



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2022 – 10:16 AM EDT

PDB ID : 7SEU
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.27
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) : 2.27

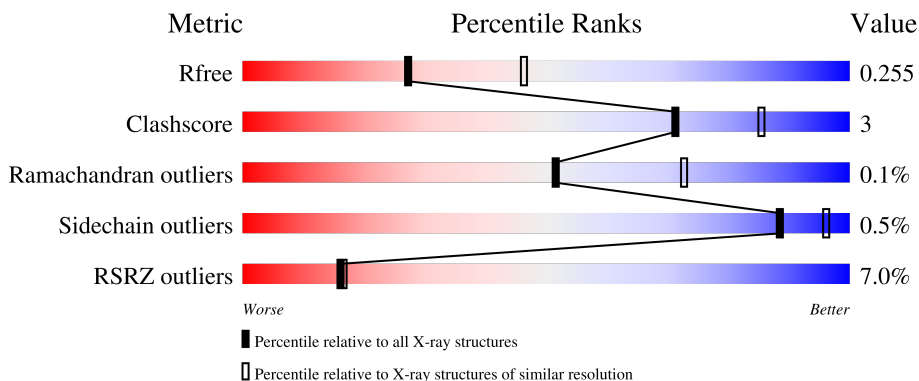
1 Overall quality at a glance

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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	 2% 84% 7% 9%
1	B	353	 4% 82% 8% 9%
1	C	353	 8% 83% 8% 9%
1	D	353	 12% 81% 8% 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
			Total	C	N	O	S			
1	A	322	Total 2482	C 1552	N 438	O 489	S 3	0	0	0
1	B	321	Total 2473	C 1547	N 437	O 486	S 3	0	0	0
1	C	321	Total 2473	C 1547	N 437	O 486	S 3	0	0	0
1	D	315	Total 2424	C 1518	N 427	O 476	S 3	0	0	0

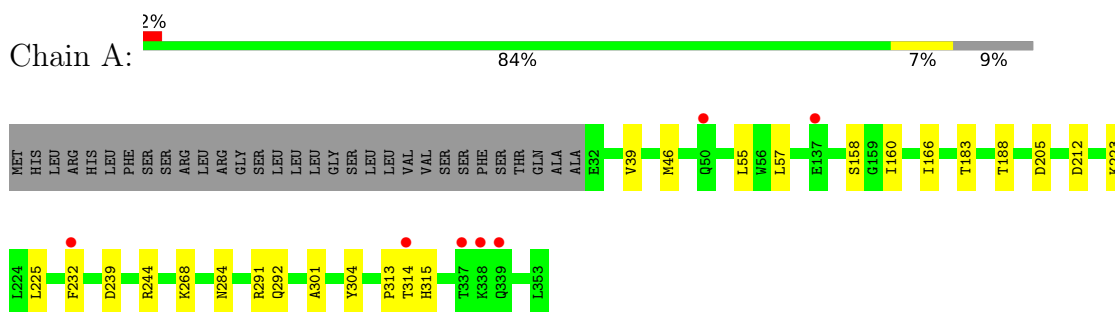
- Molecule 2 is water.

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

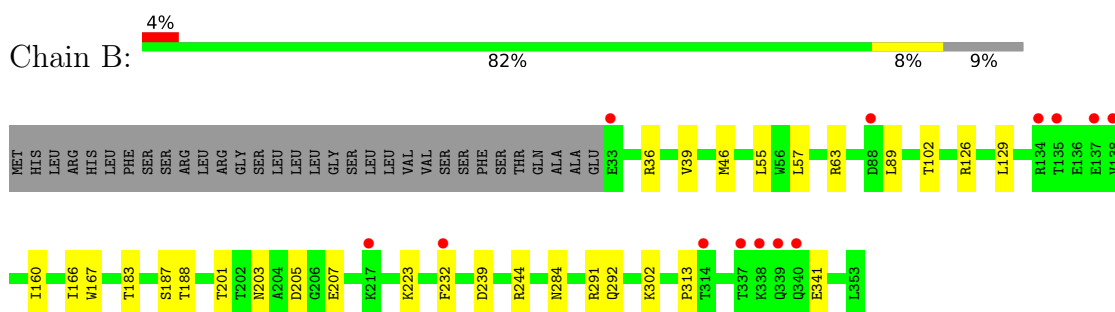
3 Residue-property plots [i](#)

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.

