



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2020 – 09:25 AM BST

PDB ID : 7BV6
Title : Crystal structure of the autophagic STX17/SNAP29/VAMP8 SNARE complex
Authors : Li, Y.; Pan, L.F.
Deposited on : 2020-04-09
Resolution : 3.05 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 : 2.14.4.dev1
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) : 2.14.4.dev1

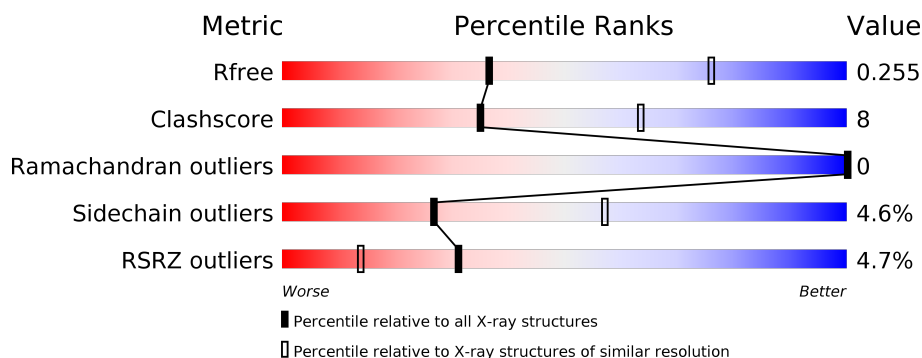
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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 on 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	68	<div> <div></div> <div>78%19%.</div> </div>
1	E	68	<div> <div>%</div> <div>82%13%.</div> </div>
1	I	68	<div> <div>%</div> <div>84%13%.</div> </div>
1	M	68	<div> <div>9%</div> <div>69%28%.</div> </div>
1	Q	68	<div> <div>12%</div> <div>68%22%10%</div> </div>
1	U	68	<div> <div>3%</div> <div>82%15%.</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	87	
2	F	87	
2	J	87	
2	N	87	
2	R	87	
2	V	87	
3	C	91	
3	G	91	
3	K	91	
3	O	91	
3	S	91	
3	W	91	
4	D	68	
4	H	68	
4	L	68	
4	P	68	
4	T	68	
4	X	68	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12345 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 Vesicle-associated membrane protein 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	66	Total	C	N	O	S	0	0	0
			547	336	106	104	1			
1	E	65	Total	C	N	O	S	0	0	0
			537	331	102	103	1			
1	I	66	Total	C	N	O	S	0	0	0
			537	330	102	104	1			
1	M	66	Total	C	N	O	S	0	0	0
			528	322	101	104	1			
1	Q	61	Total	C	N	O	S	0	0	0
			491	297	96	97	1			
1	U	66	Total	C	N	O	S	0	0	0
			539	330	104	104	1			

- Molecule 2 is a protein called Syntaxin-17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	61	Total	C	N	O	0	0	0
			459	285	75	99			
2	F	61	Total	C	N	O	0	0	0
			454	282	74	98			
2	J	59	Total	C	N	O	0	0	0
			441	272	72	97			
2	N	60	Total	C	N	O	0	0	0
			438	271	73	94			
2	R	55	Total	C	N	O	0	0	0
			413	255	67	91			
2	V	60	Total	C	N	O	0	0	0
			457	284	74	99			

- Molecule 3 is a protein called Synaptosomal-associated protein 29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	72	Total	C	N	O	S	0	0	0
			548	333	100	112	3			
3	G	74	Total	C	N	O	S	0	0	0
			560	342	102	113	3			
3	K	73	Total	C	N	O	S	0	0	0
			554	337	99	115	3			
3	O	73	Total	C	N	O	S	0	0	0
			555	336	103	113	3			
3	S	74	Total	C	N	O	S	0	0	0
			565	343	104	115	3			
3	W	72	Total	C	N	O	S	0	0	0
			541	329	97	112	3			


- Molecule 4 is a protein called Synaptosomal-associated protein 29.

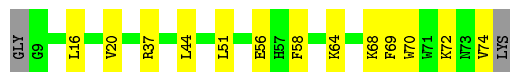
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	67	Total	C	N	O	S	0	0	0
			531	328	95	106	2			
4	H	68	Total	C	N	O	S	0	0	0
			539	332	95	110	2			
4	L	67	Total	C	N	O	S	0	0	0
			532	328	95	107	2			
4	P	65	Total	C	N	O	S	0	0	0
			525	323	94	106	2			
4	T	67	Total	C	N	O	S	0	0	0
			536	329	97	108	2			
4	X	65	Total	C	N	O	S	0	0	0
			518	319	93	104	2			

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.

