



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 02:18 AM BST

PDB ID : 6VME
Title : Human ESCRT-I heterotetramer headpiece
Authors : Flower, T.G.; Hurley, J.H.; Tjahjono, N.
Deposited on : 2020-01-27
Resolution : 2.19 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	:	2.13.1
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)	:	2.13.1

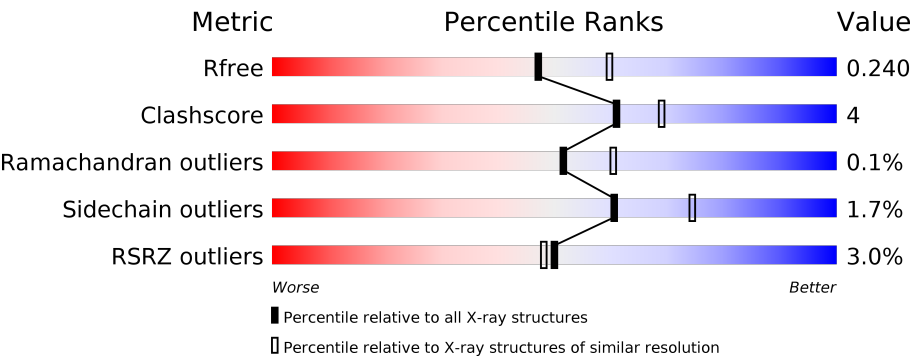
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	B	81	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>90% • 6%</div></div>
1	F	81	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>81% 11% • 5%</div></div>
1	G	81	<div><div>2%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>86% 5% • 7%</div></div>
1	H	81	<div><div>2%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>90% • 6%</div></div>
1	I	81	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>79% 11% • 7%</div></div>
1	J	81	<div><div>6%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>74% 20% 6%</div></div>

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Mol	Chain	Length	Quality of chain
2	C	71	
2	K	71	
2	L	71	
2	M	71	
2	N	71	
2	O	71	
3	A	25	
3	D	25	
3	P	25	
3	Q	25	
3	R	25	
3	T	25	
4	E	122	
4	U	122	
4	V	122	
4	W	122	
4	X	122	
4	Y	122	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12786 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 Tumor susceptibility gene 101 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	76	Total	C	N	O	S	0	0	0
			607	391	107	108	1			
1	F	77	Total	C	N	O	S	0	0	0
			615	397	108	109	1			
1	G	75	Total	C	N	O	S	0	0	0
			603	389	106	107	1			
1	H	76	Total	C	N	O	S	0	0	0
			607	392	106	108	1			
1	I	75	Total	C	N	O	S	0	0	0
			602	390	106	105	1			
1	J	76	Total	C	N	O	S	0	0	0
			604	390	107	106	1			

- Molecule 2 is a protein called Vacuolar protein sorting-associated protein 37B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	67	Total	C	N	O	S	0	0	0
			527	331	88	105	3			
2	K	65	Total	C	N	O	S	0	0	0
			521	330	87	101	3			
2	L	65	Total	C	N	O	S	0	0	0
			517	328	87	99	3			
2	M	65	Total	C	N	O	S	0	0	0
			514	326	86	99	3			
2	N	67	Total	C	N	O	S	0	0	0
			530	334	88	105	3			
2	O	62	Total	C	N	O	S	0	0	0
			488	310	82	93	3			

- Molecule 3 is a protein called Multivesicular body subunit 12A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	19	Total	C	N	O	S	0	0	0
			135	87	21	26	1			
3	P	20	Total	C	N	O	S	0	0	0
			137	89	20	27	1			
3	Q	18	Total	C	N	O	S	0	0	0
			118	75	18	24	1			
3	R	21	Total	C	N	O	S	0	0	0
			143	92	21	29	1			
3	A	20	Total	C	N	O	S	0	0	0
			135	87	20	27	1			
3	T	18	Total	C	N	O	S	0	0	0
			125	81	18	25	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	204	SER	-	expression tag	UNP Q96EY5
D	205	ASN	-	expression tag	UNP Q96EY5
P	204	SER	-	expression tag	UNP Q96EY5
P	205	ASN	-	expression tag	UNP Q96EY5
Q	204	SER	-	expression tag	UNP Q96EY5
Q	205	ASN	-	expression tag	UNP Q96EY5
R	204	SER	-	expression tag	UNP Q96EY5
R	205	ASN	-	expression tag	UNP Q96EY5
A	204	SER	-	expression tag	UNP Q96EY5
A	205	ASN	-	expression tag	UNP Q96EY5
T	204	SER	-	expression tag	UNP Q96EY5
T	205	ASN	-	expression tag	UNP Q96EY5

