wwPDB EM Map/Model Validation Report (i)

Sep 28, 2016 – 12:14 PM EDT

PDB ID	:	5L4K
EMDB ID:	:	EMD-4002
Title	:	The human 26S proteasome lid
Authors	:	Schweitzer, A.; Aufderheide, A.; Rudack, T.; Beck, F.
Deposited on	:	2016-05-25
Resolution	:	4.50 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

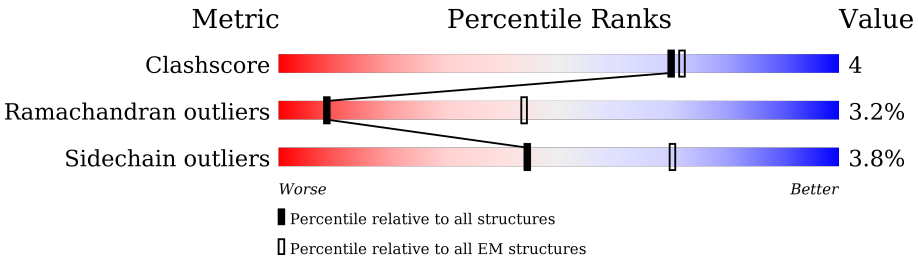
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	W	377	49% · 48%
2	V	310	72% 17% · · 5%
3	T	350	65% 10% · 22%
4	Y	70	70% 10% 20%
5	Z	908	83% 13% · ·
6	N	953	77% 14% · 8%
7	S	534	79% 11% · 8%
8	P	456	86% 14%
9	Q	422	86% 13% ·

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Mol	Chain	Length	Quality of chain
10	R	389	
11	U	324	
12	O	376	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 79649 atoms, of which 39990 are hydrogens and 0 are deuteriums.

In the tables below, 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 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	W	196	3019	927	1531	266	286	9	0	0

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	V	293	4612	1456	2311	395	431	19	0	0

- Molecule 3 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	T	272	4435	1424	2231	362	409	9	0	0

- Molecule 4 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	Y	56	848	288	374	72	113	1	0	0

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	Z	881	13583	4270	6791	1159	1318	45	0	0

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	N	876	13720	4332	6890	1158	1295	45	0	0

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	S	491	Total	C	H	N	O	S	0	0
			7977	2516	3998	707	742	14		

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	P	456	Total	C	H	N	O	S	0	0
			7525	2339	3822	635	704	25		

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	Q	422	Total	C	H	N	O	S	0	0
			6770	2116	3435	567	639	13		

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	R	389	Total	C	H	N	O	S	0	0
			6406	2041	3204	545	598	18		

- Molecule 11 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	U	292	Total	C	H	N	O	S	0	0
			4693	1488	2362	399	438	6		

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

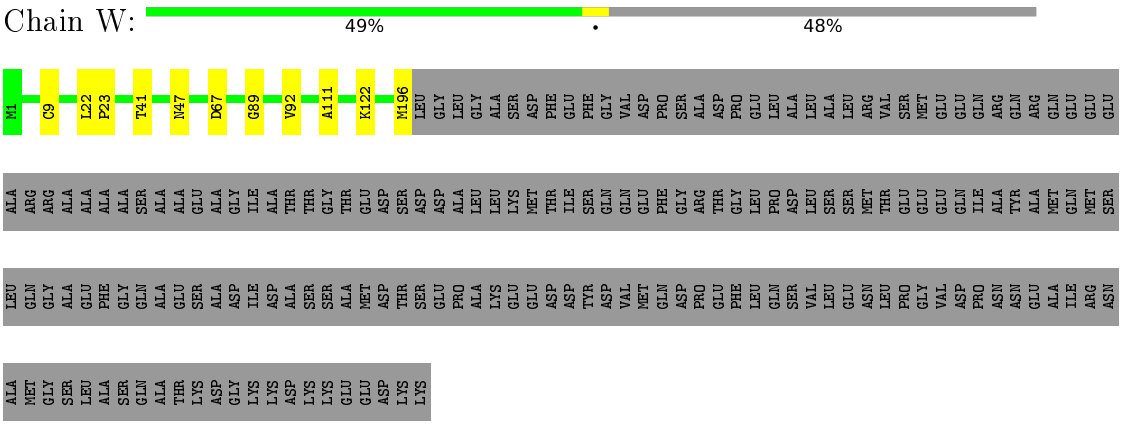
Mol	Chain	Residues	Atoms						AltConf	Trace
12	O	376	Total	C	H	N	O	S	0	0
			6061	1926	3041	514	564	16		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