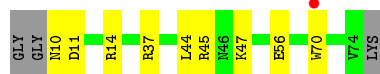
- Molecule 1: Vesicle-associated membrane protein 8

Chain A: 




- Molecule 1: Vesicle-associated membrane protein 8

Chain E: 



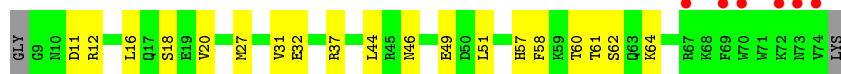
- Molecule 1: Vesicle-associated membrane protein 8

Chain I: 



- Molecule 1: Vesicle-associated membrane protein 8

Chain M: 

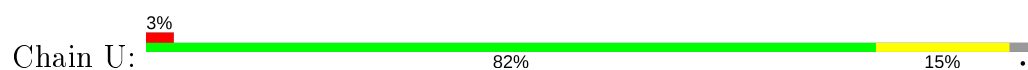


- Molecule 1: Vesicle-associated membrane protein 8

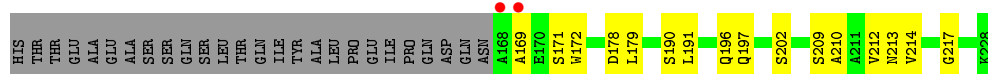
Chain Q: 



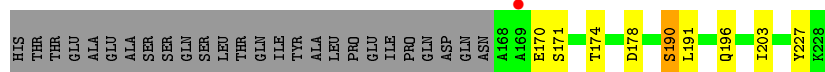
- Molecule 1: Vesicle-associated membrane protein 8



• Molecule 2: Syntaxin-17



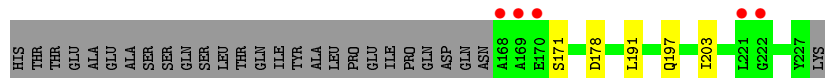
• Molecule 2: Syntaxin-17



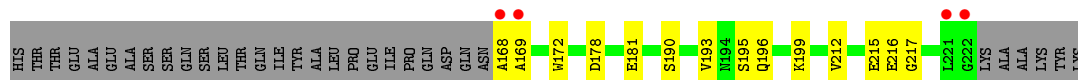
• Molecule 2: Syntaxin-17



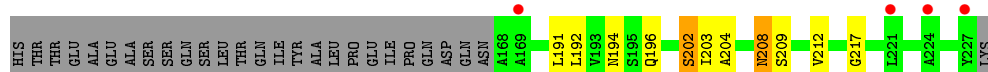
• Molecule 2: Syntaxin-17



• Molecule 2: Syntaxin-17



• Molecule 2: Syntaxin-17



- Molecule 3: Synaptosomal-associated protein 29

Chain C: 



- Molecule 3: Synaptosomal-associated protein 29

Chain G: 



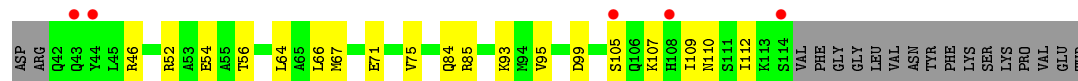
- Molecule 3: Synaptosomal-associated protein 29

Chain K: 



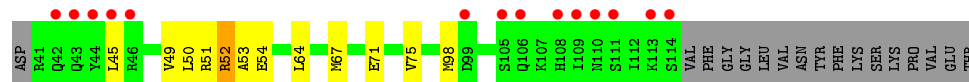
- Molecule 3: Synaptosomal-associated protein 29

Chain O: 



- Molecule 3: Synaptosomal-associated protein 29

Chain S: 



- Molecule 3: Synaptosomal-associated protein 29

Chain W: 

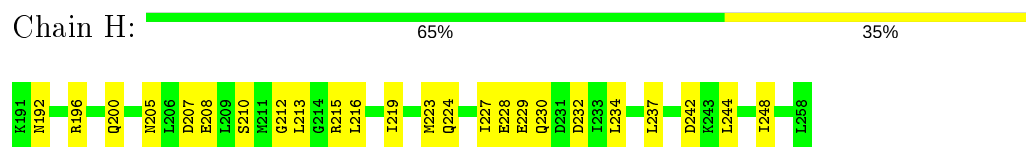


- Molecule 4: Synaptosomal-associated protein 29

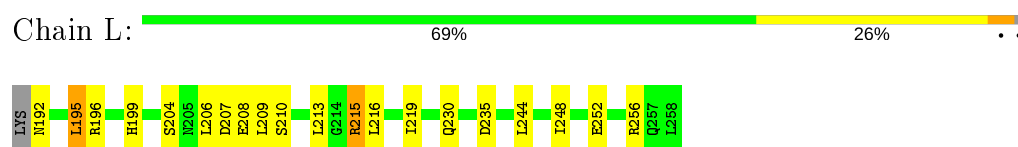
Chain D: 



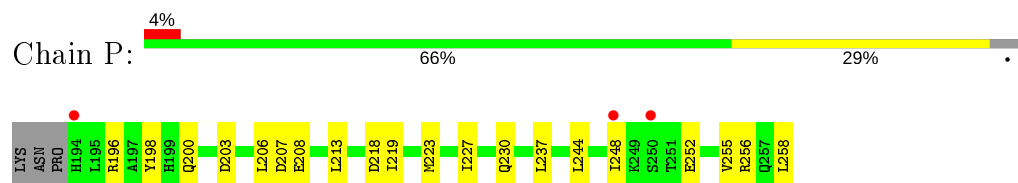
- Molecule 4: Synaptosomal-associated protein 29



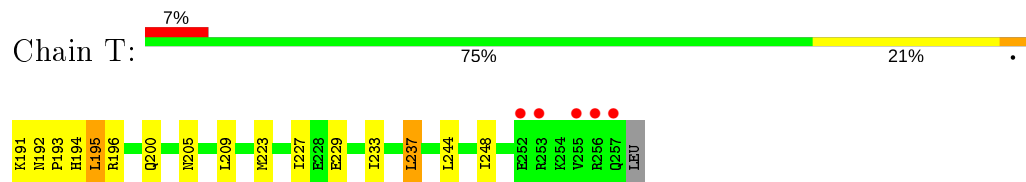
- Molecule 4: Synaptosomal-associated protein 29



