wwPDB EM Validation Summary Report

Nov 19, 2022 – 11:27 am GMT

PDB ID	:	5M32
EMDB ID	:	EMD-4146
Title	:	Human 26S proteasome in complex with Oprozomib
Authors	:	Haselbach, D.; Schrader, J.; Lambrecht, F.; Henneberg, F.; Chari, A.; Stark, H.
Deposited on	:	2016-10-14
Resolution	:	3.80 Å(reported)

This is a wwPDB EM Validation Summary 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:

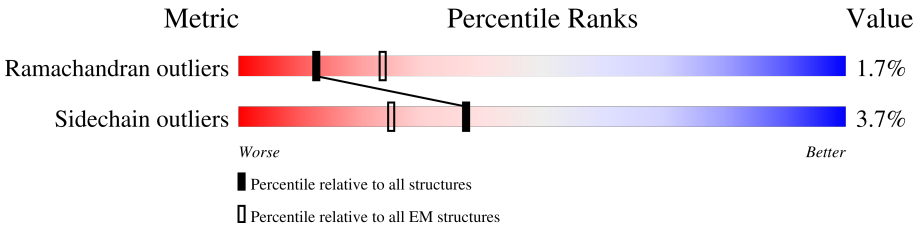
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.80 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 <=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	A	234	95%
1	O	234	95%
2	B	261	82% 6% 10%
2	P	261	5% 85% 7% 7%
3	C	234	94%
4	D	241	93%
4	R	241	94%
5	E	234	94% 5%
6	F	255	89% 9%

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Mol	Chain	Length	Quality of chain
6	T	255	91% 6%
7	G	246	91% 5%
7	U	246	94%
8	H	277	78% 20%
8	V	277	78% 21%
9	I	205	97%
9	W	205	97%
10	J	196	98%
10	X	196	98%
11	K	204	96%
11	Y	204	97%
12	L	241	87% 12%
12	Z	241	87% 12%
13	M	264	79% 18%
13	a	264	79% 18%
14	N	239	84% 15%
14	b	239	84% 15%
15	Q	235	91% 6%
16	S	238	94%
17	c	433	73% 6% 20%
18	d	428	6% 64% 11% 22%
19	e	418	78% 7% 14%
20	f	379	85% 6% 8%
21	g	439	5% 77% 5% 17%
22	h	355	81% 11% 6%

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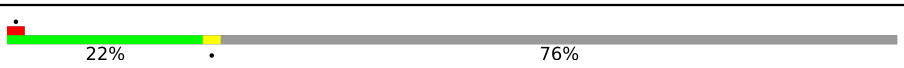
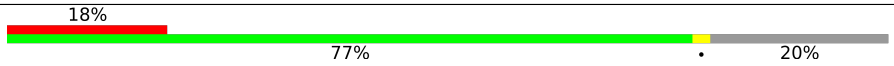
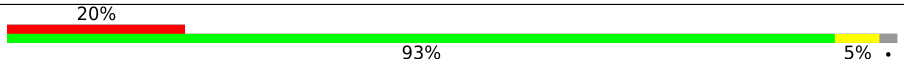
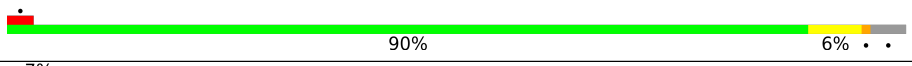
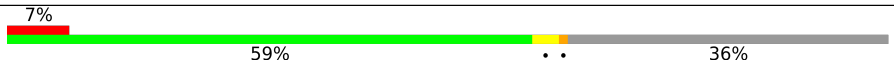
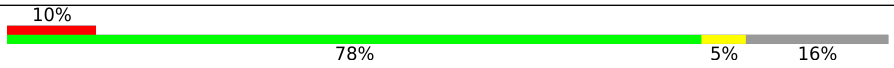
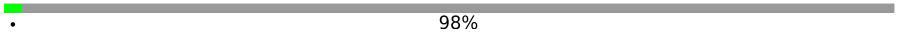
Mol	Chain	Length	Quality of chain
23	i	953	
24	j	534	
25	k	456	
26	l	422	
27	m	389	
28	n	324	
29	o	376	
30	p	377	
31	q	310	
32	r	350	
33	s	70	
34	t	4	
34	u	4	