- Molecule 4 is a protein called Vacuolar protein sorting-associated protein 28 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	102	Total	C	N	O	S	0	0	0
			822	520	138	157	7			
4	U	102	Total	C	N	O	S	0	0	0
			827	524	141	155	7			
4	V	104	Total	C	N	O	S	0	0	0
			826	523	139	157	7			
4	W	105	Total	C	N	O	S	0	0	0
			840	530	143	160	7			
4	X	101	Total	C	N	O	S	0	0	0
			820	520	137	156	7			
4	Y	100	Total	C	N	O	S	0	0	0
			815	515	138	155	7			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	10	Total O 10 10	0	0
5	C	8	Total O 8 8	0	0
5	D	3	Total O 3 3	0	0
5	E	31	Total O 31 31	0	0
5	F	18	Total O 18 18	0	0
5	G	16	Total O 16 16	0	0
5	H	5	Total O 5 5	0	0
5	I	10	Total O 10 10	0	0
5	J	5	Total O 5 5	0	0
5	K	12	Total O 12 12	0	0
5	L	3	Total O 3 3	0	0
5	M	6	Total O 6 6	0	0
5	N	15	Total O 15 15	0	0
5	O	1	Total O 1 1	0	0
5	P	7	Total O 7 7	0	0
5	Q	2	Total O 2 2	0	0
5	R	2	Total O 2 2	0	0
5	A	10	Total O 10 10	0	0
5	U	34	Total O 34 34	0	0
5	V	37	Total O 37 37	0	0
5	W	22	Total O 22 22	0	0

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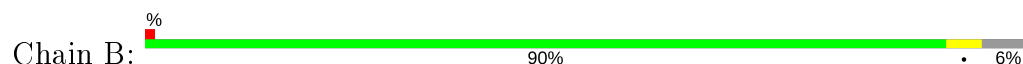
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	X	25	Total	O	0	0
			25	25		
5	Y	26	Total	O	0	0
			26	26		

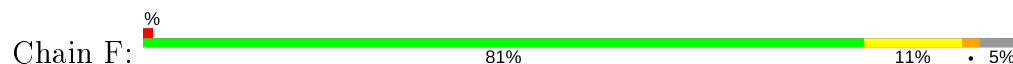
3 Residue-property plots [i](#)

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.

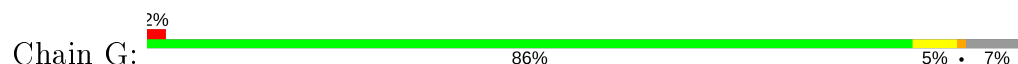
- Molecule 1: Tumor susceptibility gene 101 protein



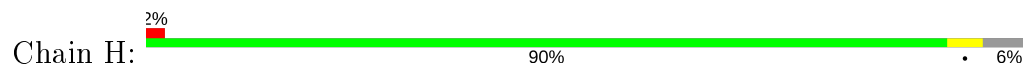
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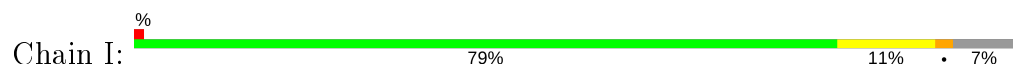
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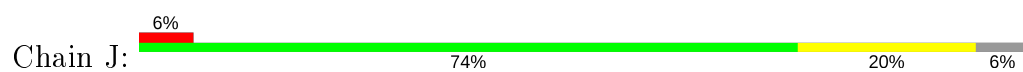
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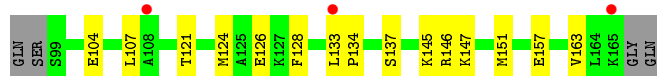
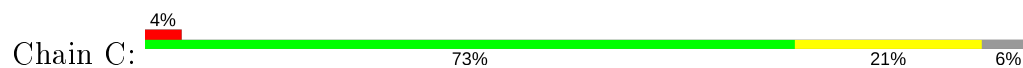
- Molecule 1: Tumor susceptibility gene 101 protein



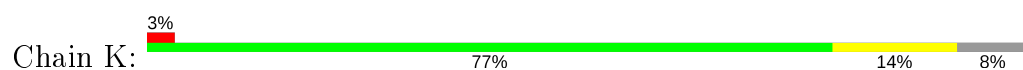
- Molecule 1: Tumor susceptibility gene 101 protein



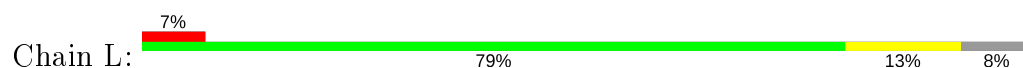
- Molecule 2: Vacuolar protein sorting-associated protein 37B



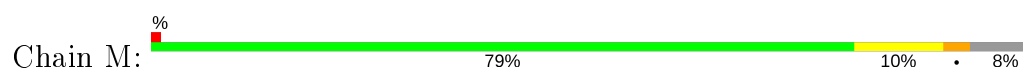
- Molecule 2: Vacuolar protein sorting-associated protein 37B



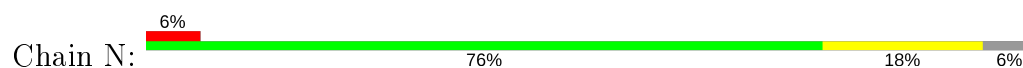
- Molecule 2: Vacuolar protein sorting-associated protein 37B



