



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:58 AM UTC

PDB ID : 7SEU / pdb_00007seu
Title : Crystal structure of E coli contaminant protein YncE co-purified with a plant protein
Authors : Chai, L.; Zhu, P.; Chai, J.; Pang, C.; Andi, B.; McsWeeney, S.; Shanklin, J.; Liu, Q.
Deposited on : 2021-10-01
Resolution : 2.50 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 ⓘ 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

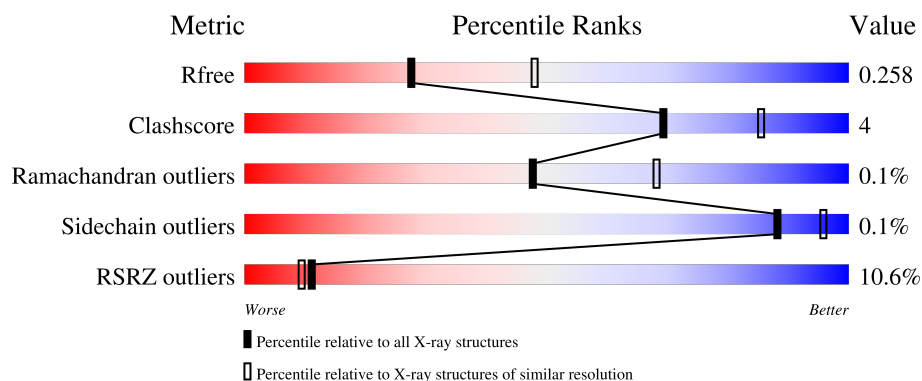
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	353	 3% 84% 7% 9%
1	B	353	 6% 82% 8% 9%
1	C	353	 10% 84% 7% 9%
1	D	353	 19% 81% 7% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10124 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 PQQ-dependent catabolism-associated beta-propeller protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2482	1552	438	489	3			
1	B	321	Total	C	N	O	S	0	0	0
			2473	1547	437	486	3			
1	C	321	Total	C	N	O	S	0	0	0
			2473	1547	437	486	3			
1	D	315	Total	C	N	O	S	0	0	0
			2424	1518	427	476	3			

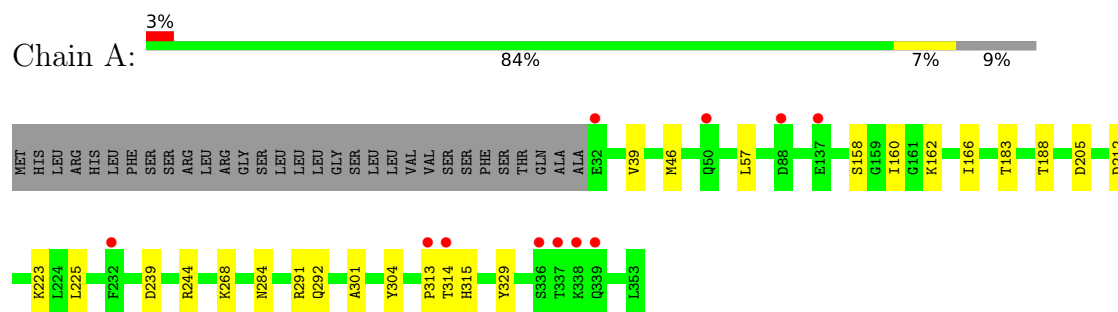
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	95	Total	O	0	0
			95	95		
2	B	90	Total	O	0	0
			90	90		
2	C	47	Total	O	0	0
			47	47		
2	D	40	Total	O	0	0
			40	40		

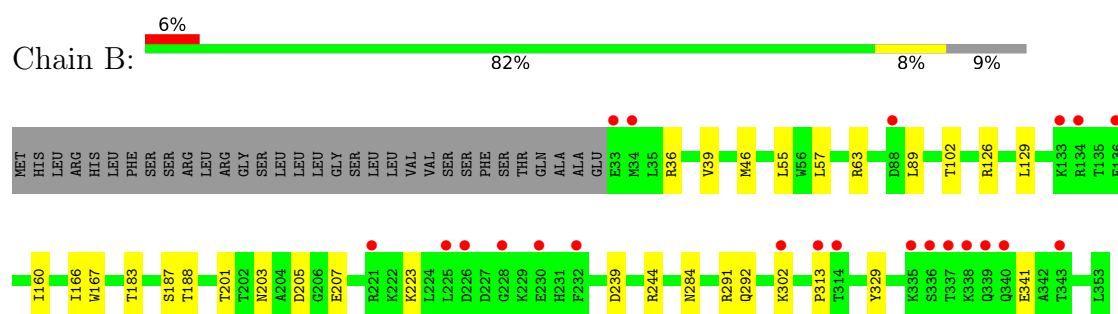
3 Residue-property plots [i](#)

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.

