Full wwPDB X-ray Structure Validation Report (i)

Dec 2, 2023 – 01:23 pm GMT

PDB ID	:	2UWM
Title	:	C-TERMINAL DOMAIN(WH2-WH4) OF ELONGATION FACTOR SELB IN COMPLEX WITH SECIS RNA
Authors	:	Ose, T.; Soler, N.; Rasubala, L.; Kuroki, K.; Kohda, D.; Fourmy, D.; Yoshizawa, S.; Maenaka, K.
Deposited on	:	2007-03-22
Resolution	:	2.31 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i) 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 (1)) were used in the production of this report:

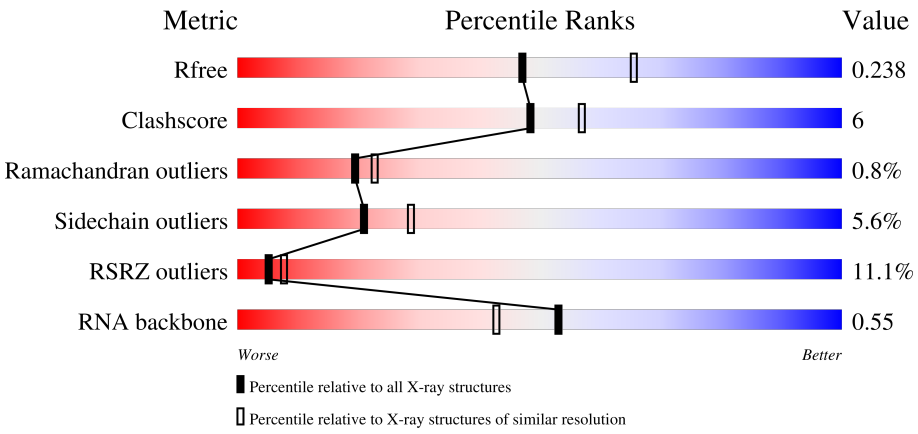
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)
RNA backbone	3102	1031 (2.70-1.94)

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 <=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	258	8% 61% 12% • 25%
1	B	258	10% 67% 11% • 21%
2	C	23	4% 48% 39% 13%
2	D	23	9% 65% 22% 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4524 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 SELENOCYSTEINE-SPECIFIC ELONGATION FACTOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	193	1585	1015	286	284	0	0	0
1	B	203	1671	1070	299	302	0	0	0

- Molecule 2 is a RNA chain called 5'-R(*GP*GP*CP*GP*UP*UP*GP*CP*CP*GP *GP*UP*CP*UP*GP*GP*CP*AP*AP*CP*GP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	23	488	218	87	161	22	0	0	0
2	D	23	488	218	87	161	22	0	0	0

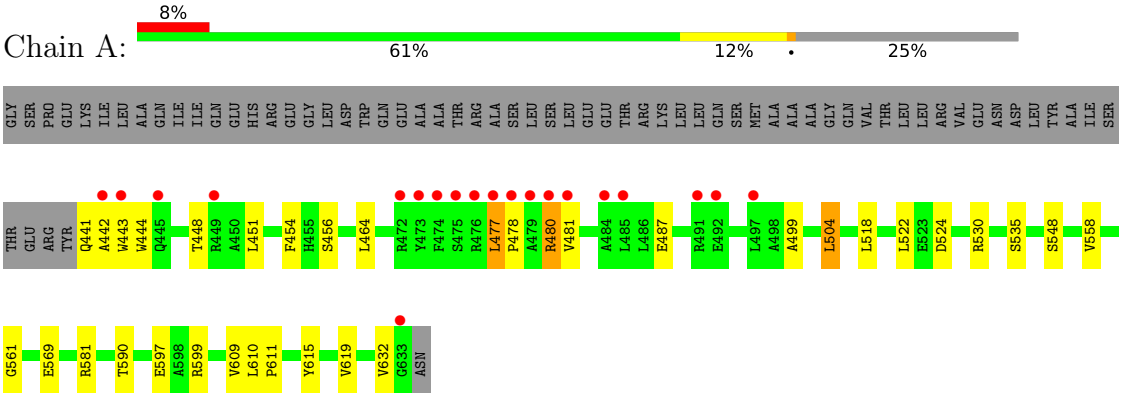
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	123	123	123	0	0
3	B	98	98	98	0	0
3	C	38	38	38	0	0
3	D	33	33	33	0	0

