



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 05:27 PM UTC

PDB ID : 6JIV / pdb_00006jiv
Title : SspE crystal structure
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Deposited on : 2019-02-23
Resolution : 3.31 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

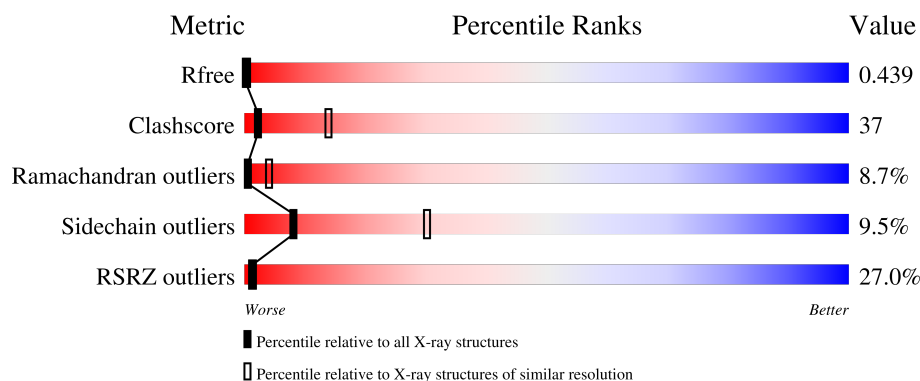
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

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	771	17% 44% 24% 5% 27%
1	B	771	25% 46% 23% . 27%
1	C	771	17% 39% 26% 7% 28%
1	D	771	18% 43% 24% 5% 27%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15028 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.

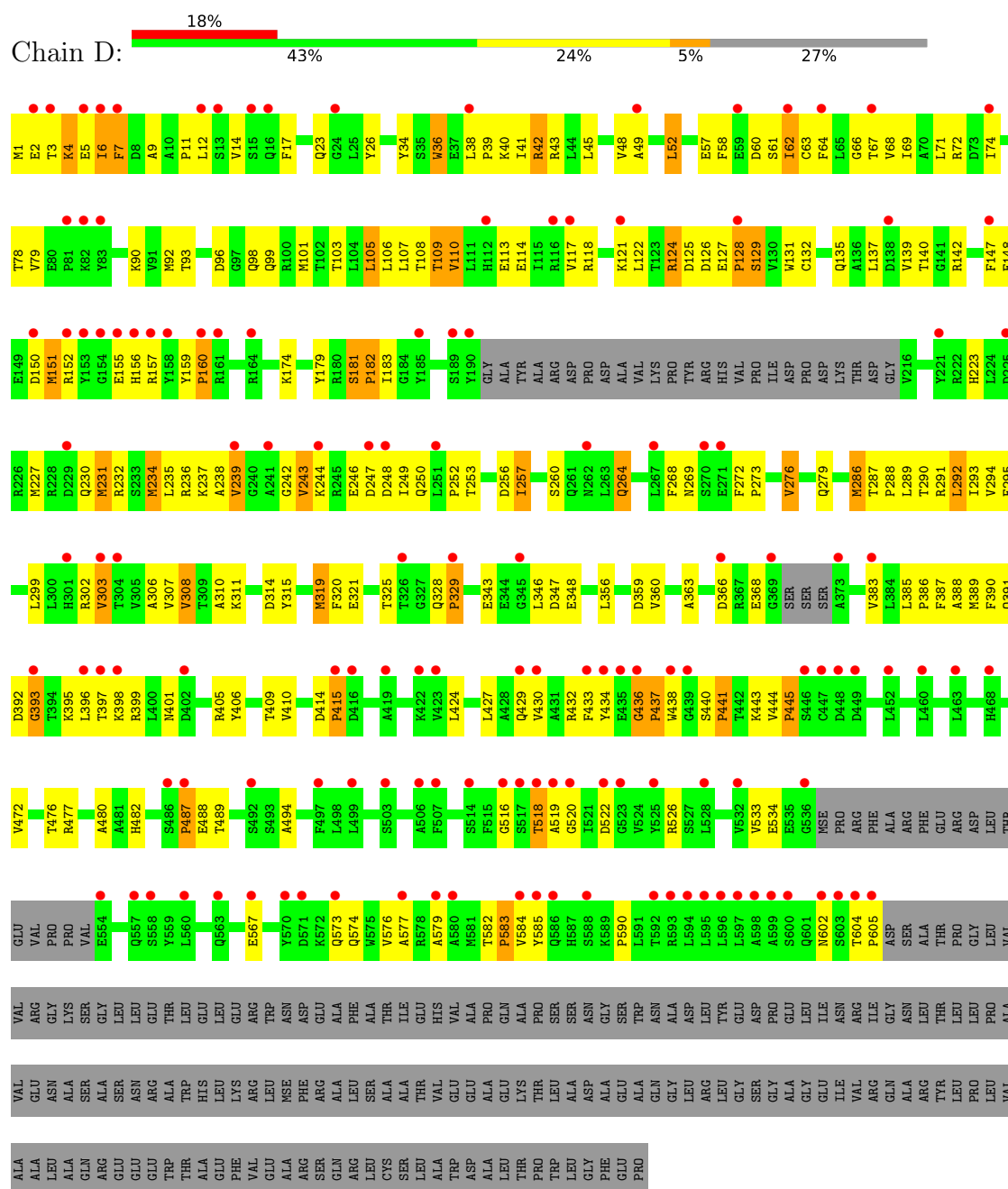
- Molecule 1 is a protein called SspE protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	D	560	Total	C	N	O	S	Se	0	0	0
			3711	2310	674	713	3	11			
1	A	560	Total	C	N	O	S	Se	0	0	0
			3711	2310	674	713	3	11			
1	B	560	Total	C	N	O	S	Se	0	0	0
			3711	2310	674	713	3	11			
1	C	557	Total	C	N	O	S	Se	0	0	0
			3895	2439	697	743	4	12			

