



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:59 AM UTC

PDB ID : 4QFK / pdb_00004qfk
Title : Crystal structure of dipeptide binding protein from pseudoalteromonas sp. SM9913
Authors : Li, C.Y.; Zhang, Y.Z.
Deposited on : 2014-05-21
Resolution : 2.29 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

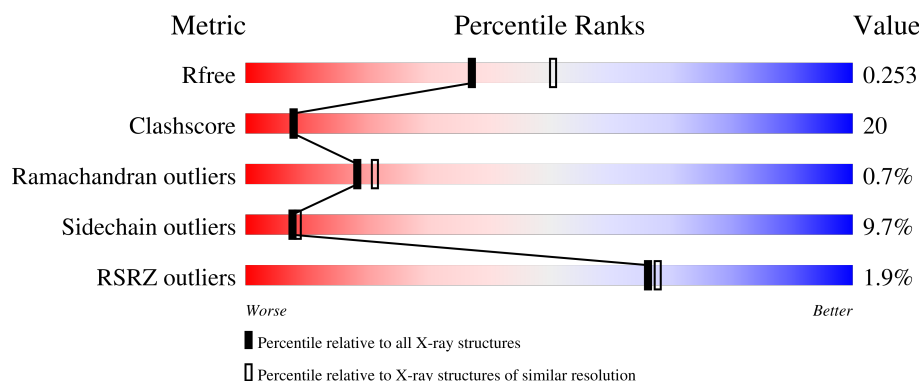
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	541	0.2% 59% 30% • 7%
1	B	541	0.2% 59% 29% 5% • 7%
1	C	541	2% 58% 29% 6% 7%
1	D	541	0.2% 63% 25% 6% 7%
1	E	541	3% 57% 31% 5% 7%

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Mol	Chain	Length	Quality of chain
1	F	541	 2% 60% 27% 6% 7%
1	G	541	 2% 60% 27% 5% 7%
1	H	541	 1% 62% 26% 6% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34170 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 ABC transporter periplasmic peptide-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	505	Total	C	N	O	S	0	0	0
			4061	2605	685	757	14			
1	A	505	Total	C	N	O	S	0	0	0
			4061	2605	685	757	14			
1	B	505	Total	C	N	O	S	0	0	0
			4061	2605	685	757	14			
1	C	505	Total	C	N	O	S	0	0	0
			4061	2605	685	757	14			
1	D	505	Total	C	N	O	S	0	0	0
			4061	2605	685	757	14			
1	E	505	Total	C	N	O	S	0	0	0
			4061	2605	685	757	14			
1	F	505	Total	C	N	O	S	0	0	0
			4061	2605	685	757	14			
1	G	505	Total	C	N	O	S	0	0	0
			4061	2605	685	757	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	536	HIS	-	expression tag	UNP A7Y7W1
H	537	HIS	-	expression tag	UNP A7Y7W1
H	538	HIS	-	expression tag	UNP A7Y7W1
H	539	HIS	-	expression tag	UNP A7Y7W1
H	540	HIS	-	expression tag	UNP A7Y7W1
H	541	HIS	-	expression tag	UNP A7Y7W1
A	536	HIS	-	expression tag	UNP A7Y7W1
A	537	HIS	-	expression tag	UNP A7Y7W1
A	538	HIS	-	expression tag	UNP A7Y7W1
A	539	HIS	-	expression tag	UNP A7Y7W1
A	540	HIS	-	expression tag	UNP A7Y7W1
A	541	HIS	-	expression tag	UNP A7Y7W1
B	536	HIS	-	expression tag	UNP A7Y7W1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	537	HIS	-	expression tag	UNP A7Y7W1
B	538	HIS	-	expression tag	UNP A7Y7W1
B	539	HIS	-	expression tag	UNP A7Y7W1
B	540	HIS	-	expression tag	UNP A7Y7W1
B	541	HIS	-	expression tag	UNP A7Y7W1
C	536	HIS	-	expression tag	UNP A7Y7W1
C	537	HIS	-	expression tag	UNP A7Y7W1
C	538	HIS	-	expression tag	UNP A7Y7W1
C	539	HIS	-	expression tag	UNP A7Y7W1
C	540	HIS	-	expression tag	UNP A7Y7W1
C	541	HIS	-	expression tag	UNP A7Y7W1
D	536	HIS	-	expression tag	UNP A7Y7W1
D	537	HIS	-	expression tag	UNP A7Y7W1
D	538	HIS	-	expression tag	UNP A7Y7W1
D	539	HIS	-	expression tag	UNP A7Y7W1
D	540	HIS	-	expression tag	UNP A7Y7W1
D	541	HIS	-	expression tag	UNP A7Y7W1
E	536	HIS	-	expression tag	UNP A7Y7W1
E	537	HIS	-	expression tag	UNP A7Y7W1
E	538	HIS	-	expression tag	UNP A7Y7W1
E	539	HIS	-	expression tag	UNP A7Y7W1
E	540	HIS	-	expression tag	UNP A7Y7W1
E	541	HIS	-	expression tag	UNP A7Y7W1
F	536	HIS	-	expression tag	UNP A7Y7W1
F	537	HIS	-	expression tag	UNP A7Y7W1
F	538	HIS	-	expression tag	UNP A7Y7W1
F	539	HIS	-	expression tag	UNP A7Y7W1
F	540	HIS	-	expression tag	UNP A7Y7W1
F	541	HIS	-	expression tag	UNP A7Y7W1
G	536	HIS	-	expression tag	UNP A7Y7W1
G	537	HIS	-	expression tag	UNP A7Y7W1
G	538	HIS	-	expression tag	UNP A7Y7W1
G	539	HIS	-	expression tag	UNP A7Y7W1
G	540	HIS	-	expression tag	UNP A7Y7W1
G	541	HIS	-	expression tag	UNP A7Y7W1

