



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 06:57 PM UTC

PDB ID : 3SYV / pdb_00003syv
Title : Crystal structure of mPACSIN 3 F-BAR domain mutant
Authors : Bai, X.
Deposited on : 2011-07-18
Resolution : 3.10 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
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

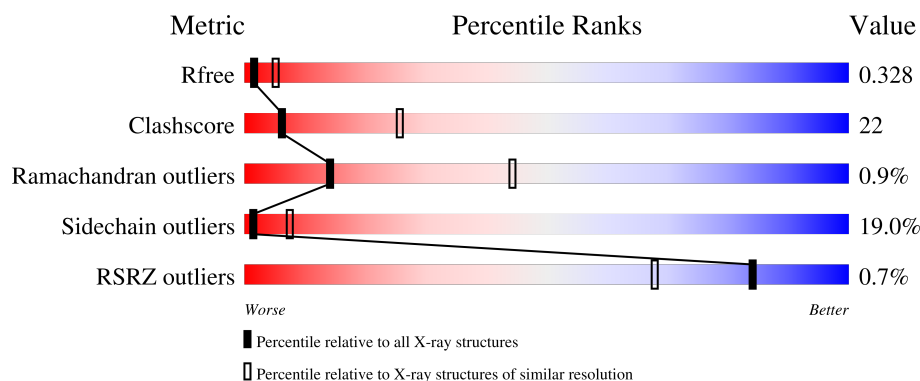
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.



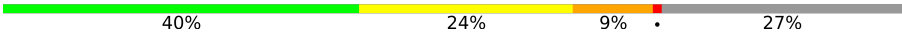
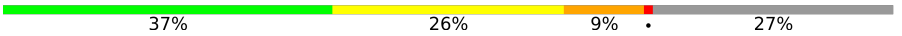
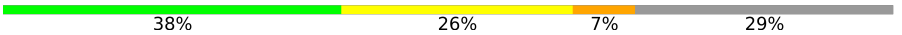
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	347	2% 37% 29% 6% 28%
1	B	347	% 41% 27% 7% 26%
1	C	347	38% 29% 6% 26%
1	D	347	35% 31% 7% 27%
1	E	347	% 33% 32% 8% 27%