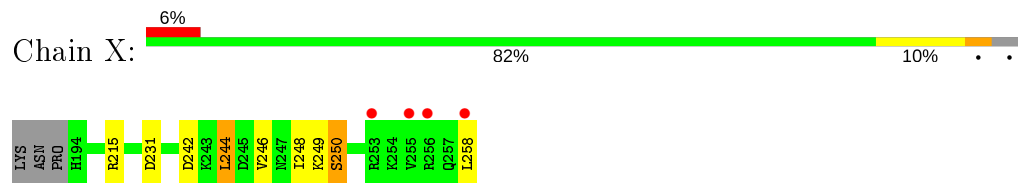
- Molecule 4: Synaptosomal-associated protein 29



- Molecule 4: Synaptosomal-associated protein 29



- Molecule 4: Synaptosomal-associated protein 29



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	143.98 Å 196.00 Å 76.14 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 3.05 49.00 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.00-3.05) 99.9 (49.00-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.07 Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.175 , 0.255 0.176 , 0.255	Depositor DCC
R_{free} test set	2088 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12345	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% 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	0.49	0/554	0.61	0/743
1	E	0.48	0/544	0.54	0/731
1	I	0.47	0/544	0.54	0/732
1	M	0.40	0/533	0.55	0/716
1	Q	0.39	0/494	0.54	0/660
1	U	0.43	0/546	0.54	0/735
2	B	0.44	0/463	0.59	0/627
2	F	0.44	0/458	0.58	0/623
2	J	0.45	0/444	0.58	0/603
2	N	0.47	0/441	0.54	0/600
2	R	0.44	0/416	0.57	0/566
2	V	0.44	0/461	0.61	0/625
3	C	0.47	0/549	0.60	0/733
3	G	0.47	0/562	0.59	0/752
3	K	0.43	0/556	0.60	0/744
3	O	0.47	0/556	0.58	0/743
3	S	0.43	0/567	0.60	1/758 (0.1%)
3	W	0.46	0/542	0.55	0/725
4	D	0.44	0/534	0.68	0/715
4	H	0.42	0/542	0.64	0/726
4	L	0.40	0/535	0.59	0/716
4	P	0.43	0/527	0.61	0/703
4	T	0.40	0/539	0.55	0/722
4	X	0.38	0/520	0.62	1/695 (0.1%)
All	All	0.44	0/12427	0.58	2/16693 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	50	LEU	CA-CB-CG	5.31	127.51	115.30
4	X	244	LEU	CB-CG-CD2	5.23	119.89	111.00

There are no chirality outliers.

There are no planarity outliers.

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	547	0	543	11	0
1	E	537	0	529	9	0
1	I	537	0	521	8	0
1	M	528	0	513	16	0
1	Q	491	0	489	14	0
1	U	539	0	521	8	0
2	B	459	0	442	16	0
2	F	454	0	431	7	0
2	J	441	0	424	8	0
2	N	438	0	418	6	0
2	R	413	0	395	17	0
2	V	457	0	444	9	0
3	C	548	0	553	15	0
3	G	560	0	555	17	0
3	K	554	0	543	21	0
3	O	555	0	555	15	0
3	S	565	0	558	6	0
3	W	541	0	537	12	0
4	D	531	0	539	15	0
4	H	539	0	542	18	0
4	L	532	0	539	22	0
4	P	525	0	538	16	0
4	T	536	0	542	11	0
4	X	518	0	528	10	0
All	All	12345	0	12199	202	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 8.