- Molecule 2 is water.

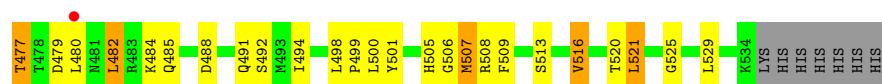
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	274	Total O 274 274	0	0
2	A	219	Total O 219 219	0	0

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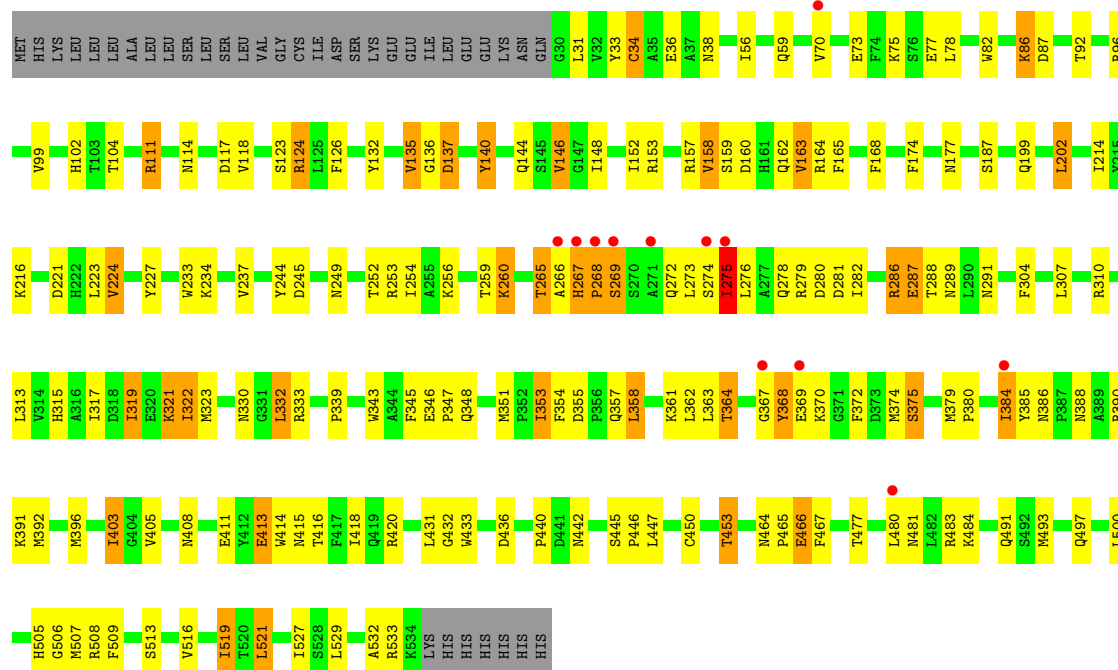
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	225	Total 225	O 225	0	0
2	C	227	Total 227	O 227	0	0
2	D	211	Total 211	O 211	0	0
2	E	159	Total 159	O 159	0	0
2	F	186	Total 186	O 186	0	0
2	G	181	Total 181	O 181	0	0