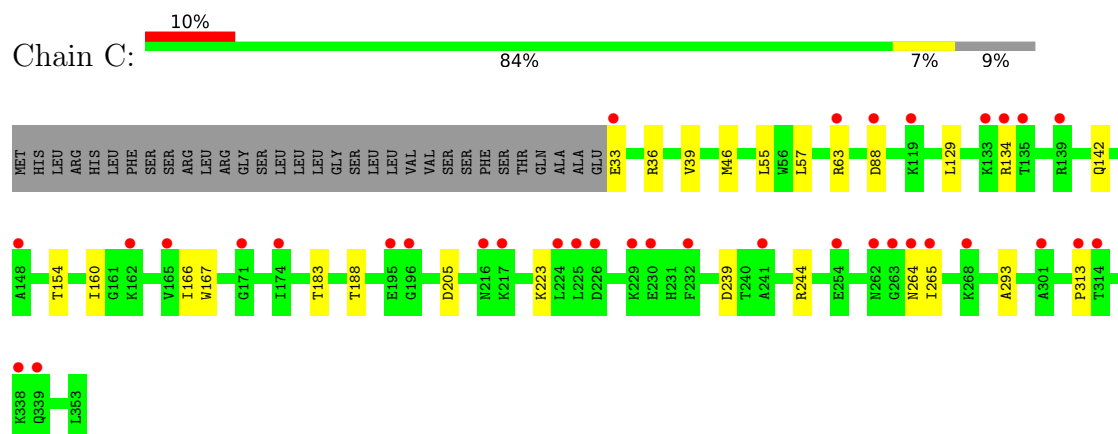
- Molecule 1: PQQ-dependent catabolism-associated beta-propeller protein



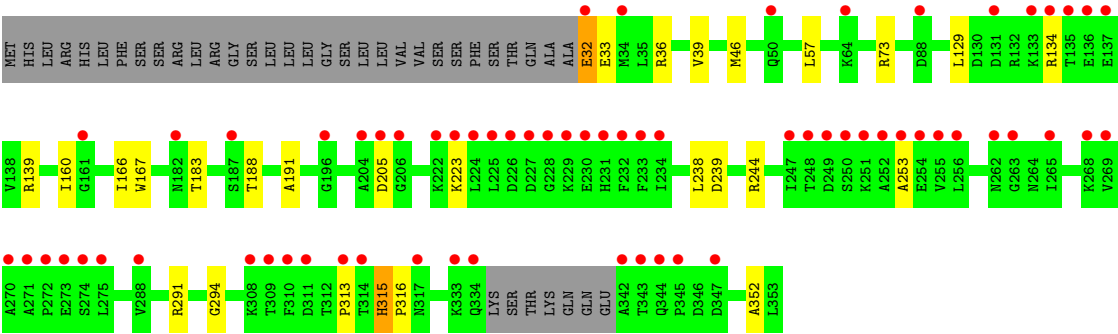
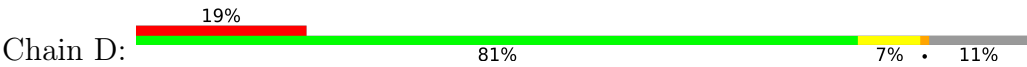
- Molecule 1: PQQ-dependent catabolism-associated beta-propeller protein



- Molecule 1: PQQ-dependent catabolism-associated beta-propeller protein



- Molecule 1: PQQ-dependent catabolism-associated beta-propeller protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.17Å 147.27Å 96.90Å 90.00° 104.40° 90.00°	Depositor
Resolution (Å)	48.61 – 2.50 48.61 – 2.50	Depositor EDS
% Data completeness (in resolution range)	88.9 (48.61-2.50) 95.7 (48.61-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.236 , 0.256 0.238 , 0.258	Depositor DCC
R_{free} test set	2296 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.695	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10124	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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 [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	0.11	0/2515	0.32	0/3406
1	B	0.11	0/2506	0.32	0/3394
1	C	0.11	0/2506	0.31	0/3394
1	D	0.13	0/2456	0.33	0/3327
All	All	0.11	0/9983	0.32	0/13521

There are no bond length outliers.

