



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 10:09 PM GMT

PDB ID : 4M6D
Title : Crystal structure of the aptamer minF-lysozyme complex.
Authors : Malashkevich, V.N.; Padlan, F.C.; Toro, R.; Girvin, M.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRG)
Deposited on : 2013-08-09
Resolution : 2.68 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

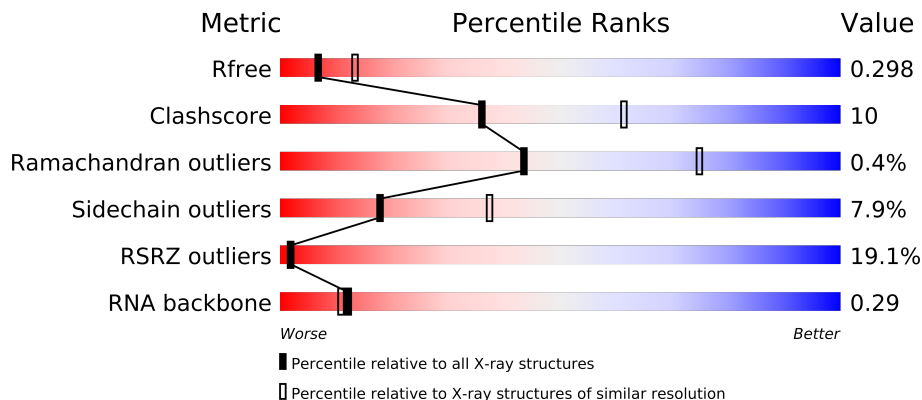
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.68 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}	66092	2010 (2.70-2.66)
Clashscore	79885	2450 (2.70-2.66)
Ramachandran outliers	78287	2410 (2.70-2.66)
Sidechain outliers	78261	2410 (2.70-2.66)
RSRZ outliers	66119	2013 (2.70-2.66)
RNA backbone	1838	1055 (3.20-2.16)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	129	
1	C	129	
1	E	129	
1	G	129	
1	I	129	
1	K	129	
2	B	45	
2	D	45	
2	F	45	
2	H	45	
2	J	45	
2	L	45	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11432 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Lysozyme C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			1001	613	193	185	10			
1	C	129	Total	C	N	O	S	0	0	0
			1001	613	193	185	10			
1	E	129	Total	C	N	O	S	0	0	0
			1001	613	193	185	10			
1	G	129	Total	C	N	O	S	0	0	0
			1001	613	193	185	10			
1	I	129	Total	C	N	O	S	1	0	0
			1001	613	193	185	10			
1	K	129	Total	C	N	O	S	0	0	0
			1001	613	193	185	10			

- Molecule 2 is a RNA chain called aptamer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	41	Total	C	N	O	P	0	0	0
			878	392	160	285	41			
2	D	42	Total	C	N	O	P	0	0	0
			901	402	165	292	42			
2	F	41	Total	C	N	O	P	0	0	0
			878	392	160	285	41			
2	H	42	Total	C	N	O	P	0	0	0
			901	402	165	292	42			
2	J	41	Total	C	N	O	P	0	0	0
			878	392	160	285	41			
2	L	43	Total	C	N	O	P	0	0	0
			921	411	168	299	43			

- Molecule 3 is water.

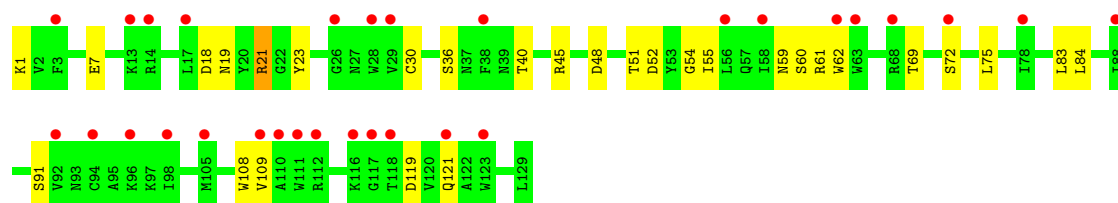
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	B	8	Total O 8 8	0	0
3	C	5	Total O 5 5	0	0
3	D	4	Total O 4 4	0	0
3	E	5	Total O 5 5	0	0
3	F	11	Total O 11 11	0	0
3	G	5	Total O 5 5	0	0
3	H	3	Total O 3 3	0	0
3	I	7	Total O 7 7	0	0
3	J	8	Total O 8 8	0	0
3	K	5	Total O 5 5	0	0
3	L	3	Total O 3 3	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

