



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 21, 2023 – 05:23 AM JST

PDB ID : 7ESO
Title : Structure and mutation analysis of the hexameric P4 from Pseudomonas aeruginosa phage phiYY
Authors : Zhang, C.Y.; Jin, T.C.
Deposited on : 2021-05-11
Resolution : 2.45 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

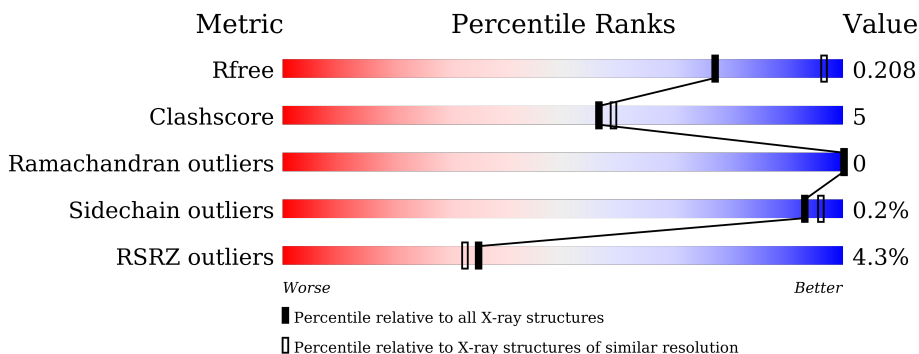
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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.



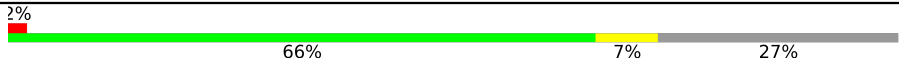

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	354	 2% 64% 11% 25%
1	B	354	 2% 63% 10% 27%
1	C	354	 3% 68% 7% 25%
1	D	354	 4% 65% 7% 27%
1	E	354	 4% 66% 9% 25%
1	F	354	 3% 66% 7% 27%

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Mol	Chain	Length	Quality of chain
1	G	354	 <p>2% 66% 7% 27%</p>
1	H	354	 <p>4% 62% 13% 25%</p>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15697 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 Packaging NTPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	266	1964	1242	339	371	12	0	0	0
1	B	257	1899	1201	325	361	12	0	0	0
1	H	266	1964	1242	339	371	12	0	0	0
1	G	257	1899	1201	325	361	12	0	0	0
1	C	266	1964	1242	339	371	12	0	0	0
1	D	257	1899	1201	325	361	12	0	0	0
1	E	266	1964	1242	339	371	12	0	0	0
1	F	257	1899	1201	325	361	12	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP A0A1U9AK63
A	-2	SER	-	expression tag	UNP A0A1U9AK63
A	-1	VAL	-	expression tag	UNP A0A1U9AK63
A	0	ASP	-	expression tag	UNP A0A1U9AK63
B	-3	GLY	-	expression tag	UNP A0A1U9AK63
B	-2	SER	-	expression tag	UNP A0A1U9AK63
B	-1	VAL	-	expression tag	UNP A0A1U9AK63
B	0	ASP	-	expression tag	UNP A0A1U9AK63
H	-3	GLY	-	expression tag	UNP A0A1U9AK63
H	-2	SER	-	expression tag	UNP A0A1U9AK63
H	-1	VAL	-	expression tag	UNP A0A1U9AK63
H	0	ASP	-	expression tag	UNP A0A1U9AK63
G	-3	GLY	-	expression tag	UNP A0A1U9AK63