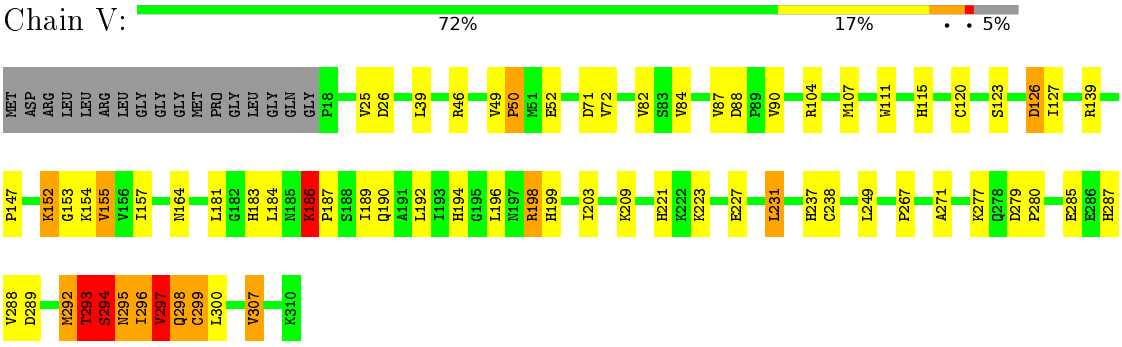
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

Chain W:



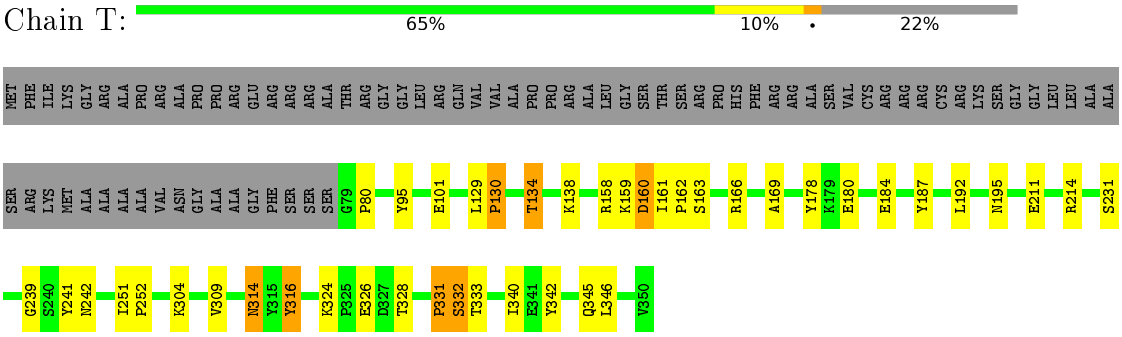
- Molecule 2: 26S proteasome non-ATPase regulatory subunit 14

Chain V:



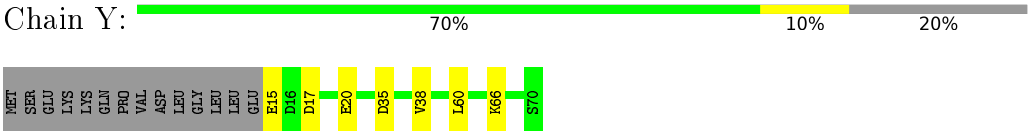
- Molecule 3: 26S proteasome non-ATPase regulatory subunit 8

Chain T:



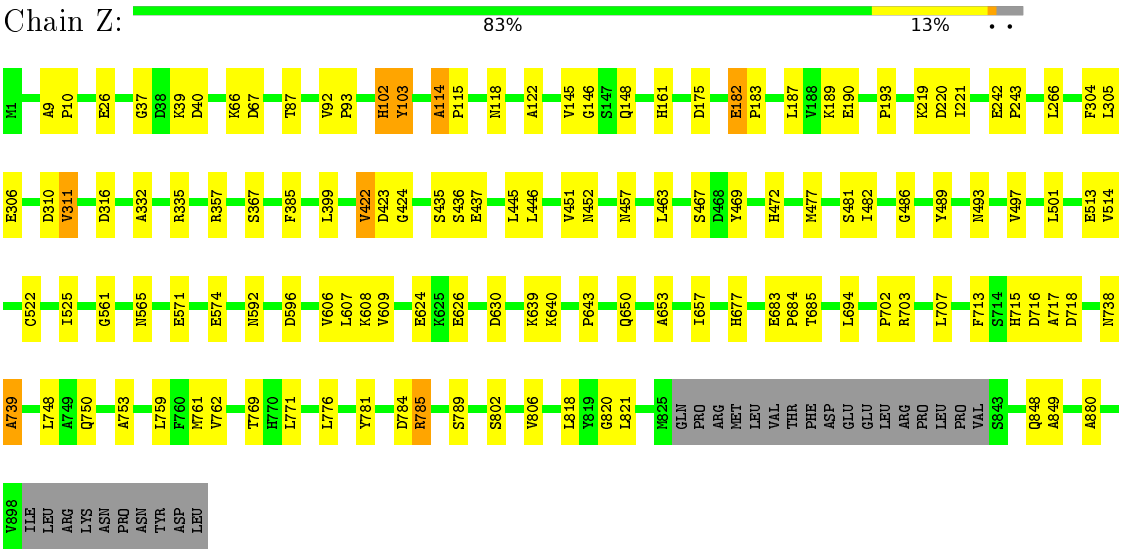
- Molecule 4: 26S proteasome complex subunit DSS1

Chain Y:



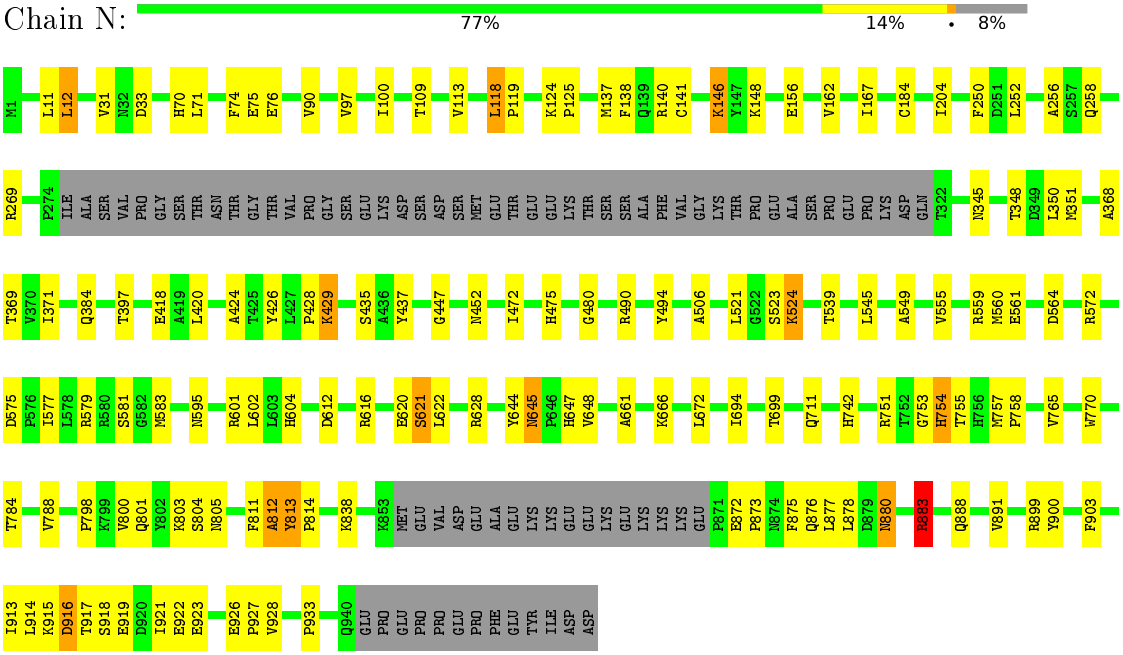
- Molecule 5: 26S proteasome non-ATPase regulatory subunit 2