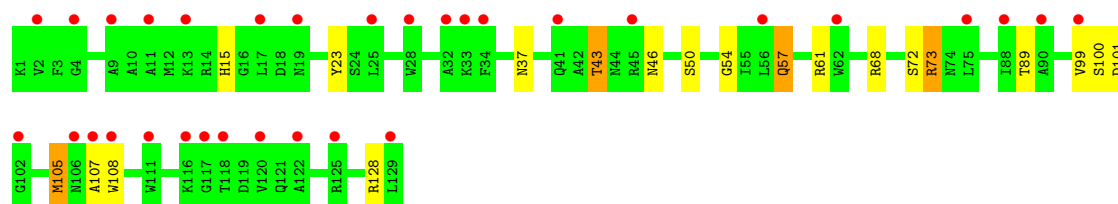
• Molecule 1: Lysozyme C

Chain A: 



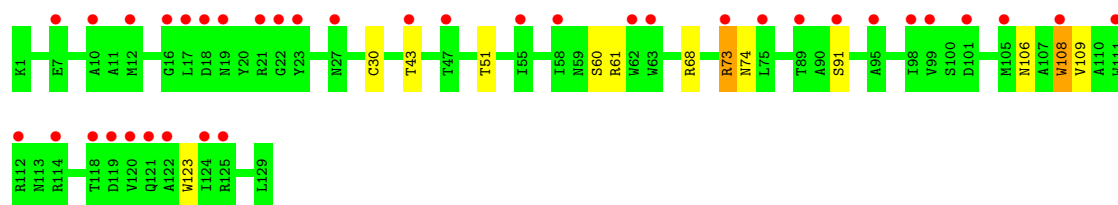
• Molecule 1: Lysozyme C

Chain C: 



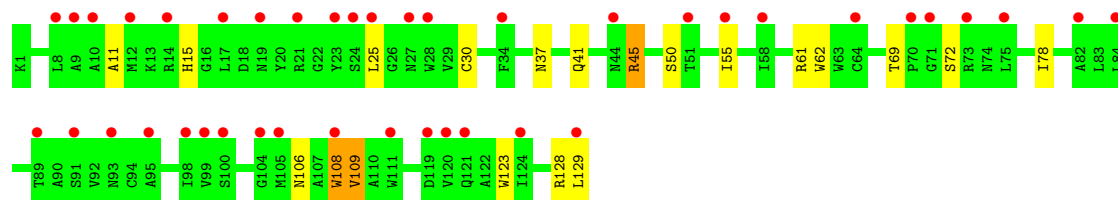
• Molecule 1: Lysozyme C

Chain E: 



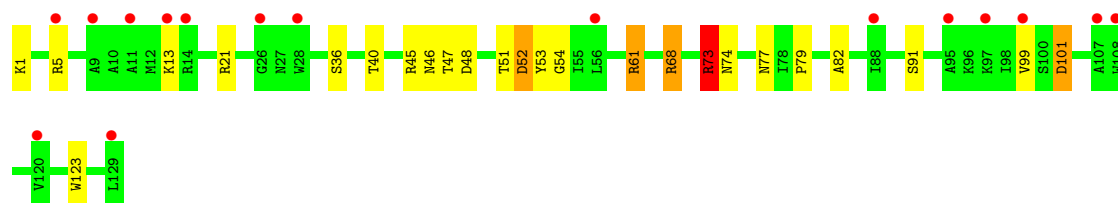
• Molecule 1: Lysozyme C

Chain G: 



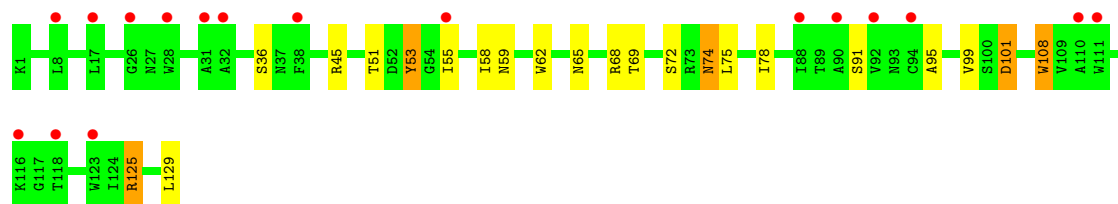
- Molecule 1: Lysozyme C

Chain I:



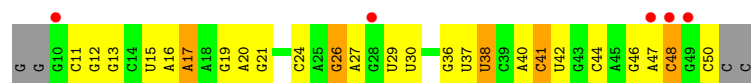
- Molecule 1: Lysozyme C

Chain K:



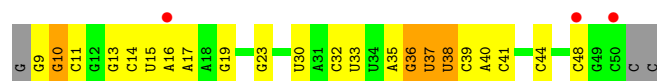
- Molecule 2: aptamer

Chain B:



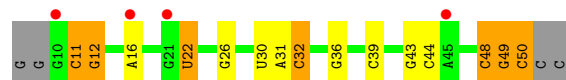
- Molecule 2: aptamer

Chain D:



- Molecule 2: aptamer

Chain F:



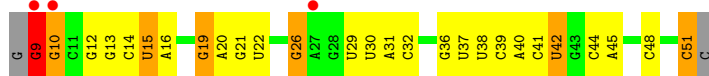
- Molecule 2: aptamer

Chain H:



- Molecule 2: aptamer

Chain J:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.91Å 132.29Å 131.54Å 118.59° 96.39° 96.27°	Depositor
Resolution (Å)	38.04 – 2.68 37.82 – 2.69	Depositor EDS
% Data completeness (in resolution range)	79.5 (38.04-2.68) 79.7 (37.82-2.69)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.165 , 0.216 0.280 , 0.298	Depositor DCC
R_{free} test set	2859 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 91.1	EDS
Estimated twinning fraction	0.351 for H, K, L 0.014 for -H, H+K+L, -L 0.015 for -H, -L, -K 0.344 for H, L, -H-K-L 0.267 for H, -H-K-L, K 0.009 for -H, -K, H+K+L 0.390 for h,-h-k-l,k 0.390 for h,l,-h-k-l 0.018 for -h,-l,-k 0.018 for -h,h+k+l,l 0.016 for -h,-k,h+k+l	Xtriage
Reported twinning fraction	0.351 for H, K, L 0.014 for -H, H+K+L, -L 0.015 for -H, -L, -K 0.344 for H, L, -H-K-L 0.267 for H, -H-K-L, K 0.009 for -H, -K, H+K+L	Depositor
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 56402 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11432	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

¹ Intensities estimated from amplitudes.

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality

5.1 Standard geometry

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	0.85	0/1021	0.82	0/1379
1	C	0.81	0/1021	0.82	2/1379 (0.1%)
1	E	0.75	0/1021	0.81	0/1379
1	G	0.69	0/1021	0.80	1/1379 (0.1%)
1	I	1.08	1/1021 (0.1%)	0.95	2/1379 (0.1%)
1	K	1.07	2/1021 (0.2%)	0.92	1/1379 (0.1%)
2	B	0.64	3/982 (0.3%)	0.73	0/1529
2	D	0.36	0/1008	0.66	0/1570
2	F	0.42	1/982 (0.1%)	0.67	0/1529
2	H	0.51	0/1008	0.72	0/1570
2	J	0.45	0/982	0.67	0/1529
2	L	0.50	0/1030	0.72	1/1604 (0.1%)
All	All	0.72	7/12118 (0.1%)	0.78	7/17605 (0.0%)

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
1	C	0	1
1	K	0	1
All	All	0	2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	20	A	O3'-P	-6.75	1.53	1.61
2	B	37	U	O3'-P	-5.93	1.54	1.61
1	K	53	TYR	CE1-CZ	-5.82	1.30	1.38
1	I	123	TRP	CE3-CZ3	5.59	1.48	1.38
1	K	101	ASP	CB-CG	5.57	1.63	1.51

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	68	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	L	9	G	C2'-C3'-O3'	5.92	123.18	113.70
1	G	25	LEU	CA-CB-CG	5.64	128.26	115.30
1	K	101	ASP	CB-CG-OD1	5.52	123.27	118.30
1	I	73	ARG	N-CA-C	5.36	125.47	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	100	SER	Peptide
1	K	101	ASP	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1001	0	0	14	0
1	C	1001	0	0	8	0
1	E	1001	0	0	4	0
1	G	1001	0	0	7	0
1	I	1001	0	0	14	0
1	K	1001	0	0	8	0
2	B	878	0	0	12	0
2	D	901	0	0	7	0
2	F	878	0	0	8	0
2	H	901	0	0	2	0
2	J	878	0	0	10	0
2	L	921	0	0	17	0
3	A	5	0	0	0	0
3	B	8	0	0	0	0
3	C	5	0	0	0	0
3	D	4	0	0	1	0
3	E	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	11	0	0	0	0
3	G	5	0	0	0	0
3	H	3	0	0	0	0
3	I	7	0	0	0	0
3	J	8	0	0	2	0
3	K	5	0	0	0	0
3	L	3	0	0	0	0
All	All	11432	0	0	105	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