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Mol	Chain	Length	Quality of chain
1	F	347	 40% 24% 9% • 27%
1	G	347	 37% 26% 9% • 27%
1	H	347	 38% 26% 7% 29%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16470 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 Protein kinase C and casein kinase II substrate protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			2047	1284	384	372	7			
1	B	257	Total	C	N	O	S	0	0	0
			2115	1317	403	387	8			
1	C	257	Total	C	N	O	S	0	0	0
			2061	1284	390	379	8			
1	D	255	Total	C	N	O	S	0	0	0
			2085	1304	396	378	7			
1	E	255	Total	C	N	O	S	0	0	1
			2044	1278	387	374	5			
1	F	255	Total	C	N	O	S	0	0	0
			2050	1283	392	369	6			
1	G	254	Total	C	N	O	S	0	0	0
			1978	1231	374	368	5			
1	H	247	Total	C	N	O	S	0	0	0
			1981	1236	378	364	3			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q99JB8
A	-4	HIS	-	expression tag	UNP Q99JB8
A	-3	HIS	-	expression tag	UNP Q99JB8
A	-2	HIS	-	expression tag	UNP Q99JB8
A	-1	HIS	-	expression tag	UNP Q99JB8
A	0	HIS	-	expression tag	UNP Q99JB8
A	121	GLN	PRO	engineered mutation	UNP Q99JB8
B	-5	HIS	-	expression tag	UNP Q99JB8
B	-4	HIS	-	expression tag	UNP Q99JB8
B	-3	HIS	-	expression tag	UNP Q99JB8
B	-2	HIS	-	expression tag	UNP Q99JB8
B	-1	HIS	-	expression tag	UNP Q99JB8
B	0	HIS	-	expression tag	UNP Q99JB8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	121	GLN	PRO	engineered mutation	UNP Q99JB8
C	-5	HIS	-	expression tag	UNP Q99JB8
C	-4	HIS	-	expression tag	UNP Q99JB8
C	-3	HIS	-	expression tag	UNP Q99JB8
C	-2	HIS	-	expression tag	UNP Q99JB8
C	-1	HIS	-	expression tag	UNP Q99JB8
C	0	HIS	-	expression tag	UNP Q99JB8
C	121	GLN	PRO	engineered mutation	UNP Q99JB8
D	-5	HIS	-	expression tag	UNP Q99JB8
D	-4	HIS	-	expression tag	UNP Q99JB8
D	-3	HIS	-	expression tag	UNP Q99JB8
D	-2	HIS	-	expression tag	UNP Q99JB8
D	-1	HIS	-	expression tag	UNP Q99JB8
D	0	HIS	-	expression tag	UNP Q99JB8
D	121	GLN	PRO	engineered mutation	UNP Q99JB8
E	-5	HIS	-	expression tag	UNP Q99JB8
E	-4	HIS	-	expression tag	UNP Q99JB8
E	-3	HIS	-	expression tag	UNP Q99JB8
E	-2	HIS	-	expression tag	UNP Q99JB8
E	-1	HIS	-	expression tag	UNP Q99JB8
E	0	HIS	-	expression tag	UNP Q99JB8
E	121	GLN	PRO	engineered mutation	UNP Q99JB8
F	-5	HIS	-	expression tag	UNP Q99JB8
F	-4	HIS	-	expression tag	UNP Q99JB8
F	-3	HIS	-	expression tag	UNP Q99JB8
F	-2	HIS	-	expression tag	UNP Q99JB8
F	-1	HIS	-	expression tag	UNP Q99JB8
F	0	HIS	-	expression tag	UNP Q99JB8
F	121	GLN	PRO	engineered mutation	UNP Q99JB8
G	-5	HIS	-	expression tag	UNP Q99JB8
G	-4	HIS	-	expression tag	UNP Q99JB8
G	-3	HIS	-	expression tag	UNP Q99JB8
G	-2	HIS	-	expression tag	UNP Q99JB8
G	-1	HIS	-	expression tag	UNP Q99JB8
G	0	HIS	-	expression tag	UNP Q99JB8
G	121	GLN	PRO	engineered mutation	UNP Q99JB8
H	-5	HIS	-	expression tag	UNP Q99JB8
H	-4	HIS	-	expression tag	UNP Q99JB8
H	-3	HIS	-	expression tag	UNP Q99JB8
H	-2	HIS	-	expression tag	UNP Q99JB8
H	-1	HIS	-	expression tag	UNP Q99JB8
H	0	HIS	-	expression tag	UNP Q99JB8

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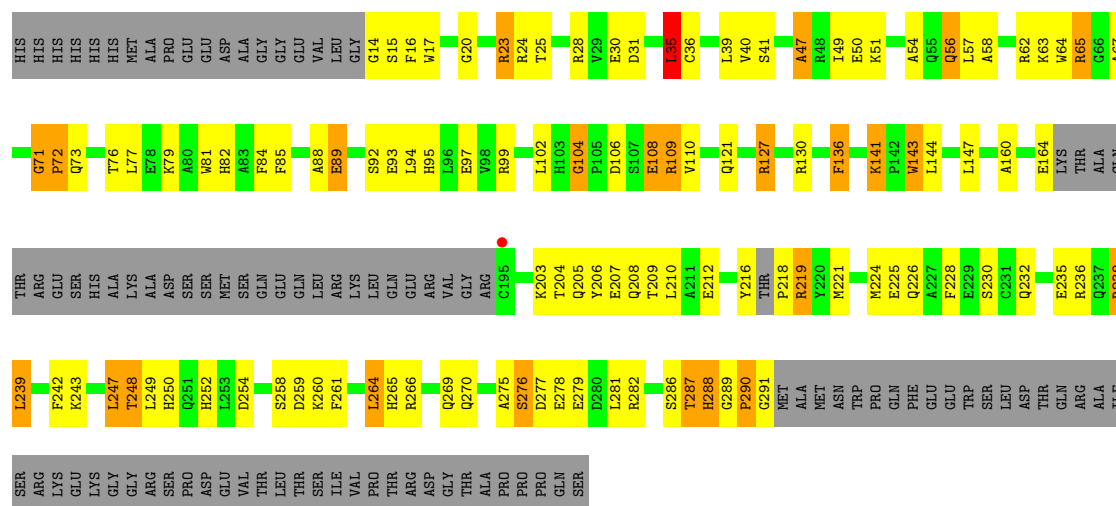
Chain	Residue	Modelled	Actual	Comment	Reference
H	121	GLN	PRO	engineered mutation	UNP Q99JB8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	14	Total O 14 14	0	0
2	B	13	Total O 13 13	0	0
2	C	19	Total O 19 19	0	0
2	D	12	Total O 12 12	0	0
2	E	12	Total O 12 12	0	0
2	F	16	Total O 16 16	0	0
2	G	10	Total O 10 10	0	0
2	H	13	Total O 13 13	0	0

