



Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 04:08 PM EST

PDB ID : 6MSG
EMDB ID : EMD-9219
Title : Cryo-EM structures and dynamics of substrate-engaged human 26S proteasome
Authors : Mao, Y.D.
Deposited on : 2018-10-16
Resolution : 3.50 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

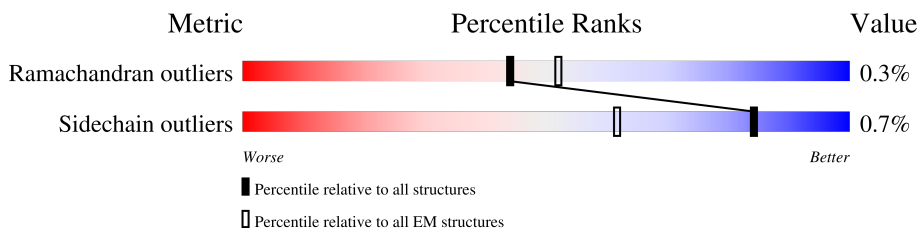
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	U	953	12% 86% 14%
2	V	533	31% 89% 10%
3	W	456	30% 99%
4	X	422	30% 90% 10%
5	Y	389	96%
6	Z	324	87% 12%
7	a	376	98%
8	b	377	51% 49%
9	c	309	88% 5% 7%

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Mol	Chain	Length	Quality of chain
10	d	349	7% 72% 26%
11	e	70	51% 6% 43%
12	f	892	66% 95%
13	A	433	8% 81% 18%
14	B	440	13% 78% 21%
15	C	398	6% 98%
16	D	418	88% 9%
17	E	403	94%
18	F	439	5% 88% 10%
19	u	76	82% 99%
20	v	24	71% 100%
21	G	245	98%
21	g	245	98%
22	H	233	100%
22	h	233	100%
23	I	260	96%
23	i	260	96%
24	J	247	97%
24	j	247	5% 97%
25	K	240	95% 5%
25	k	240	95% 5%
26	L	268	88% 11%
26	l	268	88% 11%
27	M	254	94% 6%
27	m	254	94% 6%

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Mol	Chain	Length	Quality of chain
28	N	238	 80% 20%
28	n	238	 80% 20%
29	O	276	 80% 20%
29	o	276	 80% 20%
30	P	204	 100%
30	p	204	 100%
31	Q	201	 99% .
31	q	201	 99% .
32	R	262	 77% 23%
32	r	262	 77% 23%
33	S	240	 89% 11%
33	s	240	 89% 11%
34	T	263	 81% 18%
34	t	263	 81% 18%

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 104399 atoms, of which 0 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	U	822	6414	4072	1088	1210	44	0	0

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	V	480	3852	2444	684	710	14	0	0

- Molecule 3 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	W	456	3703	2339	635	704	25	0	0

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	X	380	3009	1918	509	570	12	0	0

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	Y	378	3115	1987	533	578	17	0	0

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	Z	286	2281	1457	392	427	5	0	0

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	a	373	2995	1911	510	559	15	0	0

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	b	191	1458	910	261	279	8	0	0

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	c	287	2260	1430	389	422	19	0	0

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	d	257	2116	1371	346	390	9	0	0

- Molecule 11 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	e	40	334	200	55	77	2	0	0

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	f	889	6866	4315	1174	1331	46	0	0

- Molecule 13 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	A	356	2767	1741	488	521	17	0	0

- Molecule 14 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	B	347	2691	1694	455	530	12	0	0

- Molecule 15 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	C	396	3105	1954	558	576	17	0	0

- Molecule 16 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	D	380	3040	1923	524	580	13	0	0

- Molecule 17 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	E	389	3097	1947	552	581	17	0	0

- Molecule 18 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	F	395	3098	1951	533	596	18	0	0

- Molecule 19 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	u	76	603	378	107	117	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	63	ARG	LYS	conflict	UNP P0CG47

- Molecule 20 is a protein called substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	v	24	Total	C	N	O	0	0
			120	72	24	24		

- Molecule 21 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		
21	g	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

- Molecule 22 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	H	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		
22	h	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 23 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	I	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		
23	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 24 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	J	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		
24	j	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

- Molecule 25 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	K	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		
25	k	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 26 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	L	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		
26	l	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 27 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		
27	m	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

- Molecule 28 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	N	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		
28	n	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

- Molecule 29 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	O	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		
29	o	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

- Molecule 30 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	P	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		
30	p	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

- Molecule 31 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
31	q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 32 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
32	r	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 33 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		
33	s	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

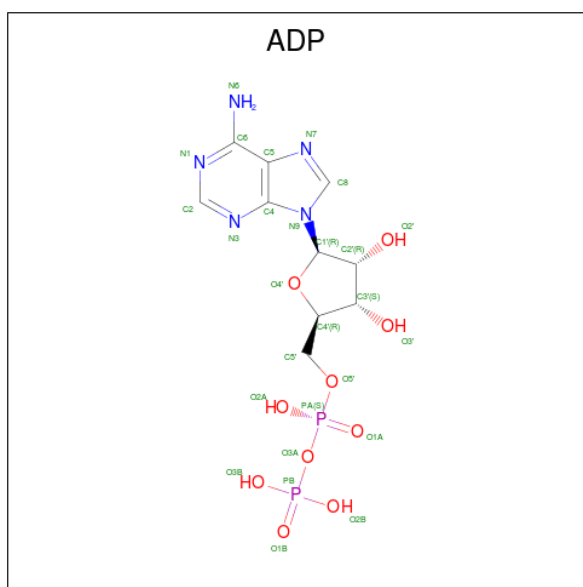
- Molecule 34 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
34	t	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn).

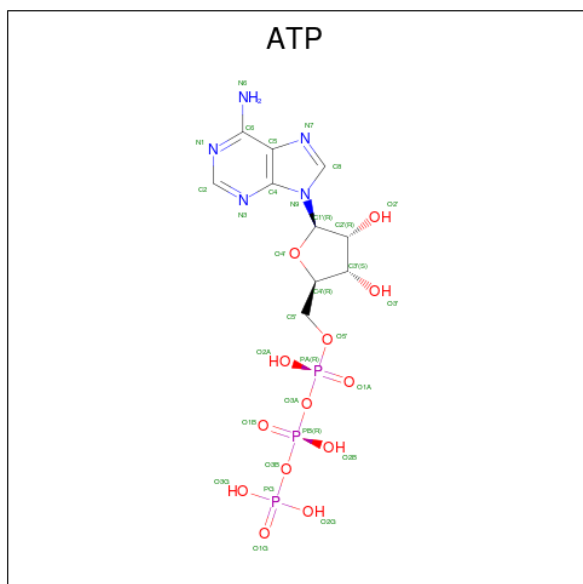
Mol	Chain	Residues	Atoms		AltConf
35	c	1	Total	Zn	0
			1	1	

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
36	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
36	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 37 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
37	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
37	D	1	Total 31	C 10	N 5	O 13	P 3	0
37	E	1	Total 31	C 10	N 5	O 13	P 3	0

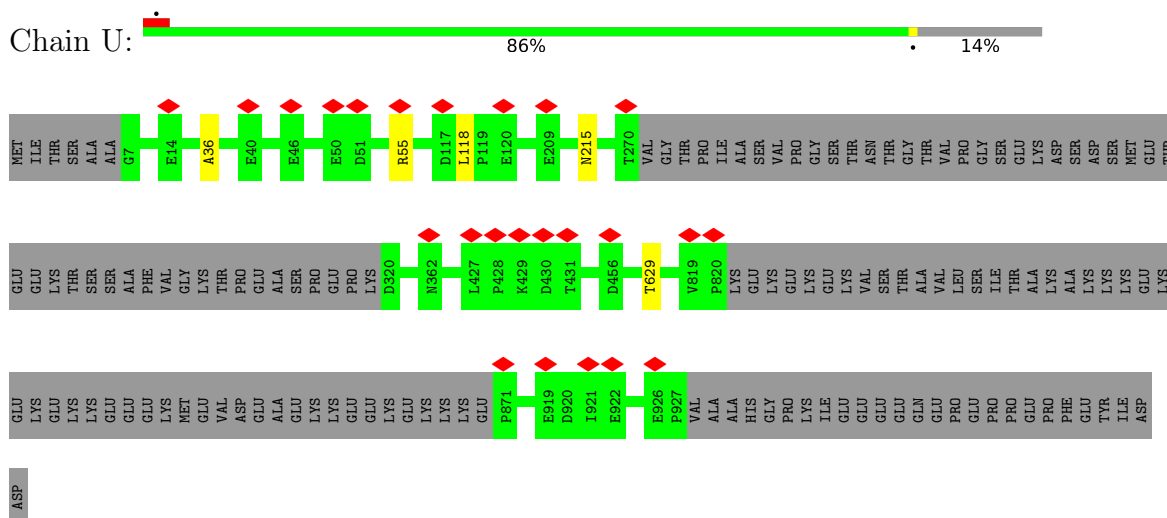
- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	C	1	Total 1	Mg 1	0
38	D	1	Total 1	Mg 1	0
38	E	1	Total 1	Mg 1	0

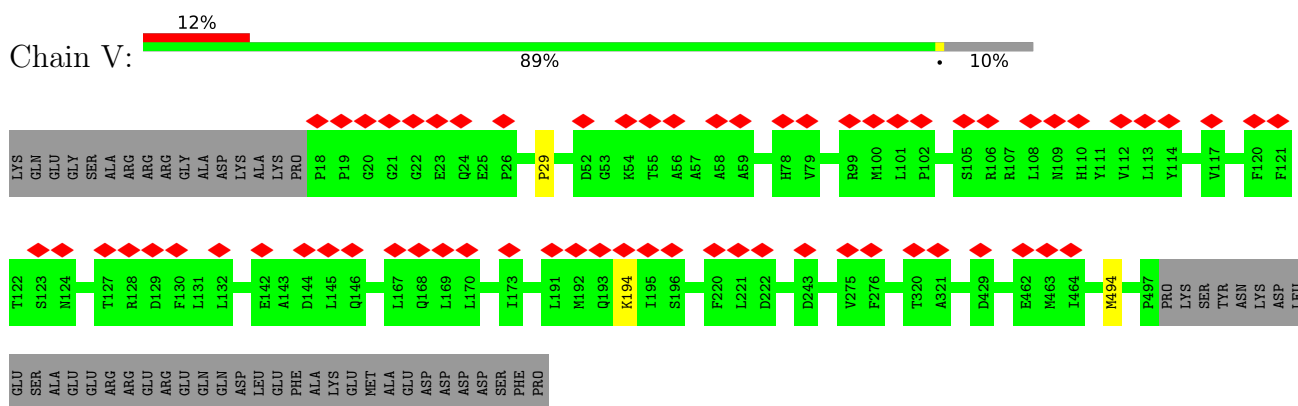
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

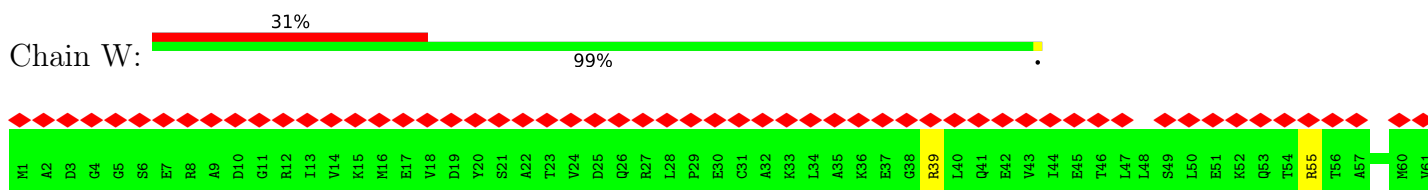
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 1