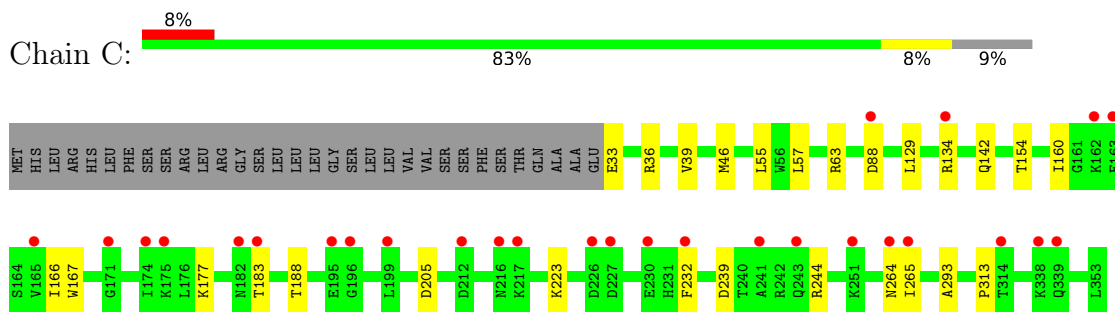
- Molecule 1: PQQ-dependent catabolism-associated beta-propeller protein



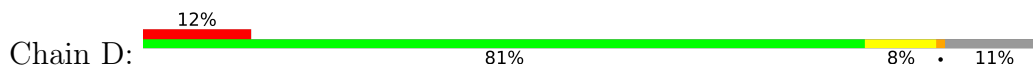
- Molecule 1: PQQ-dependent catabolism-associated beta-propeller protein

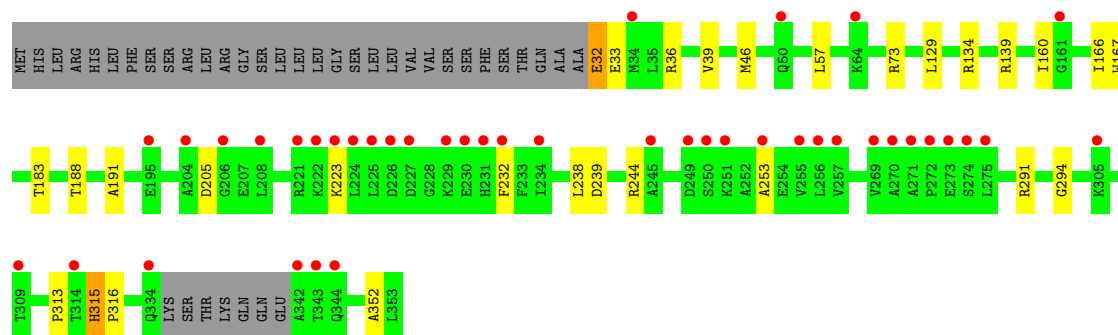


- Molecule 1: PQQ-dependent catabolism-associated beta-propeller protein



- 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) 95.8 (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)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.236 , 0.256 0.237 , 0.255	Depositor DCC
R_{free} test set	2296 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtrriage
Anisotropy	0.695	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtrriage
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

Xtrriage'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	0.24	0/2515	0.47	0/3406
1	B	0.25	0/2506	0.48	0/3394
1	C	0.24	0/2506	0.46	0/3394
1	D	0.25	0/2456	0.48	0/3327
All	All	0.25	0/9983	0.47	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	16	0
1	B	2473	0	2524	16	0
1	C	2473	0	2524	22	0
1	D	2424	0	2469	19	0
2	A	95	0	0	2	0
2	B	90	0	0	1	0
2	C	47	0	0	5	0
2	D	40	0	0	3	0
All	All	10124	0	10047	69	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 3.

All (69) 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: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:A:225:LEU:HD21	1:A:268:LYS:HZ1	1.71	0.55
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: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:C:46:MET:HE2	1:C:55:LEU:HD21	1.96	0.48
1:B:205:ASP:O	1:B:223:LYS:NZ	2.45	0.48
1:C:177:LYS:NZ	2:C:401:HOH:O	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:ASN:ND2	1:D:253:ALA:HB2	2.28	0.47
1:C:88:ASP:HA	2:C:406:HOH:O	2.14	0.47
1:A:225:LEU:HD21	1:A:268:LYS:NZ	2.30	0.46
1:A:244:ARG:NH1	1:A:304:TYR:OH	2.48	0.46
1:B:102:THR:OG1	2:B:401:HOH:O	2.21	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: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:187:SER:HG	1:B:201:THR:HG1	1.63	0.44
1:B:284:ASN:CG	1:B:302:LYS:HE3	2.35	0.44
1:D:129:LEU:HD13	1:D:167:TRP:CE3	2.53	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:B:46:MET:HE2	1:B:55:LEU:HD21	2.01	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:D:191:ALA:HB1	1:D:238:LEU:HG	2.02	0.41
1:A:46:MET:HE2	1:A:55:LEU:HD21	2.03	0.40
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%)	41	61
All	All	1269/1412 (90%)	1214 (96%)	54 (4%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	315	HIS