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.

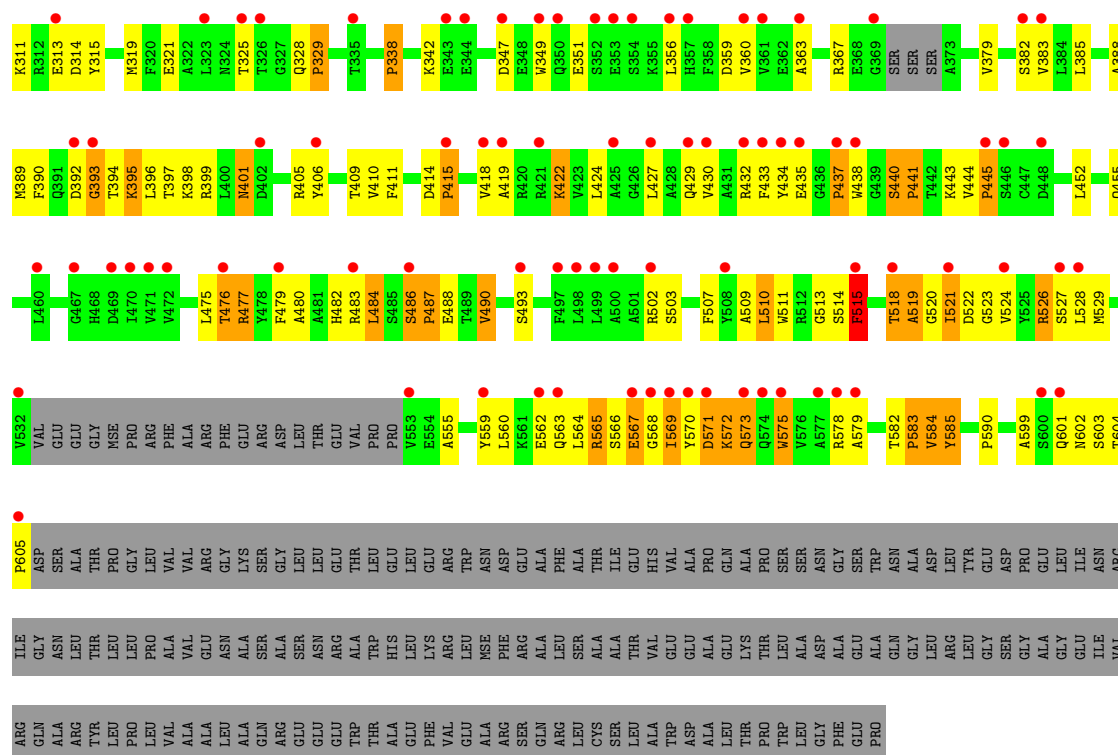
• Molecule 1: SspE protein



[illegible]

Chain B:

Component	Category	Percentage
M1	Green	1.0%
E2	Green	1.0%
T3	Green	1.0%
K4	Orange	1.0%
E5	Green	1.0%
I6	Orange	1.0%
F7	Green	1.0%
D8	Green	1.0%
A9	Green	1.0%
A10	Green	1.0%
P11	Green	1.0%
L12	Green	1.0%
S15	Green	1.0%
Q16	Green	1.0%
S19	Yellow	1.0%
Q23	Yellow	1.0%
Y26	Yellow	1.0%
I27	Yellow	1.0%
P28	Yellow	1.0%
Q31	Green	1.0%
R32	Green	1.0%
A33	Green	1.0%
Y34	Green	1.0%
S35	Green	1.0%
W36	Green	1.0%
E37	Green	1.0%
L38	Orange	1.0%
I41	Green	1.0%
R42	Green	1.0%
R43	Green	1.0%
L44	Green	1.0%
L45	Green	1.0%
S46	Green	1.0%
A49	Yellow	1.0%
L52	Orange	1.0%
L55	Green	1.0%
A56	Green	1.0%
E57	Green	1.0%
F58	Green	1.0%
E59	Green	1.0%
D60	Orange	1.0%
S61	Green	1.0%
I62	Green	1.0%
C63	Green	1.0%
F64	Green	1.0%
L65	Green	1.0%
G66	Green	1.0%
T67	Green	1.0%
V68	Green	1.0%
I69	Green	1.0%
L70	Green	1.0%
L71	Green	1.0%
R72	Green	1.0%
D73	Green	1.0%
I74	Green	1.0%
T78	Green	1.0%
V79	Green	1.0%
K82	Green	1.0%
S85	Green	1.0%
Q86	Green	1.0%
V87	Green	1.0%
P88	Green	1.0%
S89	Green	1.0%
K90	Green	1.0%
V91	Green	1.0%
I94	Green	1.0%
I95	Green	1.0%
D96	Green	1.0%
G97	Green	1.0%
Q98	Green	1.0%
Q99	Green	1.0%
R100	Green	1.0%
M101	Green	1.0%
T102	Green	1.0%
A103	Orange	1.0%