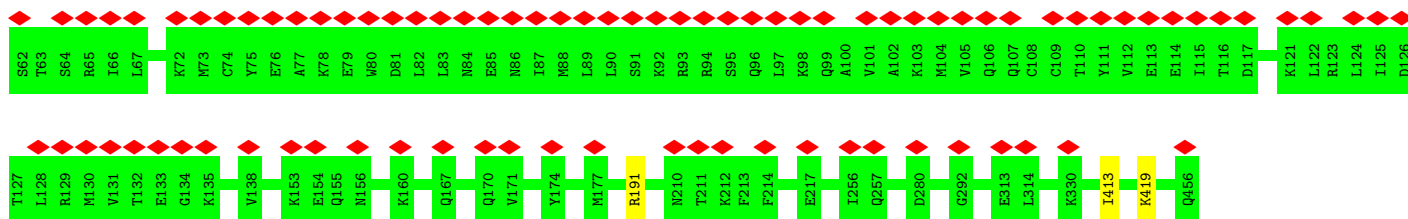


- Molecule 2: 26S proteasome non-ATPase regulatory subunit 3

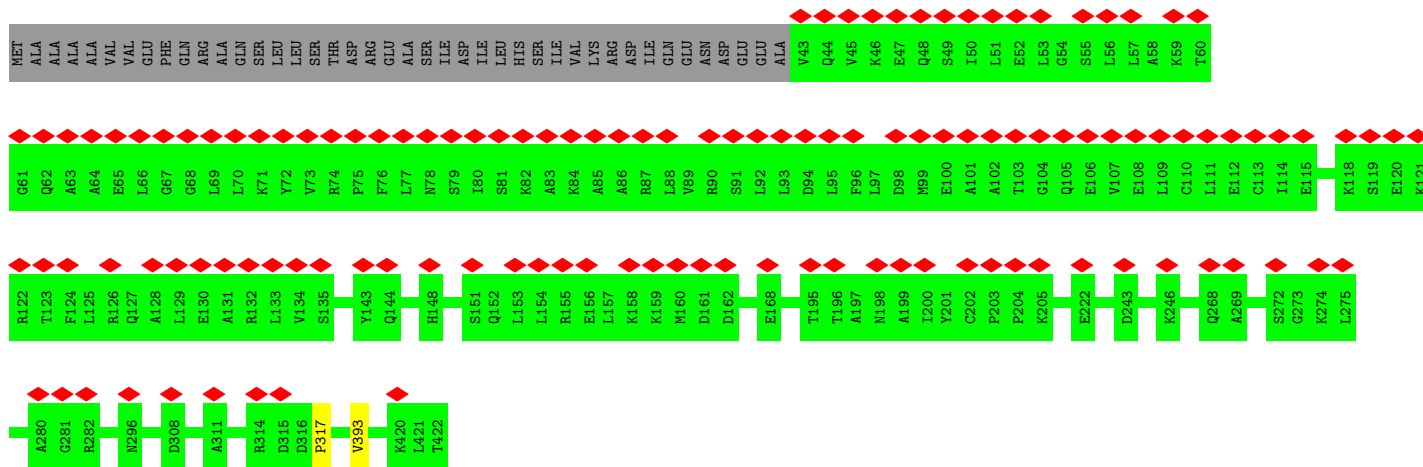
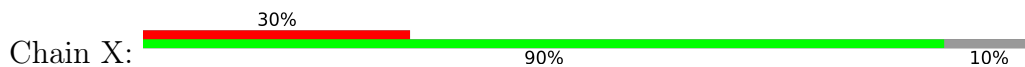


- Molecule 3: 26S proteasome non-ATPase regulatory subunit 12

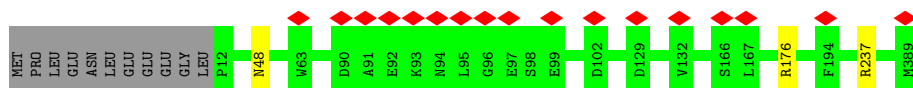




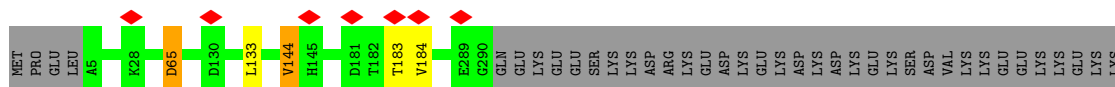
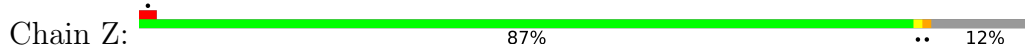
• Molecule 4: 26S proteasome non-ATPase regulatory subunit 11



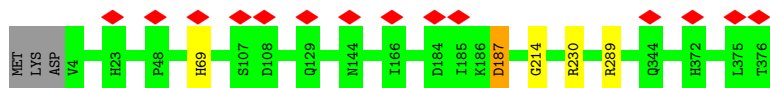
• Molecule 5: 26S proteasome non-ATPase regulatory subunit 6



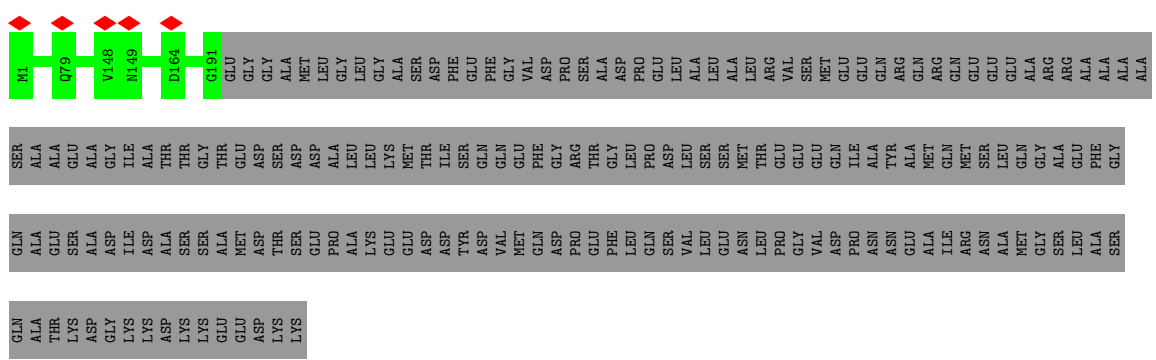
• Molecule 6: 26S proteasome non-ATPase regulatory subunit 7



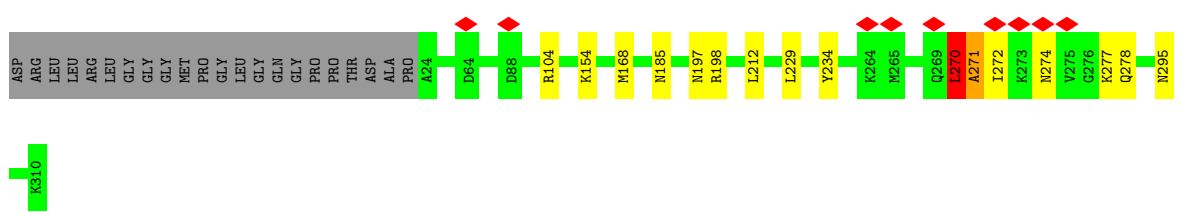
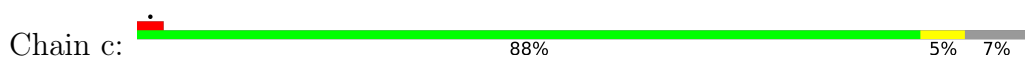
• Molecule 7: 26S proteasome non-ATPase regulatory subunit 13



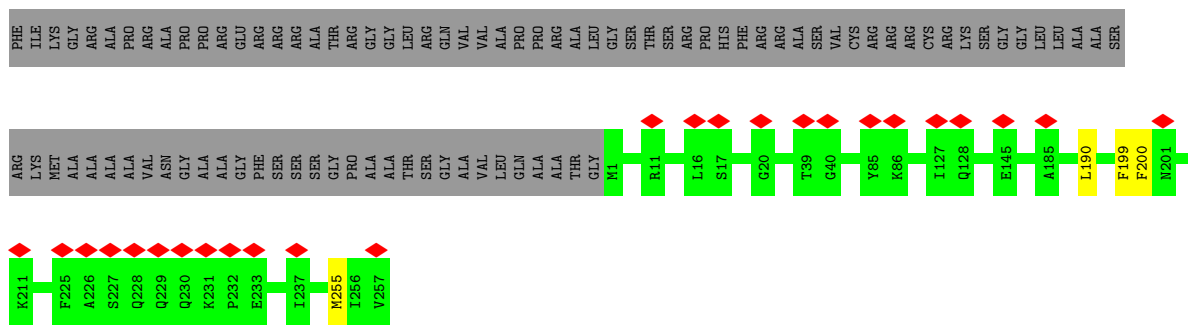
• Molecule 8: 26S proteasome non-ATPase regulatory subunit 4



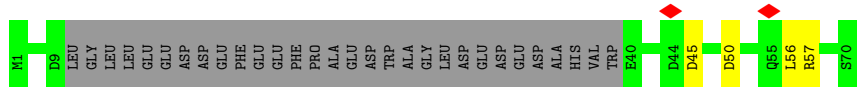
- Molecule 9: 26S proteasome non-ATPase regulatory subunit 14



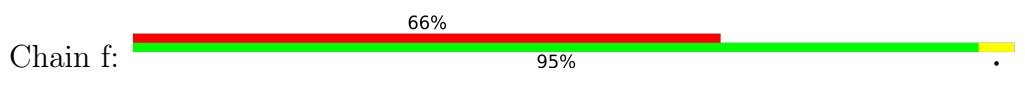
- Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

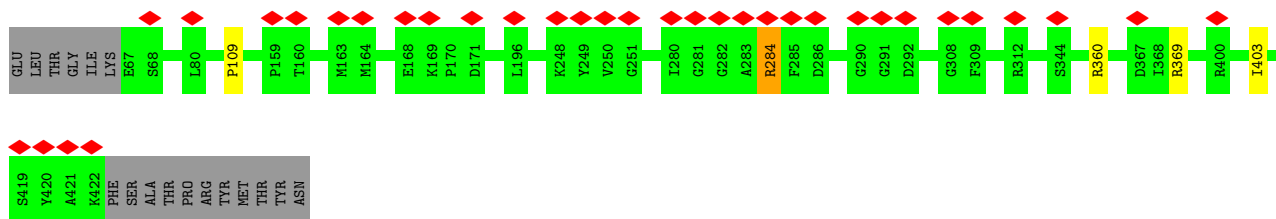


- Molecule 11: 26S proteasome complex subunit SEM1

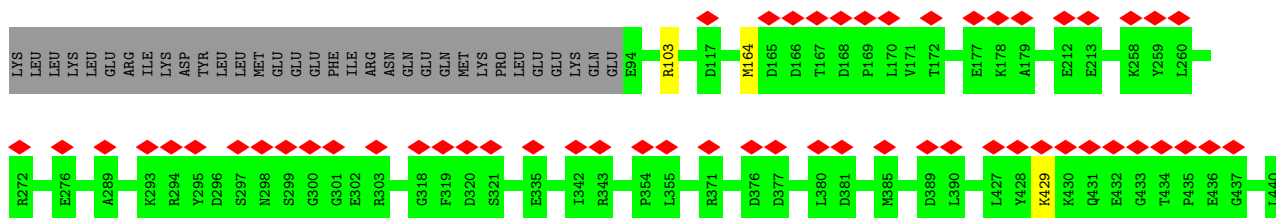
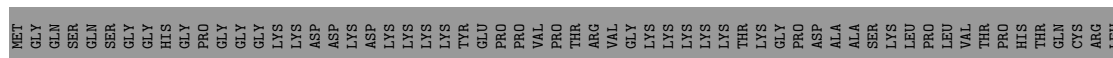
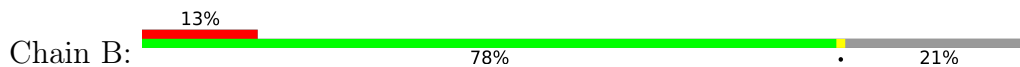


- Molecule 12: 26S proteasome non-ATPase regulatory subunit 2

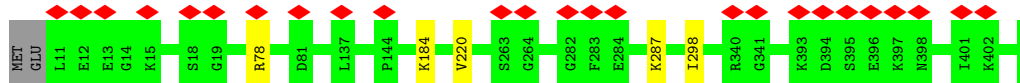




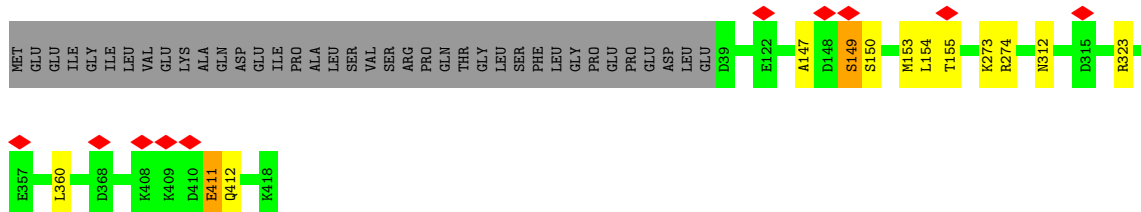
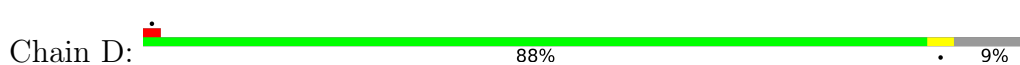
- Molecule 14: 26S proteasome regulatory subunit 4



