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

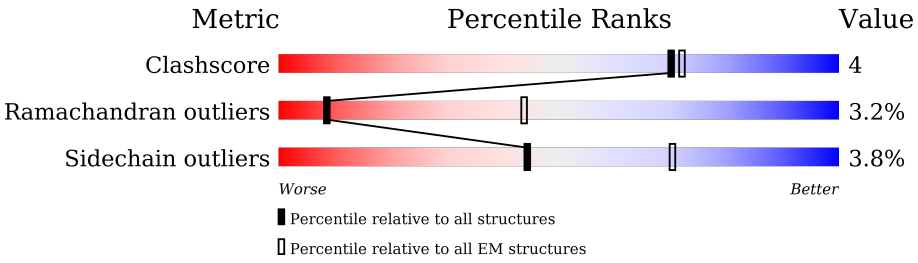
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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.

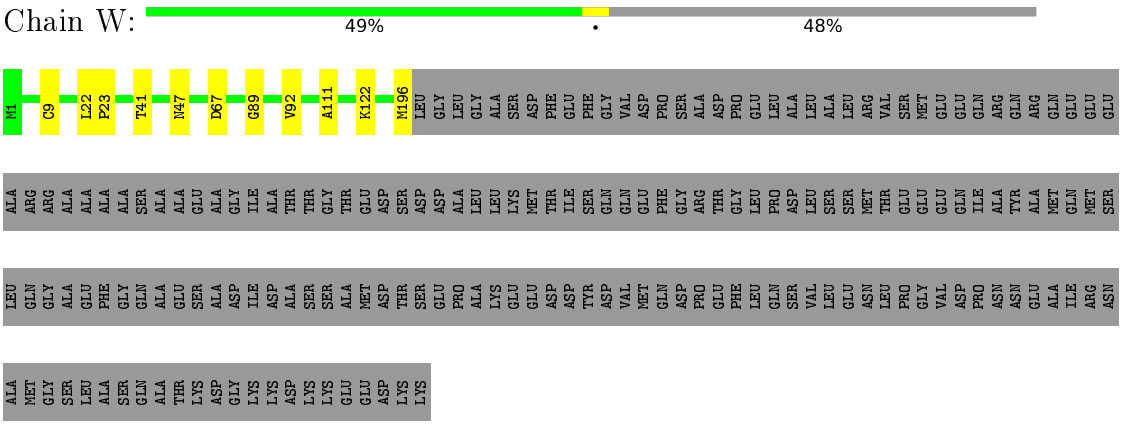
Mol	Chain	Residues	Atoms						AltConf	Trace
12	O	376	Total	C	H	N	O	S	0	0
			6061	1926	3041	514	564	16		

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.

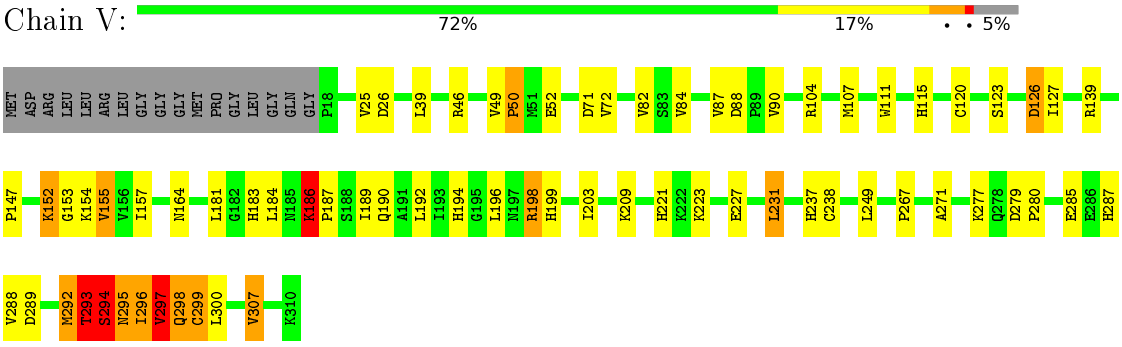
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

Chain W:



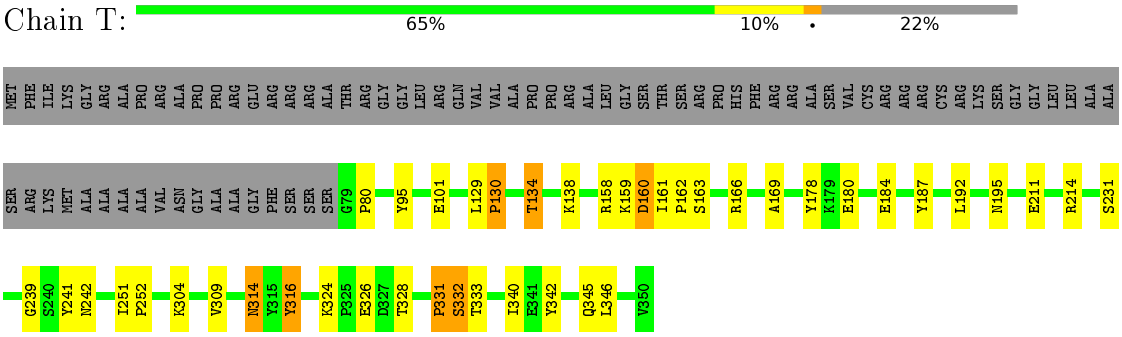
- Molecule 2: 26S proteasome non-ATPase regulatory subunit 14

Chain V:



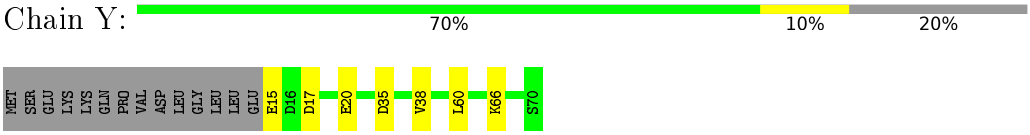
- Molecule 3: 26S proteasome non-ATPase regulatory subunit 8

Chain T:



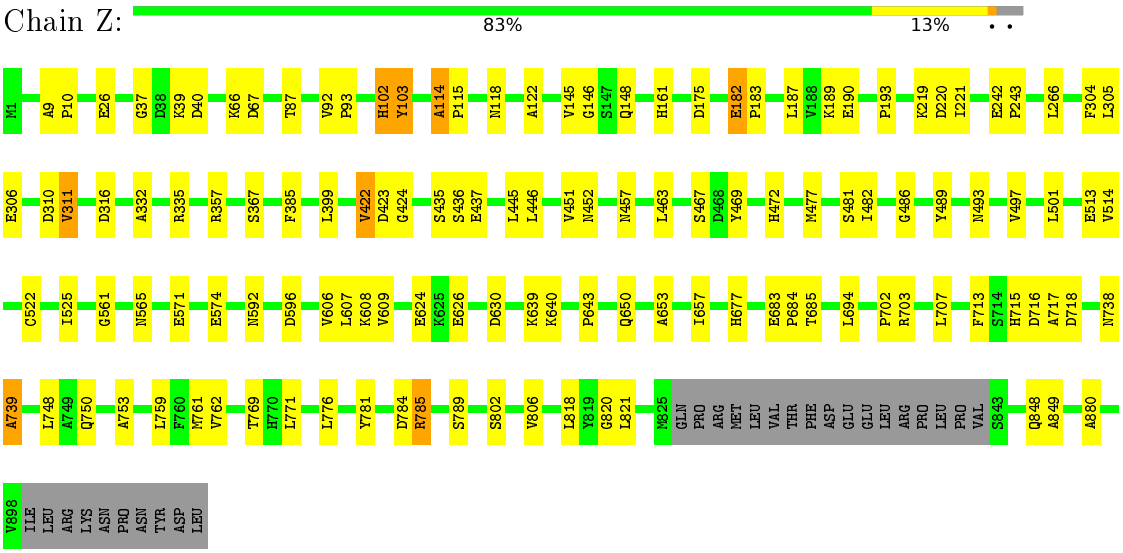
- Molecule 4: 26S proteasome complex subunit DSS1

Chain Y:



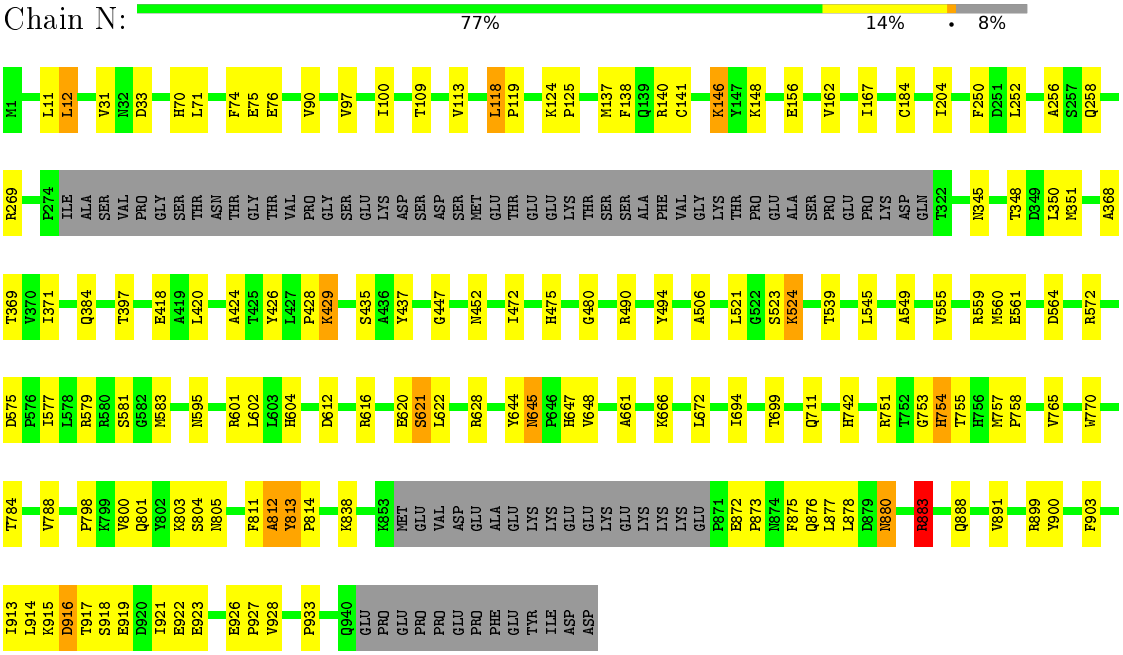
- Molecule 5: 26S proteasome non-ATPase regulatory subunit 2

Chain Z:



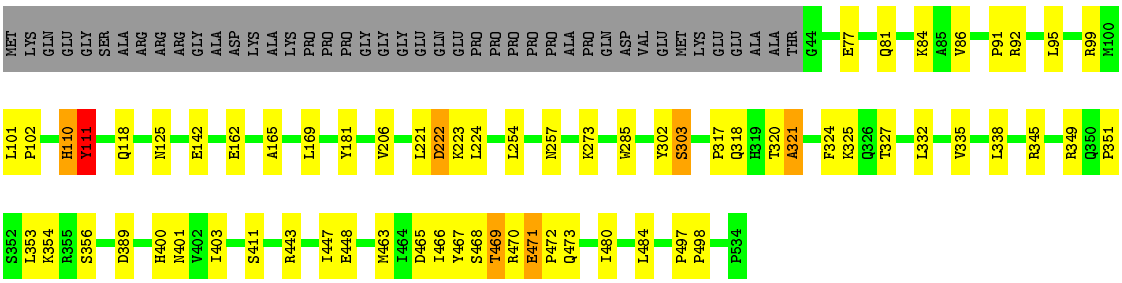
- Molecule 6: 26S proteasome non-ATPase regulatory subunit 1

Chain N:



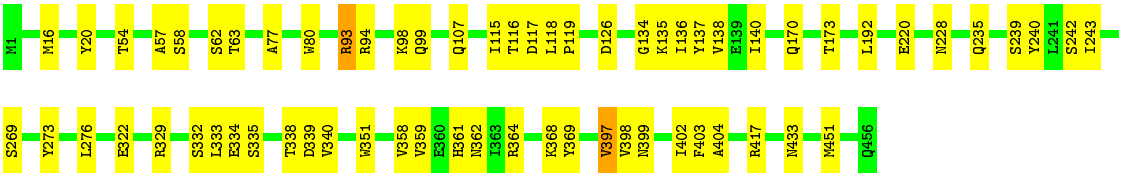
- Molecule 7: 26S proteasome non-ATPase regulatory subunit 3

Chain S:



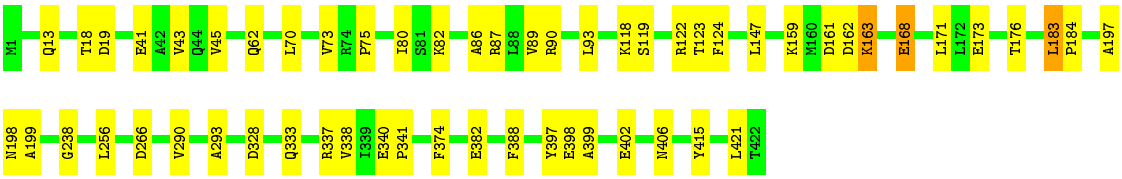
• Molecule 8: 26S proteasome non-ATPase regulatory subunit 12

Chain P:



