.72	0.48
1:A:220:C:O3'	3:C:123:C:O2'[3_454]	1.83	0.37
1:A:185:C:O2	1:A:185:C:O2[7_555]	1.87	0.33
3:C:184:A:C2	3:C:205:A:O2'[7_555]	1.99	0.21

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
2	B	104/128 (81%)	78 (75%)	18 (17%)	8 (8%)	1 15
2	D	106/128 (83%)	76 (72%)	18 (17%)	12 (11%)	0 7
All	All	210/256 (82%)	154 (73%)	36 (17%)	20 (10%)	0 11

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	64	LYS
2	B	89	GLU
2	B	96	VAL
2	D	64	LYS
2	D	77	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
2	B	94/112 (84%)	87 (93%)	7 (7%)	13 44
2	D	96/112 (86%)	90 (94%)	6 (6%)	18 49
All	All	190/224 (85%)	177 (93%)	13 (7%)	16 47

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	37	ILE
2	D	39	LYS
2	D	93	LEU
2	D	64	LYS
2	D	90	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	59	ASN
2	B	88	GLN
2	D	59	ASN
2	D	88	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	108/108 (100%)	52 (48%)	9 (8%)
3	C	106/108 (98%)	48 (45%)	13 (12%)
All	All	214/216 (99%)	100 (46%)	22 (10%)

5 of 100 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	123	C
1	A	124	G
1	A	126	C
1	A	128	U
1	A	129	C

5 of 22 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	C	181	U
3	C	185	C
3	C	184	A
3	C	186	C
1	A	186	C

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

1 non-standard protein/DNA/RNA residue 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	$\#\|Z\| > 2$
3	GDP	C	122	3	24,30,30	0.95	1 (4%)	30,47,47	1.23	4 (13%)

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
3	GDP	C	122	3	-	9/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	122	GDP	C6-N1	-2.24	1.34	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	122	GDP	PA-O3A-PB	-3.18	121.92	132.83
3	C	122	GDP	C3'-C2'-C1'	2.81	105.21	100.98
3	C	122	GDP	C8-N7-C5	2.23	107.24	102.99
3	C	122	GDP	C5-C6-N1	2.06	117.60	113.95

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	122	GDP	PA-O3A-PB-O2B
3	C	122	GDP	PA-O3A-PB-O3B
3	C	122	GDP	C5'-O5'-PA-O1A
3	C	122	GDP	O4'-C4'-C5'-O5'
3	C	122	GDP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	122	GDP	13	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	122:GDP	O3'	123:C	P	3.19

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	108/108 (100%)	-0.06	2 (1%)	66	59	42, 81, 169, 178	0
2	B	106/128 (82%)	-0.05	0	100	100	41, 63, 84, 86	0
2	D	108/128 (84%)	-0.11	0	100	100	36, 57, 78, 85	0
3	C	107/108 (99%)	-0.15	3 (2%)	53	43	39, 82, 182, 206	0
All	All	429/472 (90%)	-0.09	5 (1%)	79	72	36, 69, 156, 206	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	170	C	5.8
1	A	122	G	3.9
1	A	182	G	2.7
3	C	182	G	2.5
3	C	176	A	2.5

6.2 Non-standard residues in protein, DNA, RNA chains (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
3	GDP	C	122	28/28	0.75	0.21	123,124,125,125	0

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	K	D	129	1/1	0.81	0.29	82,82,82,82	0
4	K	A	1	1/1	0.84	0.45	75,75,75,75	0
5	MG	A	6	1/1	0.89	0.20	68,68,68,68	0
4	K	C	2	1/1	0.94	0.24	49,49,49,49	0
5	MG	C	5	1/1	0.94	0.73	30,30,30,30	0
5	MG	C	4	1/1	0.96	0.14	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.