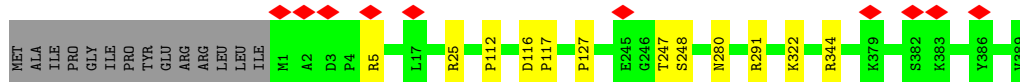
- Molecule 15: 26S proteasome regulatory subunit 8



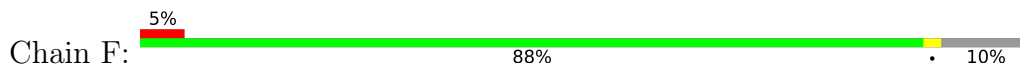
- Molecule 16: 26S proteasome regulatory subunit 6B

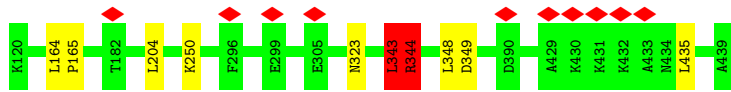
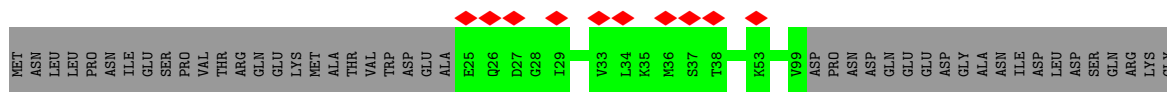


- Molecule 17: 26S proteasome regulatory subunit 10B

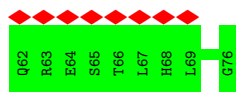
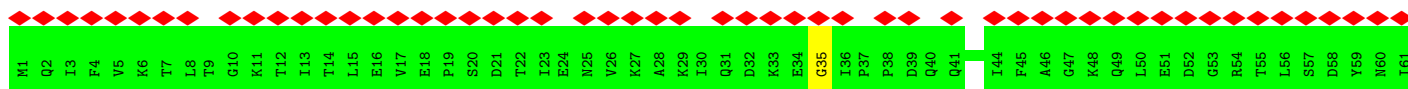
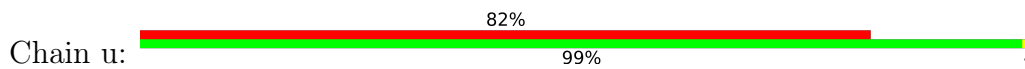


- Molecule 18: 26S proteasome regulatory subunit 6A

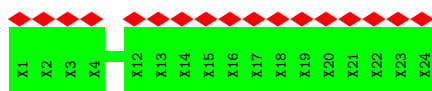




• Molecule 19: Ubiquitin



• Molecule 20: substrate



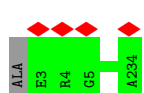
• Molecule 21: Proteasome subunit alpha type-6



• Molecule 21: Proteasome subunit alpha type-6

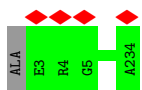


• Molecule 22: Proteasome subunit alpha type-2



• Molecule 22: Proteasome subunit alpha type-2

Chain h:  100%



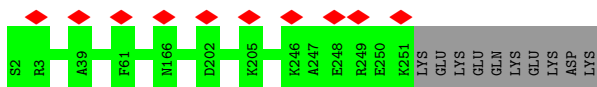
- Molecule 23: Proteasome subunit alpha type-4

Chain I:  96%



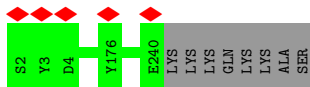
- Molecule 23: Proteasome subunit alpha type-4

Chain i:  96%



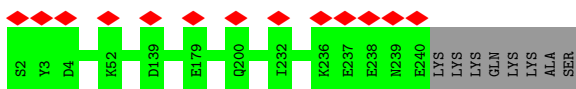
- Molecule 24: Proteasome subunit alpha type-7

Chain J:  97%



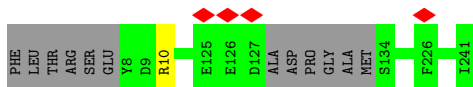
- Molecule 24: Proteasome subunit alpha type-7

Chain j:  5% 97%



- Molecule 25: Proteasome subunit alpha type-5

Chain K:  95% 5%




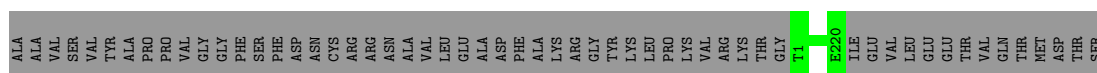
- Molecule 25: Proteasome subunit alpha type-5

Chain k:  95% 5%



- Molecule 29: Proteasome subunit beta type-7

Chain o:  80% 20%



- Molecule 30: Proteasome subunit beta type-3

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 30: Proteasome subunit beta type-3

Chain p:  100%

There are no outlier residues recorded for this chain.

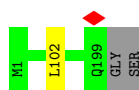
- Molecule 31: Proteasome subunit beta type-2

Chain Q:  99%




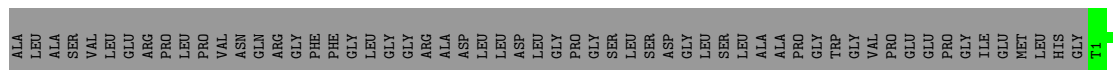
- Molecule 31: Proteasome subunit beta type-2

Chain q:  99%




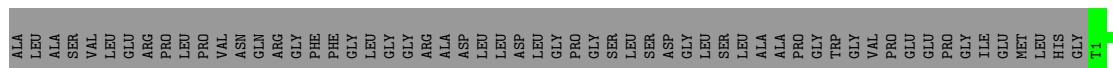
- Molecule 32: Proteasome subunit beta type-5

Chain R:  77% 23%



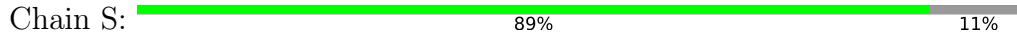
- Molecule 32: Proteasome subunit beta type-5

Chain r:  77% 23%



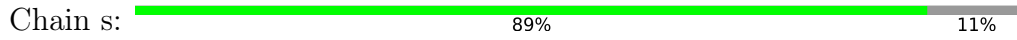
C201
SER
THR
PRO

- Molecule 33: Proteasome subunit beta type-1



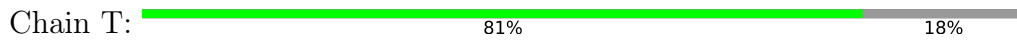
LEU SER SER THR ALA MET TYR SER PRO GLY ARG ASP LEU GLY MET MET PRO HIS ARG ALA ALA GLY PRO LEU GLN LEU R1 R213

- Molecule 33: Proteasome subunit beta type-1



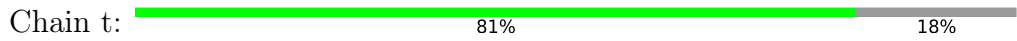
LEU SER SER THR ALA MET TYR SER PRO GLY ARG ASP LEU GLY MET MET PRO HIS ARG ALA ALA GLY PRO LEU GLN LEU R1 R213

- Molecule 34: Proteasome subunit beta type-4



GLU ALA PHE LEU GLY SER ARG SER LEU TRP ALA GLY PRO PRO GLY GLN PHE TYR ARG ILE PRO SER THR PRO ASP SER PHE MET ASP PRO ALA SER LEU TYR ARG GLY PRO ILE THR ARG TI R37 R215 SER GLY PHE GLU

- Molecule 34: Proteasome subunit beta type-4



GLU ALA PHE LEU GLY SER ARG SER LEU TRP ALA GLY PRO PRO GLY GLN PHE TYR ARG ILE PRO SER THR PRO ASP SER PHE MET ASP PRO ALA SER LEU TYR ARG GLY PRO ILE THR ARG TI R37 R215 SER GLY PHE GLU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	112776	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.014	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0035	Depositor
Map size (\AA)	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.685, 0.685, 0.685	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, ATP, ADP

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	U	0.30	0/6530	0.54	1/8840 (0.0%)
2	V	0.32	0/3929	0.59	0/5309
3	W	0.29	0/3751	0.56	0/5042
4	X	0.28	0/3053	0.52	0/4115
5	Y	0.31	0/3173	0.57	0/4273
6	Z	0.32	0/2324	0.59	2/3150 (0.1%)
7	a	0.29	0/3053	0.57	1/4133 (0.0%)
8	b	0.28	0/1478	0.55	0/2001
9	c	0.34	0/2302	0.65	3/3110 (0.1%)
10	d	0.30	0/2162	0.61	1/2919 (0.0%)
11	e	0.32	0/338	0.73	0/450
12	f	0.33	1/6980 (0.0%)	0.71	6/9433 (0.1%)
13	A	0.29	0/2814	0.53	0/3801
14	B	0.28	0/2730	0.53	0/3688
15	C	0.30	0/3146	0.54	0/4226
16	D	0.31	0/3090	0.61	0/4168
17	E	0.31	0/3145	0.59	1/4233 (0.0%)
18	F	0.30	0/3137	0.62	6/4223 (0.1%)
19	u	0.23	0/609	0.39	0/819
21	G	0.34	0/1859	0.55	1/2523 (0.0%)
21	g	0.34	0/1859	0.55	1/2523 (0.0%)
22	H	0.37	0/1743	0.53	0/2372
22	h	0.37	0/1743	0.53	0/2372
23	I	0.32	0/1942	0.53	0/2628
23	i	0.32	0/1942	0.53	0/2628
24	J	0.31	0/1728	0.51	0/2358
24	j	0.31	0/1728	0.51	0/2358
25	K	0.30	0/1747	0.53	0/2364
25	k	0.30	0/1747	0.53	0/2364
26	L	0.32	0/1885	0.54	0/2552
26	l	0.32	0/1885	0.54	0/2552
27	M	0.35	0/1891	0.53	0/2552

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	m	0.35	0/1891	0.53	0/2552
28	N	0.32	0/1454	0.49	0/1967
28	n	0.32	0/1454	0.49	0/1967
29	O	0.32	0/1670	0.51	0/2265
29	o	0.32	0/1670	0.51	0/2265
30	P	0.32	0/1614	0.50	0/2177
30	p	0.32	0/1614	0.50	0/2177
31	Q	0.34	0/1603	0.56	0/2174
31	q	0.34	0/1603	0.56	0/2174
32	R	0.35	0/1579	0.48	0/2134
32	r	0.35	0/1579	0.48	0/2134
33	S	0.32	0/1671	0.50	0/2253
33	s	0.32	0/1671	0.50	0/2253
34	T	0.33	0/1700	0.50	0/2305
34	t	0.33	0/1700	0.50	0/2305
All	All	0.32	1/105916 (0.0%)	0.56	23/143181 (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
2	V	0	1
4	X	0	1
6	Z	0	2
7	a	0	1
9	c	0	2
10	d	0	2
11	e	0	2
12	f	0	12
13	A	0	1
15	C	0	1
16	D	0	4
18	F	0	1
All	All	0	30

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	f	192	VAL	C-N	5.94	1.45	1.34