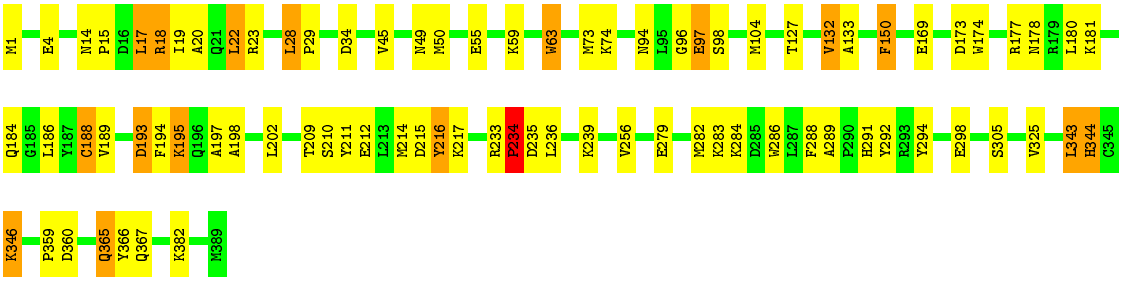
• Molecule 9: 26S proteasome non-ATPase regulatory subunit 11

Chain Q:



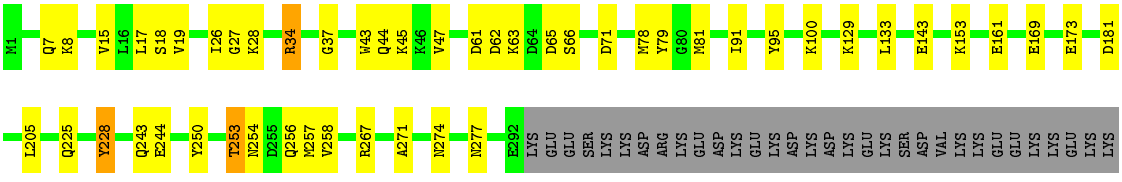
• Molecule 10: 26S proteasome non-ATPase regulatory subunit 6

Chain R:



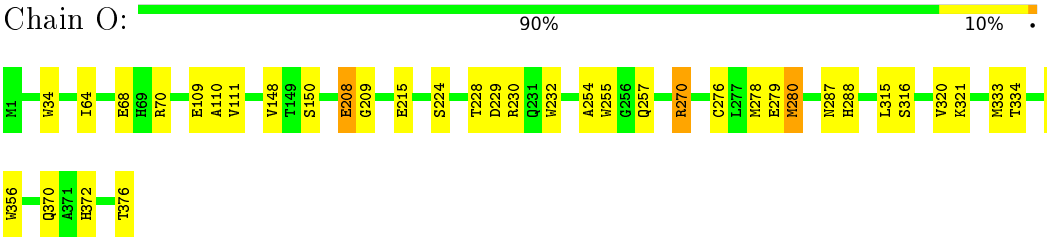
• Molecule 11: 26S proteasome non-ATPase regulatory subunit 7

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

All (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
2	V	293	THR	N-CA	-7.37	1.31	1.46
2	V	297	VAL	CA-C	-6.73	1.35	1.52
3	T	324	LYS	C-N	6.63	1.46	1.34
2	V	299	CYS	N-CA	-6.32	1.33	1.46
2	V	297	VAL	N-CA	-6.02	1.34	1.46
2	V	296	ILE	CA-C	-5.77	1.38	1.52
2	V	295	ASN	C-O	-5.51	1.12	1.23
2	V	295	ASN	CA-C	-5.40	1.39	1.52
6	N	784	THR	C-N	5.20	1.44	1.34

All (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
2	V	307	VAL	CA-CB-CG2	-7.47	99.69	110.90
2	V	293	THR	C-N-CA	-6.96	104.29	121.70
2	V	294	SER	CA-C-O	-5.96	107.58	120.10
2	V	292	MET	O-C-N	5.37	131.29	122.70
2	V	298	GLN	N-CA-C	-5.08	97.28	111.00
7	S	110	HIS	C-N-CA	5.04	134.29	121.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	O	254	ALA	Peptide
8	P	398	VAL	Peptide
10	R	234	PRO	Peptide
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
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.