- Molecule 2: Vacuolar protein sorting-associated protein 37B



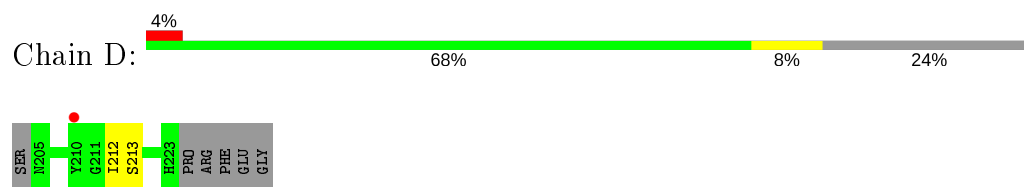
- Molecule 2: Vacuolar protein sorting-associated protein 37B



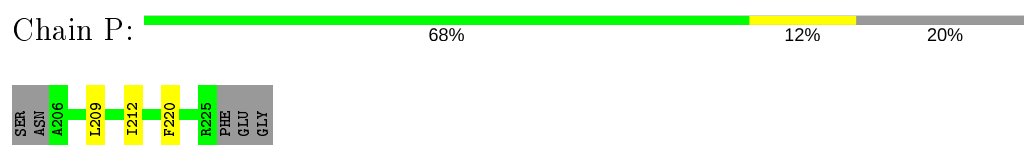
- Molecule 2: Vacuolar protein sorting-associated protein 37B



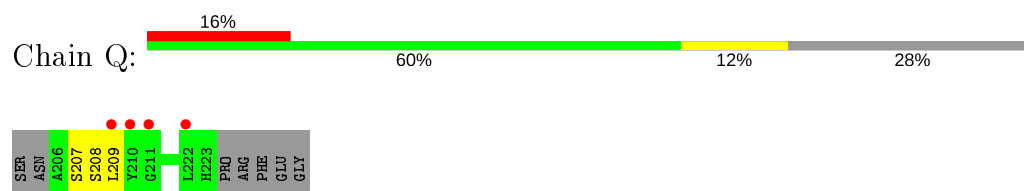
- Molecule 3: Multivesicular body subunit 12A



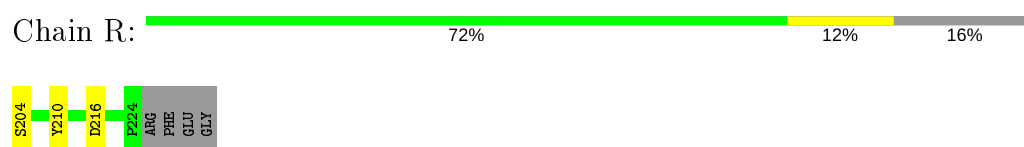
- Molecule 3: Multivesicular body subunit 12A



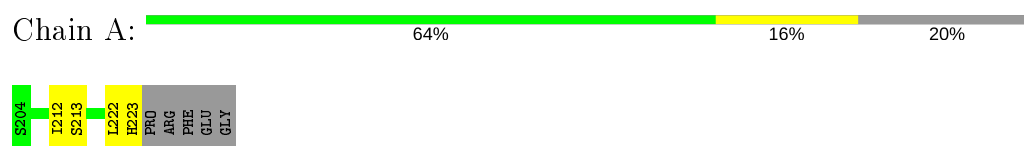
- Molecule 3: Multivesicular body subunit 12A



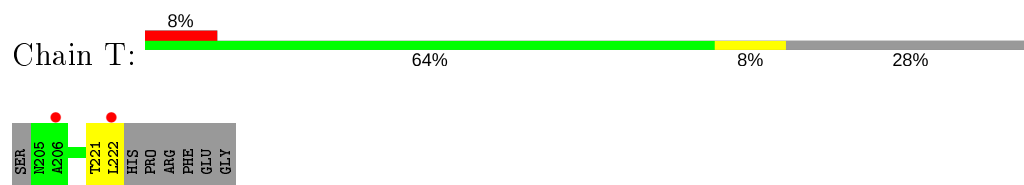
- Molecule 3: Multivesicular body subunit 12A



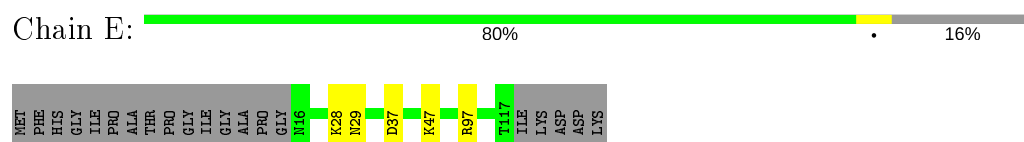
- Molecule 3: Multivesicular body subunit 12A



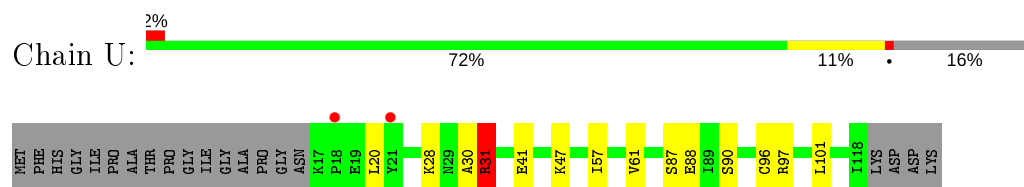
- Molecule 3: Multivesicular body subunit 12A