All (202) 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)
3:K:67:MET:HE1	4:L:216:LEU:HD12	1.45	0.98
3:K:67:MET:CE	4:L:216:LEU:HD12	1.98	0.91
3:K:67:MET:CE	4:L:216:LEU:CD1	2.55	0.83
3:K:95:VAL:HG13	4:L:244:LEU:HD12	1.64	0.78
3:G:95:VAL:HG13	4:H:244:LEU:HD12	1.66	0.77
1:E:44:LEU:HD23	2:F:203:ILE:HD13	1.66	0.76
4:D:253:ARG:HA	4:D:256:ARG:HD2	1.69	0.75
2:B:197:GLN:HG2	3:C:84:GLN:HE21	1.50	0.75
3:K:67:MET:HE1	4:L:216:LEU:CD1	2.15	0.73
3:K:67:MET:HE3	4:L:216:LEU:CD1	2.18	0.72
3:W:68:TYR:HE1	4:X:215:ARG:HH22	1.39	0.71
1:M:61:THR:HG21	4:P:256:ARG:HG2	1.72	0.70
3:W:95:VAL:HG13	4:X:244:LEU:HD12	1.74	0.68
1:M:20:VAL:HG11	2:N:178:ASP:HB3	1.77	0.67
2:B:169:ALA:HA	2:B:172:TRP:HD1	1.59	0.66
2:B:197:GLN:HG2	3:C:84:GLN:NE2	2.11	0.65
3:K:51:ARG:HA	3:K:54:GLU:HB2	1.78	0.65
1:E:37:ARG:NH2	2:F:196:GLN:OE1	2.30	0.64
3:S:51:ARG:NH2	3:S:54:GLU:OE2	2.31	0.64
3:C:72:LYS:HD3	1:U:32:GLU:OE1	1.98	0.63
2:J:181:GLU:HG2	3:O:66:LEU:HD21	1.81	0.63
1:Q:37:ARG:NH2	2:R:196:GLN:OE1	2.32	0.62
3:O:105:SER:O	3:O:109:ILE:HG12	1.99	0.62
1:A:44:LEU:HD21	4:D:237:LEU:HD13	1.82	0.62
3:G:102:LEU:HD11	4:H:248:ILE:HG12	1.81	0.62
1:I:31:VAL:O	1:I:34:ILE:HG22	2.01	0.61
4:X:244:LEU:HD22	4:X:248:ILE:HD11	1.83	0.60
4:T:223:MET:O	4:T:227:ILE:HG13	2.01	0.60
2:R:212:VAL:HA	2:R:215:GLU:HB2	1.84	0.60
3:K:67:MET:HE3	4:L:216:LEU:HD11	1.84	0.59
3:C:67:MET:HG2	4:D:216:LEU:HD11	1.83	0.59
1:E:11:ASP:OD2	1:E:14:ARG:NH2	2.35	0.59
4:D:195:LEU:HD22	4:D:199:HIS:NE2	2.17	0.59
3:W:112:ILE:HD11	4:X:258:LEU:HD13	1.85	0.58
1:M:61:THR:HG22	4:P:255:VAL:HG12	1.85	0.58
1:Q:61:THR:HG23	1:Q:64:LYS:HD2	1.85	0.58
3:C:52:ARG:O	3:C:56:THR:HG23	2.02	0.58
4:P:248:ILE:O	4:P:252:GLU:HB2	2.03	0.58
3:S:98:MET:HB3	4:T:244:LEU:HD11	1.86	0.58
1:U:48:THR:HG21	2:V:203:ILE:HG23	1.87	0.57
2:N:197:GLN:HG2	3:O:84:GLN:HE21	1.70	0.56
2:R:195:SER:HB3	2:V:194:ASN:OD1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:85:ARG:HB2	4:P:230:GLN:HE21	1.71	0.56
1:M:60:THR:HG22	1:M:64:LYS:HE3	1.88	0.56
2:N:197:GLN:HG2	3:O:84:GLN:NE2	2.21	0.55
3:O:109:ILE:HA	3:O:112:ILE:HG22	1.87	0.55
4:H:215:ARG:O	4:H:219:ILE:HG13	2.06	0.55
1:Q:61:THR:HA	1:Q:64:LYS:HB3	1.89	0.55
3:G:67:MET:SD	4:H:212:GLY:HA3	2.46	0.55
3:K:67:MET:HE3	4:L:216:LEU:HD12	1.82	0.55
1:A:70:TRP:O	1:A:74:VAL:HG22	2.08	0.54
3:S:64:LEU:HD12	4:T:205:ASN:HA	1.89	0.54
1:I:62:SER:HB3	2:J:220:ASN:HB2	1.90	0.54
4:L:192:ASN:N	4:L:196:ARG:HH11	2.05	0.53
1:A:56:GLU:HG3	2:B:213:ASN:HD21	1.74	0.53
3:W:98:MET:HB2	4:X:244:LEU:HD11	1.91	0.53
2:B:169:ALA:HA	2:B:172:TRP:CD1	2.41	0.53
3:C:102:LEU:HD11	4:D:248:ILE:HG12	1.91	0.53
1:E:37:ARG:NH1	3:G:84:GLN:OE1	2.40	0.53
1:A:58:PHE:CE2	2:B:217:GLY:HA3	2.44	0.52
3:K:85:ARG:HB2	4:L:230:GLN:HE21	1.74	0.52
3:W:52:ARG:O	3:W:56:THR:HG23	2.09	0.52
1:A:64:LYS:HD3	1:A:68:LYS:NZ	2.25	0.52
1:A:16:LEU:HD13	4:D:209:LEU:HD23	1.92	0.52
1:Q:34:ILE:HD13	2:R:193:VAL:HG22	1.90	0.52
1:U:54:THR:HG21	4:X:249:LYS:HG3	1.91	0.52