There are no bond angle outliers.

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	2482	0	2530	17	0
1	B	2473	0	2524	17	0
1	C	2473	0	2524	21	0
1	D	2424	0	2469	19	0
2	A	95	0	0	3	0
2	B	90	0	0	1	0
2	C	47	0	0	4	0
2	D	40	0	0	3	0
All	All	10124	0	10047	70	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 4.

All (70) 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:134:ARG:HH22	1:C:142:GLN:NE2	1.64	0.93
1:C:134:ARG:NH2	1:C:142:GLN:NE2	2.20	0.89
1:B:284:ASN:OD1	1:B:302:LYS:HE3	1.80	0.81
1:C:134:ARG:HH22	1:C:142:GLN:HE22	1.38	0.70
1:C:33:GLU:N	2:C:402:HOH:O	2.24	0.70
1:C:264:ASN:HD22	1:D:253:ALA:HB2	1.62	0.65
1:C:166:ILE:HG12	1:C:183:THR:HG21	1.81	0.63
1:C:63:ARG:NH1	2:C:405:HOH:O	2.32	0.62
1:A:225:LEU:HD21	1:A:268:LYS:HZ1	1.65	0.62
1:D:36:ARG:HH21	1:D:313:PRO:HD2	1.66	0.60
1:D:32:GLU:N	2:D:403:HOH:O	2.34	0.60
1:B:166:ILE:HG12	1:B:183:THR:HG21	1.84	0.60
1:D:166:ILE:HG12	1:D:183:THR:HG21	1.81	0.60
1:D:134:ARG:HH22	1:D:139:ARG:HE	1.50	0.59
1:D:73:ARG:HD3	2:D:420:HOH:O	2.03	0.58
1:D:46:MET:SD	2:D:431:HOH:O	2.58	0.55
1:C:239:ASP:HB3	1:C:244:ARG:HG3	1.89	0.55
1:D:134:ARG:NH2	1:D:139:ARG:HE	2.06	0.54
1:B:160:ILE:HG21	1:B:188:THR:HG22	1.90	0.53
1:A:160:ILE:HG21	1:A:188:THR:HG22	1.90	0.53
1:A:313:PRO:HG3	1:C:313:PRO:HG3	1.91	0.53
1:B:239:ASP:HB3	1:B:244:ARG:HG3	1.90	0.53
1:C:160:ILE:HG21	1:C:188:THR:HG22	1.91	0.52
1:D:239:ASP:HB3	1:D:244:ARG:HG3	1.92	0.52
1:D:205:ASP:O	1:D:223:LYS:NZ	2.43	0.52
1:B:284:ASN:CG	1:B:302:LYS:HE3	2.35	0.51
1:A:239:ASP:HB3	1:A:244:ARG:HG3	1.93	0.51
1:C:36:ARG:NH2	1:C:313:PRO:HD2	2.27	0.50
1:D:33:GLU:HB2	1:D:352:ALA:HB3	1.93	0.50
1:A:314:THR:OG1	1:C:293:ALA:O	2.29	0.50
1:C:264:ASN:OD1	1:C:265:ILE:N	2.46	0.49
1:C:205:ASP:O	1:C:223:LYS:NZ	2.45	0.49
1:D:160:ILE:HG21	1:D:188:THR:HG22	1.93	0.49
1:D:291:ARG:O	1:D:315:HIS:HA	2.13	0.49
1:B:205:ASP:O	1:B:223:LYS:NZ	2.45	0.48