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	g	210	PHE	C-N-CA	8.26	142.34	121.70
21	G	210	PHE	C-N-CA	8.25	142.34	121.70
12	f	830	LEU	CA-CB-CG	7.96	133.61	115.30
18	F	348	LEU	CA-CB-CG	7.24	131.94	115.30
12	f	759	LEU	CA-CB-CG	6.75	130.81	115.30
12	f	612	LEU	CA-CB-CG	6.72	130.77	115.30
18	F	164	LEU	CA-CB-CG	6.57	130.42	115.30
9	c	212	LEU	CA-CB-CG	6.16	129.47	115.30
12	f	811	LEU	CA-CB-CG	6.14	129.42	115.30
9	c	270	LEU	C-N-CA	6.10	136.94	121.70
18	F	204	LEU	CA-CB-CG	5.99	129.07	115.30
18	F	435	LEU	CA-CB-CG	5.82	128.69	115.30
10	d	190	LEU	CA-CB-CG	5.66	128.31	115.30
17	E	116	ASP	CB-CG-OD1	5.65	123.39	118.30
6	Z	133	LEU	CA-CB-CG	5.55	128.07	115.30
7	a	187	ASP	CB-CG-OD1	5.47	123.23	118.30
12	f	217	LEU	CA-CB-CG	5.43	127.80	115.30
18	F	343	LEU	C-N-CA	5.24	134.81	121.70
1	U	118	LEU	CA-CB-CG	5.14	127.12	115.30
12	f	858	LYS	C-N-CD	5.14	139.19	128.40
6	Z	65	ASP	CB-CG-OD1	5.13	122.92	118.30
9	c	229	LEU	CA-CB-CG	5.12	127.08	115.30
18	F	344	ARG	N-CA-C	5.10	124.78	111.00

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	A	284	ARG	Peptide
15	C	220	VAL	Peptide
16	D	147	ALA	Peptide
16	D	149	SER	Peptide
16	D	150	SER	Peptide
16	D	411	GLU	Peptide
18	F	343	LEU	Peptide
2	V	29	PRO	Peptide
4	X	393	VAL	Peptide
6	Z	144	VAL	Peptide
6	Z	183	THR	Peptide
7	a	214	GLY	Peptide
9	c	270	LEU	Peptide

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Mol	Chain	Res	Type	Group
9	c	271	ALA	Peptide
10	d	199	PHE	Peptide
10	d	255	MET	Peptide
11	e	45	ASP	Peptide
11	e	56	LEU	Peptide
12	f	340	MET	Peptide
12	f	642	ALA	Peptide
12	f	737	ASN	Peptide
12	f	755	ASP	Peptide
12	f	807	ARG	Peptide
12	f	809	ILE	Peptide
12	f	816	TYR	Peptide
12	f	822	VAL	Peptide
12	f	823	ALA	Peptide
12	f	854	GLY	Peptide
12	f	870	THR	Peptide
12	f	875	ALA	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	U	816/953 (86%)	753 (92%)	62 (8%)	1 (0%)	51	84
2	V	478/533 (90%)	426 (89%)	52 (11%)	0	100	100
3	W	454/456 (100%)	408 (90%)	46 (10%)	0	100	100
4	X	378/422 (90%)	357 (94%)	20 (5%)	1 (0%)	41	75
5	Y	376/389 (97%)	345 (92%)	31 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Z	284/324 (88%)	247 (87%)	34 (12%)	3 (1%)	14	52
7	a	371/376 (99%)	341 (92%)	28 (8%)	2 (0%)	29	68
8	b	189/377 (50%)	167 (88%)	22 (12%)	0	100	100
9	c	285/309 (92%)	238 (84%)	44 (15%)	3 (1%)	14	52
10	d	255/349 (73%)	212 (83%)	42 (16%)	1 (0%)	34	72
11	e	36/70 (51%)	24 (67%)	10 (28%)	2 (6%)	2	17
12	f	887/892 (99%)	712 (80%)	164 (18%)	11 (1%)	13	50
13	A	354/433 (82%)	306 (86%)	47 (13%)	1 (0%)	41	75
14	B	345/440 (78%)	305 (88%)	40 (12%)	0	100	100
15	C	394/398 (99%)	344 (87%)	50 (13%)	0	100	100
16	D	378/418 (90%)	326 (86%)	49 (13%)	3 (1%)	19	58
17	E	387/403 (96%)	340 (88%)	42 (11%)	5 (1%)	12	48
18	F	391/439 (89%)	358 (92%)	29 (7%)	4 (1%)	15	54
19	u	74/76 (97%)	67 (90%)	6 (8%)	1 (1%)	11	46
21	G	238/245 (97%)	227 (95%)	11 (5%)	0	100	100
21	g	238/245 (97%)	227 (95%)	11 (5%)	0	100	100
22	H	230/233 (99%)	216 (94%)	14 (6%)	0	100	100
22	h	230/233 (99%)	217 (94%)	13 (6%)	0	100	100
23	I	248/260 (95%)	229 (92%)	19 (8%)	0	100	100
23	i	248/260 (95%)	229 (92%)	19 (8%)	0	100	100
24	J	237/247 (96%)	223 (94%)	14 (6%)	0	100	100
24	j	237/247 (96%)	223 (94%)	14 (6%)	0	100	100
25	K	224/240 (93%)	208 (93%)	16 (7%)	0	100	100
25	k	224/240 (93%)	208 (93%)	16 (7%)	0	100	100
26	L	236/268 (88%)	225 (95%)	11 (5%)	0	100	100
26	l	236/268 (88%)	225 (95%)	11 (5%)	0	100	100
27	M	238/254 (94%)	219 (92%)	19 (8%)	0	100	100
27	m	238/254 (94%)	219 (92%)	19 (8%)	0	100	100
28	N	189/238 (79%)	184 (97%)	5 (3%)	0	100	100
28	n	189/238 (79%)	184 (97%)	5 (3%)	0	100	100
29	O	218/276 (79%)	211 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	o	218/276 (79%)	211 (97%)	7 (3%)	0	100	100
30	P	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
30	p	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
31	Q	197/201 (98%)	184 (93%)	13 (7%)	0	100	100
31	q	197/201 (98%)	184 (93%)	13 (7%)	0	100	100
32	R	199/262 (76%)	194 (98%)	5 (2%)	0	100	100
32	r	199/262 (76%)	194 (98%)	5 (2%)	0	100	100
33	S	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
33	s	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
34	T	213/263 (81%)	202 (95%)	11 (5%)	0	100	100
34	t	213/263 (81%)	202 (95%)	11 (5%)	0	100	100
All	All	13292/14919 (89%)	12109 (91%)	1145 (9%)	38 (0%)	44	75

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	c	271	ALA
9	c	272	ILE
10	d	200	PHE
12	f	808	ASN
12	f	853	VAL
17	E	248	SER
18	F	344	ARG
7	a	69	HIS
11	e	57	ARG
12	f	876	HIS
1	U	36	ALA
11	e	50	ASP
12	f	118	ASN
12	f	476	THR
12	f	664	GLU
12	f	823	ALA
12	f	859	PRO
16	D	412	GLN
17	E	127	PRO
18	F	343	LEU
4	X	317	PRO
6	Z	65	ASP

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Mol	Chain	Res	Type
7	a	187	ASP
12	f	809	ILE
16	D	149	SER
16	D	155	THR
18	F	349	ASP
19	u	35	GLY
9	c	234	TYR
12	f	475	ASN
17	E	247	THR
18	F	165	PRO
12	f	755	ASP
6	Z	184	VAL
17	E	112	PRO
17	E	117	PRO
6	Z	144	VAL
13	A	109	PRO

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	U	702/816 (86%)	699 (100%)	3 (0%)	91	96
2	V	414/459 (90%)	412 (100%)	2 (0%)	88	94
3	W	416/416 (100%)	411 (99%)	5 (1%)	71	87
4	X	327/362 (90%)	327 (100%)	0	100	100
5	Y	334/344 (97%)	331 (99%)	3 (1%)	78	90
6	Z	257/295 (87%)	257 (100%)	0	100	100
7	a	333/336 (99%)	331 (99%)	2 (1%)	86	94
8	b	167/312 (54%)	167 (100%)	0	100	100
9	c	252/267 (94%)	241 (96%)	11 (4%)	28	62
10	d	231/293 (79%)	231 (100%)	0	100	100
11	e	38/63 (60%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	f	745/748 (100%)	727 (98%)	18 (2%)	49	76
13	A	297/372 (80%)	293 (99%)	4 (1%)	69	86
14	B	300/385 (78%)	297 (99%)	3 (1%)	76	88
15	C	340/346 (98%)	336 (99%)	4 (1%)	71	87
16	D	333/366 (91%)	325 (98%)	8 (2%)	49	76
17	E	341/353 (97%)	335 (98%)	6 (2%)	59	81
18	F	340/379 (90%)	337 (99%)	3 (1%)	78	90
19	u	68/68 (100%)	68 (100%)	0	100	100
21	G	193/209 (92%)	193 (100%)	0	100	100
21	g	193/209 (92%)	193 (100%)	0	100	100
22	H	164/190 (86%)	164 (100%)	0	100	100
22	h	164/190 (86%)	164 (100%)	0	100	100
23	I	193/220 (88%)	193 (100%)	0	100	100
23	i	193/220 (88%)	193 (100%)	0	100	100
24	J	152/210 (72%)	152 (100%)	0	100	100
24	j	152/210 (72%)	152 (100%)	0	100	100
25	K	186/202 (92%)	185 (100%)	1 (0%)	88	94
25	k	186/202 (92%)	185 (100%)	1 (0%)	88	94
26	L	198/229 (86%)	197 (100%)	1 (0%)	88	94
26	l	198/229 (86%)	197 (100%)	1 (0%)	88	94
27	M	192/211 (91%)	192 (100%)	0	100	100
27	m	192/211 (91%)	192 (100%)	0	100	100
28	N	148/180 (82%)	148 (100%)	0	100	100
28	n	148/180 (82%)	148 (100%)	0	100	100
29	O	177/227 (78%)	177 (100%)	0	100	100
29	o	177/227 (78%)	177 (100%)	0	100	100
30	P	172/173 (99%)	172 (100%)	0	100	100
30	p	172/173 (99%)	172 (100%)	0	100	100
31	Q	164/171 (96%)	163 (99%)	1 (1%)	86	94
31	q	164/171 (96%)	163 (99%)	1 (1%)	86	94
32	R	153/201 (76%)	153 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	r	153/201 (76%)	153 (100%)	0	100	100
33	S	174/198 (88%)	174 (100%)	0	100	100
33	s	174/198 (88%)	174 (100%)	0	100	100
34	T	175/214 (82%)	174 (99%)	1 (1%)	86	94
34	t	175/214 (82%)	174 (99%)	1 (1%)	86	94
All	All	11117/12650 (88%)	11037 (99%)	80 (1%)	84	93

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	55	ARG
1	U	215	ASN
1	U	629	THR
2	V	194	LYS
2	V	494	MET
3	W	39	ARG
3	W	55	ARG
3	W	191	ARG
3	W	413	ILE
3	W	419	LYS
5	Y	48	ASN
5	Y	176	ARG
5	Y	237	ARG
7	a	230	ARG
7	a	289	ARG
9	c	104	ARG
9	c	154	LYS
9	c	168	MET
9	c	185	ASN
9	c	197	ASN
9	c	198	ARG
9	c	270	LEU
9	c	274	ASN
9	c	277	LYS
9	c	278	GLN
9	c	295	ASN
12	f	80	ARG
12	f	83	ARG
12	f	131	MET
12	f	267	ARG

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Mol	Chain	Res	Type
12	f	297	MET
12	f	327	ASN
12	f	344	VAL
12	f	396	ASN
12	f	457	ASN
12	f	531	ASN
12	f	565	ASN
12	f	569	LYS
12	f	660	ILE
12	f	662	MET
12	f	703	ARG
12	f	746	ARG
12	f	822	VAL
12	f	826	GLN
13	A	284	ARG
13	A	360	ARG
13	A	369	ARG
13	A	403	ILE
14	B	103	ARG
14	B	164	MET
14	B	429	LYS
15	C	78	ARG
15	C	184	LYS
15	C	287	LYS
15	C	298	ILE
16	D	153	MET
16	D	154	LEU
16	D	273	LYS
16	D	274	ARG
16	D	312	ASN
16	D	323	ARG
16	D	360	LEU
16	D	411	GLU
17	E	5	ARG
17	E	25	ARG
17	E	280	ASN
17	E	291	ARG
17	E	322	LYS
17	E	344	ARG
18	F	250	LYS
18	F	323	ASN
18	F	344	ARG

