



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 6JIV
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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

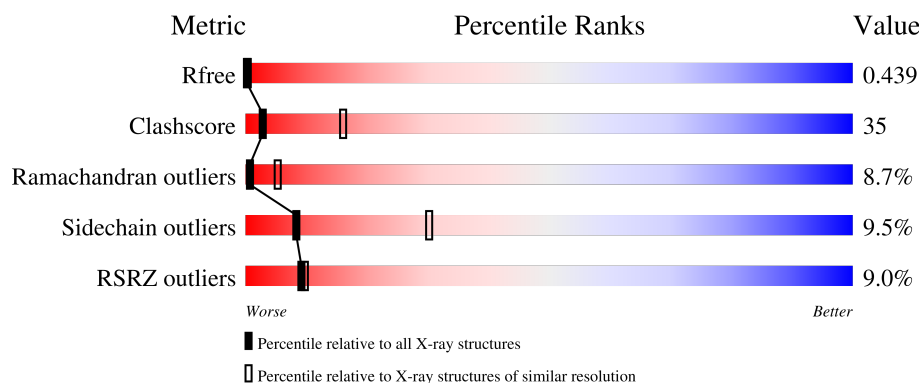
1 Overall quality at a glance

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}	130704	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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	<div> <div>5%</div> <div>44%</div> <div>23%</div> <div>5%</div> <div>27%</div> </div>
1	B	771	<div> <div>12%</div> <div>46%</div> <div>23%</div> <div>•</div> <div>27%</div> </div>
1	C	771	<div> <div>4%</div> <div>39%</div> <div>27%</div> <div>6%</div> <div>28%</div> </div>
1	D	771	<div> <div>5%</div> <div>43%</div> <div>25%</div> <div>5%</div> <div>27%</div> </div>

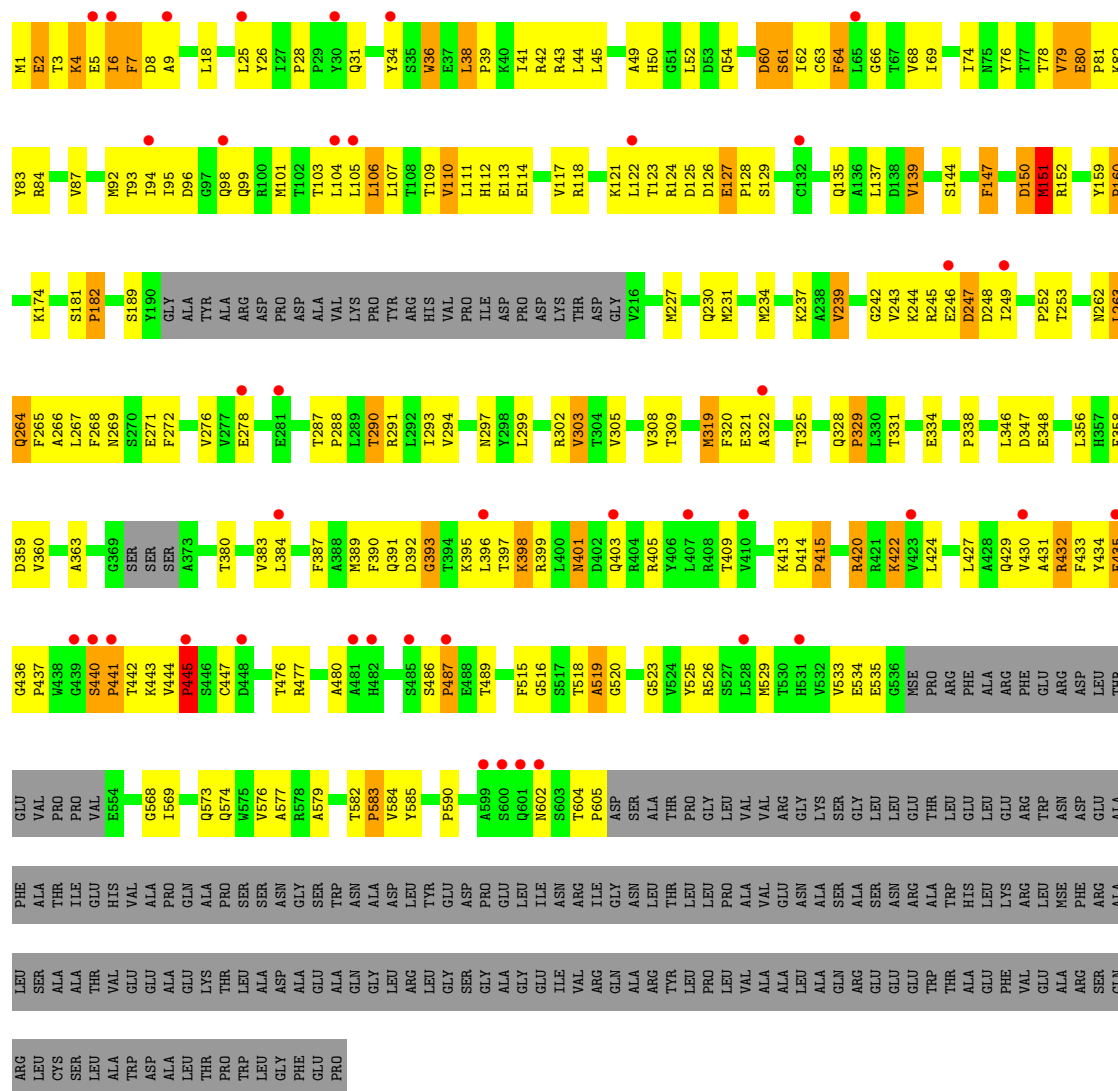
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15028 atoms, of which 0 are hydrogens and 0 are deuteriums.