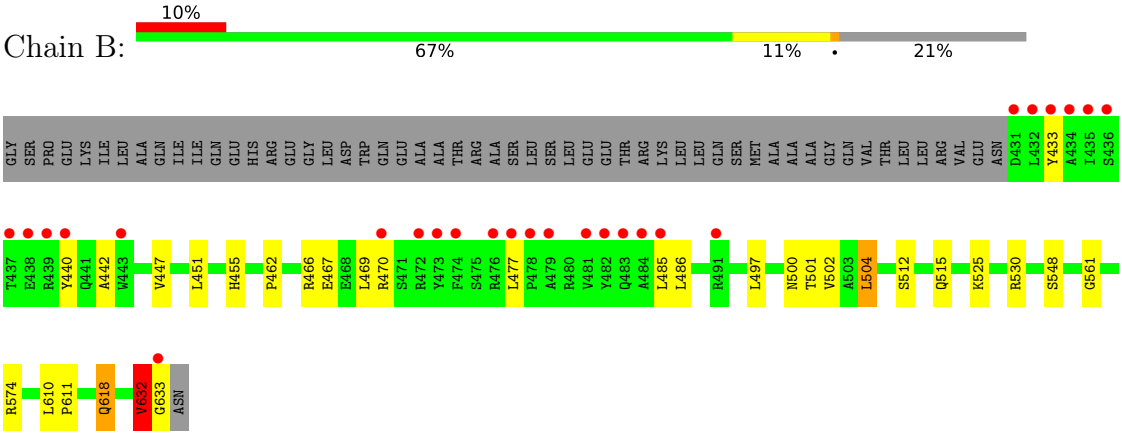
3 Residue-property plots (i)

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.

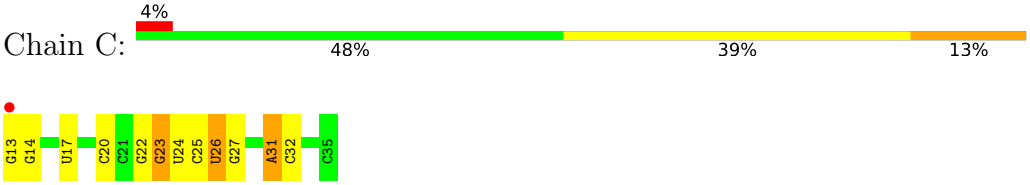
• Molecule 1: SELENOCYSTEINE-SPECIFIC ELONGATION FACTOR



• Molecule 1: SELENOCYSTEINE-SPECIFIC ELONGATION FACTOR

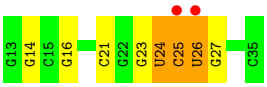


• Molecule 2: 5'-R(*GP*GP*CP*GP*UP*UP*GP*CP*CP*GP *GP*UP*CP*UP*GP*GP*CP*AP*AP*CP*GP*CP*C)-3'



• Molecule 2: 5'-R(*GP*GP*CP*GP*UP*UP*GP*CP*CP*GP *GP*UP*CP*UP*GP*GP*CP*AP*AP*CP*GP*CP*C)-3'

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	160.07Å 119.84Å 50.46Å 90.00° 100.05° 90.00°	Depositor
Resolution (Å)	50.00 – 2.31 49.69 – 2.31	Depositor EDS
% Data completeness (in resolution range)	96.8 (50.00-2.31) 96.7 (49.69-2.31)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.238 0.200 , 0.238	Depositor DCC
R_{free} test set	3558 reflections (9.00%)	wwPDB-VP
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4524	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.59	0/1623	0.70	2/2195 (0.1%)
1	B	0.55	0/1711	0.66	2/2315 (0.1%)
2	C	0.98	0/544	1.63	9/847 (1.1%)
2	D	0.93	0/544	1.52	5/847 (0.6%)
All	All	0.68	0/4422	1.01	18/6204 (0.3%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	26	U	P-O3'-C3'	9.65	131.28	119.70
1	A	530	ARG	NE-CZ-NH1	-9.23	115.69	120.30
1	A	530	ARG	NE-CZ-NH2	8.99	124.80	120.30
2	C	31	A	O4'-C1'-N9	6.79	113.64	108.20
2	D	14	G	P-O3'-C3'	6.67	127.71	119.70
2	C	23	G	O4'-C1'-N9	6.62	113.49	108.20
1	B	530	ARG	NE-CZ-NH2	6.58	123.59	120.30
2	C	26	U	O4'-C1'-N1	6.27	113.22	108.20
2	C	14	G	P-O3'-C3'	6.18	127.11	119.70
2	C	14	G	N9-C1'-C2'	5.95	121.74	114.00
1	B	530	ARG	NE-CZ-NH1	-5.75	117.42	120.30
2	D	25	C	O4'-C1'-N1	-5.64	103.69	108.20
2	C	22	G	OP2-P-O3'	5.58	117.49	105.20
2	C	20	C	O4'-C1'-N1	5.48	112.59	108.20
2	C	13	G	N1-C6-O6	5.42	123.15	119.90
2	D	21	C	C2-N3-C4	5.31	122.56	119.90
2	D	25	C	C4'-C3'-C2'	5.29	107.89	102.60
2	D	24	U	O4'-C1'-N1	5.27	112.42	108.20

There are no chirality outliers.