1:B:291:ARG:NH2	1:B:292:GLN:HE21	2.11	0.47
1:A:292:GLN:NE2	2:A:407:HOH:O	2.33	0.47
1:D:294:GLY:HA2	1:D:316:PRO:HD3	1.95	0.47
1:A:39:VAL:HG11	1:A:57:LEU:HD23	1.97	0.47
1:C:264:ASN:ND2	1:D:253:ALA:HB2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:ASP:HA	2:C:406:HOH:O	2.14	0.47
1:A:244:ARG:NH1	1:A:304:TYR:OH	2.48	0.46
1:A:225:LEU:HD21	1:A:268:LYS:NZ	2.30	0.46
1:B:102:THR:OG1	2:B:401:HOH:O	2.21	0.46
1:C:46:MET:HE2	1:C:55:LEU:HD21	1.97	0.46
1:C:134:ARG:NH2	1:C:142:GLN:HE21	2.10	0.46
1:B:129:LEU:HD13	1:B:167:TRP:CE3	2.51	0.45
1:B:187:SER:HG	1:B:201:THR:HG1	1.63	0.45
1:A:212:ASP:OD1	2:A:401:HOH:O	2.21	0.44
1:B:39:VAL:HG11	1:B:57:LEU:HD23	1.98	0.44
1:B:46:MET:HE1	1:B:329:TYR:HB3	2.00	0.44
1:A:162:LYS:NZ	2:A:415:HOH:O	2.50	0.43
1:D:129:LEU:HD13	1:D:167:TRP:CE3	2.53	0.43
1:A:46:MET:HE1	1:A:329:TYR:HB3	2.00	0.43
1:A:166:ILE:HG12	1:A:183:THR:HG21	1.99	0.43
1:C:129:LEU:HD13	1:C:167:TRP:CE3	2.53	0.43
1:A:291:ARG:HG3	1:A:315:HIS:HB3	2.00	0.43
1:D:39:VAL:HG11	1:D:57:LEU:HD23	2.01	0.43
1:B:89:LEU:HD12	1:B:126:ARG:HD3	2.02	0.42
1:B:63:ARG:N	1:B:341:GLU:OE2	2.52	0.42
1:C:154:THR:OG1	2:C:401:HOH:O	2.22	0.42
1:A:205:ASP:O	1:A:223:LYS:NZ	2.54	0.41
1:C:39:VAL:HG11	1:C:57:LEU:HD23	2.02	0.41
1:B:203:ASN:OD1	1:B:207:GLU:HG2	2.21	0.41
1:A:284:ASN:OD1	1:A:301:ALA:HB3	2.21	0.41
1:B:36:ARG:HH21	1:B:313:PRO:HD2	1.85	0.41
1:B:46:MET:HE2	1:B:55:LEU:HD21	2.01	0.41
1:D:191:ALA:HB1	1:D:238:LEU:HG	2.02	0.41
1:A:158:SER:HA	1:A:166:ILE:HD13	2.04	0.40
1:D:36:ARG:NH2	1:D:313:PRO:HD2	2.33	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	320/353 (91%)	306 (96%)	14 (4%)	0	100	100
1	B	319/353 (90%)	305 (96%)	14 (4%)	0	100	100
1	C	319/353 (90%)	306 (96%)	13 (4%)	0	100	100
1	D	311/353 (88%)	297 (96%)	13 (4%)	1 (0%)	36	55
All	All	1269/1412 (90%)	1214 (96%)	54 (4%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	315	HIS