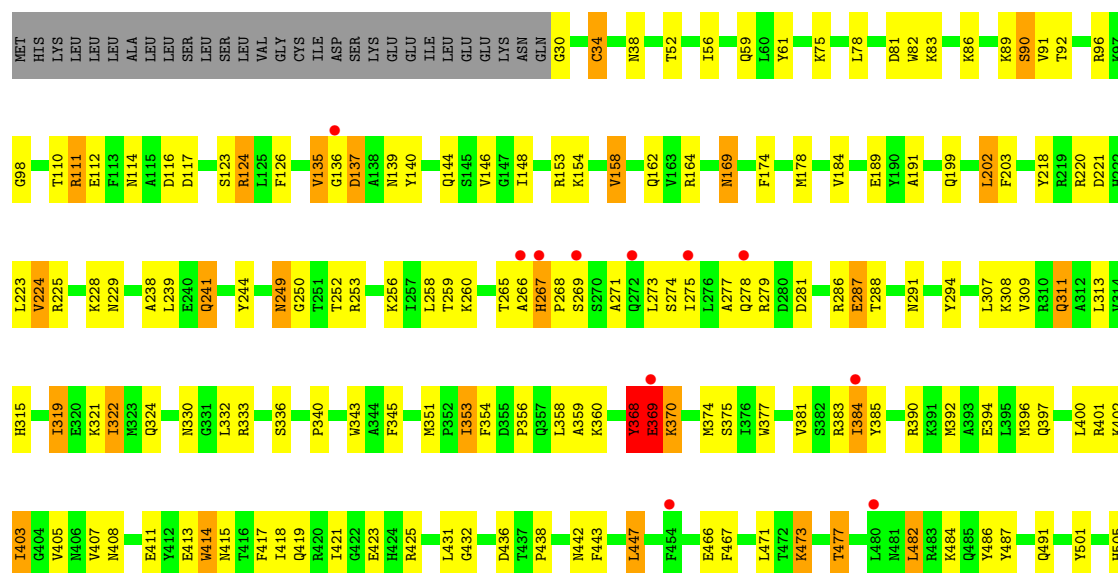




- Molecule 1: ABC transporter periplasmic peptide-binding protein



- Molecule 1: ABC transporter periplasmic peptide-binding protein



G506	M507	R508	F509	Q510		V516	E517	G518	I519	T520	L521		F524	G525		L529		A532	R533	K534	LYS	HIS	HIS	HIS	HIS	HIS	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	93.39Å 93.97Å 140.55Å 80.03° 84.43° 69.84°	Depositor
Resolution (Å)	42.63 – 2.29 42.63 – 2.29	Depositor EDS
% Data completeness (in resolution range)	88.7 (42.63-2.29) 93.0 (42.63-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.191 , 0.257 0.191 , 0.253	Depositor DCC
R_{free} test set	9376 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	34170	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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

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	0.56	2/4166 (0.0%)	0.92	9/5667 (0.2%)
1	B	0.55	2/4166 (0.0%)	0.92	14/5667 (0.2%)
1	C	0.56	2/4166 (0.0%)	0.91	11/5667 (0.2%)
1	D	0.51	0/4166	0.90	9/5667 (0.2%)
1	E	0.51	2/4166 (0.0%)	0.88	10/5667 (0.2%)
1	F	0.49	0/4166	0.89	8/5667 (0.1%)
1	G	0.49	0/4166	0.89	3/5667 (0.1%)
1	H	0.55	0/4166	0.92	8/5667 (0.1%)
All	All	0.53	8/33328 (0.0%)	0.90	72/45336 (0.2%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	386	ASN	C-N	6.92	1.40	1.34
1	A	386	ASN	C-N	6.86	1.40	1.34
1	C	386	ASN	C-N	6.47	1.41	1.34
1	A	387	PRO	N-CD	5.42	1.55	1.47
1	C	387	PRO	N-CD	5.42	1.55	1.47

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	338	LEU	CA-C-N	8.85	126.03	119.66
1	H	338	LEU	C-N-CA	8.85	126.03	119.66
1	E	78	LEU	N-CA-C	-8.17	103.45	113.50
1	B	379	MET	CA-C-N	7.93	127.85	119.05
1	B	379	MET	C-N-CA	7.93	127.85	119.05

There are no chirality outliers.