1:A:37:ARG:NH2	2:B:196:GLN:OE1	2.42	0.51
3:W:71:GLU:O	3:W:75:VAL:HG13	2.10	0.51
2:B:191:LEU:HD21	2:R:190:SER:HB3	1.92	0.51
2:B:197:GLN:CG	3:C:84:GLN:HE21	2.19	0.51
4:P:223:MET:O	4:P:227:ILE:HG13	2.11	0.51
3:K:100:GLN:HG3	3:K:103:LYS:HE3	1.93	0.51
3:K:64:LEU:O	3:K:67:MET:HB3	2.11	0.51
2:F:191:LEU:HD21	2:J:190:SER:HB3	1.92	0.51
3:C:67:MET:SD	4:D:212:GLY:HA3	2.51	0.51
3:C:92:GLU:OE2	4:D:236:ARG:HD2	2.11	0.50
1:Q:45:ARG:NH1	2:R:199:LYS:HG2	2.26	0.50
1:A:51:LEU:HD22	4:D:241:VAL:HG13	1.93	0.50
3:G:67:MET:HG2	4:H:216:LEU:HD11	1.93	0.50
3:K:100:GLN:HA	3:K:103:LYS:HE3	1.93	0.50
2:R:169:ALA:HA	2:R:172:TRP:HD1	1.76	0.50
2:F:190:SER:HB3	2:N:191:LEU:HD21	1.94	0.49
3:G:68:TYR:O	3:G:72:LYS:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:64:LEU:HD11	4:P:208:GLU:HB2	1.94	0.49
2:V:204:ALA:O	2:V:208:ASN:HB2	2.13	0.49
4:H:196:ARG:O	4:H:200:GLN:HG3	2.13	0.49
3:O:107:LYS:HA	3:O:110:ASN:HB2	1.95	0.49
3:K:85:ARG:HB2	4:L:230:GLN:NE2	2.28	0.48
1:A:56:GLU:HG3	2:B:213:ASN:ND2	2.27	0.48
3:S:45:LEU:O	3:S:49:VAL:HG23	2.14	0.48
4:P:219:ILE:O	4:P:223:MET:HG3	2.14	0.47
1:M:20:VAL:CG1	2:N:178:ASP:HB3	2.44	0.47
3:O:52:ARG:O	3:O:56:THR:HG23	2.14	0.47
1:Q:20:VAL:HG11	2:R:178:ASP:HB3	1.97	0.47
3:W:51:ARG:O	3:W:54:GLU:N	2.48	0.47
3:G:85:ARG:HH11	3:W:85:ARG:HH11	1.63	0.47
2:R:169:ALA:HA	2:R:172:TRP:CD1	2.49	0.47
3:O:71:GLU:O	3:O:75:VAL:HG13	2.15	0.47
2:F:170:GLU:O	2:F:174:THR:HG23	2.15	0.46
1:U:62:SER:OG	2:V:217:GLY:HA2	2.16	0.46
4:D:195:LEU:HD22	4:D:199:HIS:CE1	2.50	0.46
3:C:98:MET:HB2	4:D:244:LEU:HD11	1.98	0.46
3:S:71:GLU:O	3:S:75:VAL:HG13	2.16	0.46
4:D:253:ARG:O	4:D:257:GLN:HG3	2.15	0.46
4:H:223:MET:O	4:H:227:ILE:HG13	2.16	0.46
4:P:244:LEU:O	4:P:248:ILE:HG12	2.16	0.46
1:Q:42:GLU:HG2	2:R:199:LYS:HD3	1.97	0.46
3:O:64:LEU:HA	3:O:64:LEU:HD23	1.80	0.46
1:U:45:ARG:HD3	2:V:202:SER:HB3	1.97	0.46
4:H:224:GLN:O	4:H:228:GLU:HG3	2.16	0.46
4:T:195:LEU:HD23	4:T:195:LEU:HA	1.65	0.46
3:W:102:LEU:HD11	4:X:248:ILE:HG12	1.98	0.46
3:O:54:GLU:HB2	4:P:198:TYR:CE2	2.51	0.45
4:X:244:LEU:HD22	4:X:248:ILE:CD1	2.44	0.45
2:J:170:GLU:O	2:J:174:THR:HG23	2.17	0.45
1:M:46:ASN:O	1:M:49:GLU:N	2.50	0.45
2:B:190:SER:HB2	2:V:191:LEU:HD21	1.97	0.45
3:C:56:THR:O	3:C:60:THR:HG23	2.17	0.45
3:G:85:ARG:HD2	4:H:229:GLU:OE1	2.17	0.45
2:V:209:SER:O	2:V:212:VAL:HG22	2.16	0.44
3:C:64:LEU:HD11	4:D:208:GLU:HB2	2.00	0.44
3:G:83:ARG:O	3:G:87:VAL:HG23	2.18	0.44
4:T:244:LEU:O	4:T:248:ILE:N	2.46	0.44
1:U:47:LYS:HD3	4:X:242:ASP:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:102:LEU:HD11	4:L:248:ILE:HG12	1.99	0.44
3:C:93:LYS:O	3:C:97:LYS:HG3	2.18	0.44
1:M:37:ARG:NH2	3:O:84:GLN:OE1	2.43	0.44
1:Q:58:PHE:CE2	2:R:217:GLY:HA3	2.53	0.44
1:I:20:VAL:HG22	4:L:213:LEU:HD21	2.00	0.44
4:P:255:VAL:O	4:P:258:LEU:HB3	2.18	0.43
1:Q:59:LYS:HD2	2:R:216:GLU:OE1	2.18	0.43
1:U:45:ARG:HD3	2:V:202:SER:CB	2.48	0.43
3:G:85:ARG:HB2	4:H:230:GLN:HE21	1.83	0.43
4:L:196:ARG:HA	4:L:199:HIS:HD2	1.82	0.43