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	270/297 (91%)	270 (100%)	0	100	100
1	B	269/297 (91%)	269 (100%)	0	100	100
1	C	269/297 (91%)	269 (100%)	0	100	100
1	D	263/297 (89%)	262 (100%)	1 (0%)	84	93
All	All	1071/1188 (90%)	1070 (100%)	1 (0%)	88	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	32	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	235	ASN

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Mol	Chain	Res	Type
1	A	280	ASN
1	B	107	ASN
1	B	280	ASN
1	B	292	GLN
1	C	83	GLN
1	C	142	GLN
1	C	280	ASN
1	D	107	ASN

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

6.1 Protein, DNA and RNA chains

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	322/353 (91%)	0.26	11 (3%)	48	43	26, 35, 53, 86	0
1	B	321/353 (90%)	0.54	22 (6%)	23	20	27, 38, 64, 105	0
1	C	321/353 (90%)	0.89	35 (10%)	10	9	29, 52, 91, 114	0
1	D	315/353 (89%)	1.29	67 (21%)	2	2	32, 50, 84, 113	0
All	All	1279/1412 (90%)	0.74	135 (10%)	11	9	26, 41, 82, 114	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	250	SER	7.8
1	D	232	PHE	6.3
1	D	343	THR	6.2
1	D	274	SER	5.6
1	D	275	LEU	5.5
1	D	231	HIS	5.5
1	D	230	GLU	5.0
1	D	225	LEU	4.6
1	C	338	LYS	4.6
1	D	272	PRO	4.4
1	B	340	GLN	4.3
1	B	314	THR	4.3
1	B	33	GLU	4.2
1	D	342	ALA	4.2
1	B	339	GLN	4.1
1	D	228	GLY	4.0
1	D	271	ALA	4.0
1	C	264	ASN	3.9
1	D	256	LEU	3.9
1	B	338	LYS	3.9
1	D	253	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	88	ASP	3.8
1	D	254	GLU	3.8
1	A	338	LYS	3.8
1	D	229	LYS	3.7
1	D	255	VAL	3.7
1	D	273	GLU	3.6
1	B	337	THR	3.6
1	C	314	THR	3.6
1	B	88	ASP	3.5
1	D	251	LYS	3.5
1	D	34	MET	3.4
1	D	249	ASP	3.4
1	C	196	GLY	3.4
1	D	227	ASP	3.4
1	A	314	THR	3.4
1	A	50	GLN	3.3
1	C	232	PHE	3.3
1	B	232	PHE	3.2
1	B	302	LYS	3.2
1	D	344	GLN	3.2
1	D	226	ASP	3.2
1	D	223	LYS	3.2
1	D	269	VAL	3.2
1	B	221	ARG	3.1
1	C	134	ARG	3.1
1	D	204	ALA	3.1
1	C	265	ILE	3.1
1	A	232	PHE	3.1
1	B	134	ARG	3.1
1	D	234	ILE	3.0
1	D	252	ALA	2.9
1	C	241	ALA	2.9
1	D	333	LYS	2.9
1	C	226	ASP	2.9
1	C	216	ASN	2.8
1	C	225	LEU	2.8
1	D	345	PRO	2.8
1	C	165	VAL	2.8
1	C	262	ASN	2.7
1	C	224	LEU	2.7
1	D	270	ALA	2.7
1	B	335	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	88	ASP	2.6
1	D	317	ASN	2.6
1	D	334	GLN	2.5
1	C	135	THR	2.5
1	A	337	THR	2.5
1	C	174	ILE	2.5
1	B	336	SER	2.5
1	D	314	THR	2.5
1	B	230	GLU	2.5
1	D	206	GLY	2.5
1	D	136	GLU	2.4
1	D	205	ASP	2.4
1	D	262	ASN	2.4
1	C	230	GLU	2.4
1	D	50	GLN	2.4
1	D	288	VAL	2.4
1	A	336	SER	2.4
1	C	263	GLY	2.4
1	A	339	GLN	2.4
1	D	222	LYS	2.4
1	D	309	THR	2.4
1	B	225	LEU	2.4
1	C	139	ARG	2.4
1	C	268	LYS	2.3
1	C	254	GLU	2.3
1	C	63	ARG	2.3
1	D	134	ARG	2.3
1	D	224	LEU	2.3
1	D	88	ASP	2.3
1	B	343	THR	2.3
1	D	64	LYS	2.3
1	D	265	ILE	2.3
1	B	226	ASP	2.3
1	C	217	LYS	2.3
1	D	131	ASP	2.3
1	D	32	GLU	2.3
1	D	135	THR	2.2
1	B	133	LYS	2.2
1	C	119	LYS	2.2
1	D	268	LYS	2.2
1	A	137	GLU	2.2
1	A	313	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	313	PRO	2.2
1	D	182	ASN	2.2
1	D	311	ASP	2.2
1	A	32	GLU	2.2
1	D	313	PRO	2.2
1	D	133	LYS	2.2
1	D	308	LYS	2.2
1	B	228	GLY	2.2
1	D	161	GLY	2.2
1	D	196	GLY	2.2
1	C	33	GLU	2.2
1	D	233	PHE	2.2
1	C	301	ALA	2.1
1	C	339	GLN	2.1
1	D	347	ASP	2.1
1	C	133	LYS	2.1
1	C	313	PRO	2.1
1	B	34	MET	2.1
1	D	248	THR	2.1
1	D	310	PHE	2.1
1	C	195	GLU	2.1
1	D	263	GLY	2.1
1	D	137	GLU	2.1
1	C	148	ALA	2.0
1	B	136	GLU	2.0
1	C	171	GLY	2.0
1	C	162	LYS	2.0
1	C	229	LYS	2.0
1	D	247	ILE	2.0
1	D	187	SER	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 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.