Chain Z:



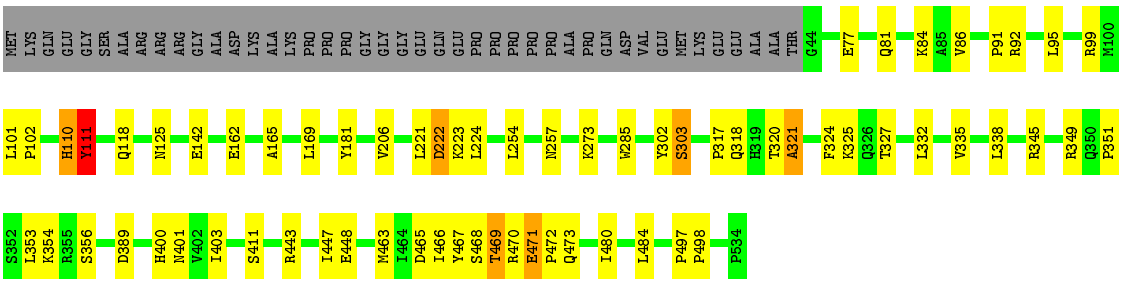
- Molecule 6: 26S proteasome non-ATPase regulatory subunit 1

Chain N:



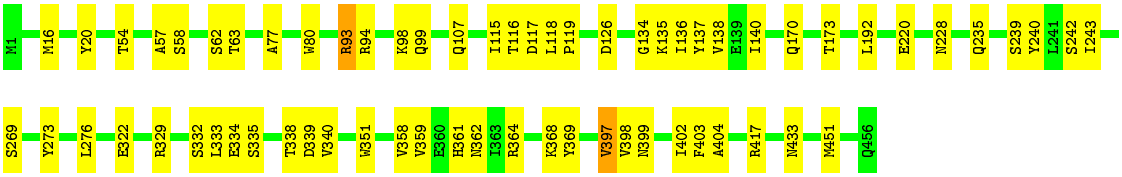
- Molecule 7: 26S proteasome non-ATPase regulatory subunit 3

Chain S:



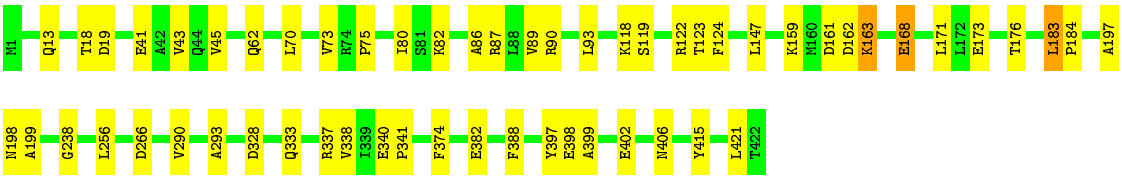
• Molecule 8: 26S proteasome non-ATPase regulatory subunit 12

Chain P:



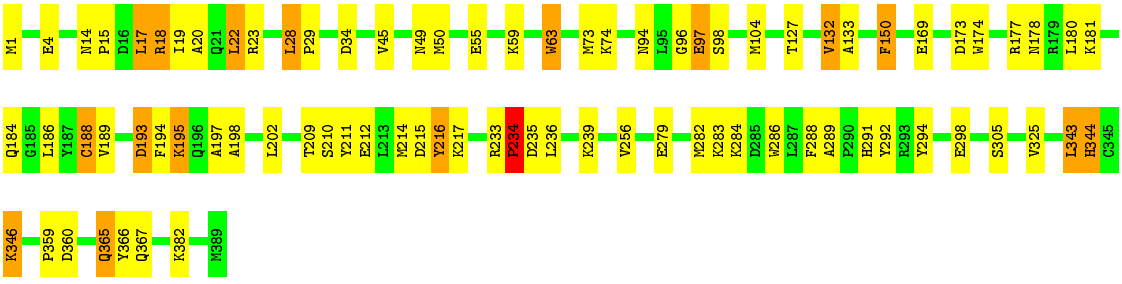
• Molecule 9: 26S proteasome non-ATPase regulatory subunit 11