- | | |
|------|-----|
| G71 | HIS |
| P72 | HIS |
| Q73 | HIS |
| T74 | HIS |
| G75 | HIS |
| T76 | HIS |
| L77 | MET |
| E78 | ALA |
| K79 | PRO |
| A80 | GLU |
| B81 | GLU |
| H82 | ASP |
| A83 | ALA |
| F84 | GLY |
| F85 | GLY |
| F86 | GLU |
| T87 | VAL |
| A88 | LEU |
| E89 | GLY |
| R90 | G14 |
| L94 | S15 |
| G95 | P16 |
| I96 | E18 |
| E97 | E19 |
| V98 | G20 |
| R99 | N21 |
| E100 | Y22 |
| K101 | R23 |
| G104 | R24 |
| P105 | T25 |
| D106 | R28 |
| S107 | V29 |
| E108 | E30 |
| R111 | H33 |
| R115 | R34 |
| Q121 | L35 |
| G125 | V40 |
| S129 | S41 |
| R130 | C42 |
| R139 | F43 |
| R140 | Q44 |
| K141 | A47 |
| V143 | E50 |
| K145 | O55 |
| R146 | R62 |
| L147 | K63 |
| K148 | W64 |
| E149 | R65 |
| V150 | V68 |
| V155 | E69 |
| | V70 |

Device Type	Percentage
Smartphone	38%
Tablet	26%
Smartwatch	7%
Other	29%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.57Å 108.90Å 222.32Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	48.90 – 3.10 48.90 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.90-3.10) 98.5 (48.90-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.281 , 0.337 0.274 , 0.328	Depositor DCC
R_{free} test set	5196 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	64.1	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	0.458 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16470	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1201e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	1.28	7/2094 (0.3%)	1.32	6/2811 (0.2%)
1	B	1.33	7/2160 (0.3%)	1.41	18/2895 (0.6%)
1	C	1.33	9/2104 (0.4%)	1.35	13/2821 (0.5%)
1	D	1.50	14/2133 (0.7%)	1.41	14/2862 (0.5%)
1	E	1.38	14/2092 (0.7%)	1.40	19/2813 (0.7%)
1	F	1.42	9/2097 (0.4%)	1.46	19/2821 (0.7%)
1	G	1.39	15/2021 (0.7%)	1.41	16/2724 (0.6%)
1	H	1.49	13/2025 (0.6%)	1.50	16/2725 (0.6%)
All	All	1.39	88/16726 (0.5%)	1.41	121/22472 (0.5%)

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	D	0	1

The worst 5 of 88 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	160	ALA	C-O	14.15	1.42	1.24
1	H	160	ALA	C-O	10.18	1.37	1.24
1	F	160	ALA	C-O	9.18	1.36	1.24
1	C	156	SER	C-O	9.13	1.35	1.24
1	H	290	PRO	N-CA	8.87	1.58	1.47

The worst 5 of 121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	289	GLY	CA-C-N	15.15	138.77	119.84
1	H	289	GLY	C-N-CA	15.15	138.77	119.84
1	B	289	GLY	CA-C-N	11.81	134.61	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	289	GLY	C-N-CA	11.81	134.61	119.84
1	G	118	PHE	N-CA-C	-11.52	96.94	112.03