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	270/297 (91%)	269 (100%)	1 (0%)	91	97
1	B	269/297 (91%)	268 (100%)	1 (0%)	91	97
1	C	269/297 (91%)	268 (100%)	1 (0%)	91	97
1	D	263/297 (89%)	261 (99%)	2 (1%)	81	93
All	All	1071/1188 (90%)	1066 (100%)	5 (0%)	88	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	232	PHE
1	B	232	PHE
1	C	232	PHE
1	D	32	GLU
1	D	232	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	HIS
1	B	292	GLN
1	B	315	HIS
1	C	142	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 [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%)	0.16	7 (2%) 62 65	26, 35, 53, 86	0
1	B	321/353 (90%)	0.35	13 (4%) 38 41	27, 38, 64, 105	0
1	C	321/353 (90%)	0.66	28 (8%) 10 10	29, 52, 91, 114	0
1	D	315/353 (89%)	0.92	42 (13%) 3 2	32, 50, 84, 113	0
All	All	1279/1412 (90%)	0.52	90 (7%) 16 16	26, 41, 82, 114	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	250	SER	8.8
1	D	230	GLU	8.2
1	D	232	PHE	6.3
1	C	338	LYS	6.1
1	B	339	GLN	5.8
1	D	343	THR	5.0
1	C	314	THR	4.9
1	D	225	LEU	4.9
1	B	338	LYS	4.9
1	A	338	LYS	4.2
1	D	231	HIS	4.2
1	D	269	VAL	4.2
1	D	344	GLN	4.1
1	D	204	ALA	4.0
1	C	232	PHE	4.0
1	C	196	GLY	4.0
1	D	227	ASP	3.9
1	D	251	LYS	3.8
1	D	253	ALA	3.8
1	C	264	ASN	3.8
1	C	226	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	229	LYS	3.7
1	B	33	GLU	3.5
1	D	255	VAL	3.5
1	D	275	LEU	3.5
1	D	256	LEU	3.5
1	C	230	GLU	3.4
1	D	226	ASP	3.2
1	B	314	THR	3.1
1	B	337	THR	3.1
1	D	249	ASP	3.1
1	D	224	LEU	3.0
1	C	88	ASP	2.9
1	C	265	ILE	2.9
1	D	234	ILE	2.9
1	A	232	PHE	2.9
1	D	342	ALA	2.9
1	C	251	LYS	2.9
1	C	216	ASN	2.9
1	D	334	GLN	2.8
1	A	339	GLN	2.8
1	D	223	LYS	2.7
1	D	206	GLY	2.7
1	D	273	GLU	2.7
1	D	274	SER	2.7
1	C	171	GLY	2.6
1	B	134	ARG	2.6
1	C	165	VAL	2.6
1	A	50	GLN	2.6
1	D	34	MET	2.6
1	D	245	ALA	2.6
1	D	272	PRO	2.6
1	C	183	THR	2.5
1	C	134	ARG	2.5
1	C	162	LYS	2.5
1	D	314	THR	2.5
1	C	174	ILE	2.5
1	C	199	LEU	2.5
1	B	137	GLU	2.5
1	D	208	LEU	2.4
1	C	217	LYS	2.4
1	D	64	LYS	2.4
1	A	314	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	340	GLN	2.4
1	D	222	LYS	2.3
1	B	232	PHE	2.3
1	A	337	THR	2.3
1	B	88	ASP	2.3
1	D	50	GLN	2.3
1	B	138	VAL	2.2
1	D	271	ALA	2.2
1	C	212	ASP	2.2
1	D	161	GLY	2.2
1	C	243	GLN	2.1
1	D	257	VAL	2.1
1	D	195	GLU	2.1
1	D	305	LYS	2.1
1	C	182	ASN	2.1
1	C	163	GLU	2.1
1	B	135	THR	2.1
1	C	339	GLN	2.1
1	C	241	ALA	2.1
1	D	309	THR	2.1
1	D	221	ARG	2.1
1	C	175	LYS	2.1
1	C	227	ASP	2.1
1	B	217	LYS	2.1
1	D	270	ALA	2.0
1	A	137	GLU	2.0
1	C	195	GLU	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.