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Mol	Chain	Res	Type
25	K	10	ARG
26	L	205	LEU
31	Q	102	LEU
34	T	37	ARG
25	k	10	ARG
26	l	205	LEU
31	q	102	LEU
34	t	37	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	218	GLN
1	U	366	HIS
1	U	377	HIS
1	U	450	HIS
1	U	707	ASN
1	U	721	HIS
1	U	888	GLN
2	V	198	GLN
2	V	281	ASN
2	V	318	GLN
2	V	319	HIS
2	V	453	HIS
3	W	107	GLN
3	W	362	ASN
3	W	454	ASN
4	X	178	HIS
4	X	292	GLN
4	X	296	ASN
4	X	406	ASN
5	Y	48	ASN
5	Y	136	HIS
5	Y	184	GLN
5	Y	291	HIS
5	Y	302	HIS
6	Z	109	ASN
6	Z	189	GLN
6	Z	229	GLN
6	Z	256	GLN
6	Z	278	ASN
7	a	18	GLN

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Mol	Chain	Res	Type
7	a	35	HIS
7	a	249	GLN
7	a	264	ASN
7	a	332	HIS
8	b	30	GLN
8	b	137	ASN
9	c	197	ASN
9	c	219	ASN
9	c	221	HIS
9	c	274	ASN
9	c	295	ASN
10	d	116	HIS
10	d	221	ASN
12	f	43	GLN
12	f	112	ASN
12	f	118	ASN
12	f	291	GLN
12	f	327	ASN
12	f	378	ASN
12	f	382	ASN
12	f	396	ASN
12	f	457	ASN
12	f	531	ASN
12	f	565	ASN
12	f	614	HIS
12	f	619	HIS
12	f	737	ASN
12	f	815	HIS
13	A	85	GLN
13	A	165	GLN
13	A	293	ASN
14	B	241	ASN
14	B	277	HIS
14	B	332	ASN
15	C	53	ASN
15	C	111	ASN
16	D	67	ASN
16	D	187	HIS
16	D	257	ASN
17	E	190	GLN
17	E	194	ASN
17	E	262	ASN

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Mol	Chain	Res	Type
17	E	271	HIS
17	E	300	HIS
17	E	364	GLN
18	F	315	ASN
18	F	323	ASN
22	H	102	GLN
22	H	112	GLN
23	I	53	HIS
23	I	109	GLN
23	I	119	GLN
24	J	18	GLN
24	J	116	GLN
24	J	175	ASN
25	K	99	HIS
25	K	155	HIS
25	K	214	ASN
26	L	146	GLN
30	P	93	ASN
31	Q	71	ASN
31	Q	82	ASN
31	Q	101	ASN
32	R	38	ASN
21	g	128	ASN
22	h	112	GLN
23	i	53	HIS
23	i	109	GLN
23	i	119	GLN
24	j	18	GLN
24	j	116	GLN
24	j	175	ASN
25	k	99	HIS
25	k	155	HIS
25	k	214	ASN
26	l	146	GLN
28	n	187	GLN
30	p	93	ASN
31	q	71	ASN
31	q	82	ASN
31	q	101	ASN
32	r	38	ASN

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](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	ATP	D	501	38	26,33,33	0.94	1 (3%)	31,52,52	1.71	5 (16%)
37	ATP	E	401	38	26,33,33	0.94	1 (3%)	31,52,52	1.68	5 (16%)
36	ADP	F	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.60	4 (13%)
36	ADP	A	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.47	4 (13%)
37	ATP	C	501	38	26,33,33	0.93	1 (3%)	31,52,52	1.52	5 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	ATP	D	501	38	-	1/18/38/38	0/3/3/3
37	ATP	E	401	38	-	2/18/38/38	0/3/3/3
36	ADP	F	501	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ADP	A	501	-	-	2/12/32/32	0/3/3/3
37	ATP	C	501	38	-	2/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A	501	ADP	C5-C4	2.53	1.47	1.40
37	C	501	ATP	C5-C4	2.47	1.47	1.40
37	E	401	ATP	C5-C4	2.42	1.47	1.40
36	F	501	ADP	C5-C4	2.41	1.47	1.40
37	D	501	ATP	C5-C4	2.39	1.47	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D	501	ATP	PA-O3A-PB	-4.83	116.24	132.83
36	F	501	ADP	PA-O3A-PB	-4.22	118.33	132.83
37	E	401	ATP	PA-O3A-PB	-4.14	118.61	132.83
37	D	501	ATP	C3'-C2'-C1'	4.08	107.12	100.98
37	E	401	ATP	PB-O3B-PG	-3.99	119.15	132.83
36	F	501	ADP	C3'-C2'-C1'	3.95	106.92	100.98
37	C	501	ATP	C3'-C2'-C1'	3.59	106.38	100.98
37	C	501	ATP	N3-C2-N1	-3.52	123.17	128.68
36	A	501	ADP	C3'-C2'-C1'	3.51	106.26	100.98
37	C	501	ATP	PB-O3B-PG	-3.51	120.79	132.83
37	E	401	ATP	C3'-C2'-C1'	3.40	106.10	100.98
36	A	501	ADP	N3-C2-N1	-3.30	123.52	128.68
36	A	501	ADP	PA-O3A-PB	-3.27	121.62	132.83
36	F	501	ADP	N3-C2-N1	-3.17	123.72	128.68
37	E	401	ATP	N3-C2-N1	-3.17	123.72	128.68
37	D	501	ATP	PB-O3B-PG	-3.13	122.09	132.83
37	D	501	ATP	N3-C2-N1	-3.11	123.82	128.68
37	D	501	ATP	C4-C5-N7	-2.48	106.81	109.40
36	A	501	ADP	C4-C5-N7	-2.48	106.81	109.40
36	F	501	ADP	C4-C5-N7	-2.47	106.83	109.40
37	E	401	ATP	C4-C5-N7	-2.33	106.97	109.40
37	C	501	ATP	C4-C5-N7	-2.27	107.03	109.40
37	C	501	ATP	PA-O3A-PB	-2.01	125.92	132.83

There are no chirality outliers.

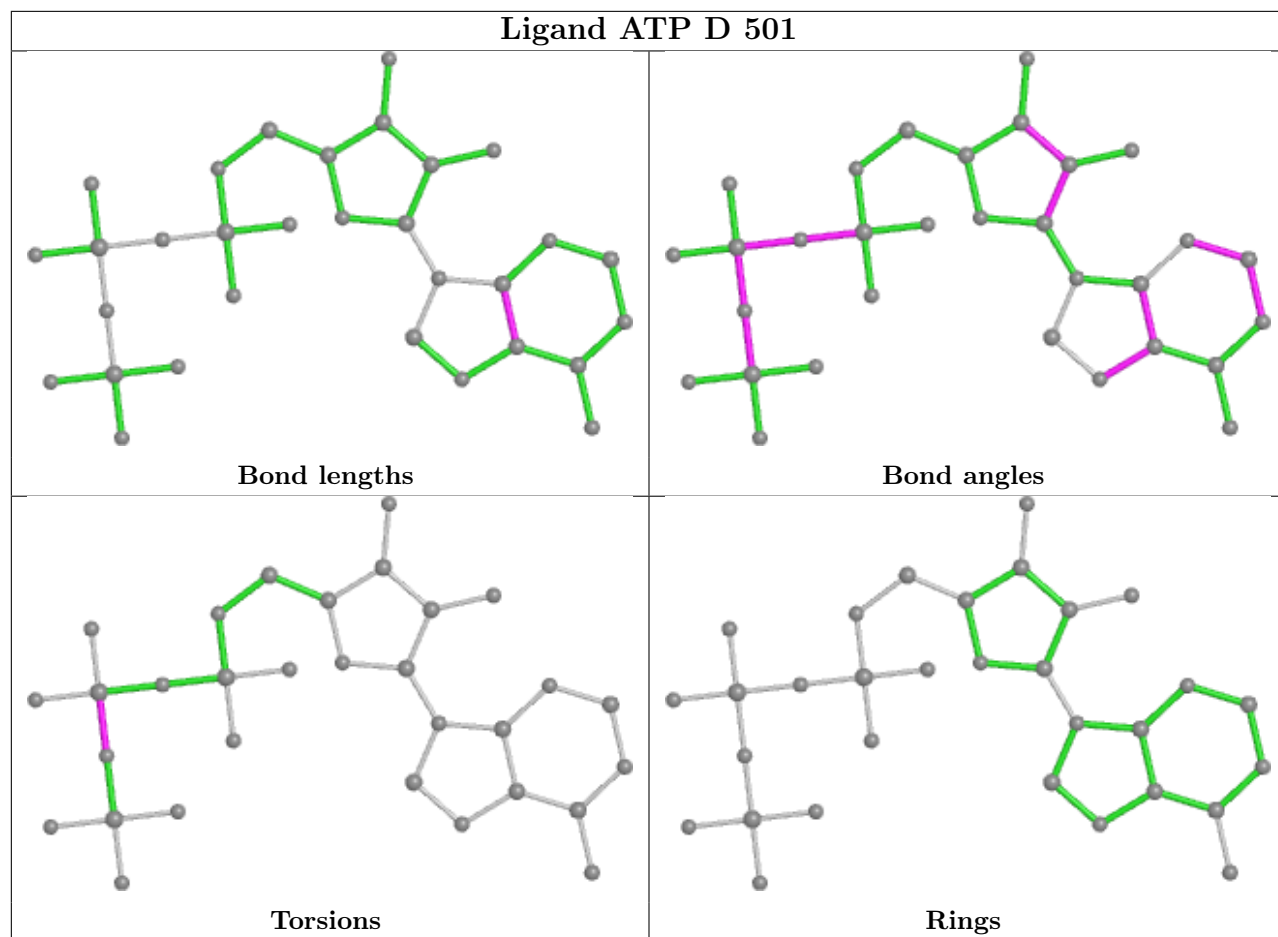
All (9) torsion outliers are listed below:

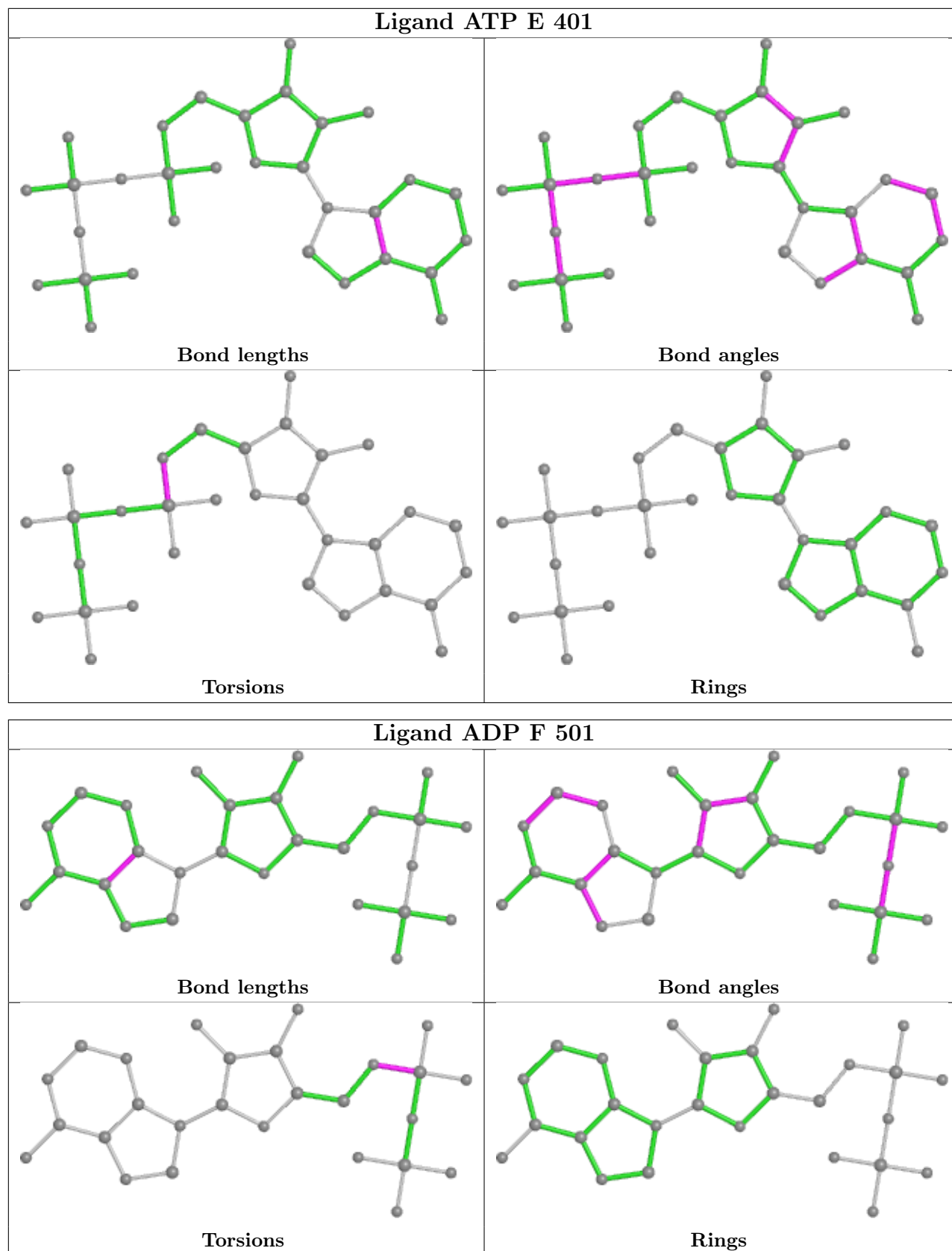
Mol	Chain	Res	Type	Atoms
36	F	501	ADP	C5'-O5'-PA-O1A
37	D	501	ATP	PG-O3B-PB-O3A
36	A	501	ADP	C5'-O5'-PA-O3A
36	F	501	ADP	C5'-O5'-PA-O3A
37	E	401	ATP	C5'-O5'-PA-O3A
37	E	401	ATP	C5'-O5'-PA-O2A
36	A	501	ADP	O4'-C4'-C5'-O5'
37	C	501	ATP	PB-O3A-PA-O1A
37	C	501	ATP	PB-O3A-PA-O2A