There are no planarity outliers.

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	1585	0	1585	28	0
1	B	1671	0	1665	18	0
2	C	488	0	251	2	0
2	D	488	0	251	3	0
3	A	123	0	0	6	0
3	B	98	0	0	1	0
3	C	38	0	0	0	0
3	D	33	0	0	0	0
All	All	4524	0	3752	48	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 6.

All (48) 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:A:442:ALA:O	1:A:444:TRP:N	2.18	0.77
1:B:466:ARG:HG2	1:B:502:VAL:HG23	1.73	0.71
1:A:597:GLU:OE2	3:A:2095:HOH:O	2.09	0.70
2:C:17:U:H3	2:C:31:A:H62	1.42	0.67
1:A:451:LEU:CB	1:A:504:LEU:HD22	2.25	0.67
1:B:618:GLN:OE1	3:B:2095:HOH:O	2.14	0.66
1:B:632:VAL:HG22	1:B:633:GLY:N	2.10	0.66
1:A:451:LEU:HB3	1:A:504:LEU:HD22	1.83	0.60
1:B:451:LEU:HD12	1:B:504:LEU:HD13	1.85	0.58
1:A:558:VAL:CG1	2:D:26:U:H5'	2.34	0.57
1:B:497:LEU:CD2	1:B:502:VAL:HG22	2.36	0.56
1:A:499:ALA:HB3	1:A:561:GLY:HA3	1.89	0.55
1:A:451:LEU:HB2	1:A:504:LEU:HD22	1.88	0.54
1:A:477:LEU:HD13	1:A:478:PRO:HD2	1.92	0.52
1:A:441:GLN:N	3:A:2003:HOH:O	2.41	0.52
1:A:441:GLN:CA	1:A:442:ALA:HB3	2.39	0.52
1:A:441:GLN:HA	1:A:442:ALA:HB3	1.93	0.51
1:B:610:LEU:HB3	1:B:611:PRO:HD3	1.93	0.51
1:A:451:LEU:HB2	1:A:504:LEU:CD2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:632:VAL:HG22	1:B:633:GLY:H	1.76	0.50
1:A:599:ARG:HA	1:A:609:VAL:HG21	1.94	0.49
1:B:561:GLY:O	1:B:574:ARG:NE	2.47	0.47
1:B:462:PRO:HG2	1:B:501:THR:HG21	1.96	0.47
1:B:455:HIS:HE1	1:B:504:LEU:H	1.63	0.47
1:A:448:THR:HG22	1:A:504:LEU:HD11	1.97	0.47
1:A:558:VAL:HG12	2:D:26:U:H5'	1.95	0.46
1:B:497:LEU:HD22	1:B:502:VAL:HG22	1.97	0.46
1:B:447:VAL:HG22	1:B:469:LEU:HD11	1.97	0.46
2:C:31:A:H2'	2:C:32:C:O4'	2.16	0.46
1:B:512:SER:H	1:B:515:GLN:HE21	1.65	0.45
1:A:590:THR:CG2	3:A:2091:HOH:O	2.64	0.45
1:A:597:GLU:CD	3:A:2095:HOH:O	2.53	0.44
1:B:466:ARG:HD3	1:B:500:ASN:HA	1.99	0.44
1:A:535:SER:HB2	1:A:569:GLU:HG3	2.00	0.44
1:A:581:ARG:HD3	3:A:2082:HOH:O	2.18	0.43
1:A:441:GLN:HA	1:A:442:ALA:C	2.37	0.43
1:A:581:ARG:NE	3:A:2082:HOH:O	2.51	0.43
1:A:610:LEU:HB3	1:A:611:PRO:HD3	2.00	0.43
1:A:480:ARG:O	1:A:481:VAL:HB	2.18	0.42
1:A:548:SER:HB2	2:D:16:G:O2'	2.19	0.42
1:B:512:SER:H	1:B:515:GLN:NE2	2.18	0.41
1:A:451:LEU:CB	1:A:504:LEU:CD2	2.98	0.41
1:B:440:TYR:CE2	1:B:442:ALA:HB3	2.56	0.41
1:B:466:ARG:CG	1:B:502:VAL:HG23	2.48	0.41
1:B:632:VAL:CG2	1:B:633:GLY:N	2.80	0.41
1:A:615:TYR:O	1:A:619:VAL:HG22	2.20	0.40
1:A:441:GLN:N	1:A:442:ALA:HB3	2.37	0.40
1:A:454:PHE:CD1	1:A:464:LEU:HD13	2.56	0.40