4:L:215:ARG:O	4:L:219:ILE:HG13	2.17	0.43
3:G:72:LYS:HE3	1:M:32:GLU:HG3	2.00	0.43
1:E:47:LYS:HD3	4:H:242:ASP:OD1	2.19	0.43
3:K:75:VAL:O	3:K:79:GLU:HG3	2.18	0.43
4:X:246:VAL:O	4:X:250:SER:HB3	2.18	0.43
1:A:69:PHE:HE2	1:A:72:LYS:HZ2	1.64	0.43
1:E:44:LEU:HD21	4:H:237:LEU:HD13	2.01	0.43
1:M:27:MET:O	1:M:31:VAL:HG23	2.19	0.43
3:K:64:LEU:HD22	3:K:68:TYR:CE2	2.54	0.43
4:T:237:LEU:HD23	4:T:237:LEU:HA	1.79	0.43
4:T:191:LYS:N	4:T:194:HIS:HB2	2.34	0.42
1:E:44:LEU:HD22	4:H:234:LEU:HD23	1.99	0.42
1:M:37:ARG:NH1	4:P:230:GLN:OE1	2.51	0.42
1:M:20:VAL:HG23	4:P:213:LEU:HD11	2.01	0.42
1:M:20:VAL:HG23	4:P:213:LEU:CD1	2.49	0.42
2:B:179:LEU:HD23	2:B:179:LEU:HA	1.75	0.42
4:D:244:LEU:HD23	4:D:244:LEU:HA	1.83	0.42
1:I:44:LEU:HD23	2:J:203:ILE:HD13	2.00	0.42
1:M:51:LEU:HD11	4:P:244:LEU:CD1	2.49	0.42
3:S:52:ARG:HH21	3:S:53:ALA:HB2	1.85	0.42
4:T:229:GLU:O	4:T:233:ILE:HG13	2.19	0.42
3:C:80:GLU:HA	3:C:83:ARG:NH1	2.34	0.42
1:Q:10:ASN:ND2	2:R:168:ALA:O	2.42	0.42
2:B:210:ALA:O	2:B:214:VAL:HG23	2.20	0.41
4:H:244:LEU:O	4:H:248:ILE:HG13	2.19	0.41
1:I:34:ILE:HA	1:I:34:ILE:HD12	1.87	0.41
2:J:210:ALA:O	2:J:214:VAL:HG23	2.20	0.41
1:Q:16:LEU:HD13	4:T:209:LEU:HD23	2.02	0.41
4:L:195:LEU:HD23	4:L:196:ARG:HD2	2.01	0.41
1:M:58:PHE:O	1:M:62:SER:OG	2.28	0.41
1:Q:34:ILE:CD1	2:R:193:VAL:HG22	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:192:LEU:O	2:V:196:GLN:HG3	2.20	0.41
3:O:93:LYS:HB2	3:O:93:LYS:HE3	1.86	0.41
1:Q:10:ASN:HA	1:Q:13:VAL:HG12	2.01	0.41
2:R:181:GLU:OE2	3:W:62:ARG:HD2	2.21	0.41
1:U:43:HIS:O	1:U:47:LYS:HG3	2.20	0.41
1:M:44:LEU:HD23	2:N:203:ILE:HD13	2.02	0.41
1:A:20:VAL:HG11	2:B:178:ASP:HB3	2.02	0.41
4:H:213:LEU:HA	4:H:213:LEU:HD23	1.75	0.41
1:I:42:GLU:OE2	2:J:199:LYS:HE2	2.21	0.41
1:Q:62:SER:OG	2:R:217:GLY:HA2	2.20	0.41
2:B:209:SER:O	2:B:212:VAL:HG22	2.20	0.41
3:C:45:LEU:O	3:C:45:LEU:HD13	2.21	0.41
3:G:87:VAL:HG13	3:G:90:ARG:NH2	2.35	0.41
4:L:207:ASP:O	4:L:210:SER:OG	2.31	0.41
3:G:68:TYR:OH	4:H:208:GLU:OE2	2.30	0.41
1:I:64:LYS:O	1:I:68:LYS:HB2	2.21	0.41
1:M:16:LEU:CD1	4:P:206:LEU:HD22	2.50	0.41
3:G:85:ARG:NH1	3:W:85:ARG:HH11	2.18	0.41
2:B:191:LEU:HD21	2:R:190:SER:CB	2.50	0.41
3:G:64:LEU:HD12	4:H:205:ASN:HA	2.03	0.41
3:K:100:GLN:HG3	3:K:103:LYS:CE	2.51	0.41
4:T:196:ARG:O	4:T:200:GLN:HG3	2.21	0.41
3:W:102:LEU:HA	3:W:102:LEU:HD23	1.66	0.41
1:E:10:ASN:CG	1:E:11:ASP:H	2.24	0.40
2:F:191:LEU:HD21	2:J:190:SER:CB	2.51	0.40
3:K:64:LEU:HD11	4:L:208:GLU:HB2	2.02	0.40
3:O:95:VAL:HG13	4:P:244:LEU:HG	2.02	0.40
3:G:85:ARG:HB2	4:H:230:GLN:NE2	2.37	0.40
1:I:16:LEU:HD11	4:L:206:LEU:HB3	2.02	0.40
3:K:108:HIS:O	3:K:112:ILE:HG13	2.21	0.40
4:L:248:ILE:O	4:L:252:GLU:HB2	2.22	0.40
4:D:213:LEU:HD23	4:D:216:LEU:HD12	2.02	0.40
4:L:209:LEU:HD12	4:L:209:LEU:HA	1.77	0.40
4:T:192:ASN:H	4:T:193:PRO:HD2	1.87	0.40
1:E:70:TRP:HB2	2:F:227:TYR:CE2	2.57	0.40
3:G:105:SER:O	3:G:109:ILE:HG13	2.21	0.40
3:K:67:MET:HE1	4:L:216:LEU:CG	2.52	0.40