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	160	ALA	Mainchain

5.2 Too-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 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	2047	0	1943	94	0
1	B	2115	0	2020	80	0
1	C	2061	0	1930	106	0
1	D	2085	0	1982	115	0
1	E	2044	0	1900	117	0
1	F	2050	0	1898	96	0
1	G	1978	0	1807	95	0
1	H	1981	0	1827	93	0
2	A	14	0	0	1	0
2	B	13	0	0	2	0
2	C	19	0	0	0	0
2	D	12	0	0	3	0
2	E	12	0	0	0	0
2	F	16	0	0	2	0
2	G	10	0	0	0	0
2	H	13	0	0	1	0
All	All	16470	0	15307	709	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 22.

The worst 5 of 709 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:D:196:THR:CB	1:D:196:THR:CG2	1.76	1.59
1:D:121:GLN:HE22	1:D:130:ARG:CD	1.42	1.33
1:D:121:GLN:NE2	1:D:130:ARG:HD3	1.46	1.30
1:E:76:THR:CG2	1:E:275:ALA:HA	1.69	1.23
1:A:76:THR:CG2	1:A:275:ALA:HA	1.74	1.18

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	243/347 (70%)	229 (94%)	10 (4%)	4 (2%)	7	30
1	B	253/347 (73%)	236 (93%)	14 (6%)	3 (1%)	10	37
1	C	251/347 (72%)	231 (92%)	20 (8%)	0	100	100
1	D	249/347 (72%)	230 (92%)	17 (7%)	2 (1%)	16	47
1	E	249/347 (72%)	232 (93%)	16 (6%)	1 (0%)	30	61
1	F	247/347 (71%)	224 (91%)	21 (8%)	2 (1%)	16	47
1	G	250/347 (72%)	222 (89%)	25 (10%)	3 (1%)	10	37
1	H	241/347 (70%)	224 (93%)	14 (6%)	3 (1%)	10	37
All	All	1983/2776 (71%)	1828 (92%)	137 (7%)	18 (1%)	14	44

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	213	LEU
1	F	297	PRO
1	B	290	PRO
1	D	71	GLY
1	H	71	GLY

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	201/294 (68%)	168 (84%)	33 (16%)	2	11
1	B	210/294 (71%)	177 (84%)	33 (16%)	2	12
1	C	197/294 (67%)	152 (77%)	45 (23%)	1	4
1	D	205/294 (70%)	172 (84%)	33 (16%)	2	11
1	E	196/294 (67%)	154 (79%)	42 (21%)	1	5
1	F	193/294 (66%)	155 (80%)	38 (20%)	1	6
1	G	182/294 (62%)	138 (76%)	44 (24%)	1	3
1	H	186/294 (63%)	155 (83%)	31 (17%)	2	10
All	All	1570/2352 (67%)	1271 (81%)	299 (19%)	1	7

5 of 299 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	49	ILE
1	H	225	GLU
1	G	90	ARG
1	G	260	LYS
1	C	219	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	226	GLN
1	G	269	GLN
1	F	250	HIS
1	G	82	HIS
1	H	119	HIS

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 oligosaccharides 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	250/347 (72%)	-0.61	6 (2%) 59 38	37, 61, 103, 129	0
1	B	257/347 (74%)	-0.74	2 (0%) 82 65	25, 55, 120, 137	0
1	C	257/347 (74%)	-0.71	0 100 100	42, 59, 97, 112	0
1	D	255/347 (73%)	-0.72	1 (0%) 88 76	34, 54, 120, 135	0
1	E	255/347 (73%)	-0.55	3 (1%) 76 58	39, 59, 108, 127	0
1	F	255/347 (73%)	-0.76	0 100 100	32, 55, 101, 114	0
1	G	254/347 (73%)	-0.71	1 (0%) 88 76	41, 59, 83, 98	0
1	H	247/347 (71%)	-0.78	1 (0%) 88 76	35, 53, 89, 102	0
All	All	2030/2776 (73%)	-0.70	14 (0%) 84 68	25, 57, 103, 137	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	158	HIS	5.3
1	A	296	TRP	5.1
1	E	162	LYS	3.4
1	A	298	GLN	3.2
1	E	293	ALA	3.2

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.