L104	Green	1.0%
S105	Green	1.0%
L106	Green	1.0%
L107	Green	1.0%
T108	Green	1.0%
T109	Green	1.0%
V110	Green	1.0%
E113	Green	1.0%
E114	Green	1.0%
I115	Green	1.0%
R116	Green	1.0%
V117	Green	1.0%
R118	Green	1.0%
R124	Green	1.0%
D125	Green	1.0%
L126	Green	1.0%
E127	Green	1.0%
P128	Orange	1.0%
S129	Green	1.0%
V130	Green	1.0%
W131	Green	1.0%
C132	Green	1.0%
Q135	Green	1.0%
A136	Green	1.0%
L137	Green	1.0%
T138	Green	1.0%
V139	Green	1.0%
T140	Orange	1.0%
L141	Green	1.0%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.07Å 138.16Å 293.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	125.33 – 3.31 125.33 – 3.31	Depositor EDS
% Data completeness (in resolution range)	99.5 (125.33-3.31) 99.5 (125.33-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.406 , 0.435 0.407 , 0.439	Depositor DCC
R_{free} test set	3357 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	122.6	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 114.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	15028	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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	0.62	1/3747 (0.0%)	0.98	14/5100 (0.3%)
1	B	0.52	0/3747	0.90	16/5100 (0.3%)
1	C	0.57	0/3943	0.95	15/5351 (0.3%)
1	D	0.72	0/3747	1.06	14/5100 (0.3%)
All	All	0.61	1/15184 (0.0%)	0.97	59/20651 (0.3%)