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 76085 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 Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	230	Total	C	N	O	S	0	0
			1763	1132	297	328	6		
1	O	230	Total	C	N	O	S	0	0
			1764	1126	301	331	6		

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	234	Total	C	N	O	S	0	0
			1836	1164	315	348	9		
2	P	244	Total	C	N	O	S	0	0
			1875	1187	323	355	10		

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	234	Total	C	N	O	S	0	0
			1771	1107	315	344	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	48	ALA	LYS	conflict	UNP O14818
C	179	ASP	GLU	conflict	UNP O14818
C	200	GLU	GLN	conflict	UNP O14818

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	233	Total	C	N	O	S	0	0
			1757	1103	290	353	11		
4	R	233	Total	C	N	O	S	0	0
			1768	1112	294	351	11		

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	234	Total	C	N	O	S	0	0
			1805	1133	321	340	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	185	ASP	ASN	conflict	UNP P25786
E	234	ASP	GLU	conflict	UNP P25786

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	232	Total	C	N	O	S	0	0
			1818	1153	310	344	11		
6	T	240	Total	C	N	O	S	0	0
			1877	1190	320	356	11		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	233	Total	C	N	O	S	0	0
			1806	1147	301	345	13		
7	U	241	Total	C	N	O	S	0	0
			1841	1168	308	352	13		

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	221	Total	C	N	O	S	0	0
			1663	1047	283	321	12		
8	V	220	Total	C	N	O	S	1	0
			1627	1025	273	318	11		

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	204	Total	C	N	O	S	0	0
			1590	1013	265	293	19		
9	W	204	Total	C	N	O	S	0	0
			1586	1010	263	294	19		

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	196	Total	C	N	O	S	0	0
			1560	1001	266	284	9		
10	X	196	Total	C	N	O	S	0	0
			1563	1002	267	285	9		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	182	VAL	ILE	conflict	UNP P49721
J	186	ASP	ASN	conflict	UNP P49721
J	190	ASN	ASP	conflict	UNP P49721
J	192	GLU	ASP	conflict	UNP P49721
J	195	ALA	SER	conflict	UNP P49721
X	182	VAL	ILE	conflict	UNP P49721
X	186	ASP	ASN	conflict	UNP P49721
X	190	ASN	ASP	conflict	UNP P49721
X	192	GLU	ASP	conflict	UNP P49721
X	195	ALA	SER	conflict	UNP P49721

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	200	Total	C	N	O	S	0	0
			1545	974	269	293	9		
11	Y	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	213	Total	C	N	O	S	1	0
			1637	1038	277	312	10		
12	Z	213	Total	C	N	O	S	0	0
			1642	1040	281	311	10		

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	216	Total	C	N	O	S	0	0
			1679	1059	290	318	12		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	202	Total	C	N	O	S	0	0
			1513	948	258	295	12		
14	b	203	Total	C	N	O	S	0	0
			1519	952	259	296	12		

- Molecule 15 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	235	Total	C	N	O	S	0	0
			1785	1118	318	344	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	179	ASP	GLU	conflict	UNP O14818

- Molecule 16 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	238	Total	C	N	O	S	0	0
			1834	1147	329	347	11		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	2	ALA	PHE	conflict	UNP P25786
S	3	ALA	ARG	conflict	UNP P25786
S	185	ASP	ASN	conflict	UNP P25786
S	234	ASP	GLU	conflict	UNP P25786

- Molecule 17 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	c	347	Total	C	N	O	S	0	0
			2728	1722	485	503	18		

- Molecule 18 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	d	333	Total	C	N	O	S	0	0
			2560	1614	433	501	12		

- Molecule 19 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	361	Total	C	N	O	S	0	0
			2776	1752	488	525	11		

- Molecule 20 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	f	348	Total	C	N	O	S	0	0
			2692	1692	483	501	16		

- Molecule 21 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	g	363	Total	C	N	O	S	0	0
			2777	1753	480	529	15		

- Molecule 22 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	h	332	Total	C	N	O	S	0	0
			2518	1589	447	466	16		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	i	230	Total	C	N	O	0	0
			1145	685	230	230		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	j	155	Total	C	N	O	0	0
			779	470	155	154		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	k	364	Total 1819	C 1092	N 364	O 363	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	l	415	Total 2572	C 1598	N 474	O 494	S 6	0	0