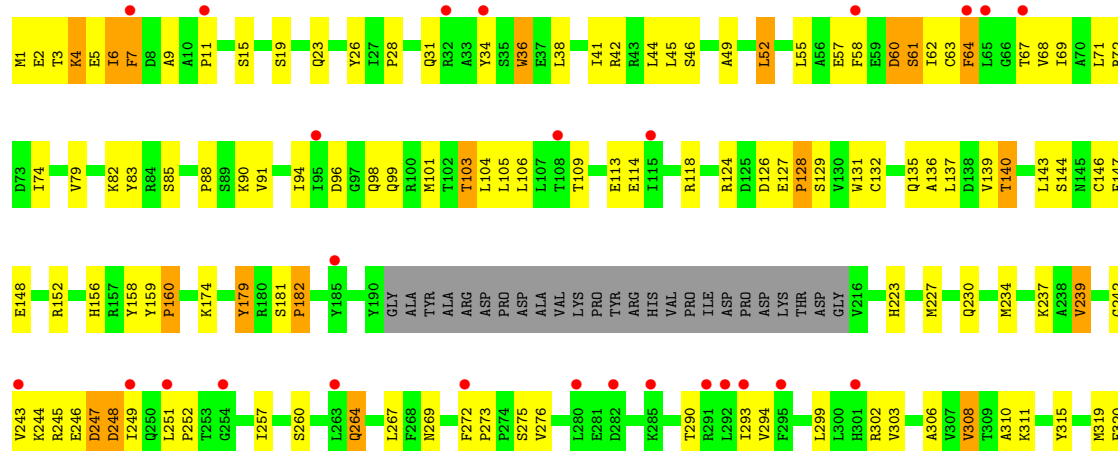
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