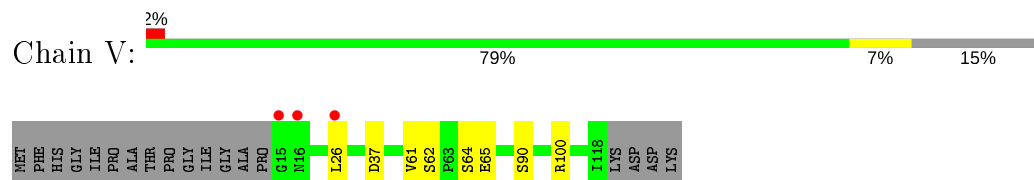
- Molecule 4: Vacuolar protein sorting-associated protein 28 homolog



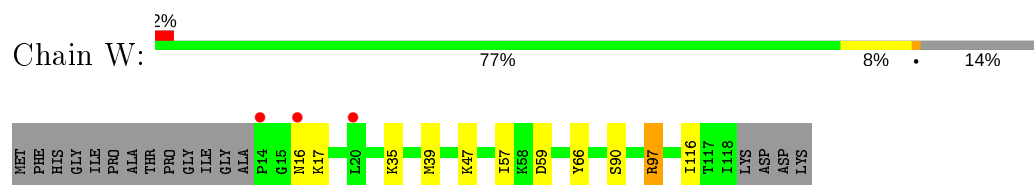
- Molecule 4: Vacuolar protein sorting-associated protein 28 homolog



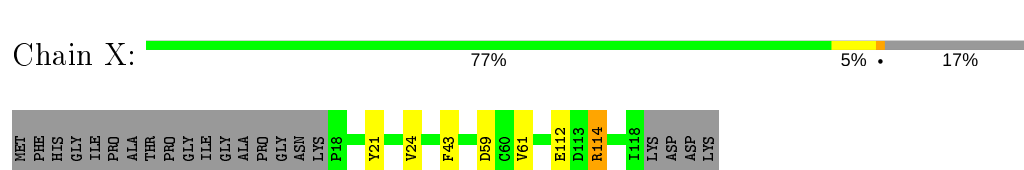
- Molecule 4: Vacuolar protein sorting-associated protein 28 homolog



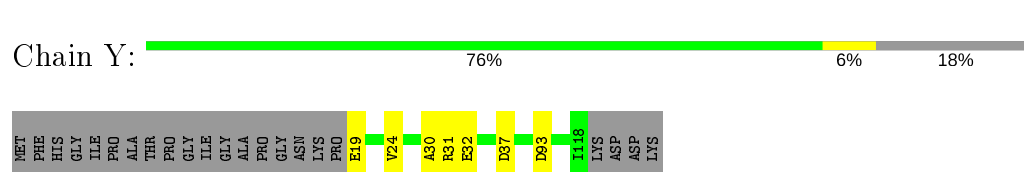
- Molecule 4: Vacuolar protein sorting-associated protein 28 homolog



- Molecule 4: Vacuolar protein sorting-associated protein 28 homolog



- Molecule 4: Vacuolar protein sorting-associated protein 28 homolog



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	162.58Å 162.58Å 139.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	99.18 – 2.19 99.18 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.2 (99.18-2.19) 90.2 (99.18-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.193 , 0.240 0.193 , 0.240	Depositor DCC
R_{free} test set	1998 reflections (1.87%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.088 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12786	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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	B	0.40	0/615	0.54	0/829
1	F	0.47	0/623	0.60	1/840 (0.1%)
1	G	0.45	0/611	0.57	0/823
1	H	0.41	0/615	0.48	0/830
1	I	0.44	0/610	0.60	1/822 (0.1%)
1	J	0.43	0/612	0.52	0/825
2	C	0.39	0/531	0.54	0/710
2	K	0.41	0/525	0.57	1/700 (0.1%)
2	L	0.39	0/521	0.55	0/695
2	M	0.34	0/518	0.45	0/693
2	N	0.41	0/534	0.53	0/714
2	O	0.37	0/492	0.53	0/659
3	A	0.43	0/137	0.69	0/186
3	D	0.48	0/138	0.60	0/187
3	P	0.39	0/140	0.59	0/191
3	Q	0.55	0/119	0.76	0/161
3	R	0.37	0/146	0.56	0/199
3	T	0.31	0/127	0.53	0/172
4	E	0.41	0/835	0.52	0/1122
4	U	0.51	0/840	0.68	3/1128 (0.3%)
4	V	0.45	0/839	0.57	0/1129
4	W	0.42	0/854	0.53	0/1148
4	X	0.44	0/833	0.53	0/1118
4	Y	0.44	0/827	0.52	0/1110
All	All	0.43	0/12642	0.56	6/16991 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	31	ARG	NE-CZ-NH2	-10.29	115.16	120.30
4	U	31	ARG	CG-CD-NE	7.53	127.61	111.80
4	U	31	ARG	NE-CZ-NH1	5.87	123.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	364	ARG	NE-CZ-NH1	-5.78	117.41	120.30
2	K	164	LEU	CA-CB-CG	5.67	128.33	115.30
1	F	364	ARG	NE-CZ-NH1	-5.45	117.58	120.30