All (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
2:V:296:ILE:O	2:V:299:CYS:CB	2.01	1.07
2:V:289:ASP:O	2:V:293:THR:CG2	2.09	1.00
2:V:293:THR:O	2:V:294:SER:C	1.91	0.92
2:V:296:ILE:C	2:V:299:CYS:HB2	1.94	0.86
2:V:297:VAL:O	2:V:299:CYS:N	2.13	0.81
2:V:237:HIS:CE1	2:V:298:GLN:HG2	2.16	0.80
2:V:299:CYS:SG	11:U:256:GLN:HG2	2.22	0.79
10:R:365:GLN:O	10:R:367:GLN:N	2.17	0.78
2:V:71:ASP:OD2	2:V:72:VAL:N	2.18	0.76
2:V:299:CYS:SG	11:U:256:GLN:CG	2.74	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:295:ASN:HB3	11:U:256:GLN:OE1	1.86	0.75
8:P:403:PHE:O	8:P:417:ARG:NH1	2.19	0.75
2:V:297:VAL:O	2:V:298:GLN:O	2.04	0.75
2:V:52:GLU:OE2	2:V:52:GLU:N	2.20	0.74
2:V:295:ASN:O	2:V:298:GLN:HB3	1.91	0.71
6:N:524:LYS:O	6:N:559:ARG:NH1	2.24	0.69
2:V:295:ASN:HA	2:V:298:GLN:HB2	1.72	0.69
2:V:237:HIS:NE2	2:V:298:GLN:CG	2.44	0.69
10:R:193:ASP:O	10:R:195:LYS:N	2.26	0.68
2:V:293:THR:O	2:V:295:ASN:N	2.25	0.68
7:S:465:ASP:O	7:S:467:TYR:N	2.25	0.68
2:V:237:HIS:CD2	2:V:298:GLN:HG2	2.28	0.67
2:V:292:MET:O	2:V:295:ASN:N	2.28	0.66
10:R:289:ALA:O	10:R:291:HIS:N	2.29	0.65
2:V:153:GLY:N	11:U:173:GLU:OE1	2.28	0.65
2:V:115:HIS:NE2	2:V:126:ASP:OD2	2.29	0.64
9:Q:197:ALA:O	9:Q:199:ALA:N	2.29	0.64
4:Y:17:ASP:O	7:S:99:ARG:NH1	2.32	0.64
2:V:293:THR:O	2:V:294:SER:O	2.17	0.63
6:N:258:GLN:OE1	6:N:452:ASN:ND2	2.32	0.63
2:V:299:CYS:SG	11:U:256:GLN:HG3	2.40	0.62
8:P:58:SER:O	8:P:63:THR:OG1	2.17	0.62
3:T:184:GLU:N	3:T:184:GLU:OE2	2.33	0.61
2:V:237:HIS:CE1	2:V:298:GLN:CG	2.83	0.61
2:V:152:LYS:NZ	11:U:169:GLU:OE2	2.26	0.61
6:N:348:THR:HA	6:N:742:HIS:NE2	2.15	0.61
7:S:162:GLU:N	7:S:162:GLU:OE2	2.34	0.60
2:V:294:SER:O	2:V:298:GLN:HB2	2.02	0.59
10:R:194:PHE:O	10:R:198:ALA:N	2.32	0.59
10:R:96:GLY:O	10:R:98:SER:N	2.36	0.59
2:V:194:HIS:O	2:V:198:ARG:HB3	2.04	0.57
10:R:233:ARG:HB3	10:R:234:PRO:HD2	1.87	0.57
2:V:295:ASN:HA	2:V:298:GLN:CB	2.34	0.56
3:T:342:TYR:CZ	7:S:480:ILE:HD11	2.41	0.56
5:Z:187:LEU:O	5:Z:190:GLU:N	2.39	0.56
5:Z:422:VAL:HG13	5:Z:423:ASP:H	1.71	0.55
2:V:296:ILE:CA	2:V:299:CYS:HB2	2.37	0.55
6:N:250:PHE:CE2	6:N:913:ILE:HD11	2.41	0.55
3:T:251:ILE:N	3:T:252:PRO:CD	2.70	0.55
5:Z:316:ASP:OD1	5:Z:493:ASN:N	2.40	0.55
2:V:88:ASP:HB3	2:V:90:VAL:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z:522:CYS:O	5:Z:525:ILE:HG22	2.07	0.54
10:R:173:ASP:N	10:R:173:ASP:OD1	2.41	0.54
5:Z:715:HIS:CB	5:Z:753:ALA:HB1	2.38	0.54
6:N:583:MET:HG3	6:N:602:LEU:HD11	1.89	0.54
6:N:545:LEU:HG	6:N:577:ILE:HG21	1.89	0.54
11:U:78:MET:O	11:U:81:MET:N	2.41	0.54
6:N:368:ALA:O	6:N:371:ILE:HG12	2.08	0.54
8:P:57:ALA:O	8:P:62:SER:N	2.41	0.53
6:N:804:SER:OG	6:N:876:GLN:N	2.40	0.53
2:V:71:ASP:OD1	2:V:104:ARG:NH1	2.42	0.53
5:Z:423:ASP:OD2	5:Z:424:GLY:N	2.41	0.53
9:Q:399:ALA:O	9:Q:402:GLU:N	2.41	0.53
2:V:237:HIS:CE1	2:V:298:GLN:CD	2.83	0.52
6:N:118:LEU:HB2	6:N:119:PRO:HD3	1.92	0.52
6:N:575:ASP:O	6:N:579:ARG:NH1	2.43	0.52
6:N:915:LYS:O	6:N:917:THR:N	2.42	0.52
10:R:17:LEU:O	10:R:19:ILE:N	2.43	0.52
6:N:803:LYS:HE2	6:N:875:PHE:CD1	2.44	0.52
6:N:813:TYR:OH	6:N:883:ARG:HB3	2.10	0.52
8:P:136:ILE:O	8:P:138:VAL:N	2.44	0.51
7:S:338:LEU:O	7:S:401:ASN:ND2	2.43	0.51
2:V:186:LYS:H	2:V:187:PRO:HD2	1.74	0.51
12:O:109:GLU:HG2	12:O:110:ALA:N	2.26	0.51
7:S:497:PRO:HB2	7:S:498:PRO:HD3	1.93	0.51
2:V:277:LYS:O	2:V:280:PRO:HD2	2.11	0.51
7:S:317:PRO:O	7:S:325:LYS:NZ	2.45	0.50
5:Z:486:GLY:HA2	5:Z:525:ILE:HB	1.92	0.50
3:T:328:THR:HA	3:T:331:PRO:HD2	1.92	0.50
2:V:296:ILE:O	2:V:299:CYS:CA	2.59	0.50
12:O:228:THR:O	12:O:230:ARG:N	2.45	0.50
7:S:470:ARG:O	7:S:473:GLN:N	2.45	0.50
5:Z:624:GLU:O	5:Z:626:GLU:N	2.41	0.50
10:R:343:LEU:O	10:R:344:HIS:HB2	2.12	0.49
6:N:137:MET:O	6:N:140:ARG:HB3	2.12	0.49
6:N:74:PHE:O	6:N:76:GLU:N	2.45	0.49
2:V:115:HIS:CE1	2:V:126:ASP:OD2	2.65	0.49
10:R:215:ASP:O	10:R:216:TYR:CB	2.60	0.49
9:Q:397:TYR:CE2	11:U:258:VAL:HG21	2.47	0.49
10:R:211:TYR:O	10:R:212:GLU:HB3	2.12	0.49
10:R:217:LYS:HD2	10:R:217:LYS:H	1.78	0.48
10:R:96:GLY:O	10:R:97:GLU:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:404:ALA:HA	8:P:417:ARG:HH12	1.79	0.48
10:R:202:LEU:HD21	10:R:239:LYS:HB3	1.95	0.48
7:S:92:ARG:NH1	7:S:95:LEU:HB2	2.28	0.48
2:V:192:LEU:HG	2:V:196:LEU:HB2	1.95	0.48
2:V:298:GLN:HA	2:V:298:GLN:NE2	2.28	0.48
5:Z:114:ALA:H	5:Z:115:PRO:CD	2.27	0.48
5:Z:561:GLY:O	5:Z:565:ASN:ND2	2.42	0.48
7:S:111:TYR:N	7:S:111:TYR:CD2	2.80	0.48
7:S:222:ASP:O	7:S:224:LEU:N	2.46	0.48
5:Z:463:LEU:O	5:Z:467:SER:OG	2.29	0.48
6:N:252:LEU:O	6:N:256:ALA:HB3	2.13	0.48
3:T:342:TYR:O	3:T:346:LEU:HG	2.14	0.48
11:U:15:VAL:O	11:U:18:SER:N	2.45	0.48
6:N:742:HIS:CE1	6:N:814:PRO:HG2	2.49	0.48
12:O:372:HIS:HA	12:O:376:THR:O	2.14	0.48
6:N:146:LYS:HA	6:N:146:LYS:HE3	1.94	0.48
6:N:437:TYR:HA	6:N:472:ILE:HG21	1.95	0.48
11:U:225:GLN:O	11:U:228:TYR:HB2	2.14	0.48
10:R:174:TRP:CE3	10:R:177:ARG:NH1	2.82	0.48
6:N:109:THR:HG21	6:N:156:GLU:HB3	1.96	0.47
6:N:601:ARG:HA	6:N:604:HIS:NE2	2.29	0.47
8:P:116:THR:OG1	8:P:117:ASP:N	2.47	0.47
6:N:644:TYR:O	6:N:645:ASN:CB	2.63	0.47
2:V:154:LYS:O	2:V:155:VAL:HB	2.14	0.47
8:P:358:VAL:O	8:P:361:HIS:HB3	2.14	0.47
10:R:20:ALA:HA	10:R:23:ARG:HE	1.78	0.47
11:U:257:MET:O	11:U:258:VAL:C	2.52	0.47