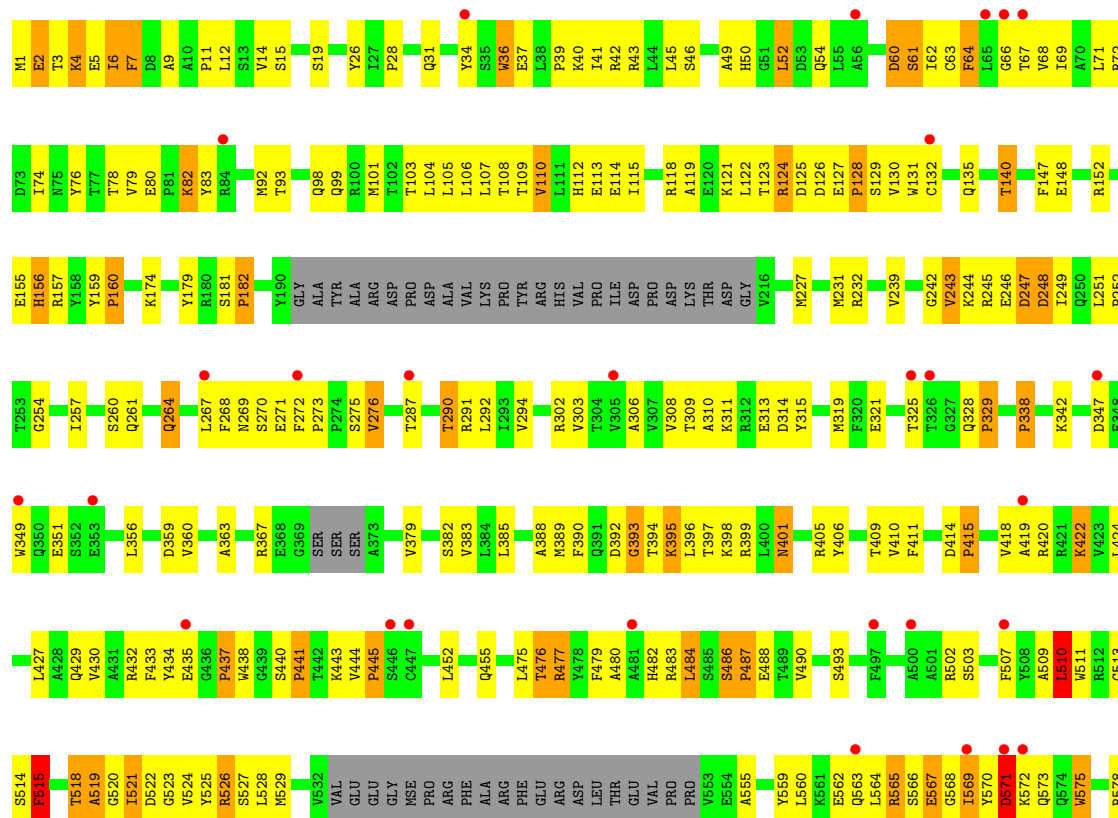
- Molecule 1 is a protein called SspE protein.

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			



• Molecule 1: SspE protein





GLU	ALA	SER	A579
ALA	TRP	TRP	
GLN	ASN	ASN	T582
GLY	ALA	ALA	P583
LEU	LEU	ASP	V584
ARG	LEU	LEU	Y585
LEU	LEU	TYR	
GLY	GLU	GLU	P590
SER	ASP	ASP	
GLY	PRO	PRO	A599
ALA	ALA	GLU	S600
GLY	GLY	LEU	Q601
GLU	ILE	ILE	N602
ILE	ASN	ASN	S603
VAL	ARG	ARG	T604
ARG	ILE	ILE	P605
GLN	GLY	GLY	ASP
ALA	ALA	SER	SER
ARG	LEU	ALA	ALA
TYR	THR	THR	THR
LEU	LEU	LEU	PRO
PRO	LEU	LEU	GLY
LEU	PRO	PRO	LEU
VAL	VAL	ALA	VAL
ALA	VAL	VAL	VAL
ALA	GLU	GLU	ARG
LEU	ASN	ASN	GLY
ALA	ALA	LYS	LYS
GLN	SER	SER	SER
ARG	ALA	ALA	GLY
GLU	GLU	ASN	LEU
GLU	ARG	ARG	LEU
TRP	ALA	ALA	GLU
THR	TRP	THR	THR
ALA	ALA	HIS	GLU
GLU	LEU	LEU	LEU
PHE	PHE	LYS	GLU
VAL	ARG	ARG	ARG
GLU	LEU	LEU	TRP
ALA	ALA	NSE	ASN
ALA	ALA	PHE	ASP
ARG	ARG	ARG	GLU
SER	SER	ALA	ALA
GLN	GLN	LEU	PHE
ARG	ARG	SER	ALA
LEU	LEU	ALA	THR
CYS	CYS	ALA	ILE
SER	SER	ALA	ILE
LEU	LEU	THR	GLU
ALA	ALA	VAL	HIS
TRP	TRP	GLU	VAL
ASP	ASP	GLU	ALA
ALA	ALA	ALA	ALA
LEU	LEU	GLN	PRO
THR	THR	LYS	ALA
PRO	PRO	THR	PRO
TRP	TRP	LEU	SER
LEU	LEU	ALA	SER
GLY	GLY	ASP	ASN
PHE	PHE	ALA	GLY