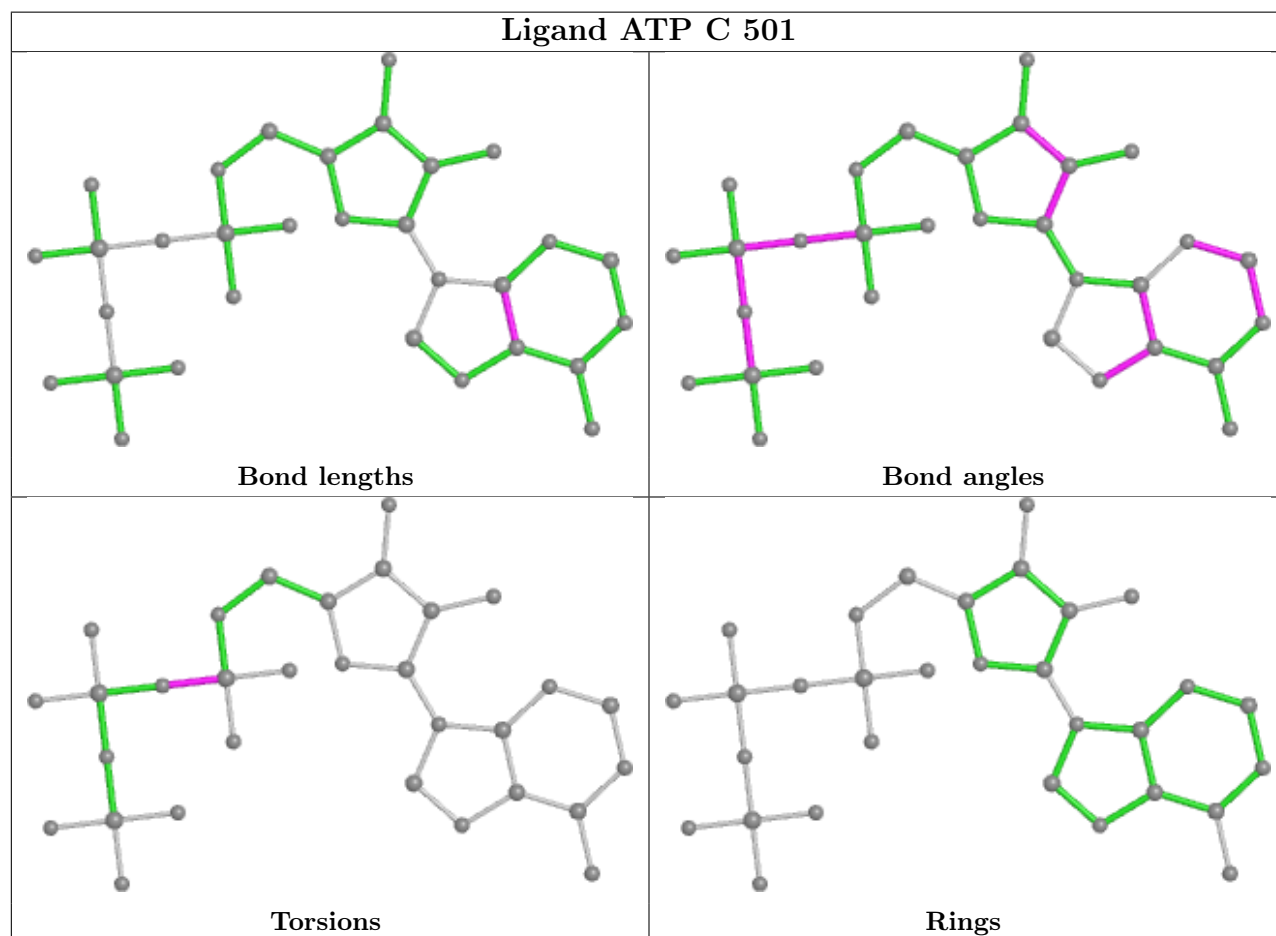
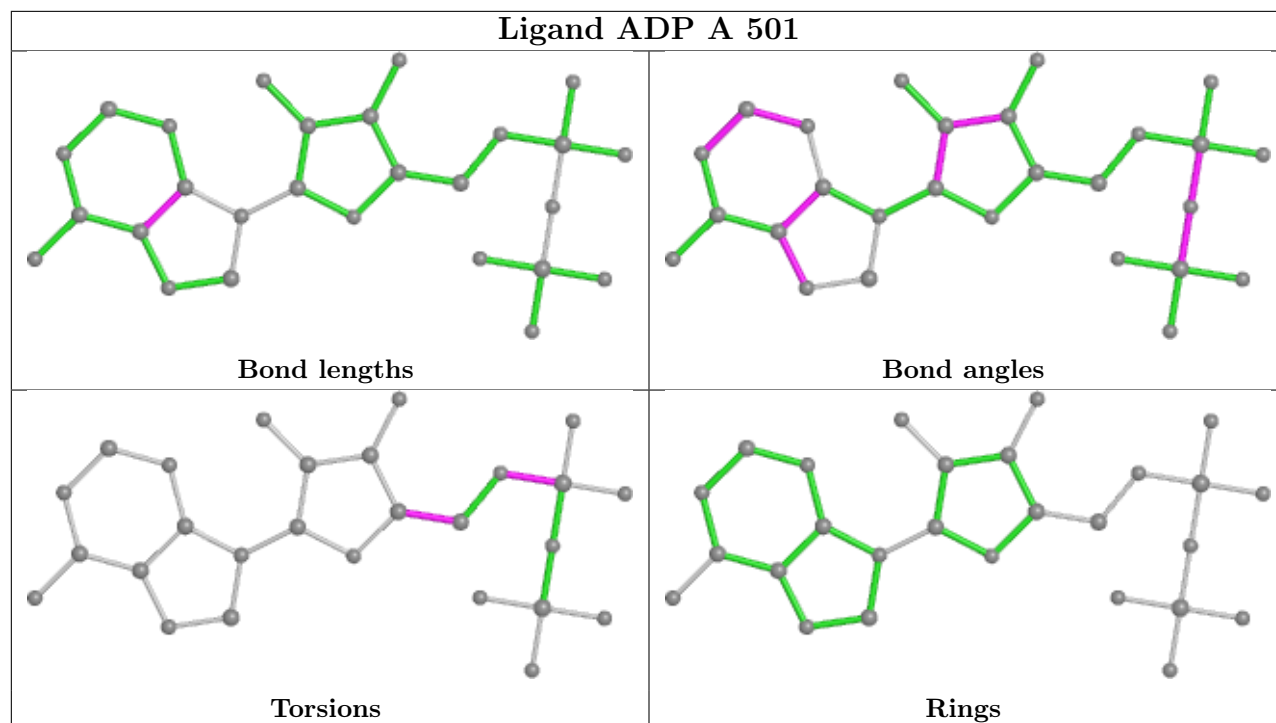
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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.

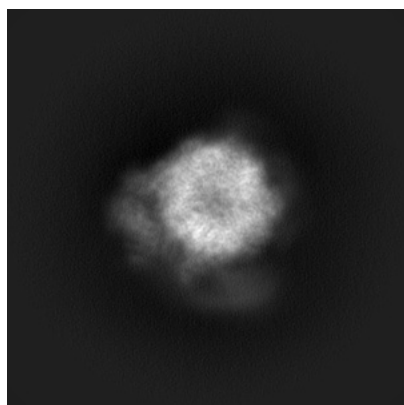
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9219. These allow visual inspection of the internal detail of the map and identification of artifacts.

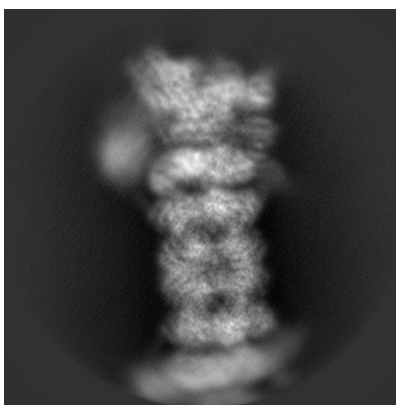
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

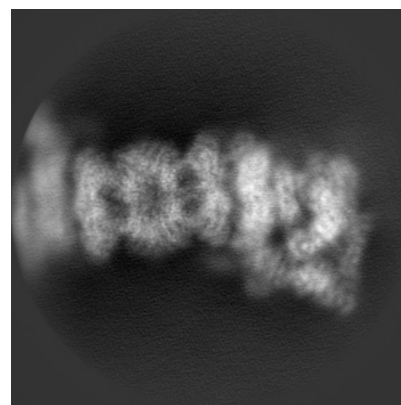
6.1.1 Primary map



X



Y

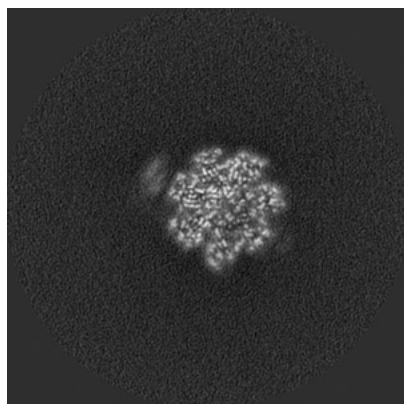


Z

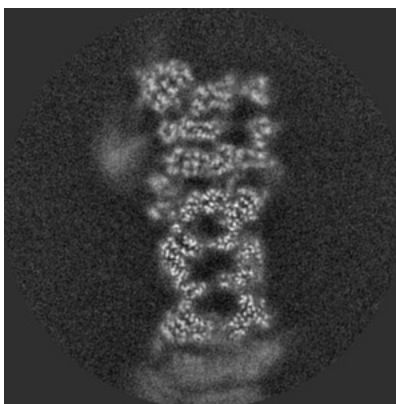
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

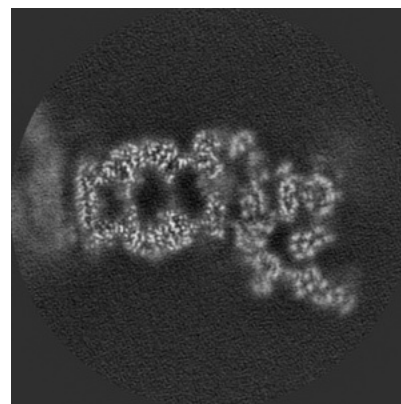
6.2.1 Primary map



X Index: 300



Y Index: 300

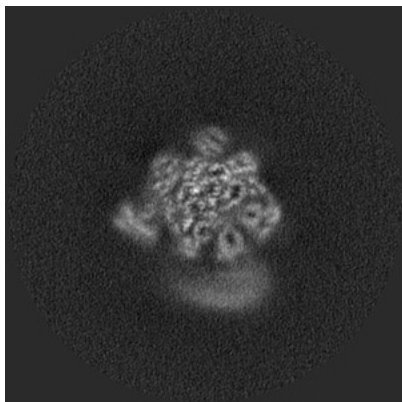


Z Index: 300

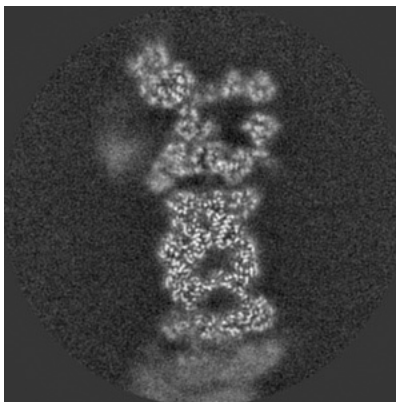
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