2:V:292:MET:O	2:V:293:THR:C	2.52	0.47
12:O:208:GLU:OE1	12:O:209:GLY:N	2.47	0.47
2:V:87:VAL:O	2:V:87:VAL:HG12	2.14	0.47
6:N:138:PHE:O	6:N:141:CYS:N	2.48	0.47
6:N:523:SER:O	6:N:559:ARG:NH1	2.47	0.47
6:N:899:ARG:NE	6:N:916:ASP:OD2	2.45	0.47
10:R:178:ASN:O	10:R:181:LYS:HB2	2.15	0.47
6:N:428:PRO:O	6:N:429:LYS:HB2	2.15	0.46
10:R:132:VAL:HG13	10:R:133:ALA:N	2.31	0.46
6:N:148:LYS:HD2	6:N:148:LYS:N	2.30	0.46
6:N:742:HIS:CD2	6:N:814:PRO:HD2	2.51	0.46
9:Q:86:ALA:O	9:Q:89:VAL:HG12	2.15	0.46
8:P:333:LEU:O	8:P:340:VAL:HG22	2.14	0.46
10:R:289:ALA:HB1	10:R:291:HIS:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z:316:ASP:OD2	5:Z:316:ASP:N	2.41	0.46
5:Z:718:ASP:N	5:Z:718:ASP:OD1	2.49	0.46
6:N:148:LYS:HD2	6:N:148:LYS:H	1.80	0.46
6:N:804:SER:HG	6:N:876:GLN:H	1.63	0.46
6:N:923:GLU:O	6:N:928:VAL:HG22	2.16	0.46
8:P:136:ILE:HG13	8:P:138:VAL:HG22	1.98	0.46
7:S:349:ARG:NH1	7:S:349:ARG:HA	2.29	0.46
6:N:124:LYS:HB2	6:N:125:PRO:HD3	1.97	0.46
6:N:90:VAL:HA	6:N:97:VAL:HG21	1.97	0.46
11:U:79:TYR:CE1	11:U:91:ILE:HG13	2.50	0.45
8:P:134:GLY:O	8:P:136:ILE:N	2.49	0.45
2:V:296:ILE:O	2:V:299:CYS:N	2.49	0.45
9:Q:163:LYS:N	9:Q:163:LYS:HD2	2.31	0.45
7:S:484:LEU:HD21	11:U:267:ARG:NH1	2.31	0.45
11:U:19:VAL:HG12	11:U:95:TYR:CZ	2.52	0.45
12:O:270:ARG:HE	12:O:270:ARG:HA	1.82	0.45
8:P:369:TYR:CE2	12:O:315:LEU:HB2	2.52	0.45
7:S:165:ALA:O	7:S:169:LEU:HG	2.17	0.45
3:T:309:VAL:O	3:T:314:ASN:ND2	2.50	0.45
11:U:19:VAL:HG12	11:U:95:TYR:CE1	2.51	0.45
2:V:84:VAL:HG13	2:V:87:VAL:HB	1.99	0.45
6:N:872:GLU:HB3	6:N:873:PRO:HA	1.99	0.45
10:R:178:ASN:O	10:R:181:LYS:N	2.48	0.45
5:Z:92:VAL:N	5:Z:93:PRO:CD	2.80	0.45
2:V:46:ARG:HG2	2:V:46:ARG:O	2.17	0.45
5:Z:39:LYS:O	5:Z:40:ASP:HB2	2.17	0.45
6:N:644:TYR:O	6:N:645:ASN:HB3	2.17	0.45
6:N:788:VAL:O	6:N:880:ASN:O	2.34	0.45
11:U:8:LYS:O	11:U:47:VAL:HA	2.16	0.45
6:N:549:ALA:HB1	6:N:581:SER:HB2	1.99	0.44
8:P:16:MET:O	8:P:20:TYR:N	2.48	0.44
8:P:77:ALA:HA	8:P:80:TRP:CE2	2.52	0.44
10:R:180:LEU:O	10:R:180:LEU:HD13	2.17	0.44
6:N:621:SER:OG	6:N:622:LEU:N	2.51	0.44
5:Z:482:ILE:HD11	5:Z:514:VAL:HG21	2.00	0.44
10:R:104:MET:HB3	10:R:127:THR:HG22	1.99	0.44
10:R:215:ASP:O	10:R:216:TYR:HB2	2.17	0.44
2:V:285:GLU:HA	2:V:288:VAL:HG22	2.00	0.44
5:Z:761:MET:HB3	5:Z:806:VAL:HG11	1.99	0.44
9:Q:338:VAL:O	9:Q:341:PRO:HD2	2.17	0.44
3:T:159:LYS:O	3:T:160:ASP:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:157:ILE:HG23	2:V:157:ILE:O	2.17	0.44
6:N:899:ARG:NE	6:N:923:GLU:HB2	2.33	0.44
5:Z:750:GLN:O	5:Z:753:ALA:HB3	2.17	0.44
6:N:447:GLY:HA3	6:N:480:GLY:HA2	2.00	0.44
6:N:801:GLN:CB	6:N:877:LEU:HB3	2.48	0.44
5:Z:114:ALA:H	5:Z:115:PRO:HD2	1.83	0.44
6:N:801:GLN:HA	6:N:878:LEU:O	2.18	0.43
6:N:917:THR:HA	6:N:922:GLU:HB3	1.99	0.43
6:N:926:GLU:HB3	6:N:927:PRO:HD2	2.00	0.43
7:S:324:PHE:O	7:S:327:THR:HG22	2.18	0.43
3:T:192:LEU:O	3:T:195:ASN:HB3	2.17	0.43
3:T:211:GLU:O	3:T:214:ARG:HG2	2.18	0.43
10:R:194:PHE:HA	10:R:197:ALA:HB3	1.99	0.43
2:V:221:HIS:HB2	2:V:223:LYS:HE3	2.00	0.43
6:N:755:THR:HG23	6:N:755:THR:O	2.17	0.43
8:P:368:LYS:C	8:P:369:TYR:CD1	2.92	0.43
7:S:92:ARG:HH21	7:S:206:VAL:HA	1.81	0.43
11:U:43:TRP:HB2	11:U:47:VAL:O	2.18	0.43
5:Z:9:ALA:N	5:Z:10:PRO:HD2	2.34	0.43
6:N:921:ILE:O	6:N:922:GLU:C	2.57	0.43
10:R:294:TYR:O	10:R:298:GLU:HG2	2.19	0.43
7:S:484:LEU:O	7:S:484:LEU:HD13	2.19	0.43
5:Z:640:LYS:HA	5:Z:771:LEU:HD22	2.00	0.43
6:N:583:MET:CG	6:N:602:LEU:HD11	2.49	0.43
10:R:63:TRP:CE3	10:R:63:TRP:HA	2.53	0.43
2:V:139:ARG:HA	2:V:139:ARG:NE	2.33	0.43
5:Z:219:LYS:O	5:Z:220:ASP:HB2	2.19	0.43
5:Z:522:CYS:HA	5:Z:525:ILE:HG22	1.99	0.43
6:N:368:ALA:O	6:N:371:ILE:CG1	2.66	0.43
6:N:71:LEU:HD13	7:S:273:LYS:HE3	2.00	0.43
6:N:903:PHE:CE2	6:N:915:LYS:HB3	2.54	0.43
8:P:334:GLU:HA	8:P:339:ASP:HA	2.00	0.43
7:S:221:LEU:N	7:S:221:LEU:HD23	2.33	0.43
2:V:300:LEU:HD22	3:T:340:ILE:HD11	2.01	0.43
11:U:26:ILE:O	11:U:28:LYS:N	2.52	0.43
6:N:612:ASP:HB3	6:N:647:HIS:ND1	2.32	0.43
6:N:800:VAL:HG11	6:N:914:LEU:HD13	2.01	0.43
12:O:34:TRP:CD1	12:O:70:ARG:NH2	2.87	0.43
11:U:253:THR:HG22	11:U:254:ASN:N	2.33	0.43
2:V:279:ASP:N	2:V:280:PRO:CD	2.81	0.43
3:T:331:PRO:O	3:T:332:SER:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:167:ILE:HD11	6:N:204:ILE:HG21	2.00	0.43
9:Q:168:GLU:O	9:Q:171:LEU:N	2.52	0.43
10:R:45:VAL:HA	10:R:49:ASN:HB2	2.00	0.43
7:S:81:GLN:HG3	7:S:91:PRO:HG2	1.99	0.43
11:U:271:ALA:O	11:U:274:ASN:HB3	2.19	0.43
5:Z:489:TYR:CD2	5:Z:497:VAL:HG21	2.54	0.43
6:N:899:ARG:O	6:N:917:THR:N	2.52	0.43
6:N:798:PRO:HB3	6:N:900:TYR:CE1	2.54	0.43
9:Q:80:ILE:O	9:Q:82:LYS:HG3	2.19	0.43
10:R:284:LYS:HD2	10:R:292:TYR:CD1	2.54	0.43
5:Z:190:GLU:HA	5:Z:193:PRO:HD2	2.01	0.43
6:N:11:LEU:O	6:N:12:LEU:CB	2.67	0.42
11:U:205:LEU:HD21	12:O:356:TRP:CH2	2.54	0.42
7:S:471:GLU:HB3	7:S:472:PRO:CD	2.49	0.42
2:V:296:ILE:O	2:V:297:VAL:C	2.50	0.42
6:N:524:LYS:HB2	6:N:555:VAL:HB	2.01	0.42
8:P:118:LEU:HB3	8:P:119:PRO:HD3	2.01	0.42
9:Q:122:ARG:C	9:Q:124:PHE:H	2.23	0.42
5:Z:266:LEU:HD11	5:Z:305:LEU:HD12	2.00	0.42
3:T:134:THR:O	3:T:138:LYS:HG3	2.20	0.42
11:U:61:ASP:OD2	11:U:62:ASP:N	2.52	0.42
2:V:194:HIS:O	2:V:199:HIS:N	2.52	0.42
5:Z:469:TYR:HB3	5:Z:481:SER:OG	2.19	0.42
