



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:01 AM UTC

PDB ID : 3F73 / pdb_00003f73
Title : Alignment of guide-target seed duplex within an argonaute silencing complex
Authors : Wang, Y.; Li, H.; Sheng, G.; Juranek, S.; Tuschl, T.; Patel, D.J.
Deposited on : 2008-11-07
Resolution : 3.00 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 ⓘ 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

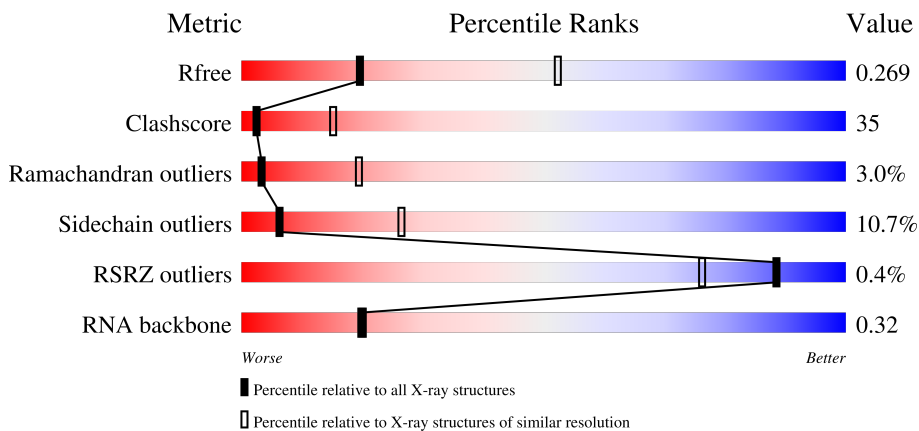
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



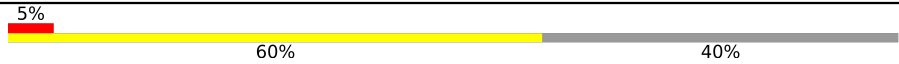
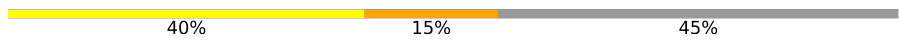
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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	685	
1	B	685	
2	C	21	
2	X	21	

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Mol	Chain	Length	Quality of chain
3	H	20	
3	Y	20	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11048 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 ARGONAUTE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	678	Total	C	N	O	S	13	0	0
			5075	3261	944	864	6			
1	B	670	Total	C	N	O	S	21	0	0
			4969	3193	912	857	7			

- Molecule 2 is a DNA chain called DNA (5'-D(P*DTP*DGP*DAP*DGP*DGP*DTP*DAP*DGP*DTP*DAP*DGP*DGP*DTP*DTP*DGP*DTP*DA*DTP*DAP*DGP*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	16	Total	C	N	O	P	0	0	1
			292	135	54	88	15			
2	X	15	Total	C	N	O	P	0	0	1
			296	140	55	87	14			

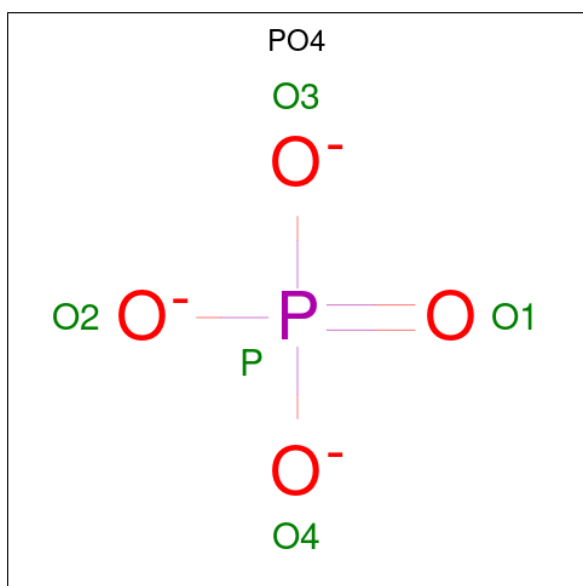
- Molecule 3 is a RNA chain called RNA (5'-R(*UP*AP*UP*AP*CP*AP*A*CP*UP*CP*A*P*CP*UP*AP*CP*CP*UP*CP*GP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	H	12	Total	C	N	O	P	0	0	1
			203	89	28	75	11			
3	Y	11	Total	C	N	O	P	0	0	1
			189	84	26	69	10			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	X	1	Total	Mg	0	0
			1	1		

