



wwPDB X-ray Structure Validation Summary Report ⓘ

May 7, 2026 – 09:30 AM EDT

PDB ID : 5ITU / pdb_00005itu
Title : Crystal Structure of Human NEIL1(242K) bound to duplex DNA containing THF
Authors : Zhu, C.; Lu, L.; Zhang, J.; Yue, Z.; Song, J.; Zong, S.; Liu, M.; Stovicek, O.; Gao, Y.; Yi, C.
Deposited on : 2016-03-17
Resolution : 2.41 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

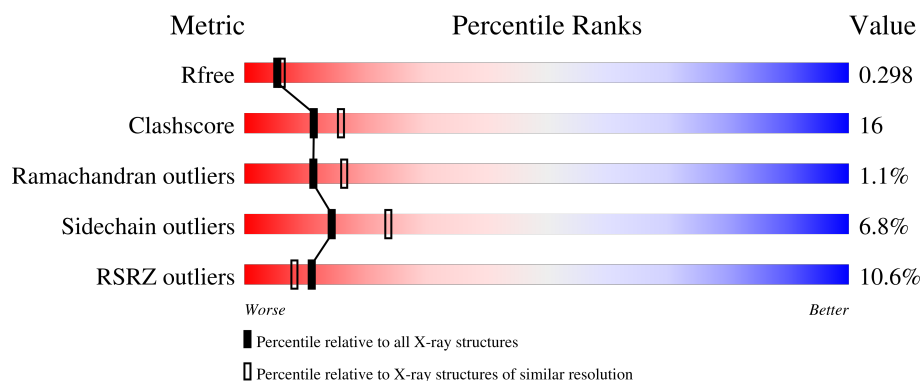
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	400	 2% 50% 12% 33%
1	B	400	 2% 48% 13% 36%
1	C	400	 18% 46% 20% 32%
2	D	13	 8% 46% 38% 15%
2	F	13	 31% 62% 8%

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Mol	Chain	Length	Quality of chain
2	H	13	
3	E	13	
3	G	13	
3	I	13	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8023 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 Endonuclease 8-like 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	1	0
			2120	1355	382	372	11			
1	B	255	Total	C	N	O	S	0	0	0
			2033	1302	371	350	10			
1	C	271	Total	C	N	O	S	0	0	0
			2143	1373	382	378	10			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	391	ALA	-	expression tag	UNP Q96FI4
A	392	ALA	-	expression tag	UNP Q96FI4
A	393	LEU	-	expression tag	UNP Q96FI4
A	394	GLY	-	expression tag	UNP Q96FI4
A	395	HIS	-	expression tag	UNP Q96FI4
A	396	HIS	-	expression tag	UNP Q96FI4
A	397	HIS	-	expression tag	UNP Q96FI4
A	398	HIS	-	expression tag	UNP Q96FI4
A	399	HIS	-	expression tag	UNP Q96FI4
A	400	HIS	-	expression tag	UNP Q96FI4
B	391	ALA	-	expression tag	UNP Q96FI4
B	392	ALA	-	expression tag	UNP Q96FI4
B	393	LEU	-	expression tag	UNP Q96FI4
B	394	GLY	-	expression tag	UNP Q96FI4
B	395	HIS	-	expression tag	UNP Q96FI4
B	396	HIS	-	expression tag	UNP Q96FI4
B	397	HIS	-	expression tag	UNP Q96FI4
B	398	HIS	-	expression tag	UNP Q96FI4
B	399	HIS	-	expression tag	UNP Q96FI4
B	400	HIS	-	expression tag	UNP Q96FI4
C	391	ALA	-	expression tag	UNP Q96FI4
C	392	ALA	-	expression tag	UNP Q96FI4
C	393	LEU	-	expression tag	UNP Q96FI4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	394	GLY	-	expression tag	UNP Q96FI4
C	395	HIS	-	expression tag	UNP Q96FI4
C	396	HIS	-	expression tag	UNP Q96FI4
C	397	HIS	-	expression tag	UNP Q96FI4
C	398	HIS	-	expression tag	UNP Q96FI4
C	399	HIS	-	expression tag	UNP Q96FI4
C	400	HIS	-	expression tag	UNP Q96FI4