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	B	607	0	629	2	1
1	F	615	0	640	11	0
1	G	603	0	629	4	0
1	H	607	0	629	2	0
1	I	602	0	634	9	0
1	J	604	0	627	12	0
2	C	527	0	533	11	0
2	K	521	0	541	8	0
2	L	517	0	537	5	0
2	M	514	0	528	6	0
2	N	530	0	542	7	0
2	O	488	0	494	8	0
3	A	135	0	123	2	0
3	D	135	0	126	5	0
3	P	137	0	128	4	0
3	Q	118	0	112	2	2
3	R	143	0	133	0	0
3	T	125	0	119	3	0
4	E	822	0	815	4	0
4	U	827	0	831	14	2
4	V	826	0	814	9	0
4	W	840	0	828	7	1
4	X	820	0	823	6	0
4	Y	815	0	815	4	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	8	0	0	0	0
5	D	3	0	0	0	0
5	E	31	0	0	1	0
5	F	18	0	0	0	0
5	G	16	0	0	0	0
5	H	5	0	0	0	0
5	I	10	0	0	0	0
5	J	5	0	0	0	0
5	K	12	0	0	0	0
5	L	3	0	0	0	0
5	M	6	0	0	0	0
5	N	15	0	0	0	0
5	O	1	0	0	0	0
5	P	7	0	0	0	0
5	Q	2	0	0	0	0
5	R	2	0	0	0	0
5	U	34	0	0	2	0
5	V	37	0	0	2	0
5	W	22	0	0	1	0
5	X	25	0	0	1	0
5	Y	26	0	0	0	0
All	All	12786	0	12630	112	3