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	64/68 (94%)	62 (97%)	2 (3%)	0	100	100
1	E	63/68 (93%)	62 (98%)	1 (2%)	0	100	100
1	I	64/68 (94%)	60 (94%)	4 (6%)	0	100	100
1	M	64/68 (94%)	62 (97%)	2 (3%)	0	100	100
1	Q	59/68 (87%)	58 (98%)	1 (2%)	0	100	100
1	U	64/68 (94%)	64 (100%)	0	0	100	100
2	B	59/87 (68%)	58 (98%)	1 (2%)	0	100	100
2	F	59/87 (68%)	57 (97%)	2 (3%)	0	100	100
2	J	57/87 (66%)	56 (98%)	1 (2%)	0	100	100
2	N	58/87 (67%)	55 (95%)	3 (5%)	0	100	100
2	R	53/87 (61%)	51 (96%)	2 (4%)	0	100	100
2	V	58/87 (67%)	57 (98%)	1 (2%)	0	100	100
3	C	70/91 (77%)	67 (96%)	3 (4%)	0	100	100
3	G	72/91 (79%)	72 (100%)	0	0	100	100
3	K	71/91 (78%)	71 (100%)	0	0	100	100
3	O	71/91 (78%)	68 (96%)	3 (4%)	0	100	100
3	S	72/91 (79%)	71 (99%)	1 (1%)	0	100	100
3	W	70/91 (77%)	69 (99%)	1 (1%)	0	100	100
4	D	65/68 (96%)	64 (98%)	1 (2%)	0	100	100
4	H	66/68 (97%)	63 (96%)	3 (4%)	0	100	100
4	L	65/68 (96%)	63 (97%)	2 (3%)	0	100	100
4	P	63/68 (93%)	63 (100%)	0	0	100	100
4	T	65/68 (96%)	63 (97%)	2 (3%)	0	100	100
4	X	63/68 (93%)	62 (98%)	1 (2%)	0	100	100
All	All	1535/1884 (82%)	1498 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	60/61 (98%)	60 (100%)	0	100	100
1	E	59/61 (97%)	57 (97%)	2 (3%)	37	67
1	I	58/61 (95%)	58 (100%)	0	100	100
1	M	57/61 (93%)	53 (93%)	4 (7%)	15	41
1	Q	54/61 (88%)	52 (96%)	2 (4%)	34	64
1	U	58/61 (95%)	55 (95%)	3 (5%)	23	52
2	B	49/74 (66%)	47 (96%)	2 (4%)	30	61
2	F	48/74 (65%)	45 (94%)	3 (6%)	18	45
2	J	48/74 (65%)	44 (92%)	4 (8%)	11	35
2	N	46/74 (62%)	45 (98%)	1 (2%)	52	76
2	R	46/74 (62%)	46 (100%)	0	100	100
2	V	50/74 (68%)	48 (96%)	2 (4%)	31	62
3	C	59/80 (74%)	57 (97%)	2 (3%)	37	67
3	G	58/80 (72%)	57 (98%)	1 (2%)	60	82
3	K	58/80 (72%)	54 (93%)	4 (7%)	15	42
3	O	59/80 (74%)	56 (95%)	3 (5%)	24	53
3	S	59/80 (74%)	57 (97%)	2 (3%)	37	67
3	W	57/80 (71%)	53 (93%)	4 (7%)	15	41
4	D	59/63 (94%)	56 (95%)	3 (5%)	24	53
4	H	60/63 (95%)	56 (93%)	4 (7%)	16	43
4	L	59/63 (94%)	54 (92%)	5 (8%)	10	34
4	P	59/63 (94%)	53 (90%)	6 (10%)	7	24
4	T	60/63 (95%)	58 (97%)	2 (3%)	38	67
4	X	58/63 (92%)	56 (97%)	2 (3%)	37	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1338/1668 (80%)	1277 (95%)	61 (5%)	27 57