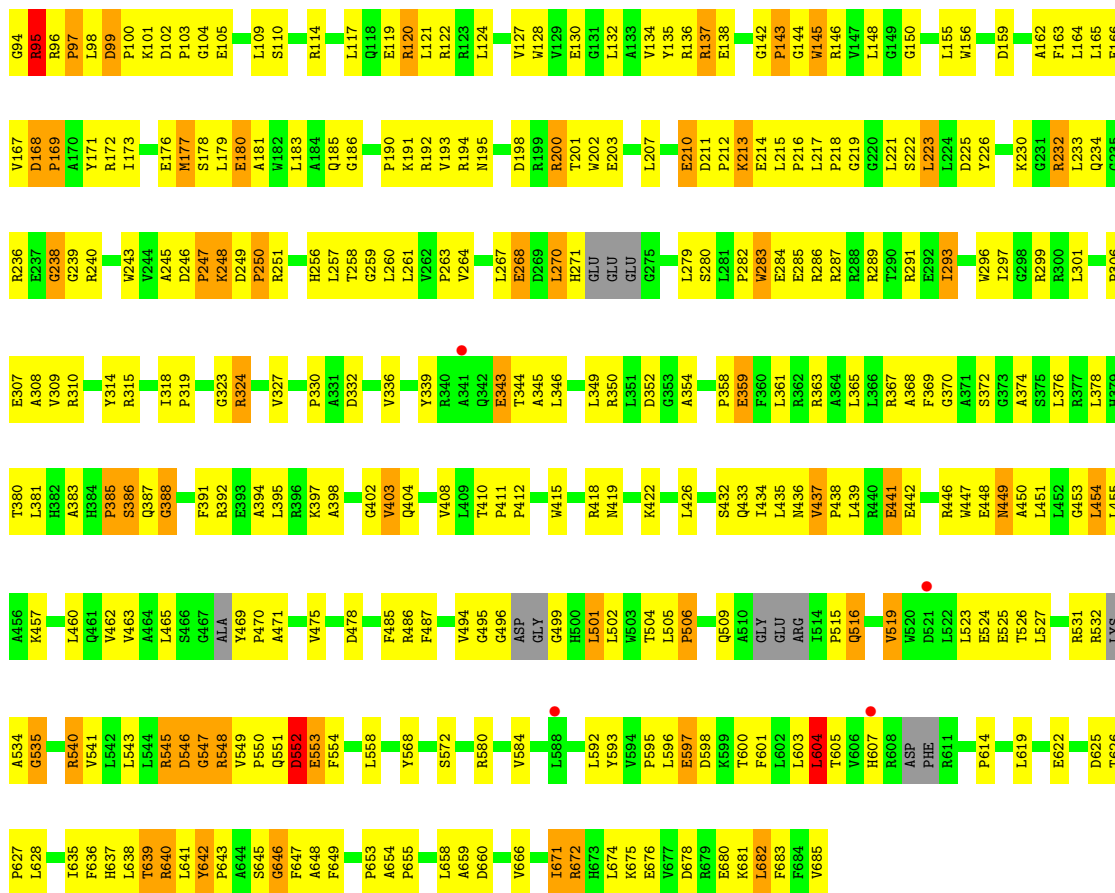
- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



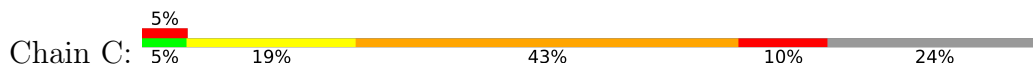
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	O P	0	0
			5	4 1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		
6	B	8	Total	O	0	0
			8	8		



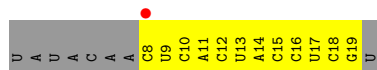
• Molecule 2: DNA (5'-D(P*DTP*DGP*DAP*DGP*DGP*DTP*DAP*DGP*DTP*DAP*DGP*DGP*DTP*DTP*DGP*DTP*DA*DTP*DAP*DGP*DT)-3')



• Molecule 2: DNA (5'-D(P*DTP*DGP*DAP*DGP*DGP*DTP*DAP*DGP*DTP*DAP*DGP*DGP*DTP*DTP*DGP*DTP*DA*DTP*DAP*DGP*DT)-3')



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



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

Chain Y:  40% 15% 45%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.16Å 120.53Å 109.08Å 90.00° 105.30° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (30.00-3.00) 97.2 (30.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.81Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.282 (Not available) , 0.269	Depositor DCC
R_{free} test set	2512 reflections (7.00%)	wwPDB-VP
Wilson B-factor (Å ²)	64.7	Xtrriage
Anisotropy	0.309	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11048	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PO4

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	0.59	2/5197 (0.0%)	1.17	43/7084 (0.6%)
1	B	0.56	1/5084 (0.0%)	1.14	40/6934 (0.6%)
2	C	0.78	1/326 (0.3%)	1.85	19/501 (3.8%)
2	X	0.65	1/331 (0.3%)	1.90	17/508 (3.3%)
3	H	0.73	1/223 (0.4%)	1.13	2/345 (0.6%)
3	Y	1.00	3/208 (1.4%)	1.03	2/321 (0.6%)
All	All	0.60	9/11369 (0.1%)	1.21	123/15693 (0.8%)