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*GP*TP*CP*CP*AP*CP*GP*TP*CP*TP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	13	Total	C	N	O	P	0	0	0
			249	120	41	76	12			
2	F	13	Total	C	N	O	P	0	0	0
			249	120	41	76	12			
2	H	13	Total	C	N	O	P	0	0	0
			249	120	41	76	12			

- Molecule 3 is a DNA chain called DNA (5'-D(*TP*AP*GP*AP*CP*CP*TP*GP*GP*AP*CP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	13	Total	C	N	O	P	0	0	0
			267	127	53	75	12			
3	G	13	Total	C	N	O	P	0	0	0
			267	127	53	75	12			
3	I	13	Total	C	N	O	P	0	0	0
			267	127	53	75	12			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	97	Total	O	0	0
			97	97		
4	B	58	Total	O	0	0
			58	58		
4	D	6	Total	O	0	0
			6	6		
4	E	8	Total	O	0	0
			8	8		

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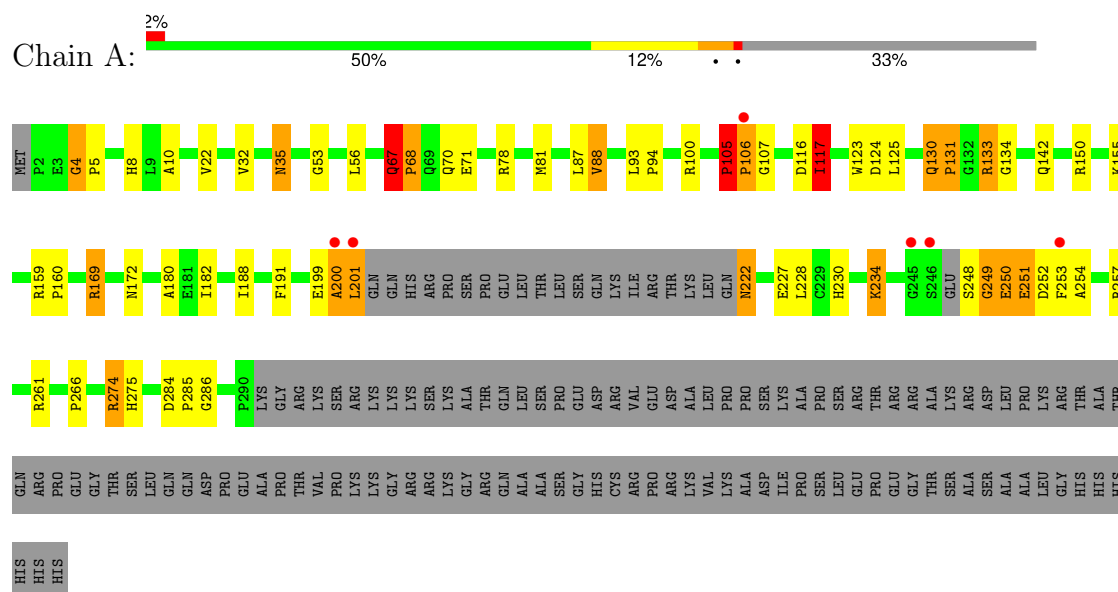
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	6	Total	O	0	0
			6	6		
4	G	4	Total	O	0	0
			4	4		