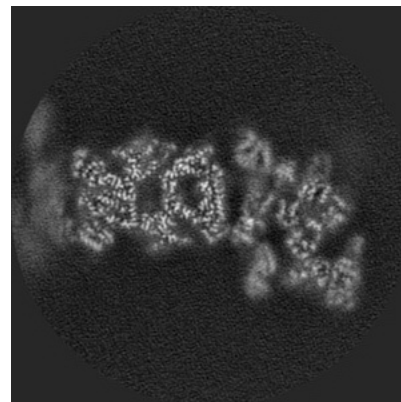
6.3.1 Primary map



X Index: 362



Y Index: 284



Z Index: 278

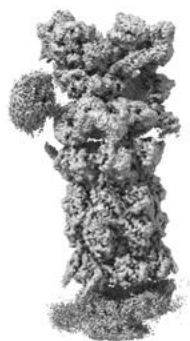
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

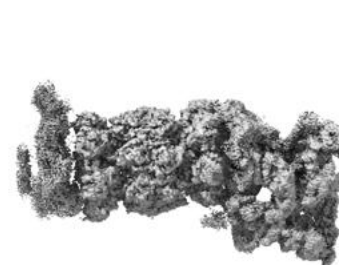
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

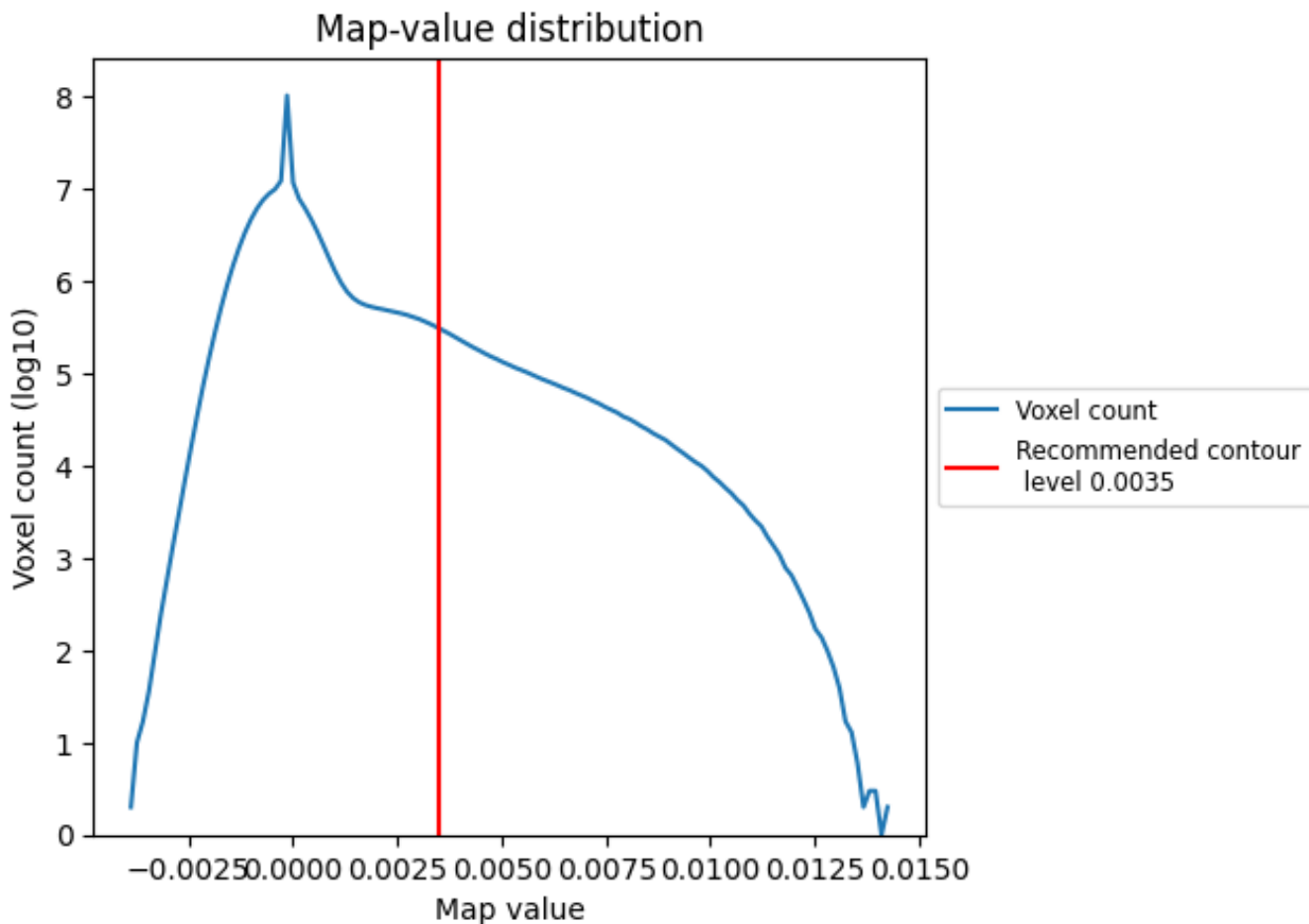
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

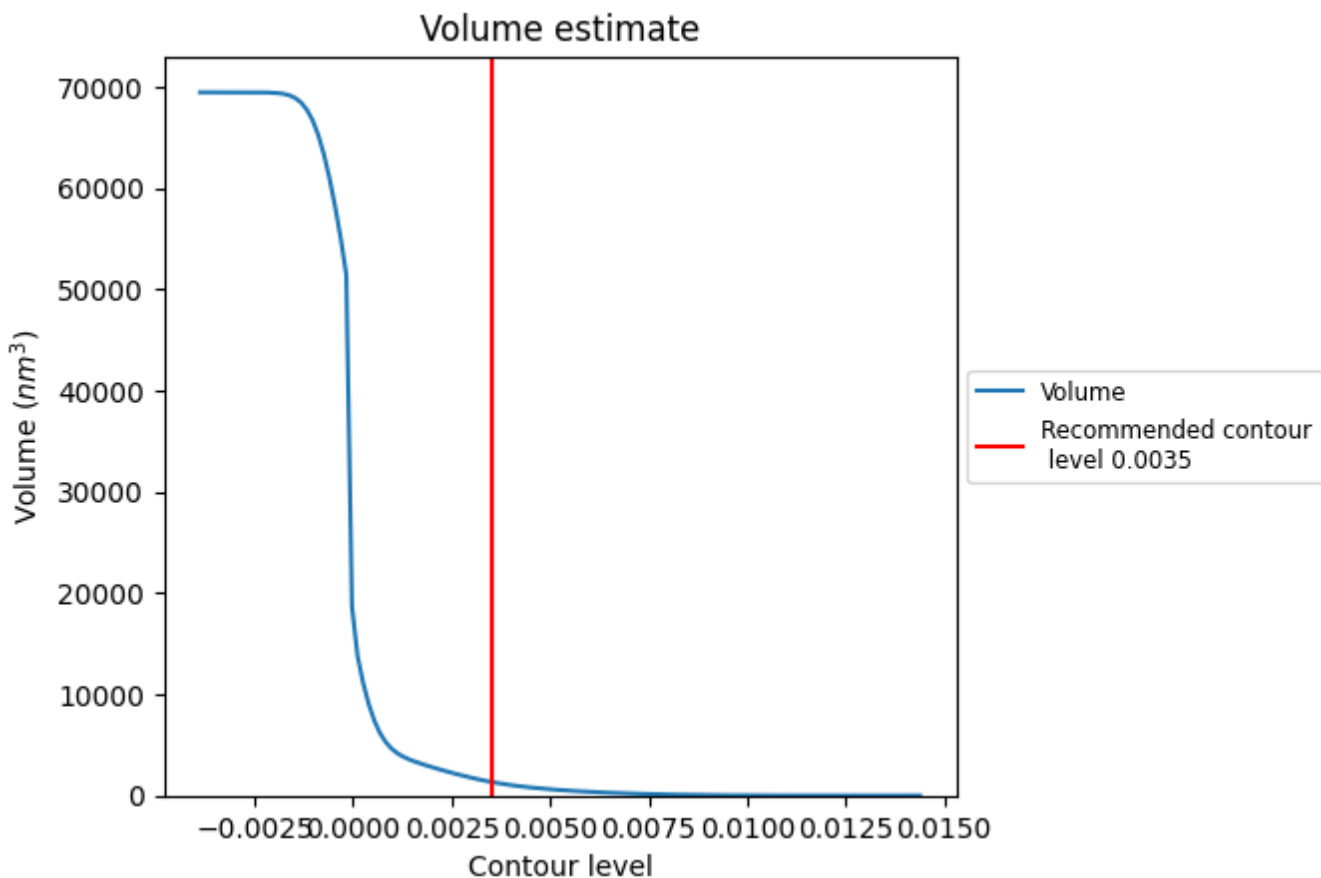
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

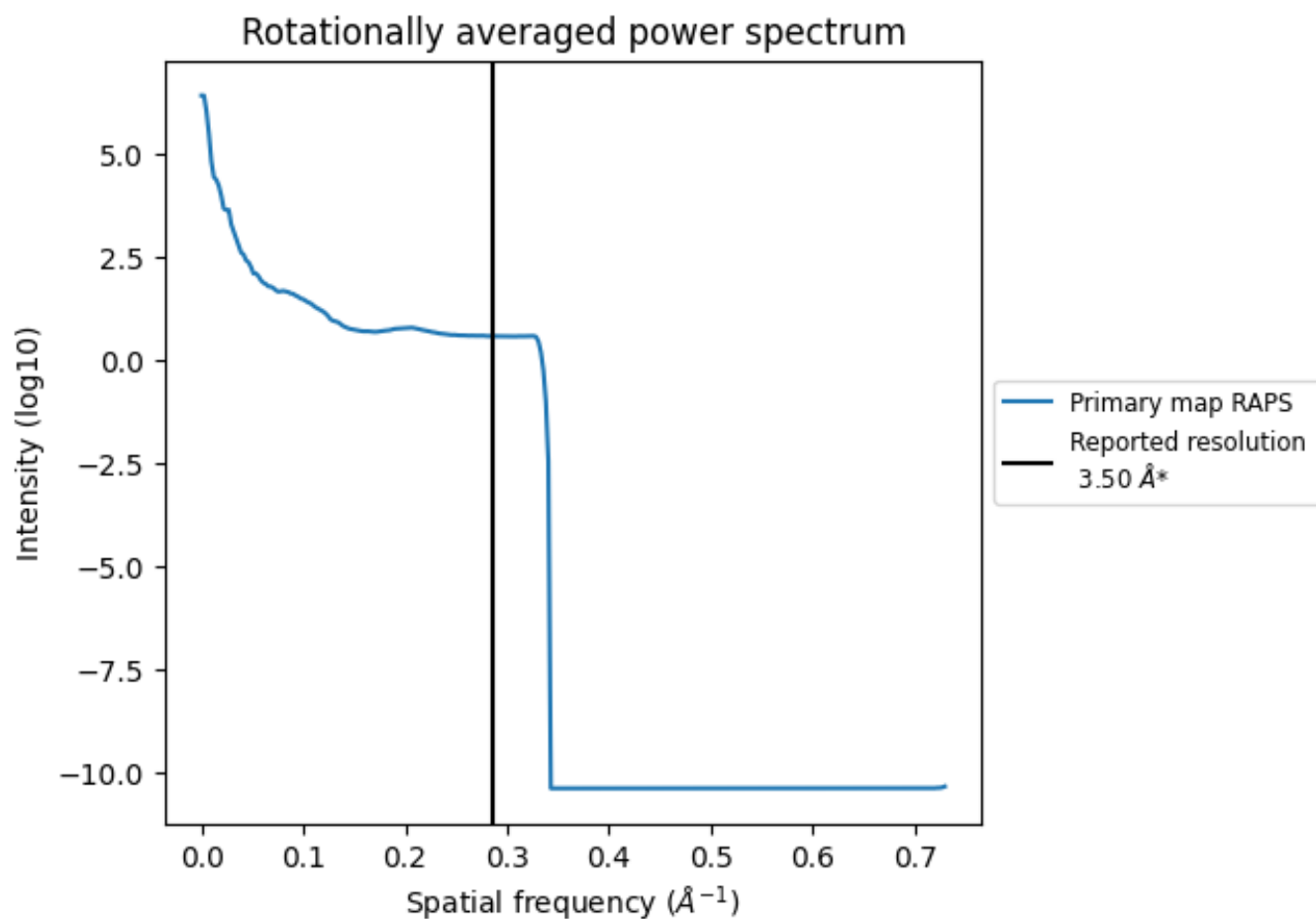
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1352 nm³; this corresponds to an approximate mass of 1222 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