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	1
1	C	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	MSE	SE-CE	-6.20	1.76	1.95

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	160	PRO	N-CA-CB	10.75	114.54	103.25
1	A	160	PRO	N-CA-CB	9.27	112.98	103.25
1	A	329	PRO	N-CA-CB	8.99	112.69	103.25
1	B	329	PRO	N-CA-CB	8.66	112.35	103.25
1	C	329	PRO	N-CA-CB	8.54	112.22	103.25

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	GLU	Peptide
1	C	477	ARG	Peptide
1	C	584	VAL	Peptide

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	3711	0	3036	223	0
1	B	3711	0	3038	229	0
1	C	3895	0	3376	335	0
1	D	3711	0	3038	257	0
All	All	15028	0	12488	1009	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 37.

The worst 5 of 1009 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:515:PHE:CZ	1:C:578:ARG:HD3	1.32	1.63
1:D:356:LEU:CA	1:D:427:LEU:HD11	1.17	1.59
1:A:356:LEU:CA	1:A:427:LEU:HD11	1.16	1.59
1:D:356:LEU:HA	1:D:427:LEU:CD1	1.30	1.55
1:D:395:LYS:CE	1:D:526:ARG:HD3	1.37	1.55

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	552/771 (72%)	429 (78%)	73 (13%)	50 (9%)	0	3
1	B	552/771 (72%)	437 (79%)	70 (13%)	45 (8%)	0	5
1	C	549/771 (71%)	423 (77%)	80 (15%)	46 (8%)	0	4
1	D	552/771 (72%)	427 (77%)	75 (14%)	50 (9%)	0	3
All	All	2205/3084 (72%)	1716 (78%)	298 (14%)	191 (9%)	0	4

5 of 191 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	2	GLU
1	D	4	LYS
1	D	6	ILE
1	D	61	SER
1	D	129	SER

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	268/637 (42%)	244 (91%)	24 (9%)	9	32
1	B	268/637 (42%)	243 (91%)	25 (9%)	8	31
1	C	322/637 (50%)	291 (90%)	31 (10%)	8	29
1	D	268/637 (42%)	241 (90%)	27 (10%)	7	27
All	All	1126/2548 (44%)	1019 (90%)	107 (10%)	8	30

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	103	THR
1	B	401	ASN
1	C	515	PHE
1	B	110	VAL

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Mol	Chain	Res	Type
1	B	269	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	429	GLN
1	C	391	GLN
1	C	482	HIS
1	C	324	ASN
1	A	156	HIS

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 ⓘ

There are no oligosaccharides 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 [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	548/771 (71%)	1.29	129 (23%) 2 2	53, 109, 176, 219	0
1	B	548/771 (71%)	1.78	193 (35%) 1 1	62, 120, 274, 329	0
1	C	545/771 (70%)	1.38	130 (23%) 2 1	30, 104, 136, 171	0
1	D	548/771 (71%)	1.31	139 (25%) 1 1	37, 91, 169, 223	0
All	All	2189/3084 (70%)	1.44	591 (26%) 1 1	30, 106, 216, 329	0

The worst 5 of 591 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	514	SER	8.9
1	B	591	LEU	7.7
1	C	325	THR	7.1
1	D	3	THR	7.0
1	B	593	ARG	7.0

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.