



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 15, 2018 – 01:58 PM EST

PDB ID : 1GL9
Title : Archaeoglobus fulgidus reverse gyrase complexed with ADPNP
Authors : Rodriguez, A.C.; Stock, D.
Deposited on : 2001-08-30
Resolution : 3.20 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

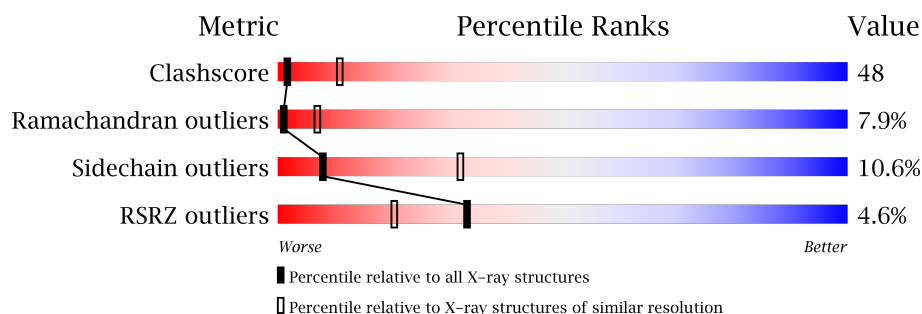
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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. 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	B	1054	 2% 35% 50% 11% ..
1	C	1054	 7% 35% 50% 9% . 5%

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
2	ANP	B	2055	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 16398 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.

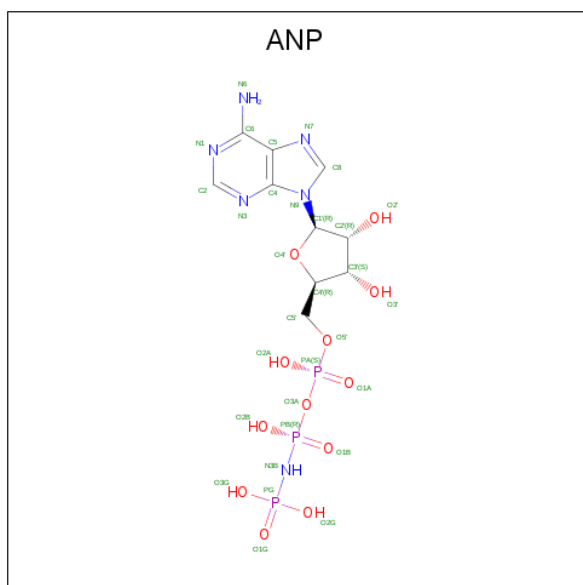
- Molecule 1 is a protein called REVERSE GYRASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1020	Total	C	N	O	S	0	0	0
			8226	5246	1450	1505	25			
1	C	1005	Total	C	N	O	S	0	0	0
			8108	5169	1430	1483	26			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	719	LEU	PRO	engineered mutation	UNP O29238
B	1046	MET	LEU	engineered mutation	UNP O29238
C	719	LEU	PRO	engineered mutation	UNP O29238
C	1046	MET	LEU	engineered mutation	UNP O29238