6:N:811:PHE:O	6:N:812:ALA:HB3	2.18	0.42
12:O:320:VAL:HG13	12:O:333:MET:HE3	2.00	0.42
8:P:240:TYR:O	8:P:243:ILE:N	2.52	0.42
10:R:14:ASN:HB2	10:R:15:PRO:HD3	2.00	0.42
7:S:101:LEU:N	7:S:102:PRO:HD2	2.33	0.42
5:Z:592:ASN:O	5:Z:596:ASP:HB2	2.19	0.42
6:N:888:GLN:HG2	6:N:888:GLN:O	2.20	0.42
9:Q:290:VAL:O	9:Q:293:ALA:HB3	2.19	0.42
10:R:104:MET:HB3	10:R:127:THR:CG2	2.49	0.42
2:V:46:ARG:HB2	2:V:147:PRO:HB3	2.02	0.42
5:Z:469:TYR:CB	5:Z:481:SER:OG	2.68	0.42
6:N:420:LEU:O	6:N:424:ALA:HB2	2.20	0.42
8:P:235:GLN:HE22	8:P:338:THR:HB	1.83	0.42
7:S:332:LEU:HA	7:S:335:VAL:HG22	2.00	0.42
7:S:469:THR:HG22	7:S:471:GLU:H	1.85	0.42
6:N:616:ARG:HD2	6:N:770:TRP:CZ3	2.55	0.42
10:R:18:ARG:O	10:R:22:LEU:N	2.43	0.42
7:S:77:GLU:O	7:S:81:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:U:65:ASP:N	11:U:65:ASP:OD1	2.50	0.42
2:V:111:TRP:CG	2:V:111:TRP:O	2.72	0.42
5:Z:118:ASN:H	5:Z:122:ALA:HB2	1.84	0.42
3:T:316:TYR:N	3:T:316:TYR:CD2	2.86	0.42
1:W:89:GLY:O	1:W:92:VAL:HG22	2.19	0.42
6:N:100:ILE:HG22	6:N:100:ILE:O	2.19	0.42
6:N:661:ALA:HA	6:N:694:ILE:HA	2.01	0.42
10:R:50:MET:SD	10:R:74:LYS:HB2	2.59	0.42
10:R:150:PHE:O	10:R:150:PHE:CD1	2.73	0.42
10:R:169:GLU:HA	10:R:169:GLU:OE1	2.20	0.42
3:T:158:ARG:O	3:T:159:LYS:HB2	2.20	0.42
2:V:237:HIS:HE1	2:V:294:SER:OG	2.02	0.42
5:Z:653:ALA:O	5:Z:657:ILE:HG12	2.19	0.42
5:Z:781:TYR:O	5:Z:784:ASP:N	2.53	0.42
8:P:170:GLN:NE2	8:P:173:THR:O	2.53	0.41
10:R:279:GLU:O	10:R:283:LYS:HB2	2.20	0.41
2:V:203:ILE:HD12	2:V:203:ILE:N	2.34	0.41
4:Y:60:LEU:HB3	4:Y:66:LYS:HB2	2.01	0.41
5:Z:182:GLU:HB3	5:Z:183:PRO:CD	2.50	0.41
5:Z:762:VAL:HG13	5:Z:762:VAL:O	2.20	0.41
12:O:64:ILE:O	12:O:64:ILE:HG22	2.20	0.41
8:P:273:TYR:O	8:P:276:LEU:N	2.53	0.41
7:S:400:HIS:O	7:S:403:ILE:HG22	2.20	0.41
7:S:81:GLN:HA	7:S:84:LYS:HB2	2.01	0.41
5:Z:316:ASP:OD1	5:Z:493:ASN:HB2	2.20	0.41
6:N:918:SER:O	6:N:919:GLU:HB2	2.20	0.41
11:U:133:LEU:CD1	11:U:161:GLU:HA	2.50	0.41
5:Z:650:GLN:O	5:Z:653:ALA:N	2.53	0.41
5:Z:683:GLU:N	5:Z:684:PRO:HD3	2.35	0.41
6:N:883:ARG:H	6:N:883:ARG:HD3	1.85	0.41
8:P:93:ARG:HG2	8:P:94:ARG:N	2.36	0.41
10:R:184:GLN:O	10:R:188:CYS:HB2	2.20	0.41
10:R:20:ALA:HA	10:R:23:ARG:NE	2.35	0.41
2:V:267:PRO:O	2:V:271:ALA:HB2	2.20	0.41
6:N:138:PHE:CZ	6:N:162:VAL:HG13	2.55	0.41
8:P:329:ARG:HH22	8:P:351:TRP:HE1	1.69	0.41
9:Q:183:LEU:H	9:Q:184:PRO:HD2	1.86	0.41
8:P:397:VAL:HG11	9:Q:341:PRO:HB3	2.02	0.41
10:R:174:TRP:O	10:R:177:ARG:N	2.54	0.41
11:U:253:THR:O	11:U:256:GLN:N	2.53	0.41
5:Z:310:ASP:O	5:Z:311:VAL:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:645:ASN:O	6:N:648:VAL:N	2.51	0.41
6:N:753:GLY:O	6:N:754:HIS:HB2	2.21	0.41
9:Q:337:ARG:HA	9:Q:340:GLU:OE1	2.20	0.41
9:Q:147:LEU:HG	9:Q:176:THR:HG21	2.03	0.41
10:R:18:ARG:O	10:R:22:LEU:HB2	2.21	0.41
2:V:231:LEU:O	2:V:231:LEU:HD12	2.21	0.41
5:Z:820:GLY:HA3	5:Z:848:GLN:HB2	2.02	0.41
3:T:129:LEU:O	3:T:130:PRO:C	2.59	0.41
5:Z:776:LEU:O	5:Z:802:SER:O	2.39	0.41
6:N:118:LEU:HB2	6:N:119:PRO:CD	2.51	0.41
8:P:57:ALA:HB1	8:P:62:SER:H	1.86	0.41
10:R:346:LYS:HB3	10:R:346:LYS:HZ3	1.85	0.41
7:S:86:VAL:HG21	7:S:91:PRO:HD2	2.03	0.41
2:V:49:VAL:HB	2:V:50:PRO:CD	2.51	0.41
5:Z:684:PRO:HD2	5:Z:713:PHE:CE1	2.56	0.41
5:Z:738:ASN:O	5:Z:739:ALA:HB2	2.21	0.41
5:Z:677:HIS:CE1	5:Z:785:ARG:O	2.74	0.41
6:N:561:GLU:HA	6:N:564:ASP:HB2	2.03	0.41
6:N:742:HIS:CG	6:N:814:PRO:HG2	2.55	0.41
9:Q:118:LYS:O	9:Q:119:SER:HB2	2.21	0.41
7:S:320:THR:O	7:S:321:ALA:HB2	2.20	0.41
11:U:243:GLN:HG3	11:U:244:GLU:N	2.36	0.41
2:V:39:LEU:HD12	11:U:17:LEU:HD12	2.02	0.41
2:V:84:VAL:HA	2:V:87:VAL:HB	2.03	0.41
5:Z:445:LEU:HD13	5:Z:481:SER:OG	2.21	0.41
9:Q:397:TYR:O	9:Q:398:GLU:C	2.58	0.40
4:Y:15:GLU:OE2	7:S:92:ARG:CG	2.69	0.40
3:T:161:ILE:HB	3:T:162:PRO:HD3	2.03	0.40
3:T:332:SER:OG	3:T:333:THR:N	2.52	0.40
5:Z:607:LEU:O	5:Z:607:LEU:HG	2.21	0.40
6:N:805:ASN:HB2	6:N:891:VAL:HA	2.03	0.40
9:Q:90:ARG:O	9:Q:93:LEU:HB3	2.20	0.40
12:O:321:LYS:O	12:O:334:THR:OG1	2.34	0.40
9:Q:70:LEU:O	9:Q:73:VAL:HG22	2.21	0.40
10:R:282:MET:HA	10:R:286:TRP:CD1	2.56	0.40
10:R:55:GLU:O	10:R:59:LYS:HB2	2.22	0.40
11:U:37:GLY:HA3	11:U:95:TYR:CE2	2.56	0.40
2:V:123:SER:H	2:V:126:ASP:HB2	1.86	0.40
5:Z:242:GLU:N	5:Z:243:PRO:CD	2.85	0.40
5:Z:482:ILE:HB	5:Z:501:LEU:HG	2.02	0.40
6:N:348:THR:CA	6:N:742:HIS:NE2	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:923:GLU:HA	6:N:926:GLU:HB2	2.03	0.40
12:O:276:CYS:O	12:O:280:MET:HB2	2.21	0.40
8:P:359:VAL:O	8:P:362:ASN:HB2	2.22	0.40
7:S:470:ARG:O	7:S:471:GLU:C	2.59	0.40
11:U:34:ARG:CD	11:U:34:ARG:H	2.35	0.40
1:W:9:CYS:HB2	1:W:111:ALA:HA	2.03	0.40
6:N:549:ALA:HB2	6:N:577:ILE:CG2	2.51	0.40
6:N:757:MET:N	6:N:758:PRO:CD	2.85	0.40
12:O:229:ASP:O	12:O:232:TRP:CD1	2.74	0.40
8:P:57:ALA:HB1	8:P:62:SER:HB2	2.03	0.40
3:T:345:GLN:OE1	7:S:484:LEU:HD12	2.21	0.40
2:V:189:ILE:HA	2:V:192:LEU:HB3	2.04	0.40
2:V:249:LEU:HD13	9:Q:402:GLU:HG3	2.04	0.40
5:Z:716:ASP:O	5:Z:761:MET:HG3	2.22	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 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
9	Q	420/422 (100%)	349 (83%)	59 (14%)	12 (3%)	6 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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