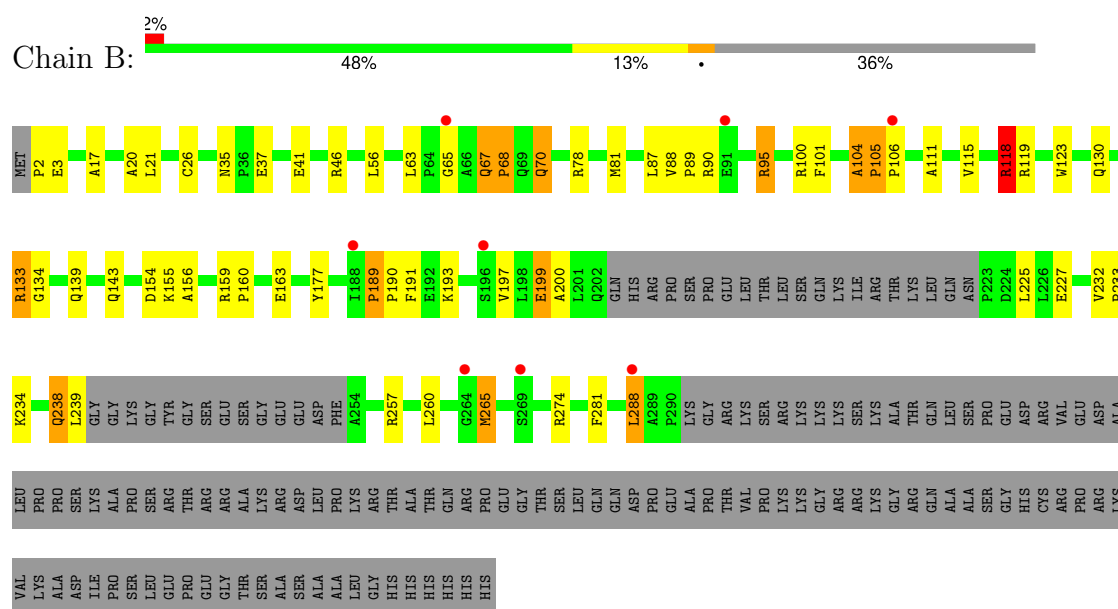
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Endonuclease 8-like 1



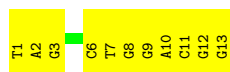
• Molecule 1: Endonuclease 8-like 1



• Molecule 1: Endonuclease 8-like 1

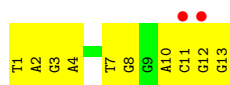
- Molecule 3: DNA (5'-D(*TP*AP*GP*AP*CP*CP*TP*GP*GP*AP*CP*GP*G)-3')

Chain G:  15% 85%



- Molecule 3: DNA (5'-D(*TP*AP*GP*AP*CP*CP*TP*GP*GP*AP*CP*GP*G)-3')

Chain I:  15% 23% 77%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.70Å 109.29Å 171.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.23 – 2.41 92.22 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.8 (92.23-2.41) 98.8 (92.22-2.41)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.210 , 0.260 0.263 , 0.298	Depositor DCC
R_{free} test set	2721 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8023	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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	1.34	12/2181 (0.6%)	1.46	28/2949 (0.9%)
1	B	1.22	5/2089 (0.2%)	1.33	16/2826 (0.6%)
1	C	0.71	1/2192 (0.0%)	1.10	15/2952 (0.5%)
2	D	0.46	0/277	1.04	3/424 (0.7%)
2	F	0.52	0/277	1.00	2/424 (0.5%)
2	H	0.41	0/277	0.91	2/424 (0.5%)
3	E	0.41	0/300	0.95	2/462 (0.4%)
3	G	0.46	0/300	0.97	2/462 (0.4%)
3	I	0.33	0/300	0.74	0/462
All	All	1.02	18/8193 (0.2%)	1.23	70/11385 (0.6%)

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	A	0	3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	115	VAL	CA-C	-7.55	1.43	1.52
1	A	10	ALA	CA-C	7.54	1.62	1.52
1	A	10	ALA	C-O	7.05	1.32	1.24
1	A	134	GLY	N-CA	6.60	1.51	1.43
1	A	228	LEU	C-O	-6.20	1.16	1.24