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

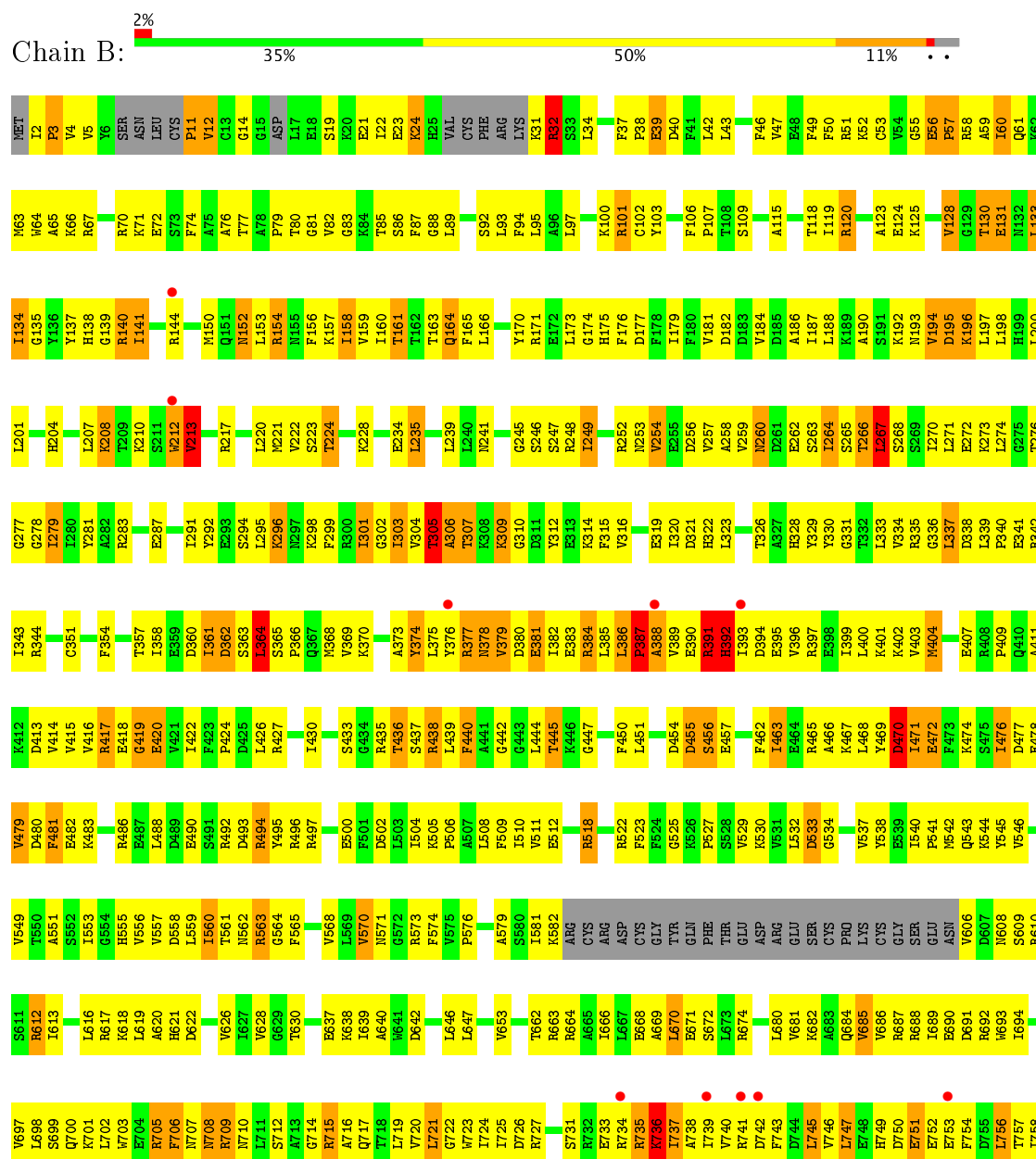
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: REVERSE GYRASE





F1008	R942	R810	L667	CYS
L1009	R943	R811	E668	PRO
V1010	R944	R812	A669	LYS
R1011	A945	D813		CYS
R1012	R946	S814	L673	GLY
Y1013	R947	R815		SER
A1014	R948	R816	V681	GLU
	S949	V617	A682	ASN
	R950	S818	A683	V606
	R951	D819	Q684	D607
	R952	A888	V685	N608
	R953	A889	V686	S609
		S890	R687	S610
		Q891	A688	S611
		C892	E689	R612
		R893	E690	R613
		R894	D691	E614
		R895		A615
		R896	L684	L616
		R897	G895	L617
		R898	R696	R618
		R899	V697	L619
		R900	Q700	A620
		R901	K701	H621
		R902	L702	D622
		S903	E703	A623
		T904	E704	E624
		F905	E766	
		F906	R767	L627
		D907	R768	V628
		GLY	T769	A629
		LYS	P770	T630
		THR	L771	
		ALA		T634
		R912	Y774	E635
		E913	T775	E636
		E914	T776	E637
		R915	E777	E638
				E639
		E920	D782	
		G921	A783	L646
		R922	T784	L647
		A923		S648
		Y924	L787	E649
		E925	R788	C650
		R926	F789	
		R927	S790	
		R928	V791	
		A929	K792	
		V930	I795	
		W931	T796	
		V932		
		R933	Q796	
		N934	I797	
		L935		
		R936	L801	
		P937		
		D1004	L806	
		F1005	I807	
		V1006	T808	
		R1007	K736	
			T737	
			A738	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	132.41Å 68.69Å 134.00Å 90.00° 99.70° 90.00°	Depositor
Resolution (Å)	34.00 – 3.20 34.40 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.6 (34.00-3.20) 96.7 (34.40-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 3.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.256 , 0.332 0.249 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	69.1	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 87.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16398	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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, ANP