There are no planarity outliers.

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	4061	0	3968	169	0
1	B	4061	0	3968	158	0
1	C	4061	0	3968	180	0
1	D	4061	0	3968	149	0
1	E	4061	0	3968	157	0
1	F	4061	0	3968	175	0
1	G	4061	0	3968	143	0
1	H	4061	0	3968	147	0
2	A	219	0	0	11	0
2	B	225	0	0	10	0
2	C	227	0	0	3	0
2	D	211	0	0	5	0
2	E	159	0	0	4	0
2	F	186	0	0	7	0
2	G	181	0	0	3	0
2	H	274	0	0	8	0
All	All	34170	0	31744	1263	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 20.

The worst 5 of 1263 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:275:ILE:HD11	1:C:274:SER:HB2	1.30	1.12
1:D:279:ARG:HB2	1:D:280:ASP:CA	1.76	1.12
1:C:84:ILE:HD11	1:C:88:GLY:HA2	1.27	1.10
1:H:384:ILE:HD13	1:H:384:ILE:H	1.12	1.08
1:E:368:TYR:HA	1:E:369:GLU:HB2	1.20	1.07

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	503/541 (93%)	474 (94%)	25 (5%)	4 (1%)	16	18
1	B	503/541 (93%)	478 (95%)	21 (4%)	4 (1%)	16	18
1	C	503/541 (93%)	470 (93%)	29 (6%)	4 (1%)	16	18
1	D	503/541 (93%)	470 (93%)	30 (6%)	3 (1%)	21	25
1	E	503/541 (93%)	471 (94%)	29 (6%)	3 (1%)	21	25
1	F	503/541 (93%)	473 (94%)	28 (6%)	2 (0%)	30	36
1	G	503/541 (93%)	474 (94%)	24 (5%)	5 (1%)	12	13
1	H	503/541 (93%)	481 (96%)	18 (4%)	4 (1%)	16	18
All	All	4024/4328 (93%)	3791 (94%)	204 (5%)	29 (1%)	18	21

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	266	ALA
1	H	268	PRO
1	A	276	LEU
1	B	267	HIS
1	B	268	PRO

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	438/472 (93%)	397 (91%)	41 (9%)	8	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	438/472 (93%)	397 (91%)	41 (9%)	8	9
1	C	438/472 (93%)	398 (91%)	40 (9%)	9	10
1	D	438/472 (93%)	400 (91%)	38 (9%)	9	11
1	E	438/472 (93%)	393 (90%)	45 (10%)	7	7
1	F	438/472 (93%)	395 (90%)	43 (10%)	7	8
1	G	438/472 (93%)	391 (89%)	47 (11%)	6	7
1	H	438/472 (93%)	394 (90%)	44 (10%)	7	8
All	All	3504/3776 (93%)	3165 (90%)	339 (10%)	8	8

5 of 339 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	358	LEU
1	F	453	THR
1	E	408	ASN
1	F	158	VAL
1	G	135	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 146 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	205	GLN
1	G	348	GLN
1	F	291	ASN
1	F	505	HIS
1	B	442	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 [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	505/541 (93%)	-0.13	7 (1%) 73 75	13, 25, 45, 63	0
1	B	505/541 (93%)	-0.16	8 (1%) 70 72	14, 24, 46, 71	0
1	C	505/541 (93%)	-0.13	10 (1%) 65 66	14, 25, 45, 66	0
1	D	505/541 (93%)	-0.04	8 (1%) 70 72	15, 27, 51, 72	0
1	E	505/541 (93%)	0.14	14 (2%) 55 56	17, 31, 59, 78	0
1	F	505/541 (93%)	0.05	12 (2%) 59 61	18, 30, 53, 72	0
1	G	505/541 (93%)	0.05	11 (2%) 62 64	17, 30, 56, 82	0
1	H	505/541 (93%)	-0.24	8 (1%) 70 72	13, 22, 41, 55	0
All	All	4040/4328 (93%)	-0.06	78 (1%) 66 68	13, 27, 51, 82	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	266	ALA	5.8
1	C	267	HIS	4.6
1	D	267	HIS	4.5
1	G	275	ILE	4.4
1	G	454	PHE	4.2

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.