GLU

PRO

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 – 3.31 125.02 – 3.31	Depositor EDS
% Data completeness (in resolution range)	99.5 (125.33-3.31) 99.5 (125.02-3.31)	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 (4.96%)	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)	0.29 , 110.6	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	0.80	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	0.60	0/3747	0.84	17/5100 (0.3%)
1	B	0.52	0/3747	0.75	16/5100 (0.3%)
1	C	0.57	0/3943	0.82	15/5351 (0.3%)
1	D	0.73	5/3747 (0.1%)	0.90	16/5100 (0.3%)
All	All	0.61	5/15184 (0.0%)	0.83	64/20651 (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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	146	CYS	CB-SG	-10.19	1.65	1.82
1	D	110	VAL	CB-CG1	-5.86	1.40	1.52
1	D	133	TYR	CE1-CZ	-5.46	1.31	1.38
1	D	260	SER	CA-CB	-5.23	1.45	1.52
1	D	68	VAL	CB-CG1	-5.01	1.42	1.52

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	484	LEU	CB-CG-CD1	-9.98	94.03	111.00
1	D	160	PRO	N-CA-CB	9.37	114.54	103.30
1	A	160	PRO	N-CA-CB	8.07	112.98	103.30
1	A	329	PRO	N-CA-CB	7.82	112.69	103.30
1	B	329	PRO	N-CA-CB	7.54	112.35	103.30

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

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	217	0
1	B	3711	0	3038	219	0
1	C	3895	0	3376	323	0
1	D	3711	0	3038	246	0
All	All	15028	0	12488	970	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 35.

The worst 5 of 970 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 ⓘ

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	552/771 (72%)	429 (78%)	73 (13%)	50 (9%)	1	5
1	B	552/771 (72%)	437 (79%)	70 (13%)	45 (8%)	1	6
1	C	549/771 (71%)	423 (77%)	80 (15%)	46 (8%)	1	6
1	D	552/771 (72%)	427 (77%)	75 (14%)	50 (9%)	1	5
All	All	2205/3084 (72%)	1716 (78%)	298 (14%)	191 (9%)	1	5

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%)	241 (90%)	27 (10%)	7	28
1	B	268/637 (42%)	245 (91%)	23 (9%)	10	36
1	C	322/637 (50%)	293 (91%)	29 (9%)	9	33
1	D	268/637 (42%)	240 (90%)	28 (10%)	7	26
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	52	LEU
1	B	358	PHE
1	C	518	THR
1	B	67	THR
1	B	140	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	391	GLN
1	B	429	GLN
1	C	482	HIS
1	C	156	HIS
1	A	391	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 monosaccharides 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 ⓘ

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%)	0.30	41 (7%) 14 14	53, 109, 176, 219	0
1	B	548/771 (71%)	0.87	92 (16%) 1 1	62, 120, 274, 329	0
1	C	545/771 (70%)	0.37	28 (5%) 28 27	30, 104, 136, 171	0
1	D	548/771 (71%)	0.36	36 (6%) 18 19	37, 91, 169, 223	0
All	All	2189/3084 (70%)	0.47	197 (8%) 9 10	30, 106, 216, 329	0

The worst 5 of 197 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	446	SER	14.8
1	B	448	ASP	12.9
1	B	533	VAL	10.3
1	B	522	ASP	9.0
1	B	532	VAL	8.3

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 monosaccharides 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.