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 (112) 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)
4:U:31:ARG:HD2	4:U:31:ARG:H	1.22	1.01
2:M:124:MET:HE1	2:M:145:LYS:HD2	1.55	0.89
4:U:31:ARG:HD2	4:U:31:ARG:N	2.00	0.75
4:X:114:ARG:NH1	5:X:201:HOH:O	2.22	0.72
2:L:102:SER:OG	2:L:103:LEU:N	2.24	0.71
2:C:124:MET:HE1	2:C:145:LYS:HD2	1.73	0.70
4:U:31:ARG:CD	4:U:31:ARG:H	2.04	0.70
2:C:128:PHE:HB2	2:C:133:LEU:HD23	1.79	0.65
1:I:356:LEU:HD22	4:X:61:VAL:HG21	1.79	0.65
2:C:104:GLU:OE2	2:C:163:VAL:HG11	1.97	0.64
4:U:28:LYS:NZ	5:U:201:HOH:O	2.30	0.64
2:C:157:GLU:OE1	3:D:212:ILE:HD13	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:ARG:NH2	4:E:37:ASP:OD1	2.24	0.62
1:F:324:LEU:HD23	4:U:20:LEU:HD13	1.81	0.62
1:H:314:ILE:HD12	1:H:317:VAL:HG11	1.80	0.61
3:T:221:THR:HG22	3:T:222:LEU:H	1.66	0.61
2:C:133:LEU:HD12	2:C:134:PRO:HD2	1.82	0.60
4:U:30:ALA:HB3	4:U:31:ARG:NH1	2.16	0.60
4:U:90:SER:OG	4:W:97:ARG:NE	2.23	0.59
2:C:121:THR:HA	2:C:124:MET:HE3	1.86	0.58
1:F:314:ILE:HG21	2:K:113:GLU:HG3	1.87	0.57
1:J:357:ASP:OD1	1:J:357:ASP:N	2.34	0.56
1:I:371:PHE:HB2	4:X:43:PHE:CD1	2.41	0.55
4:Y:31:ARG:NH1	4:Y:32:GLU:HG3	2.22	0.55
4:E:97:ARG:NH1	4:V:90:SER:OG	2.37	0.54
4:V:100:ARG:NH2	5:V:203:HOH:O	2.41	0.53
4:W:47:LYS:NZ	5:W:201:HOH:O	2.38	0.52
3:D:212:ILE:HD12	3:D:213:SER:N	2.25	0.51
2:O:139:ILE:O	2:O:143:GLN:HB2	2.10	0.51
1:J:368:ARG:NH2	4:Y:37:ASP:OD1	2.30	0.51
4:W:66:TYR:CE2	4:W:116:ILE:HG22	2.46	0.51
2:K:154:VAL:HA	3:P:212:ILE:HD11	1.93	0.50
4:W:16:ASN:C	4:W:17:LYS:HD2	2.32	0.50
1:I:323:PRO:HD2	4:X:21:TYR:HA	1.93	0.50
2:N:125:ALA:O	2:N:129:LEU:HG	2.11	0.50
4:W:35:LYS:O	4:W:39:MET:HG3	2.12	0.50
1:G:379:LYS:HD2	1:G:382:LYS:HE3	1.95	0.49
1:G:356:LEU:HD13	4:V:61:VAL:HG11	1.94	0.49
3:D:212:ILE:C	3:D:212:ILE:HD12	2.32	0.49
1:J:381:ARG:NH2	1:J:387:SER:O	2.43	0.49
1:J:378:GLN:O	1:J:382:LYS:HG2	2.13	0.49
4:X:112:GLU:O	4:X:114:ARG:HG3	2.12	0.49
2:L:127:LYS:HG2	2:L:132:GLU:HB2	1.95	0.48
3:Q:207:SER:HB3	4:V:100:ARG:HD2	1.94	0.48
1:F:356:LEU:HD13	4:U:61:VAL:HG11	1.95	0.48
1:J:319:ILE:HG12	1:J:320:PRO:HD2	1.95	0.48
1:I:376:LEU:HD22	4:X:24:VAL:HG23	1.95	0.48
4:V:61:VAL:HB	4:V:65:GLU:HG3	1.94	0.48
1:F:361:LYS:HD2	1:F:361:LYS:HA	1.63	0.48
2:N:154:VAL:HA	3:A:212:ILE:HD11	1.95	0.47
2:O:123:ASN:O	2:O:127:LYS:HG2	2.14	0.47
2:O:114:GLY:O	2:O:118:GLU:HG2	2.15	0.47
2:C:147:LYS:O	2:C:151:MET:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:349:LEU:HD22	1:J:359:PHE:CD2	2.49	0.47
2:N:133:LEU:HD12	2:N:134:PRO:HD2	1.96	0.47
4:U:96:CYS:HB3	4:U:101:LEU:O	2.15	0.47
2:C:157:GLU:OE1	3:D:212:ILE:CD1	2.64	0.46
1:F:334:GLU:HG2	2:K:147:LYS:HD2	1.96	0.46
2:M:127:LYS:HB3	2:M:127:LYS:HE2	1.66	0.46
2:L:124:MET:HE1	2:L:142:TYR:N	2.30	0.46
1:F:320:PRO:HA	3:P:220:PHE:HA	1.99	0.45
2:M:137:SER:O	2:M:141:VAL:HG22	2.17	0.45
1:F:364:ARG:HD3	4:U:41:GLU:OE1	2.17	0.45
4:E:28:LYS:HG3	4:E:29:ASN:ND2	2.31	0.45
1:I:381:ARG:HH21	1:I:387:SER:HA	1.81	0.45
2:O:103:LEU:HD12	2:O:104:GLU:HG2	1.99	0.45
2:K:102:SER:O	2:K:106:LEU:HG	2.17	0.44
1:F:338:ILE:HD11	1:F:369:LYS:HE2	1.99	0.44
1:B:376:LEU:HD23	1:B:376:LEU:HA	1.82	0.44
3:T:221:THR:HG22	3:T:222:LEU:N	2.30	0.44
2:C:104:GLU:OE1	2:C:107:LEU:HD23	2.17	0.44
2:O:107:LEU:O	2:O:111:GLN:HG3	2.17	0.44
2:N:105:THR:O	2:N:109:LEU:HG	2.18	0.44
4:U:87:SER:O	4:W:97:ARG:NH1	2.51	0.44
2:C:146:ARG:HD2	2:C:146:ARG:HA	1.77	0.43
2:C:157:GLU:CD	3:D:212:ILE:HD13	2.38	0.43
1:F:314:ILE:HG21	2:K:113:GLU:CG	2.49	0.43
2:O:117:ILE:HD11	2:O:145:LYS:HB3	2.00	0.43
1:H:314:ILE:HA	1:H:317:VAL:HG13	2.01	0.43
2:M:116:LYS:HD2	2:M:116:LYS:HA	1.74	0.43
3:Q:209:LEU:HB2	5:V:227:HOH:O	2.18	0.43
1:I:382:LYS:N	1:I:382:LYS:HD3	2.34	0.43
1:I:364:ARG:HH11	1:I:364:ARG:HD3	1.65	0.42
1:J:333:ALA:HB2	2:O:151:MET:HG3	2.02	0.42
2:K:127:LYS:HB3	2:K:133:LEU:HD12	2.02	0.42
1:G:368:ARG:NH2	4:V:37:ASP:OD1	2.43	0.42
2:L:103:LEU:HD23	2:L:163:VAL:HG12	2.01	0.42
1:F:348:ALA:HB2	2:K:128:PHE:CE2	2.55	0.41
1:J:317:VAL:O	3:T:222:LEU:HD23	2.20	0.41
2:M:107:LEU:HA	2:M:159:LEU:HD23	2.02	0.41
4:U:47:LYS:NZ	5:U:202:HOH:O	2.53	0.41
2:N:124:MET:HE1	2:N:145:LYS:HD2	2.01	0.41
4:V:100:ARG:HB2	4:V:100:ARG:HE	1.60	0.41
4:E:47:LYS:NZ	5:E:204:HOH:O	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:103:LEU:HD23	2:N:103:LEU:HA	1.85	0.41
1:I:339:GLU:HG2	4:Y:30:ALA:HB1	2.02	0.41
4:V:26:LEU:HA	4:V:26:LEU:HD12	1.89	0.41
1:I:324:LEU:CD2	1:I:384:ALA:HB2	2.51	0.41
1:J:319:ILE:HG23	1:J:320:PRO:O	2.21	0.41
4:V:62:SER:OG	4:V:65:GLU:HG2	2.21	0.41
2:K:158:LYS:HG3	3:P:220:PHE:CD1	2.55	0.41
1:F:335:GLU:HG2	3:P:209:LEU:HD21	2.03	0.41
1:G:364:ARG:NH1	4:U:57:ILE:O	2.54	0.41
4:U:97:ARG:NH2	4:W:90:SER:OG	2.54	0.41
2:M:159:LEU:O	2:M:163:VAL:HG13	2.21	0.41
2:N:116:LYS:O	2:N:120:ASP:HB2	2.21	0.40
3:A:222:LEU:HD22	3:A:223:HIS:H	1.86	0.40
1:J:369:LYS:HE3	1:J:373:LEU:HD21	2.03	0.40
2:L:146:ARG:HA	2:L:146:ARG:HD2	1.92	0.40
2:O:125:ALA:O	2:O:129:LEU:HG	2.21	0.40
1:J:379:LYS:HB3	4:Y:24:VAL:HG11	2.03	0.40
1:J:334:GLU:HB3	1:J:373:LEU:HD13	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:208:SER:O	4:U:31:ARG:NH2[5_554]	1.56	0.64
3:Q:209:LEU:CA	4:U:31:ARG:NH2[5_554]	2.12	0.08
1:B:364:ARG:NH2	4:W:57:ILE:O[5_554]	2.19	0.01