All (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	Z	422	VAL
5	Z	739	ALA
6	N	12	LEU
6	N	33	ASP
6	N	645	ASN
6	N	916	ASP
7	S	111	TYR
7	S	321	ALA
7	S	351	PRO
7	S	466	ILE
8	P	93	ARG
8	P	397	VAL
8	P	399	ASN
9	Q	161	ASP
10	R	18	ARG
10	R	97	GLU
10	R	132	VAL
10	R	234	PRO
10	R	359	PRO
10	R	366	TYR
11	U	63	LYS
12	O	224	SER
12	O	255	TRP
2	V	183	HIS
2	V	227	GLU
3	T	242	ASN
4	Y	20	GLU
5	Z	66	LYS

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Mol	Chain	Res	Type
5	Z	145	VAL
5	Z	182	GLU
5	Z	357	ARG
5	Z	513	GLU
5	Z	571	GLU
6	N	118	LEU
6	N	435	SER
6	N	506	ALA
6	N	572	ARG
6	N	699	THR
6	N	812	ALA
6	N	880	ASN
7	S	223	LYS
7	S	447	ILE
7	S	463	MET
8	P	99	GLN
9	Q	43	VAL
9	Q	183	LEU
9	Q	198	ASN
9	Q	374	PHE
10	R	17	LEU
10	R	94	ASN
10	R	193	ASP
10	R	216	TYR
10	R	344	HIS
10	R	365	GLN
11	U	7	GLN
11	U	27	GLY
11	U	45	LYS
2	V	50	PRO
2	V	152	LYS
2	V	186	LYS
2	V	198	ARG
2	V	231	LEU
3	T	160	ASP
3	T	163	SER
3	T	239	GLY
4	Y	38	VAL
5	Z	67	ASP
5	Z	102	HIS
5	Z	103	TYR
5	Z	114	ALA