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
2	C	0	2
2	X	0	4
All	All	0	6

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	18	DT	O3'-P	-10.13	1.46	1.61
3	Y	9	U	O3'-P	-8.50	1.48	1.61
1	A	221	LEU	C-O	7.86	1.33	1.23
1	A	437	VAL	CA-CB	6.85	1.57	1.54
3	Y	10	C	P-OP2	6.29	1.61	1.49

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	607	HIS	N-CA-C	-11.50	91.66	107.88
2	C	10	DA	N9-C1'-C2'	11.26	130.39	113.50
2	X	9	DT	O3'-P-O5'	11.04	120.56	104.00
1	B	386	SER	N-CA-C	11.03	122.87	111.07
2	X	19	DA	C2'-C3'-O3'	-10.40	95.89	111.50

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	2	DG	Sidechain
2	C	9	DT	Sidechain
2	X	6	DT	Sidechain
2	X	8	DG	Sidechain
2	X	9	DT	Sidechain

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	5075	0	5007	335	2
1	B	4969	0	4842	335	2
2	C	292	0	155	35	0
2	X	296	0	161	39	0
3	H	203	0	107	29	0
3	Y	189	0	99	15	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	X	1	0	0	0	0
5	C	5	0	0	0	0
6	A	8	0	0	1	0
6	B	8	0	0	0	0
All	All	11048	0	10371	740	2

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 35.

The worst 5 of 740 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:102:ASP:OD1	1:B:103:PRO:HD2	1.39	1.19
1:A:561:LEU:HD22	1:A:566:ILE:HD11	1.29	1.15
1:B:545:ARG:HE	1:B:547:GLY:HA2	1.08	1.12
1:A:396:ARG:HH11	1:A:396:ARG:HB3	1.07	1.11
2:C:10:DA:H4'	2:C:11:DG:OP1	1.32	1.09

All (2) 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:236:ARG:NH1	1:B:234:GLN:O[2_755]	2.05	0.15
1:A:234:GLN:O	1:B:236:ARG:NH1[2_755]	2.18	0.02

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	672/685 (98%)	577 (86%)	78 (12%)	17 (2%)	4	23
1	B	656/685 (96%)	545 (83%)	88 (13%)	23 (4%)	3	16
All	All	1328/1370 (97%)	1122 (84%)	166 (12%)	40 (3%)	3	19

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	PRO
1	A	675	LYS
1	B	143	PRO
1	B	387	GLN
1	B	547	GLY

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	256/549 (47%)	226 (88%)	30 (12%)	5	23
1	B	457/549 (83%)	411 (90%)	46 (10%)	7	29
All	All	713/1098 (65%)	637 (89%)	76 (11%)	6	26

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	361	LEU
1	B	600	THR
1	B	432	SER
1	B	516	GLN
1	B	672	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	634	GLN
1	B	621	HIS
1	B	256	HIS
1	B	436	ASN
1	B	48	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	H	10/20 (50%)	1 (10%)	0
3	Y	9/20 (45%)	2 (22%)	0
All	All	19/40 (47%)	3 (15%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	H	19	G
3	Y	11	A
3	Y	19	G

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 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	$\# Z > 2$
5	PO4	C	23	-	4,4,4	1.75	1 (25%)	6,6,6	0.47	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	23	PO4	P-O2	-2.01	1.48	1.54

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	677/685 (98%)	-0.19	0 100 100	29, 67, 99, 111	3 (0%)
1	B	670/685 (97%)	-0.15	4 (0%) 85 69	36, 68, 100, 115	5 (0%)
2	C	16/21 (76%)	0.39	1 (6%) 26 13	48, 74, 129, 134	0
2	X	15/21 (71%)	0.31	0 100 100	44, 57, 137, 148	0
3	H	12/20 (60%)	0.71	1 (8%) 17 9	85, 103, 129, 130	0
3	Y	11/20 (55%)	0.51	0 100 100	91, 100, 134, 139	0
All	All	1401/1452 (96%)	-0.14	6 (0%) 88 76	29, 68, 101, 148	8 (0%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	521	ASP	3.8
1	B	607	HIS	2.7
1	B	341	ALA	2.4
2	C	11	DG	2.3
1	B	588	LEU	2.2

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 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(Å ²)	Q<0.9
5	PO4	C	23	5/5	0.57	0.09	125,125,125,125	4
4	MG	X	22	1/1	0.91	0.14	47,47,47,47	0
4	MG	A	686	1/1	0.93	0.05	62,62,62,62	0
4	MG	C	22	1/1	0.96	0.13	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.