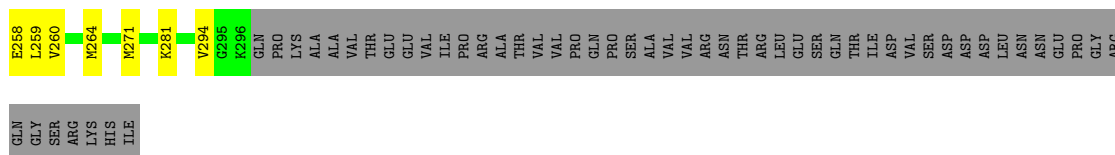
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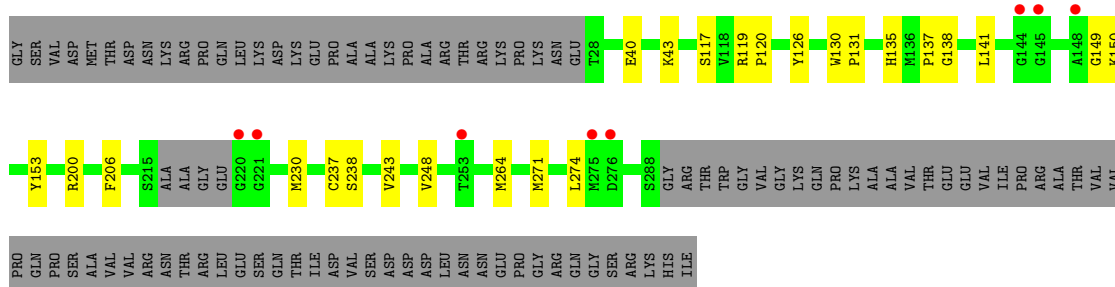
Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	SER	-	expression tag	UNP A0A1U9AK63
G	-1	VAL	-	expression tag	UNP A0A1U9AK63
G	0	ASP	-	expression tag	UNP A0A1U9AK63
C	-3	GLY	-	expression tag	UNP A0A1U9AK63
C	-2	SER	-	expression tag	UNP A0A1U9AK63
C	-1	VAL	-	expression tag	UNP A0A1U9AK63
C	0	ASP	-	expression tag	UNP A0A1U9AK63
D	-3	GLY	-	expression tag	UNP A0A1U9AK63
D	-2	SER	-	expression tag	UNP A0A1U9AK63
D	-1	VAL	-	expression tag	UNP A0A1U9AK63
D	0	ASP	-	expression tag	UNP A0A1U9AK63
E	-3	GLY	-	expression tag	UNP A0A1U9AK63
E	-2	SER	-	expression tag	UNP A0A1U9AK63
E	-1	VAL	-	expression tag	UNP A0A1U9AK63
E	0	ASP	-	expression tag	UNP A0A1U9AK63
F	-3	GLY	-	expression tag	UNP A0A1U9AK63
F	-2	SER	-	expression tag	UNP A0A1U9AK63
F	-1	VAL	-	expression tag	UNP A0A1U9AK63
F	0	ASP	-	expression tag	UNP A0A1U9AK63

- Molecule 2 is water.

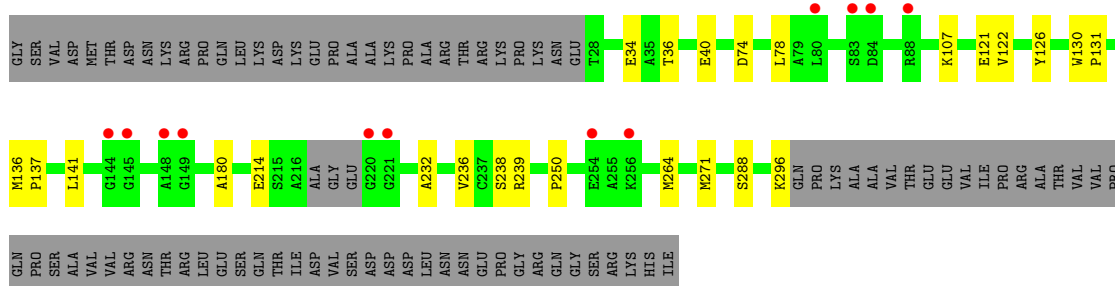
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	37	Total O 37 37	0	0
2	B	39	Total O 39 39	0	0
2	H	24	Total O 24 24	0	0
2	G	34	Total O 34 34	0	0
2	C	33	Total O 33 33	0	0
2	D	25	Total O 25 25	0	0
2	E	27	Total O 27 27	0	0
2	F	26	Total O 26 26	0	0