The worst 5 of 105 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:12:G:O6	2:J:48:C:N3	2.04	0.89
2:L:14:C:N3	2:L:15:U:C5	2.45	0.84
2:L:14:C:C2	2:L:15:U:C5	2.66	0.83
2:L:26:G:N2	2:L:42:U:C2	2.53	0.76
1:I:46:ASN:ND2	1:I:52:ASP:OD1	2.24	0.69

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	127/129 (98%)	108 (85%)	19 (15%)	0	100	100
1	C	127/129 (98%)	114 (90%)	12 (9%)	1 (1%)	27	56
1	E	127/129 (98%)	112 (88%)	14 (11%)	1 (1%)	27	56
1	G	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	27	56
1	I	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
1	K	127/129 (98%)	114 (90%)	13 (10%)	0	100	100
All	All	762/774 (98%)	679 (89%)	80 (10%)	3 (0%)	43	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	109	VAL
1	C	107	ALA
1	E	109	VAL

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	105/105 (100%)	99 (94%)	6 (6%)	29	56
1	C	105/105 (100%)	96 (91%)	9 (9%)	15	31
1	E	105/105 (100%)	98 (93%)	7 (7%)	23	47
1	G	105/105 (100%)	95 (90%)	10 (10%)	12	26
1	I	105/105 (100%)	97 (92%)	8 (8%)	19	40
1	K	105/105 (100%)	95 (90%)	10 (10%)	12	26
All	All	630/630 (100%)	580 (92%)	50 (8%)	18	37

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	37	ASN
1	G	61	ARG
1	K	99	VAL
1	G	41	GLN
1	G	50	SER

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	40/45 (88%)	14 (35%)	1 (2%)
2	D	41/45 (91%)	17 (41%)	2 (4%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	F	40/45 (88%)	10 (25%)	1 (2%)
2	H	42/45 (93%)	13 (30%)	5 (11%)
2	J	40/45 (88%)	12 (30%)	4 (10%)
2	L	43/45 (95%)	18 (41%)	5 (11%)
All	All	246/270 (91%)	84 (34%)	18 (7%)

5 of 84 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	11	C
2	B	15	U
2	B	17	A
2	B	24	C
2	B	26	G

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	H	40	A
2	J	22	U
2	L	36	G
2	H	30	U
2	H	37	U

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	129/129 (100%)	1.23	30 (23%) 1 1	57, 90, 131, 171	0
1	C	129/129 (100%)	1.58	32 (24%) 1 1	60, 97, 140, 160	1 (0%)
1	E	129/129 (100%)	1.56	37 (28%) 1 1	57, 103, 154, 169	0
1	G	129/129 (100%)	1.56	41 (31%) 1 1	71, 101, 146, 162	1 (0%)
1	I	129/129 (100%)	1.17	16 (12%) 5 4	44, 72, 108, 136	0
1	K	129/129 (100%)	1.20	17 (13%) 4 4	44, 71, 115, 132	1 (0%)
2	B	41/45 (91%)	1.16	5 (12%) 5 4	106, 151, 230, 278	0
2	D	42/45 (93%)	0.77	3 (7%) 16 16	134, 180, 212, 234	0
2	F	41/45 (91%)	0.72	4 (9%) 8 8	110, 154, 202, 231	0
2	H	42/45 (93%)	0.61	5 (11%) 5 5	105, 135, 186, 229	0
2	J	41/45 (91%)	0.77	3 (7%) 15 15	83, 129, 204, 207	0
2	L	43/45 (95%)	0.81	3 (6%) 16 17	106, 140, 194, 221	0
All	All	1024/1044 (98%)	1.24	196 (19%) 2 2	44, 100, 186, 278	3 (0%)

The worst 5 of 196 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	23	TYR	11.6
1	C	99	VAL	10.3
1	C	107	ALA	7.4
1	E	124	ILE	6.8
1	C	117	GLY	6.8

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 carbohydrates 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.