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	m	375	Total 2421	C 1513	N 434	O 468	S 6	0	0

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	n	206	Total 1030	C 618	N 206	O 206	0	0

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	o	75	Total 377	C 227	N 75	O 75	0	0

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	p	101	Total 504	C 303	N 101	O 100	0	0

- Molecule 31 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	q	259	Total 1311	C 789	N 261	O 261	0	0

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	r	8	Total	C	N	O	0	0
			40	25	8	7		

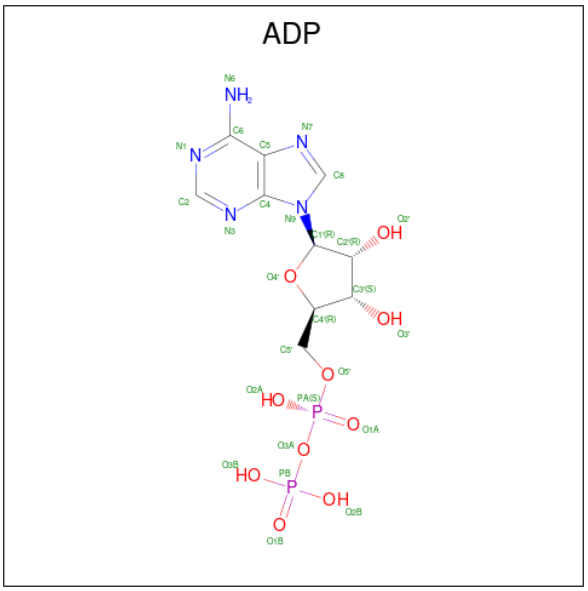
- Molecule 33 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	s	26	Total	C	N	O	0	0
			130	79	26	25		

- Molecule 34 is a protein called bound Oprozomib.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	t	4	Total	C	N	O	S	0	0
			37	25	4	7	1		
34	u	4	Total	C	N	O	S	0	0
			37	25	4	7	1		

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
35	c	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	d	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	e	1	Total	C	N	O	P	0
			27	10	5	10	2	

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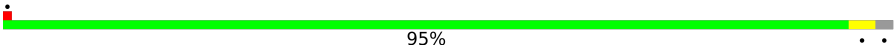
Mol	Chain	Residues	Atoms					AltConf
35	g	1	Total	C	N	O	P	0
			54	20	10	20	4	
35	g	1	Total	C	N	O	P	0
			54	20	10	20	4	
35	h	1	Total	C	N	O	P	0
			27	10	5	10	2	

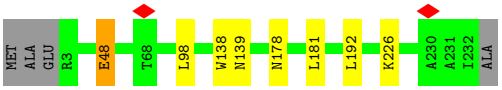
3 Residue-property plots

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: Proteasome subunit alpha type-2

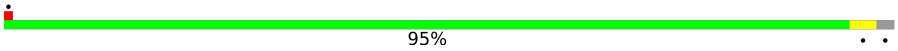
Chain A:

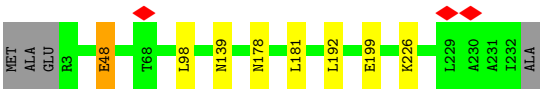




• Molecule 1: Proteasome subunit alpha type-2

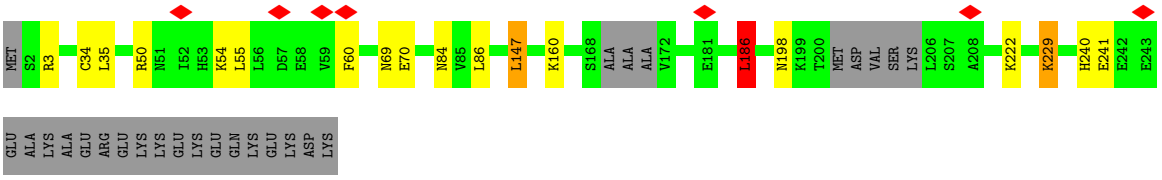
Chain O:





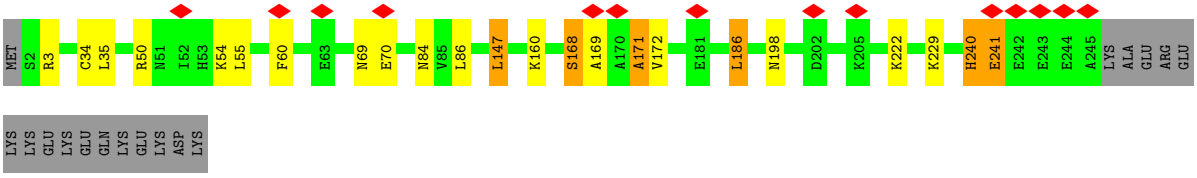
• Molecule 2: Proteasome subunit alpha type-4

Chain B:



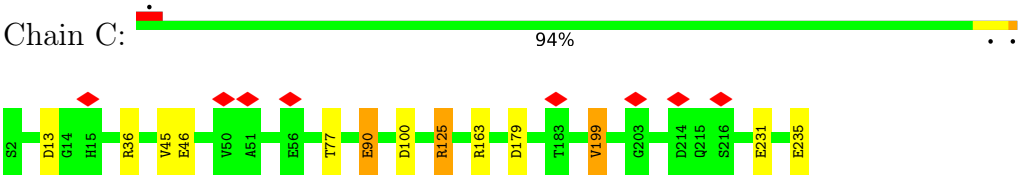
• Molecule 2: Proteasome subunit alpha type-4

Chain P:



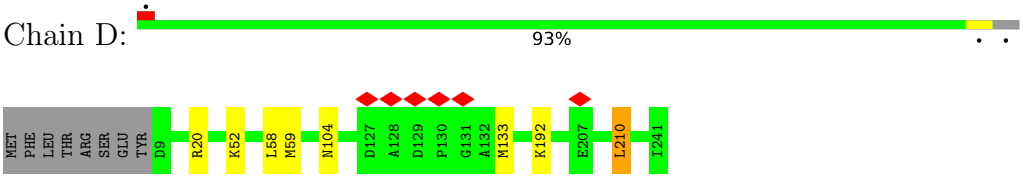
• Molecule 3: Proteasome subunit alpha type-7

Chain C:



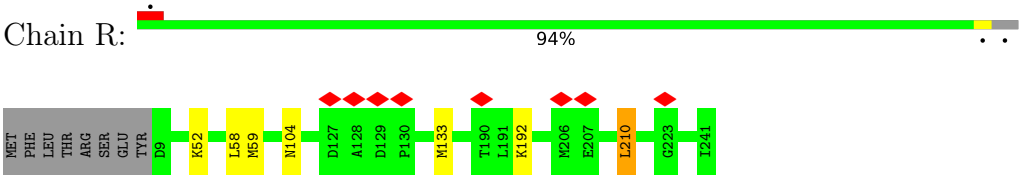
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



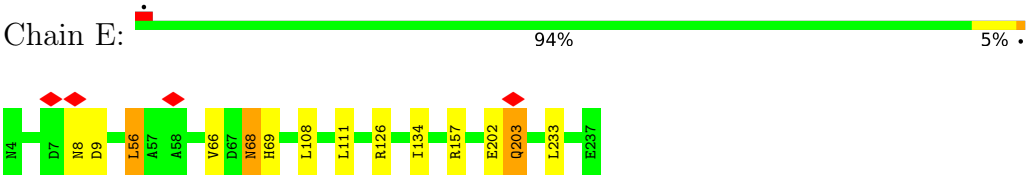
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



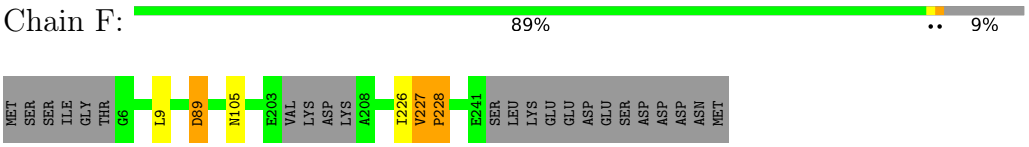
• Molecule 5: Proteasome subunit alpha type-1

Chain E:



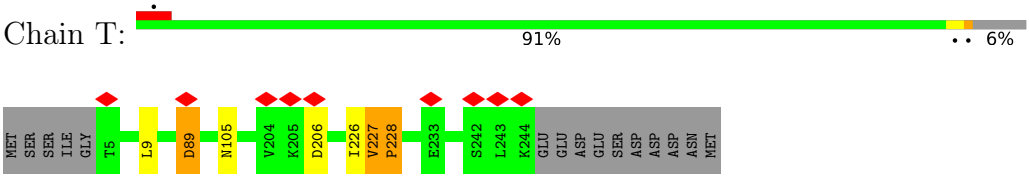
• Molecule 6: Proteasome subunit alpha type-3

Chain F:



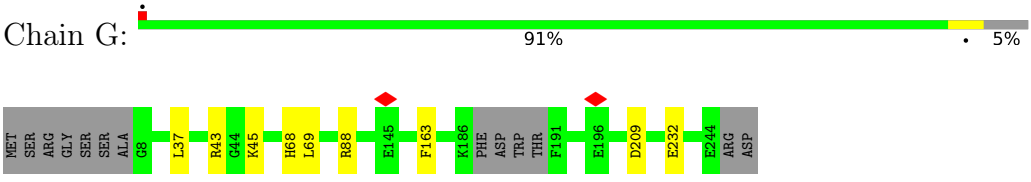
• Molecule 6: Proteasome subunit alpha type-3

Chain T:



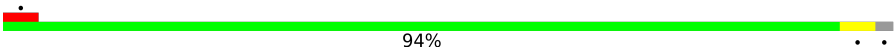
• Molecule 7: Proteasome subunit alpha type-6

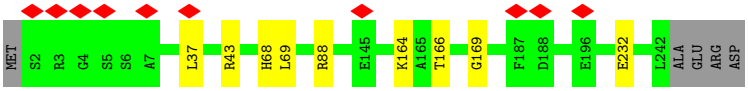
Chain G:



• Molecule 7: Proteasome subunit alpha type-6

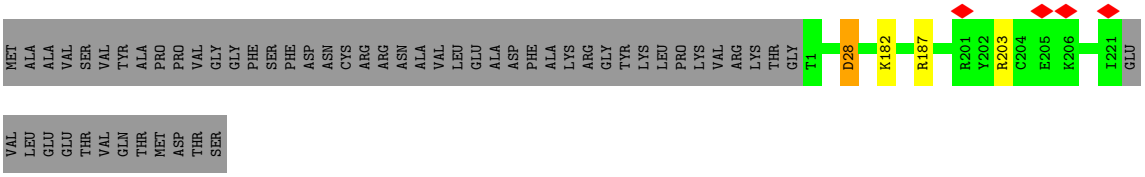
Chain U:





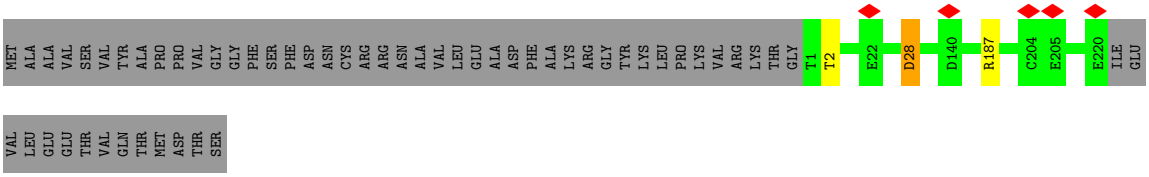
• Molecule 8: Proteasome subunit beta type-7

Chain H:



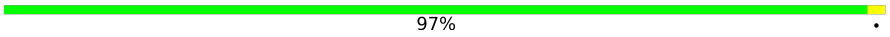
• Molecule 8: Proteasome subunit beta type-7

Chain V:



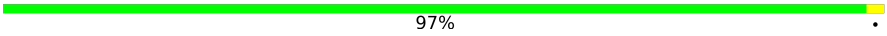
• Molecule 9: Proteasome subunit beta type-3

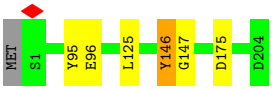
Chain I:



• Molecule 9: Proteasome subunit beta type-3

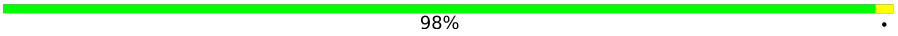
Chain W:





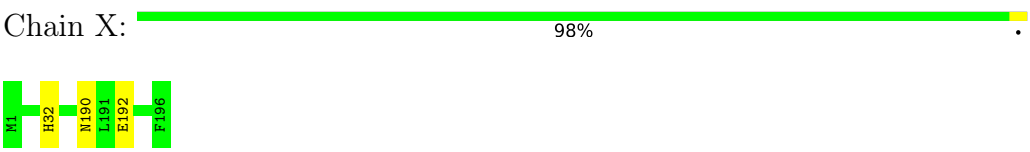
• Molecule 10: Proteasome subunit beta type-2

Chain J:



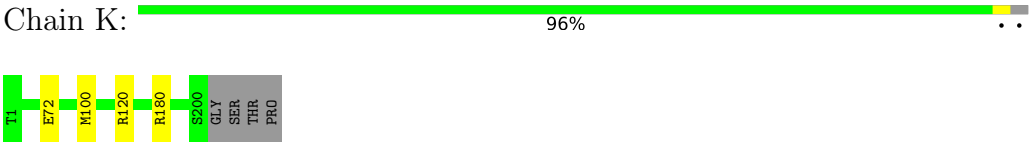
• Molecule 10: Proteasome subunit beta type-2

Chain X:



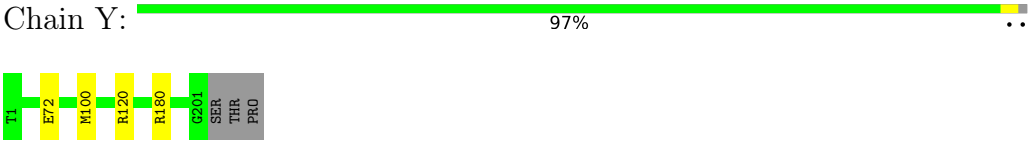
• Molecule 11: Proteasome subunit beta type-5

Chain K:



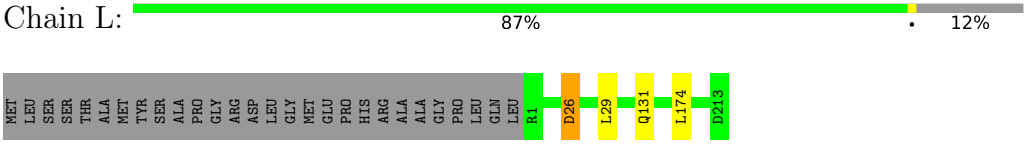
• Molecule 11: Proteasome subunit beta type-5

Chain Y:



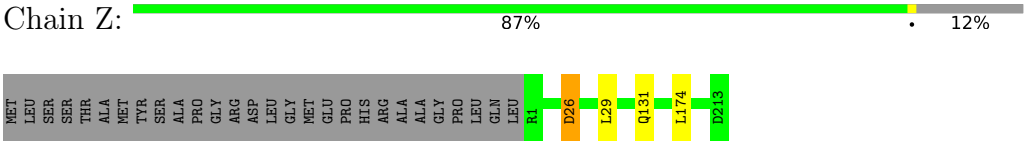
• Molecule 12: Proteasome subunit beta type-1

Chain L:



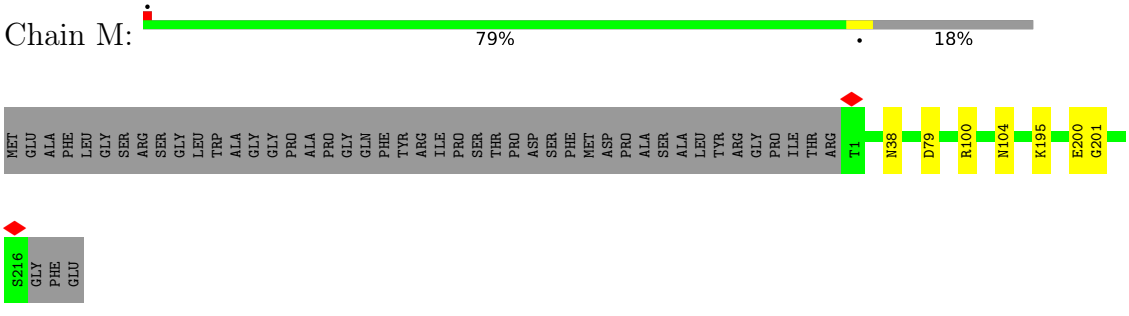
• Molecule 12: Proteasome subunit beta type-1