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	PRO	N-CA-C	11.64	124.91	110.70
1	C	128	LYS	N-CA-CB	-11.53	90.90	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	LYS	N-CA-C	10.77	141.15	111.00
1	A	133	ARG	NE-CZ-NH2	-8.91	111.18	119.20
1	B	104	ALA	CA-C-N	8.30	128.93	120.38

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	248	SER	Peptide
1	A	67	GLN	Mainchain,Peptide

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	2120	0	2091	49	1
1	B	2033	0	2026	41	1
1	C	2143	0	2109	81	0
2	D	249	0	143	7	0
2	F	249	0	143	14	0
2	H	249	0	143	27	0
3	E	267	0	147	19	0
3	G	267	0	147	12	0
3	I	267	0	147	44	0
4	A	97	0	0	4	1
4	B	58	0	0	1	0
4	D	6	0	0	0	0
4	E	8	0	0	0	0
4	F	6	0	0	0	0
4	G	4	0	0	0	0
All	All	8023	0	7096	240	2

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 16.

The worst 5 of 240 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:C:118:ARG:NH2	2:H:6:DA:C2	1.83	1.45
1:C:118:ARG:NH2	2:H:6:DA:N1	1.74	1.35
1:C:117:ILE:CD1	3:I:8:DG:H5'	1.60	1.30
2:H:2:DG:H1	3:I:11:DC:N4	1.43	1.14
3:E:1:DT:H5''	3:I:13:DG:H2''	1.30	1.09

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:501:HOH:O	4:A:503:HOH:O[3_554]	1.99	0.21
1:A:284:ASP:OD2	1:B:95:ARG:NH2[3_454]	2.09	0.11

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	263/400 (66%)	249 (95%)	8 (3%)	6 (2%)	5	5
1	B	249/400 (62%)	232 (93%)	16 (6%)	1 (0%)	30	42
1	C	249/400 (62%)	217 (87%)	31 (12%)	1 (0%)	30	42
All	All	761/1200 (63%)	698 (92%)	55 (7%)	8 (1%)	11	16

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	PRO
1	A	105	PRO
1	A	200	ALA
1	A	250	GLU
1	A	251	GLU

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	222/335 (66%)	212 (96%)	10 (4%)	24	40
1	B	214/335 (64%)	201 (94%)	13 (6%)	17	28
1	C	225/335 (67%)	203 (90%)	22 (10%)	7	11
All	All	661/1005 (66%)	616 (93%)	45 (7%)	14	24

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	78	ARG
1	C	138	LEU
1	C	90	ARG
1	C	113	CYS
1	C	211	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	275	HIS
1	C	151	ASN
1	C	282	GLN
1	A	139	GLN
1	A	86	GLN

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 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	268/400 (67%)	-0.03	6 (2%) 62 59	2, 9, 34, 60	1 (0%)
1	B	255/400 (63%)	0.23	8 (3%) 51 48	4, 17, 41, 52	0
1	C	271/400 (67%)	1.59	74 (27%) 1 1	38, 62, 111, 169	0
2	D	13/13 (100%)	0.26	1 (7%) 19 16	11, 30, 65, 66	0
2	F	13/13 (100%)	0.09	0 100 100	17, 33, 46, 59	0
2	H	13/13 (100%)	0.75	1 (7%) 19 16	26, 39, 59, 62	0
3	E	13/13 (100%)	-0.05	0 100 100	16, 31, 48, 50	0
3	G	13/13 (100%)	0.44	0 100 100	12, 33, 44, 54	0
3	I	13/13 (100%)	0.81	2 (15%) 5 4	33, 48, 70, 70	0
All	All	872/1278 (68%)	0.59	92 (10%) 11 8	2, 25, 84, 169	1 (0%)

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	152	LEU	6.4
1	C	218	THR	5.9
1	C	30	SER	4.8
1	C	249	GLY	4.7
1	C	128	LYS	4.7

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 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.