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	B	74/81 (91%)	74 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	75/81 (93%)	75 (100%)	0	0	100	100
1	G	73/81 (90%)	73 (100%)	0	0	100	100
1	H	74/81 (91%)	74 (100%)	0	0	100	100
1	I	73/81 (90%)	72 (99%)	1 (1%)	0	100	100
1	J	74/81 (91%)	74 (100%)	0	0	100	100
2	C	65/71 (92%)	62 (95%)	3 (5%)	0	100	100
2	K	63/71 (89%)	61 (97%)	2 (3%)	0	100	100
2	L	63/71 (89%)	61 (97%)	1 (2%)	1 (2%)	9	7
2	M	63/71 (89%)	63 (100%)	0	0	100	100
2	N	65/71 (92%)	65 (100%)	0	0	100	100
2	O	60/71 (84%)	59 (98%)	1 (2%)	0	100	100
3	A	18/25 (72%)	17 (94%)	1 (6%)	0	100	100
3	D	17/25 (68%)	17 (100%)	0	0	100	100
3	P	18/25 (72%)	18 (100%)	0	0	100	100
3	Q	16/25 (64%)	14 (88%)	2 (12%)	0	100	100
3	R	19/25 (76%)	18 (95%)	1 (5%)	0	100	100
3	T	16/25 (64%)	16 (100%)	0	0	100	100
4	E	100/122 (82%)	99 (99%)	1 (1%)	0	100	100
4	U	100/122 (82%)	99 (99%)	1 (1%)	0	100	100
4	V	102/122 (84%)	102 (100%)	0	0	100	100
4	W	103/122 (84%)	100 (97%)	3 (3%)	0	100	100
4	X	99/122 (81%)	99 (100%)	0	0	100	100
4	Y	98/122 (80%)	98 (100%)	0	0	100	100
All	All	1528/1794 (85%)	1510 (99%)	17 (1%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	165	LYS

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	B	63/71 (89%)	63 (100%)	0	100	100
1	F	64/71 (90%)	63 (98%)	1 (2%)	62	76
1	G	63/71 (89%)	62 (98%)	1 (2%)	62	76
1	H	63/71 (89%)	62 (98%)	1 (2%)	62	76
1	I	63/71 (89%)	62 (98%)	1 (2%)	62	76
1	J	62/71 (87%)	62 (100%)	0	100	100
2	C	57/62 (92%)	55 (96%)	2 (4%)	36	46
2	K	57/62 (92%)	57 (100%)	0	100	100
2	L	56/62 (90%)	56 (100%)	0	100	100
2	M	55/62 (89%)	53 (96%)	2 (4%)	35	45
2	N	58/62 (94%)	57 (98%)	1 (2%)	60	74
2	O	51/62 (82%)	50 (98%)	1 (2%)	55	69
3	A	13/20 (65%)	12 (92%)	1 (8%)	13	13
3	D	14/20 (70%)	14 (100%)	0	100	100
3	P	14/20 (70%)	14 (100%)	0	100	100
3	Q	12/20 (60%)	12 (100%)	0	100	100
3	R	15/20 (75%)	12 (80%)	3 (20%)	1	1
3	T	13/20 (65%)	13 (100%)	0	100	100
4	E	88/105 (84%)	88 (100%)	0	100	100
4	U	89/105 (85%)	87 (98%)	2 (2%)	52	65
4	V	87/105 (83%)	86 (99%)	1 (1%)	73	85
4	W	89/105 (85%)	87 (98%)	2 (2%)	52	65
4	X	89/105 (85%)	87 (98%)	2 (2%)	52	65
4	Y	88/105 (84%)	86 (98%)	2 (2%)	50	63
All	All	1323/1548 (86%)	1300 (98%)	23 (2%)	60	74