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	B	0.47	0/8371	0.72	5/11265 (0.0%)
1	C	0.35	0/8246	0.61	3/11090 (0.0%)
All	All	0.41	0/16617	0.67	8/22355 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	391	ARG	N-CA-C	-7.20	91.57	111.00
1	C	305	THR	N-CA-C	6.94	129.73	111.00
1	B	388	ALA	N-CA-C	-6.79	92.68	111.00
1	B	3	PRO	N-CA-CB	5.77	110.23	103.30
1	C	11	PRO	N-CA-CB	5.54	109.95	103.30

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	B	8226	0	8310	830	0
1	C	8108	0	8178	754	0
2	B	31	0	13	5	0
2	C	31	0	13	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
All	All	16398	0	16514	1581	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 48.

The worst 5 of 1581 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:379:VAL:HG12	1:B:380:ASP:H	1.12	1.12
1:B:386:LEU:HD23	1:B:386:LEU:H	1.19	1.06
1:B:638:LYS:HB2	1:B:684:GLN:HG3	1.38	1.06
1:C:192:LYS:HB3	1:C:196:LYS:HE3	1.43	1.00
1:B:540:ILE:HG13	1:B:541:PRO:HD2	1.46	0.97

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	B	1010/1054 (96%)	752 (74%)	177 (18%)	81 (8%)	1	7
1	C	987/1054 (94%)	696 (70%)	214 (22%)	77 (8%)	1	7
All	All	1997/2108 (95%)	1448 (72%)	391 (20%)	158 (8%)	1	7

5 of 158 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	PRO
1	B	5	VAL

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Mol	Chain	Res	Type
1	B	12	VAL
1	B	24	LYS
1	B	32	ARG

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	B	876/925 (95%)	782 (89%)	94 (11%)	8	31
1	C	863/925 (93%)	773 (90%)	90 (10%)	8	33
All	All	1739/1850 (94%)	1555 (89%)	184 (11%)	8	32

5 of 184 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	886	ARG
1	C	131	GLU
1	C	873	ARG
1	B	934	ASN
1	B	1050	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	934	ASN
1	C	152	ASN
1	C	876	HIS
1	B	963	GLN
1	C	164	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
2	ANP	B	2055	-	29,33,33	2.13	7 (24%)	28,52,52	2.84	9 (32%)
2	ANP	C	2055	-	29,33,33	2.55	9 (31%)	28,52,52	2.80	10 (35%)

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
2	ANP	B	2055	-	1/1/7/8	1/13/38/38	0/3/3/3
2	ANP	C	2055	-	-	0/13/38/38	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2055	ANP	C2'-C1'	-4.62	1.46	1.53
2	C	2055	ANP	C2'-C1'	-4.22	1.46	1.53
2	B	2055	ANP	PB-O2B	-3.88	1.46	1.56
2	C	2055	ANP	PB-O2B	-3.67	1.46	1.56
2	C	2055	ANP	PB-N3B	-2.14	1.57	1.63

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2055	ANP	O1B-PB-N3B	-5.48	103.59	111.79
2	B	2055	ANP	O1B-PB-N3B	-5.39	103.73	111.79
2	B	2055	ANP	O1G-PG-N3B	-5.36	103.78	111.79
2	C	2055	ANP	O1G-PG-N3B	-5.29	103.87	111.79
2	B	2055	ANP	N3-C2-N1	-4.76	124.71	128.86

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	2055	ANP	C2'

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2055	ANP	O1G-PG-N3B-PB

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2055	ANP	5	0
2	C	2055	ANP	5	0

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
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	15:GLY	C	16:ASP	N	13.42

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	B	1020/1054 (96%)	-0.31	16 (1%) 72 59	1, 38, 137, 192	0
1	C	1005/1054 (95%)	0.32	78 (7%) 14 8	24, 92, 160, 195	0
All	All	2025/2108 (96%)	0.00	94 (4%) 33 20	1, 68, 153, 195	0

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	942	ARG	7.9
1	C	140	ARG	6.4
1	C	139	GLY	6.2
1	C	381	GLU	5.5
1	C	907	ASP	5.5

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	ANP	C	2055	31/31	0.88	0.23	0.23	38,57,75,77	0
2	ANP	B	2055	31/31	0.95	0.20	0.16	24,34,69,77	0
3	MG	C	2056	1/1	0.32	1.04	-	70,70,70,70	0
3	MG	B	2056	1/1	0.83	0.38	-	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.