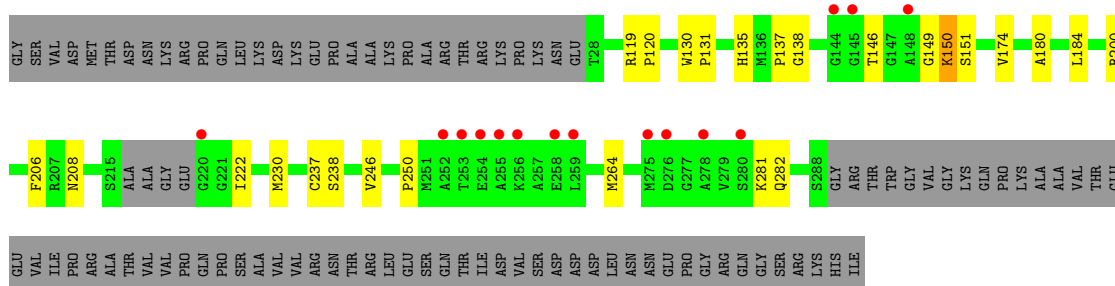
Molecule 1: Packaging NTPase



Molecule 1: Packaging NTPase

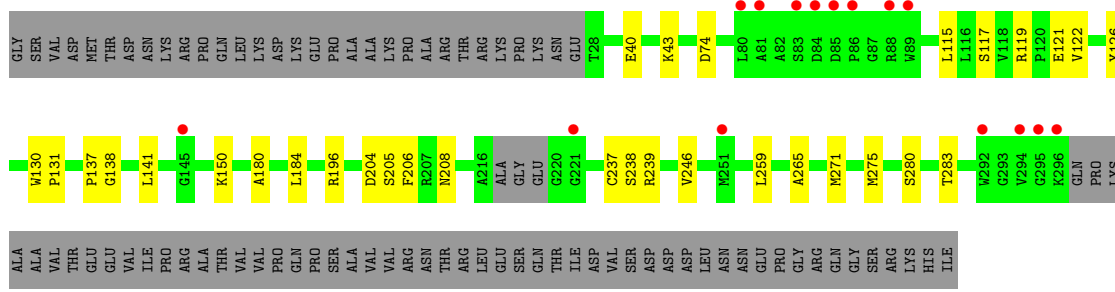


Molecule 1: Packaging NTPase

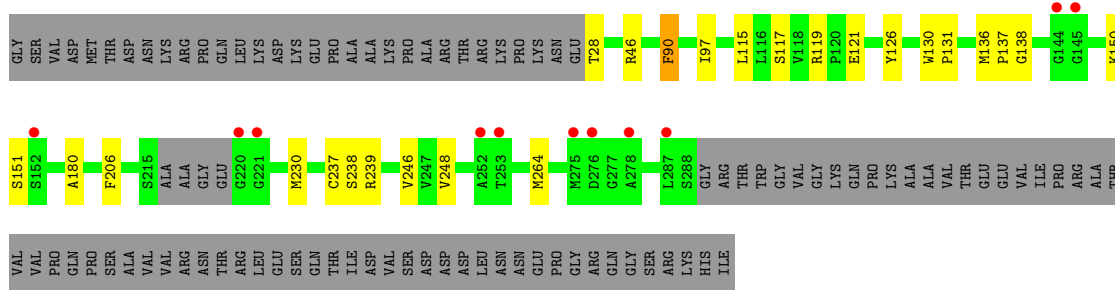


Molecule 1: Packaging NTPase





● Molecule 1: Packaging NTPase



4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	241.07Å 241.07Å 152.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.13 – 2.45 49.40 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.7 (41.13-2.45) 96.0 (49.40-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.180 , 0.208 0.180 , 0.208	Depositor DCC
R_{free} test set	6068 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for $-1/3^*h+1/3^*k+4/3^*l,-k,2/3^*h+1/3^*k+1/3^*l$ 0.008 for $-2/3^*h-1/3^*k-4/3^*l,-1/3^*h-2/3^*k+4/3^*l,-1/3^*h+1/3^*k+1/3^*l$ 0.008 for $-h,1/3^*h-1/3^*k-4/3^*l,-1/3^*h-2/3^*k+1/3^*l$ 0.059 for $-1/3^*h-2/3^*k+4/3^*l,-2/3^*h-1/3^*k-4/3^*l,1/3^*h-1/3^*k-1/3^*l$ 0.039 for $-h,2/3^*h+1/3^*k+4/3^*l,1/3^*h+2/3^*k-1/3^*l$ 0.023 for $1/3^*h+2/3^*k-4/3^*l,-k,-2/3^*h-1/3^*k-1/3^*l$ 0.018 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15697	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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](#)