Chain Q:



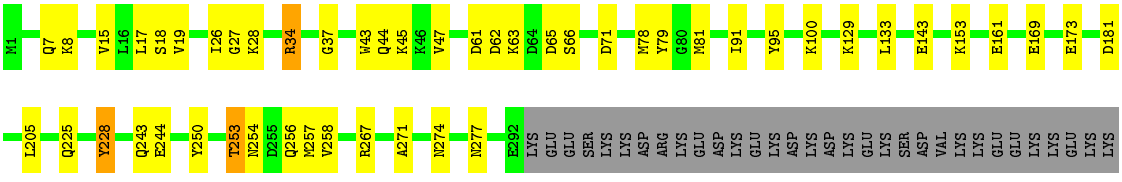
• Molecule 10: 26S proteasome non-ATPase regulatory subunit 6

Chain R:



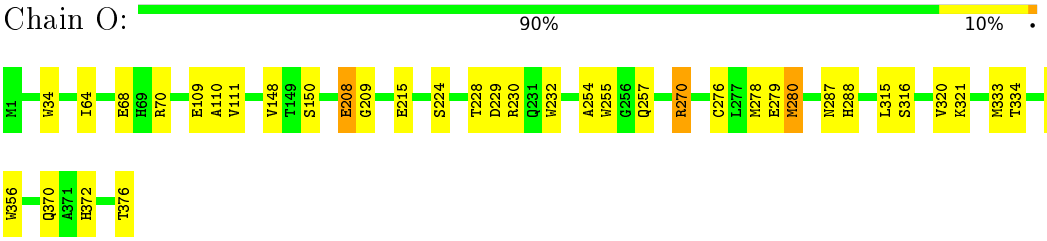
• Molecule 11: 26S proteasome non-ATPase regulatory subunit 7

Chain U:



- Molecule 12: 26S proteasome non-ATPase regulatory subunit 13

Chain O:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	461402	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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	#$\|Z\|$ >2	RMSZ	#$\|Z\|$ >2
1	W	0.31	0/1508	0.51	0/2040
10	R	0.68	1/3261 (0.0%)	0.55	0/4393
11	U	0.37	0/2375	0.53	0/3219
12	O	0.32	0/3078	0.48	0/4165
2	V	0.76	11/2346 (0.5%)	0.77	10/3173 (0.3%)
3	T	0.36	1/2251 (0.0%)	0.49	0/3042
4	Y	0.37	0/486	0.53	0/658
5	Z	0.29	0/6903	0.48	0/9327
6	N	0.33	1/6949 (0.0%)	0.49	0/9395
7	S	0.34	0/4053	0.52	1/5465 (0.0%)
8	P	0.35	0/3751	0.51	0/5042
9	Q	0.34	0/3381	0.49	0/4558
All	All	0.41	14/40342 (0.0%)	0.52	11/54477 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
10	R	0	1
12	O	0	1
2	V	0	3
3	T	0	1
5	Z	0	1
8	P	0	1
All	All	0	8

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	R	28	LEU	C-N	31.06	1.93	1.34
2	V	295	ASN	N-CA	-12.65	1.21	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	294	SER	CA-C	-10.17	1.26	1.52
2	V	298	GLN	N-CA	-8.17	1.30	1.46
2	V	294	SER	N-CA	-7.93	1.30	1.46

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V	294	SER	C-N-CA	-8.56	100.31	121.70
2	V	296	ILE	C-N-CA	-8.19	101.22	121.70
2	V	293	THR	O-C-N	-8.11	109.72	122.70
2	V	293	THR	CA-C-O	7.72	136.31	120.10
2	V	297	VAL	O-C-N	-7.66	110.44	122.70