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	191/258 (74%)	183 (96%)	7 (4%)	1 (0%)	29	35
1	B	201/258 (78%)	189 (94%)	10 (5%)	2 (1%)	15	17
All	All	392/516 (76%)	372 (95%)	17 (4%)	3 (1%)	19	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	443	TRP
1	B	433	TYR
1	B	632	VAL

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	165/219 (75%)	156 (94%)	9 (6%)	21	29
1	B	174/219 (80%)	164 (94%)	10 (6%)	20	28
All	All	339/438 (77%)	320 (94%)	19 (6%)	21	29

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	456	SER
1	A	477	LEU
1	A	480	ARG
1	A	487	GLU
1	A	504	LEU
1	A	518	LEU
1	A	522	LEU
1	A	524	ASP
1	A	632	VAL
1	B	467	GLU
1	B	470	ARG
1	B	477	LEU
1	B	485	LEU

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Mol	Chain	Res	Type
1	B	486	LEU
1	B	504	LEU
1	B	525	LYS
1	B	548	SER
1	B	618	GLN
1	B	632	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	496	GLN
1	A	515	GLN
1	A	532	GLN
1	A	544	ASN
1	A	586	ASN
1	A	618	GLN
1	B	455	HIS
1	B	483	GLN
1	B	515	GLN
1	B	532	GLN
1	B	618	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	22/23 (95%)	4 (18%)	2 (9%)
2	D	22/23 (95%)	5 (22%)	1 (4%)
All	All	44/46 (95%)	9 (20%)	3 (6%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	23	G
2	C	24	U
2	C	26	U
2	C	27	G
2	D	23	G
2	D	24	U
2	D	25	C
2	D	26	U

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Mol	Chain	Res	Type
2	D	27	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	25	C
2	C	26	U
2	D	25	C

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 (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	193/258 (74%)	0.83	20 (10%)	6	9	18, 25, 37, 40	0
1	B	203/258 (78%)	0.92	26 (12%)	3	5	19, 26, 42, 48	0
2	C	23/23 (100%)	0.95	1 (4%)	35	42	16, 24, 34, 43	0
2	D	23/23 (100%)	0.53	2 (8%)	10	14	18, 25, 39, 52	0
All	All	442/562 (78%)	0.86	49 (11%)	5	8	16, 26, 40, 52	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	478	PRO	11.4
1	B	437	THR	9.2
1	B	477	LEU	7.0
1	B	433	TYR	6.6
1	B	476	ARG	6.4
1	B	440	TYR	6.3
1	A	473	TYR	5.9
1	A	475	SER	5.9
1	A	443	TRP	5.7
1	B	435	ILE	5.5
1	B	443	TRP	5.5
1	A	477	LEU	5.4
1	A	476	ARG	5.3
1	A	472	ARG	4.9
1	A	478	PRO	4.8
1	B	436	SER	4.7
1	A	481	VAL	4.7
1	B	431	ASP	4.7
1	A	491	ARG	4.3
1	B	485	LEU	4.2
1	B	491	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	485	LEU	4.1
1	A	474	PHE	3.8
1	A	442	ALA	3.6
1	B	432	LEU	3.5
1	B	470	ARG	3.3
1	A	479	ALA	3.3
1	B	434	ALA	3.3
1	B	438	GLU	3.3
1	B	481	VAL	3.3
1	B	439	ARG	3.1
1	B	633	GLY	2.9
1	A	492	GLU	2.9
1	B	473	TYR	2.8
1	A	633	GLY	2.7
1	B	482	TYR	2.6
1	A	445	GLN	2.5
1	A	484	ALA	2.4
1	B	479	ALA	2.4
1	A	449	ARG	2.4
1	A	480	ARG	2.3
2	D	26	U	2.3
1	B	483	GLN	2.3
1	B	472	ARG	2.3
1	A	497	LEU	2.3
1	B	484	ALA	2.2
1	B	474	PHE	2.1
2	C	13	G	2.0
2	D	25	C	2.0

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 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.