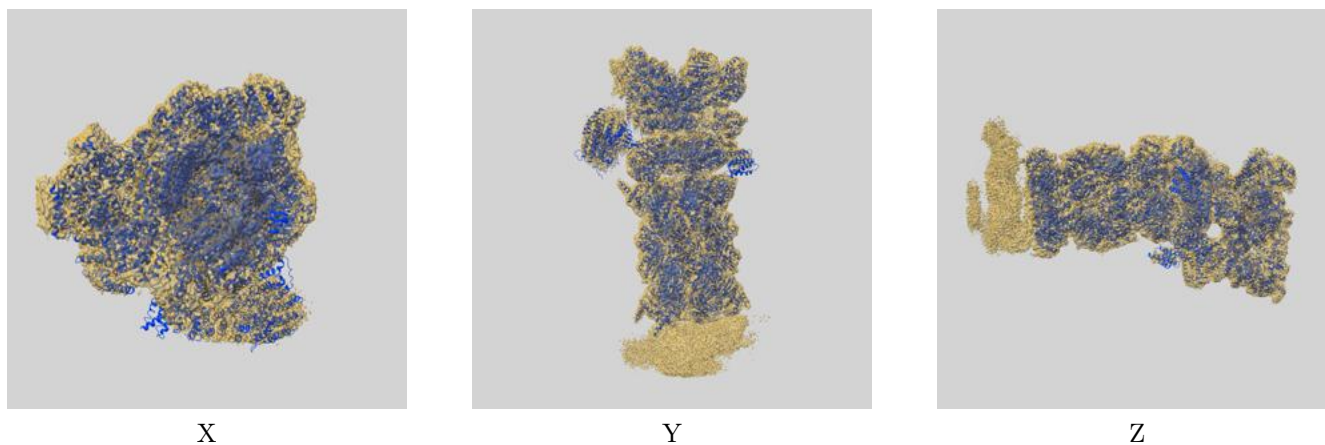
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

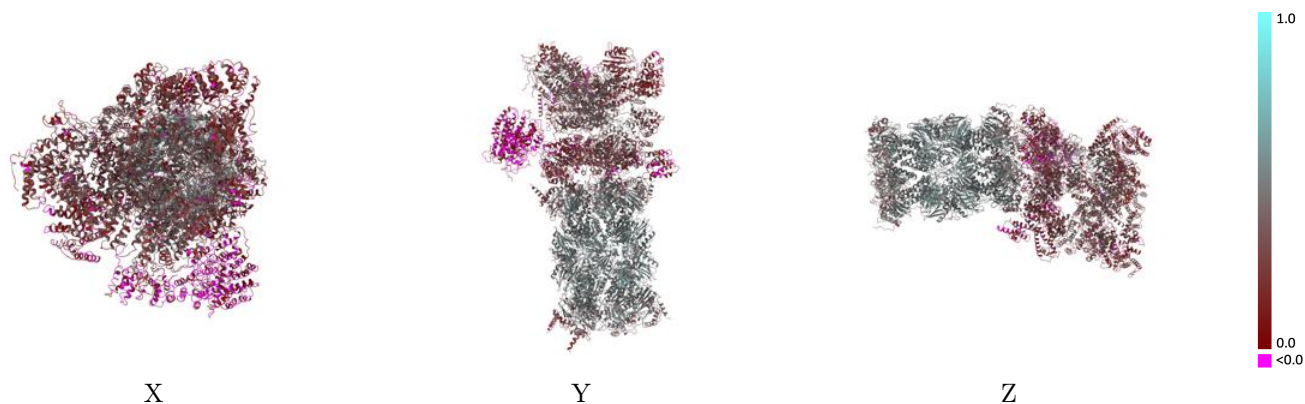
This section contains information regarding the fit between EMDB map EMD-9219 and PDB model 6MSG. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



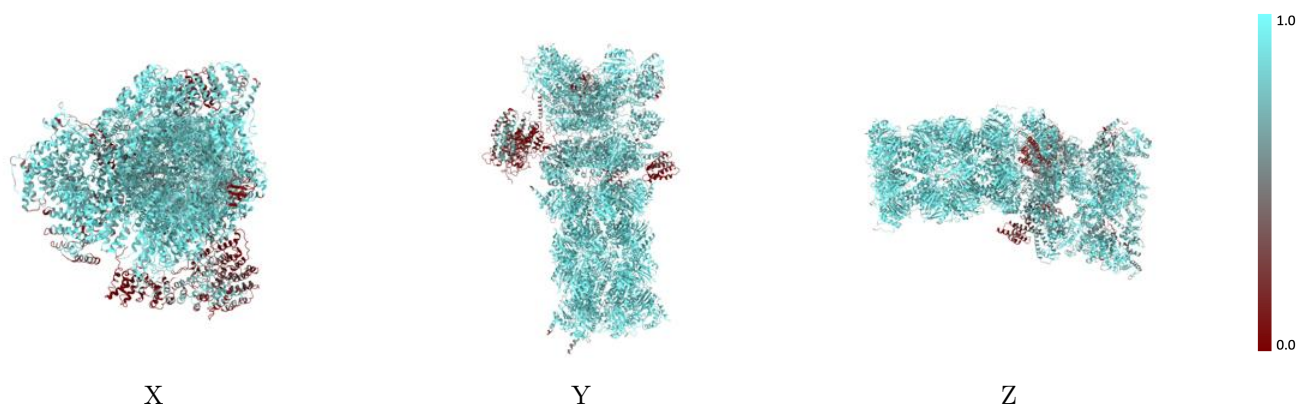
The images above show the 3D surface view of the map at the recommended contour level 0.0035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



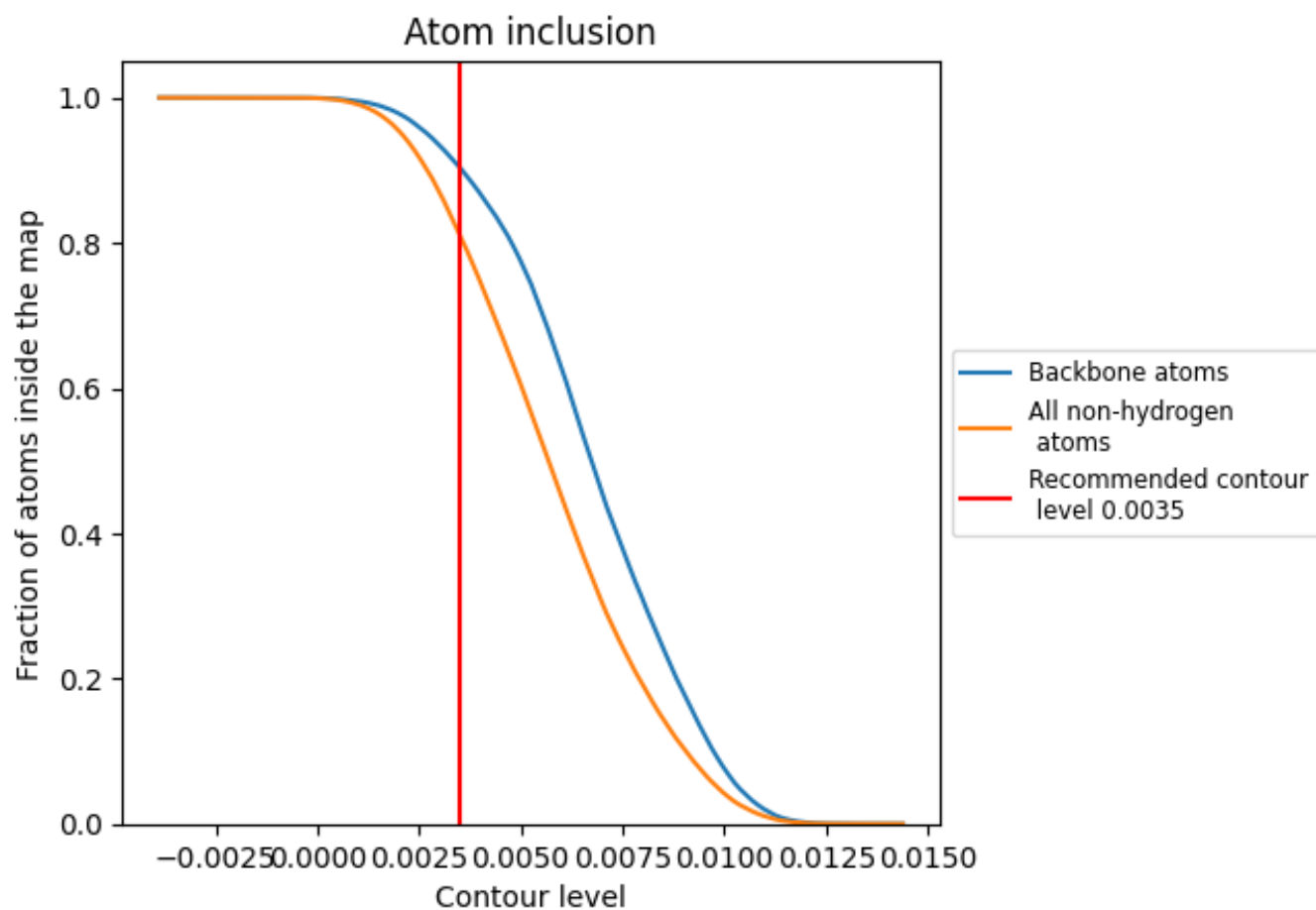
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0035).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





























The table lists the average atom inclusion at the recommended contour level (0.0035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8118	 0.3400
A	 0.7840	 0.2280
B	 0.7096	 0.1780
C	 0.7902	 0.2810
D	 0.8188	 0.3180
E	 0.8411	 0.3340
F	 0.8109	 0.2800
G	 0.9298	 0.4630
H	 0.9237	 0.4670
I	 0.8981	 0.4230
J	 0.9160	 0.4030
K	 0.8992	 0.4320
L	 0.9402	 0.4680
M	 0.9086	 0.4370
N	 0.9592	 0.5140
O	 0.9591	 0.4980
P	 0.9602	 0.5120
Q	 0.9394	 0.4780
R	 0.9660	 0.5100
S	 0.9470	 0.5030
T	 0.9618	 0.5140
U	 0.8541	 0.2990
V	 0.7461	 0.2340
W	 0.6096	 0.2230
X	 0.5849	 0.2290
Y	 0.8360	 0.2470
Z	 0.8457	 0.3130
a	 0.8264	 0.2290
b	 0.8487	 0.2310
c	 0.8342	 0.3370
d	 0.7461	 0.2130
e	 0.8061	 0.2130
f	 0.3013	 0.0250
g	 0.9115	 0.4520
h	 0.9046	 0.4530



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Chain	Atom inclusion	Q-score
i	 0.8613	 0.4120
j	 0.8745	 0.3810
k	 0.8834	 0.4350
l	 0.9286	 0.4660
m	 0.8921	 0.4310
n	 0.9542	 0.5100
o	 0.9517	 0.5030
p	 0.9551	 0.5070
q	 0.9401	 0.4830
r	 0.9626	 0.5200
s	 0.9502	 0.5070
t	 0.9643	 0.5150
u	 0.1858	 0.1850
v	 0.3083	 0.2510