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	T	241	TYR	Peptide
2	V	293	THR	Mainchain
2	V	294	SER	Mainchain
2	V	297	VAL	Mainchain
5	Z	102	HIS	Peptide

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	W	1488	1531	1531	2	0
2	V	2301	2311	2314	67	0
3	T	2204	2231	2231	18	0
4	Y	474	374	374	3	0
5	Z	6792	6791	6790	48	0
6	N	6830	6890	6890	76	0
7	S	3979	3998	3998	32	0
8	P	3703	3822	3822	26	0
9	Q	3335	3435	3435	19	0
10	R	3202	3204	3204	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	U	2331	2362	2362	29	0
12	O	3020	3041	3041	13	0
All	All	39659	39990	39992	357	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.

The worst 5 of 357 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)
2:V:289:ASP:O	2:V:293:THR:HG23	1.31	1.28
2:V:296:ILE:O	2:V:299:CYS:HB2	1.13	1.22
2:V:237:HIS:NE2	2:V:298:GLN:HG2	1.50	1.22
10:R:28:LEU:C	10:R:29:PRO:N	1.93	1.20
2:V:297:VAL:O	2:V:298:GLN:C	1.81	1.11

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 PDB entries followed by that with respect to all EM entries.

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	W	194/377 (52%)	171 (88%)	21 (11%)	2 (1%)	19 65
2	V	291/310 (94%)	236 (81%)	41 (14%)	14 (5%)	3 32
3	T	270/350 (77%)	242 (90%)	17 (6%)	11 (4%)	3 36
4	Y	54/70 (77%)	46 (85%)	6 (11%)	2 (4%)	4 39
5	Z	877/908 (97%)	737 (84%)	108 (12%)	32 (4%)	4 40
6	N	870/953 (91%)	741 (85%)	104 (12%)	25 (3%)	6 45
7	S	489/534 (92%)	425 (87%)	52 (11%)	12 (2%)	7 48
8	P	454/456 (100%)	384 (85%)	57 (13%)	13 (3%)	6 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	Q	420/422 (100%)	349 (83%)	59 (14%)	12 (3%)	6	45
10	R	387/389 (100%)	321 (83%)	48 (12%)	18 (5%)	3	32
11	U	290/324 (90%)	245 (84%)	38 (13%)	7 (2%)	7	49
12	O	374/376 (100%)	329 (88%)	36 (10%)	9 (2%)	7	49
All	All	4970/5469 (91%)	4226 (85%)	587 (12%)	157 (3%)	8	43

5 of 157 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	W	23	PRO
3	T	180	GLU
3	T	332	SER
5	Z	311	VAL
5	Z	367	SER

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 PDB entries followed by that with respect to all EM entries.

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	W	169/312 (54%)	164 (97%)	5 (3%)	48	78
2	V	257/268 (96%)	247 (96%)	10 (4%)	39	73
3	T	238/294 (81%)	228 (96%)	10 (4%)	36	72
4	Y	50/63 (79%)	49 (98%)	1 (2%)	63	86
5	Z	736/763 (96%)	707 (96%)	29 (4%)	39	73
6	N	747/816 (92%)	723 (97%)	24 (3%)	46	77
7	S	428/460 (93%)	408 (95%)	20 (5%)	32	69
8	P	416/416 (100%)	404 (97%)	12 (3%)	50	79
9	Q	362/362 (100%)	345 (95%)	17 (5%)	32	69
10	R	344/344 (100%)	325 (94%)	19 (6%)	27	66
11	U	263/295 (89%)	253 (96%)	10 (4%)	40	74
12	O	336/336 (100%)	326 (97%)	10 (3%)	48	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4346/4729 (92%)	4179 (96%)	167 (4%)	44 74

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	N	751	ARG
7	S	356	SER
11	U	250	TYR
6	N	838	LYS
7	S	254	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	V	237	HIS

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 carbohydrates 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 (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	28:LEU	C	29:PRO	N	1.93