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Mol	Chain	Res	Type
5	Z	437	GLU
5	Z	643	PRO
5	Z	703	ARG
5	Z	789	SER
5	Z	849	ALA
5	Z	880	ALA
6	N	397	THR
6	N	429	LYS
6	N	490	ARG
6	N	539	THR
6	N	560	MET
7	S	303	SER
8	P	239	SER
8	P	335	SER
9	Q	18	THR
9	Q	62	GLN
10	R	4	GLU
10	R	34	ASP
10	R	195	LYS
10	R	288	PHE
10	R	360	ASP
11	U	71	ASP
12	O	288	HIS
1	W	22	LEU
2	V	164	ASN
2	V	181	LEU
2	V	184	LEU
2	V	190	GLN
5	Z	146	GLY
5	Z	221	ILE
5	Z	436	SER
5	Z	717	ALA
5	Z	821	LEU
6	N	75	GLU
6	N	475	HIS
6	N	524	LYS
6	N	754	HIS
7	S	448	GLU
8	P	98	LYS
8	P	135	LYS
8	P	220	GLU
8	P	322	GLU

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Mol	Chain	Res	Type
11	U	129	LYS
11	U	228	TYR
12	O	68	GLU
12	O	280	MET
2	V	155	VAL
3	T	134	THR
3	T	169	ALA
5	Z	87	THR
5	Z	332	ALA
5	Z	457	ASN
5	Z	818	LEU
6	N	628	ARG
6	N	883	ARG
6	N	933	PRO
7	S	181	TYR
8	P	115	ILE
8	P	402	ILE
9	Q	123	THR
9	Q	159	LYS
9	Q	162	ASP
12	O	150	SER
12	O	370	GLN
6	N	813	TYR
7	S	222	ASP
8	P	137	TYR
9	Q	75	PRO
5	Z	37	GLY
12	O	111	VAL
2	V	25	VAL
2	V	127	ILE
3	T	130	PRO
5	Z	702	PRO
7	S	471	GLU
9	Q	238	GLY
12	O	148	VAL
5	Z	451	VAL
6	N	113	VAL
3	T	80	PRO
3	T	331	PRO
10	R	325	VAL

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 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
All	All	4346/4729 (92%)	4179 (96%)	167 (4%)	44 74

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W	41	THR
1	W	47	ASN
1	W	67	ASP
1	W	122	LYS
1	W	196	MET
2	V	26	ASP
2	V	82	VAL
2	V	107	MET
2	V	120	CYS
2	V	126	ASP
2	V	186	LYS
2	V	209	LYS
2	V	238	CYS
2	V	287	HIS

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Mol	Chain	Res	Type
2	V	307	VAL
3	T	95	TYR
3	T	101	GLU
3	T	166	ARG
3	T	178	TYR
3	T	187	TYR
3	T	231	SER
3	T	304	LYS
3	T	314	ASN
3	T	316	TYR
3	T	326	GLU
4	Y	35	ASP
5	Z	26	GLU
5	Z	103	TYR
5	Z	148	GLN
5	Z	161	HIS
5	Z	175	ASP
5	Z	189	LYS
5	Z	304	PHE
5	Z	306	GLU
5	Z	335	ARG
5	Z	385	PHE
5	Z	399	LEU
5	Z	435	SER
5	Z	446	LEU
5	Z	452	ASN
5	Z	472	HIS
5	Z	477	MET
5	Z	574	GLU
5	Z	606	VAL
5	Z	608	LYS
5	Z	609	VAL
5	Z	630	ASP
5	Z	639	LYS
5	Z	685	THR
5	Z	694	LEU
5	Z	707	LEU
5	Z	748	LEU
5	Z	759	LEU
5	Z	769	THR
5	Z	785	ARG
6	N	31	VAL

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Mol	Chain	Res	Type
6	N	70	HIS
6	N	146	LYS
6	N	184	CYS
6	N	269	ARG
6	N	345	ASN
6	N	350	LEU
6	N	351	MET
6	N	369	THR
6	N	384	GLN
6	N	418	GLU
6	N	426	TYR
6	N	494	TYR
6	N	521	LEU
6	N	595	ASN
6	N	620	GLU
6	N	621	SER
6	N	666	LYS
6	N	672	LEU
6	N	711	GLN
6	N	751	ARG
6	N	765	VAL
6	N	838	LYS
6	N	883	ARG
7	S	110	HIS
7	S	111	TYR
7	S	118	GLN
7	S	125	ASN
7	S	142	GLU
7	S	254	LEU
7	S	257	ASN
7	S	285	TRP
7	S	302	TYR
7	S	303	SER
7	S	318	GLN
7	S	345	ARG
7	S	353	LEU
7	S	354	LYS
7	S	356	SER
7	S	389	ASP
7	S	411	SER
7	S	443	ARG
7	S	468	SER

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Mol	Chain	Res	Type
7	S	469	THR
8	P	54	THR
8	P	107	GLN
8	P	126	ASP
8	P	140	ILE
8	P	192	LEU
8	P	228	ASN
8	P	242	SER
8	P	269	SER
8	P	332	SER
8	P	364	ARG
8	P	433	ASN
8	P	451	MET
9	Q	13	GLN
9	Q	19	ASP
9	Q	41	GLU
9	Q	45	VAL
9	Q	87	ARG
9	Q	163	LYS
9	Q	168	GLU
9	Q	173	GLU
9	Q	256	LEU
9	Q	266	ASP
9	Q	328	ASP
9	Q	333	GLN
9	Q	382	GLU
9	Q	388	PHE
9	Q	406	ASN
9	Q	415	TYR
9	Q	421	LEU
10	R	1	MET
10	R	22	LEU
10	R	63	TRP
10	R	73	MET
10	R	150	PHE
10	R	186	LEU
10	R	188	CYS
10	R	189	VAL
10	R	209	THR
10	R	210	SER
10	R	214	MET
10	R	234	PRO

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Mol	Chain	Res	Type
10	R	235	ASP
10	R	236	LEU
10	R	256	VAL
10	R	305	SER
10	R	343	LEU
10	R	346	LYS
10	R	382	LYS
11	U	34	ARG
11	U	44	GLN
11	U	66	SER
11	U	100	LYS
11	U	143	GLU
11	U	153	LYS
11	U	181	ASP
11	U	250	TYR
11	U	253	THR
11	U	277	ASN
12	O	208	GLU
12	O	215	GLU
12	O	257	GLN
12	O	270	ARG
12	O	278	MET
12	O	279	GLU
12	O	287	ASN
12	O	316	SER
12	O	339	ARG
12	O	350	LYS

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 (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 carbohydrates 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)

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