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	126	GLU

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Mol	Chain	Res	Type
2	C	137	SER
1	F	361	LYS
1	G	382	LYS
1	H	382	LYS
1	I	382	LYS
2	M	124	MET
2	M	127	LYS
2	N	136	ASP
2	O	137	SER
3	R	204	SER
3	R	210	TYR
3	R	216	ASP
3	A	213	SER
4	U	31	ARG
4	U	88	GLU
4	V	64	SER
4	W	59	ASP
4	W	97	ARG
4	X	59	ASP
4	X	114	ARG
4	Y	19	GLU
4	Y	93	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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 ⓘ

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	B	76/81 (93%)	0.20	1 (1%) 77 75	39, 54, 80, 98	0
1	F	77/81 (95%)	0.19	1 (1%) 77 75	36, 48, 76, 117	0
1	G	75/81 (92%)	0.20	2 (2%) 54 52	39, 48, 91, 122	0
1	H	76/81 (93%)	0.28	2 (2%) 56 53	43, 57, 94, 109	0
1	I	75/81 (92%)	0.20	1 (1%) 77 75	39, 49, 74, 100	0
1	J	76/81 (93%)	0.33	5 (6%) 18 17	43, 62, 104, 142	0
2	C	67/71 (94%)	0.37	3 (4%) 33 32	42, 61, 90, 119	0
2	K	65/71 (91%)	0.17	2 (3%) 49 47	42, 56, 91, 122	0
2	L	65/71 (91%)	0.40	5 (7%) 13 12	44, 62, 115, 137	0
2	M	65/71 (91%)	0.23	1 (1%) 73 72	53, 73, 90, 107	0
2	N	67/71 (94%)	0.21	4 (5%) 21 20	43, 59, 84, 146	0
2	O	62/71 (87%)	0.64	5 (8%) 12 10	58, 84, 111, 122	0
3	A	20/25 (80%)	0.08	0 100 100	47, 58, 102, 107	0
3	D	19/25 (76%)	0.16	1 (5%) 26 25	45, 59, 83, 112	0
3	P	20/25 (80%)	0.08	0 100 100	41, 55, 131, 134	0
3	Q	18/25 (72%)	1.79	4 (22%) 0 0	57, 73, 119, 127	0
3	R	21/25 (84%)	0.61	0 100 100	47, 72, 115, 125	0
3	T	18/25 (72%)	0.52	2 (11%) 5 4	51, 84, 108, 112	0
4	E	102/122 (83%)	0.09	0 100 100	36, 54, 85, 99	0
4	U	102/122 (83%)	0.14	2 (1%) 65 63	37, 50, 74, 140	0
4	V	104/122 (85%)	0.23	3 (2%) 51 49	36, 50, 75, 145	0
4	W	105/122 (86%)	0.21	3 (2%) 51 49	40, 56, 95, 139	0
4	X	101/122 (82%)	0.08	0 100 100	40, 54, 79, 90	0
4	Y	100/122 (81%)	0.06	0 100 100	41, 55, 89, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
All	All	1576/1794 (87%)	0.24	47 (2%)	50 48	36, 57, 98, 146	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	209	LEU	20.6
4	V	15	GLY	13.1
2	L	164	LEU	5.0
4	V	16	ASN	4.8
2	C	165	LYS	4.3
4	W	14	PRO	3.8
1	G	386	LEU	3.8
1	J	384	ALA	3.8
2	L	103	LEU	3.7
3	T	222	LEU	3.7
3	Q	210	TYR	3.7
2	L	162	MET	3.3
1	B	388	ASP	3.3
1	J	386	LEU	3.3
1	H	318	ILE	3.2
2	C	108	ALA	3.2
2	O	138	PHE	3.1
2	K	166	GLY	3.0
3	Q	211	GLY	2.9
1	G	387	SER	2.9
1	H	329	LEU	2.8
2	L	106	LEU	2.8
4	V	26	LEU	2.8
1	J	376	LEU	2.8
2	O	131	GLY	2.7
2	O	110	LEU	2.7
2	N	99	SER	2.6
2	N	139	ILE	2.6
4	U	21	TYR	2.5
1	J	345	LEU	2.5
3	T	206	ALA	2.4
3	D	210	TYR	2.4
4	U	18	PRO	2.4
3	Q	222	LEU	2.4
1	F	312	ASN	2.3
1	J	318	ILE	2.3
4	W	16	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	386	LEU	2.3
2	O	135	LEU	2.3
2	N	140	ASP	2.2
2	M	164	LEU	2.2
4	W	20	LEU	2.2
2	C	133	LEU	2.1
2	O	103	LEU	2.1
2	N	119	GLU	2.1
2	L	163	VAL	2.1
2	K	163	VAL	2.1

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.