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	0.32	0/2000	0.54	1/2724 (0.0%)
1	B	0.38	0/1933	0.58	1/2634 (0.0%)
1	C	0.36	0/2000	0.54	0/2724
1	D	0.33	0/1933	0.56	0/2634
1	E	0.34	0/2000	0.55	1/2724 (0.0%)
1	F	0.34	0/1933	0.56	1/2634 (0.0%)
1	G	0.35	0/1933	0.56	0/2634
1	H	0.33	0/2000	0.54	0/2724
All	All	0.34	0/15732	0.55	4/21432 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	90	PHE	CB-CG-CD2	-6.12	116.52	120.80
1	A	118	VAL	C-N-CA	-5.78	107.24	121.70
1	E	259	LEU	CB-CG-CD2	5.72	120.72	111.00
1	B	90	PHE	CB-CG-CD2	-5.24	117.13	120.80

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	1964	0	1977	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1899	0	1911	21	0
1	C	1964	0	1977	17	0
1	D	1899	0	1911	23	0
1	E	1964	0	1977	22	0
1	F	1899	0	1911	18	0
1	G	1899	0	1911	17	0
1	H	1964	0	1977	31	0
2	A	37	0	0	0	0
2	B	39	0	0	0	0
2	C	33	0	0	1	0
2	D	25	0	0	0	0
2	E	27	0	0	0	0
2	F	26	0	0	0	0
2	G	34	0	0	1	0
2	H	24	0	0	0	0
All	All	15697	0	15552	154	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 5.

The worst 5 of 154 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:H:181:VAL:HB	1:H:186:GLU:HG3	1.66	0.77
1:A:181:VAL:HB	1:A:186:GLU:HG3	1.65	0.77
1:B:137:PRO:HB2	1:B:238:SER:HA	1.74	0.69
1:F:137:PRO:HB2	1:F:238:SER:HA	1.75	0.68
1:B:174:VAL:HG22	1:C:122:VAL:HG11	1.74	0.67

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	262/354 (74%)	253 (97%)	9 (3%)	0	100	100
1	B	253/354 (72%)	246 (97%)	7 (3%)	0	100	100
1	C	262/354 (74%)	256 (98%)	6 (2%)	0	100	100
1	D	253/354 (72%)	247 (98%)	6 (2%)	0	100	100
1	E	262/354 (74%)	257 (98%)	5 (2%)	0	100	100
1	F	253/354 (72%)	250 (99%)	3 (1%)	0	100	100
1	G	253/354 (72%)	247 (98%)	6 (2%)	0	100	100
1	H	262/354 (74%)	255 (97%)	7 (3%)	0	100	100
All	All	2060/2832 (73%)	2011 (98%)	49 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	205/281 (73%)	205 (100%)	0	100	100
1	B	200/281 (71%)	199 (100%)	1 (0%)	88	93
1	C	205/281 (73%)	205 (100%)	0	100	100
1	D	200/281 (71%)	199 (100%)	1 (0%)	88	93
1	E	205/281 (73%)	205 (100%)	0	100	100
1	F	200/281 (71%)	200 (100%)	0	100	100
1	G	200/281 (71%)	199 (100%)	1 (0%)	88	93
1	H	205/281 (73%)	205 (100%)	0	100	100
All	All	1620/2248 (72%)	1617 (100%)	3 (0%)	93	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	150	LYS
1	G	150	LYS

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Mol	Chain	Res	Type
1	D	150	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	266/354 (75%)	-0.02	7 (2%) 56 52	38, 52, 88, 103	0
1	B	257/354 (72%)	-0.03	8 (3%) 49 45	35, 50, 87, 105	0
1	C	266/354 (75%)	0.06	12 (4%) 33 30	37, 53, 94, 109	0
1	D	257/354 (72%)	0.07	15 (5%) 23 20	40, 54, 94, 107	0
1	E	266/354 (75%)	0.09	15 (5%) 24 21	41, 59, 95, 110	0
1	F	257/354 (72%)	-0.01	11 (4%) 35 32	39, 52, 90, 108	0
1	G	257/354 (72%)	-0.09	8 (3%) 49 45	38, 53, 92, 109	0
1	H	266/354 (75%)	0.09	15 (5%) 24 21	40, 57, 95, 113	0
All	All	2092/2832 (73%)	0.02	91 (4%) 35 32	35, 54, 93, 113	0

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	220	GLY	9.0
1	G	220	GLY	8.4
1	B	220	GLY	6.0
1	E	292	TRP	5.7
1	H	221	GLY	5.7

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.