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	171	SER
2	B	202	SER
3	C	51	ARG
3	C	67	MET
4	D	243	LYS
4	D	244	LEU
4	D	250	SER
1	E	45	ARG
1	E	56	GLU
2	F	171	SER
2	F	178	ASP
2	F	190	SER
3	G	81	LEU
4	H	192	ASN
4	H	207	ASP
4	H	210	SER
4	H	232	ASP
2	J	171	SER
2	J	178	ASP
2	J	194	ASN
2	J	205	ASP
3	K	43	GLN
3	K	44	TYR
3	K	59	SER
3	K	85	ARG
4	L	195	LEU
4	L	204	SER
4	L	215	ARG
4	L	235	ASP
4	L	256	ARG
1	M	11	ASP
1	M	12	ARG
1	M	18	SER
1	M	57	HIS
2	N	171	SER
3	O	46	ARG
3	O	67	MET

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Mol	Chain	Res	Type
3	O	99	ASP
4	P	196	ARG
4	P	200	GLN
4	P	203	ASP
4	P	207	ASP
4	P	218	ASP
4	P	237	LEU
1	Q	11	ASP
1	Q	69	PHE
3	S	52	ARG
3	S	67	MET
4	T	195	LEU
4	T	237	LEU
1	U	11	ASP
1	U	12	ARG
1	U	71	TRP
2	V	202	SER
2	V	208	ASN
3	W	45	LEU
3	W	51	ARG
3	W	67	MET
3	W	78	SER
4	X	231	ASP
4	X	250	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	84	GLN
2	F	184	GLN
2	R	197	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	66/68 (97%)	-0.20	0 100 100	25, 47, 97, 129	0
1	E	65/68 (95%)	-0.40	1 (1%) 73 51	25, 50, 90, 124	0
1	I	66/68 (97%)	-0.12	1 (1%) 73 51	28, 52, 147, 184	0
1	M	66/68 (97%)	-0.02	6 (9%) 9 3	27, 59, 123, 147	0
1	Q	61/68 (89%)	0.16	8 (13%) 3 1	30, 69, 144, 185	0
1	U	66/68 (97%)	-0.04	2 (3%) 50 25	25, 62, 112, 153	0
2	B	61/87 (70%)	-0.17	2 (3%) 46 23	24, 38, 83, 148	0
2	F	61/87 (70%)	-0.20	1 (1%) 72 49	27, 42, 97, 177	0
2	J	59/87 (67%)	-0.02	0 100 100	25, 46, 121, 124	0
2	N	60/87 (68%)	0.10	5 (8%) 11 4	24, 47, 127, 180	0
2	R	55/87 (63%)	0.13	4 (7%) 15 5	29, 54, 133, 182	0
2	V	60/87 (68%)	0.01	4 (6%) 17 7	29, 50, 116, 151	0
3	C	72/91 (79%)	-0.14	0 100 100	29, 44, 98, 137	0
3	G	74/91 (81%)	-0.32	0 100 100	27, 44, 94, 106	0
3	K	73/91 (80%)	0.22	4 (5%) 25 10	26, 52, 124, 171	0
3	O	73/91 (80%)	0.18	5 (6%) 17 6	24, 53, 137, 157	0
3	S	74/91 (81%)	0.53	14 (18%) 1 0	30, 57, 156, 170	0
3	W	72/91 (79%)	0.09	6 (8%) 11 4	31, 52, 117, 133	0
4	D	67/68 (98%)	-0.42	0 100 100	28, 46, 74, 106	0
4	H	68/68 (100%)	-0.23	0 100 100	31, 49, 83, 114	0
4	L	67/68 (98%)	-0.11	0 100 100	29, 51, 109, 140	0
4	P	65/68 (95%)	0.06	3 (4%) 32 15	28, 55, 115, 137	0
4	T	67/68 (98%)	0.15	5 (7%) 14 5	28, 54, 124, 152	0
4	X	65/68 (95%)	0.09	4 (6%) 20 8	31, 59, 109, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	1583/1884 (84%)	-0.03	75 (4%) 31 14	24, 51, 126, 185	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	44	TYR	5.7
2	B	168	ALA	5.5
2	N	169	ALA	5.3
3	O	44	TYR	4.7
2	R	168	ALA	4.2
3	S	99	ASP	4.0
3	S	106	GLN	3.7
3	S	113	LYS	3.6
3	W	106	GLN	3.6
1	Q	65	VAL	3.6
3	S	110	ASN	3.5
4	T	257	GLN	3.5
3	S	44	TYR	3.5
2	R	222	GLY	3.4
3	S	108	HIS	3.4
2	N	221	LEU	3.2
3	S	109	ILE	3.2
3	K	45	LEU	3.1
1	I	71	TRP	3.1
1	Q	68	LYS	3.1
2	R	169	ALA	3.1
3	W	44	TYR	3.0
3	W	112	ILE	3.0
2	V	227	TYR	3.0
3	S	42	GLN	2.9
2	B	169	ALA	2.9
1	M	72	LYS	2.9
3	S	111	SER	2.8
3	S	114	SER	2.8
2	N	168	ALA	2.8
4	X	255	VAL	2.8
1	M	70	TRP	2.7
1	M	69	PHE	2.6
1	U	73	ASN	2.6
2	R	221	LEU	2.6
1	Q	64	LYS	2.6
2	F	169	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	V	169	ALA	2.5
4	X	256	ARG	2.5
3	S	45	LEU	2.5
4	T	253	ARG	2.5
1	M	73	ASN	2.4
3	S	43	GLN	2.4
3	O	43	GLN	2.4
1	M	74	VAL	2.4
3	S	105	SER	2.4
3	W	105	SER	2.4
3	W	43	GLN	2.4
3	S	46	ARG	2.3
2	V	221	LEU	2.3
1	Q	9	GLY	2.3
4	T	255	VAL	2.3
1	Q	69	PHE	2.3
3	O	105	SER	2.3
4	X	258	LEU	2.3
3	K	47	GLN	2.3
3	O	114	SER	2.2
3	K	42	GLN	2.2
1	Q	67	ARG	2.2
4	T	256	ARG	2.2
3	W	45	LEU	2.1
4	P	248	ILE	2.1
2	N	222	GLY	2.1
1	M	67	ARG	2.1
4	P	250	SER	2.1
4	P	194	HIS	2.1
2	V	224	ALA	2.1
1	Q	57	HIS	2.1
1	E	70	TRP	2.0
1	Q	66	ALA	2.0
1	U	74	VAL	2.0
3	O	108	HIS	2.0
4	T	252	GLU	2.0
4	X	253	ARG	2.0
2	N	170	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.