Chain Z:



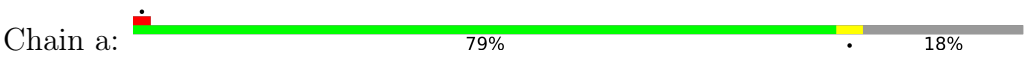
• Molecule 13: Proteasome subunit beta type-4

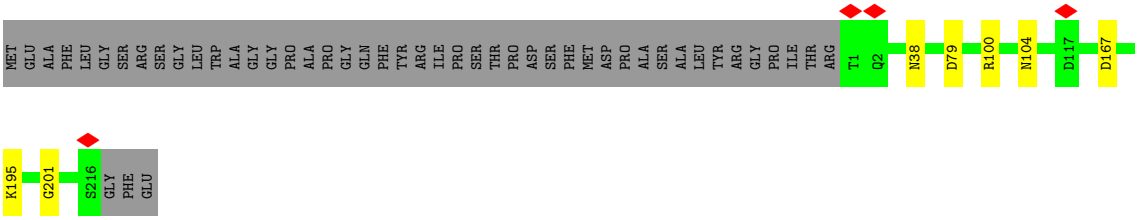
Chain M:



• Molecule 13: Proteasome subunit beta type-4

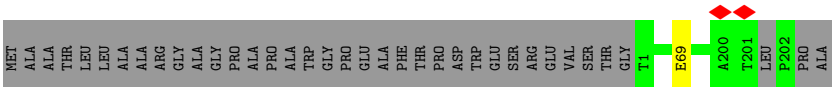
Chain a:





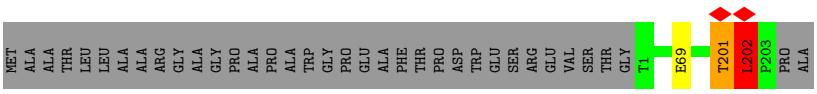
• Molecule 14: Proteasome subunit beta type-6

Chain N:



• Molecule 14: Proteasome subunit beta type-6

Chain b:

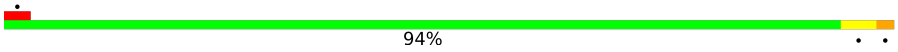


• Molecule 15: Proteasome subunit alpha type-7

Chain Q:

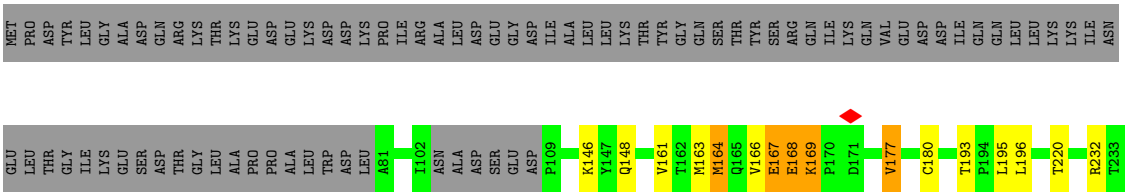
• Molecule 16: Proteasome subunit alpha type-1

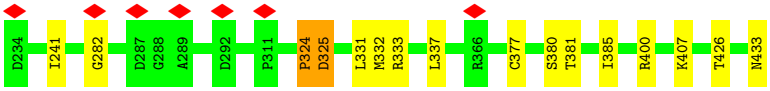
Chain S:



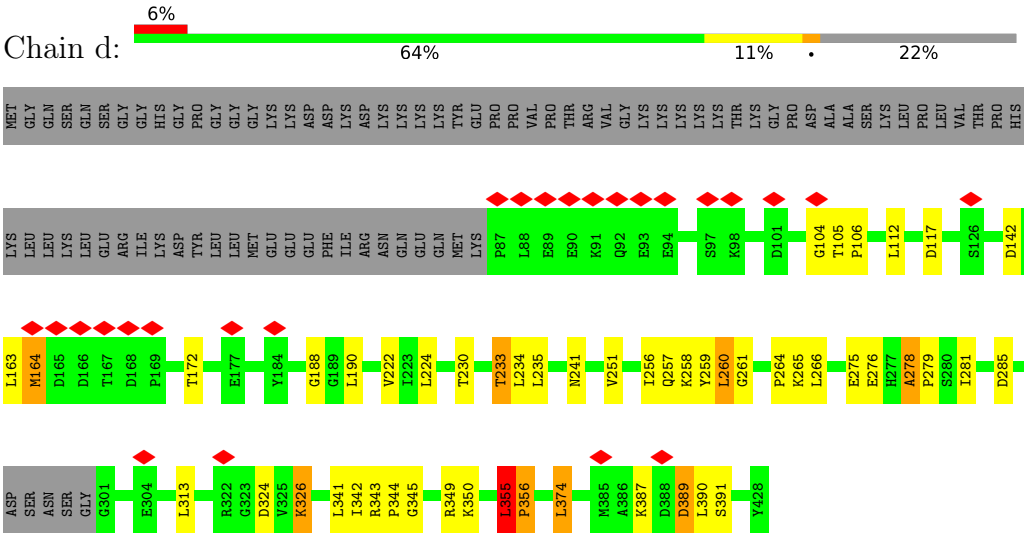
• Molecule 17: 26S protease regulatory subunit 7

Chain c:

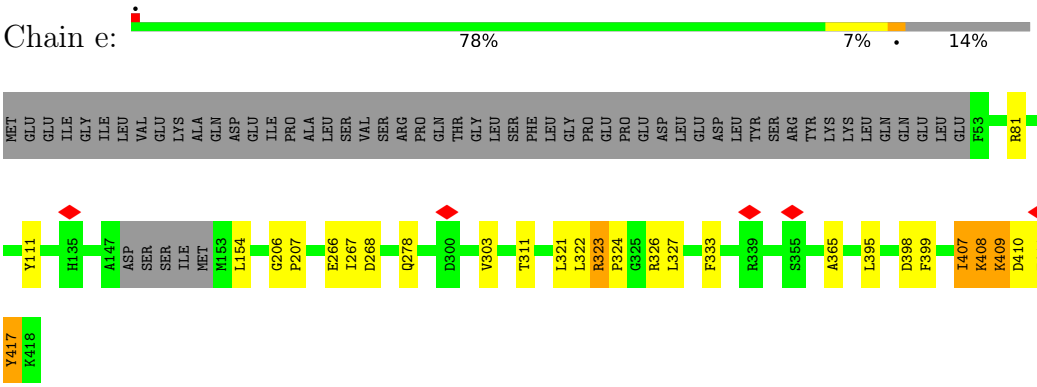




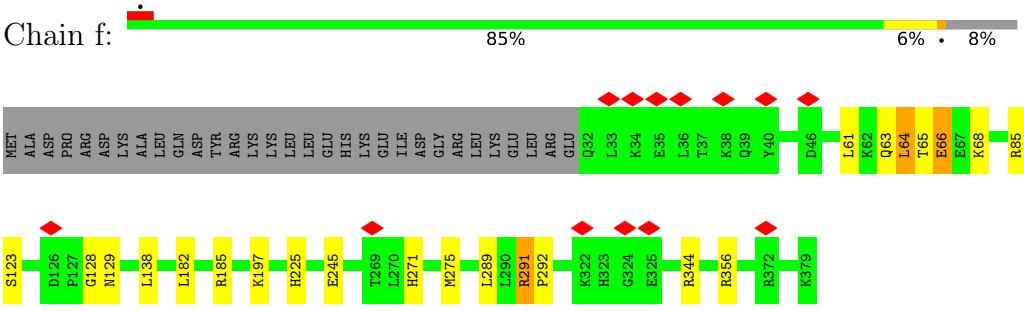
• Molecule 18: 26S protease regulatory subunit 4



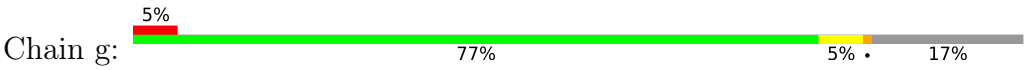
• Molecule 19: 26S protease regulatory subunit 6B

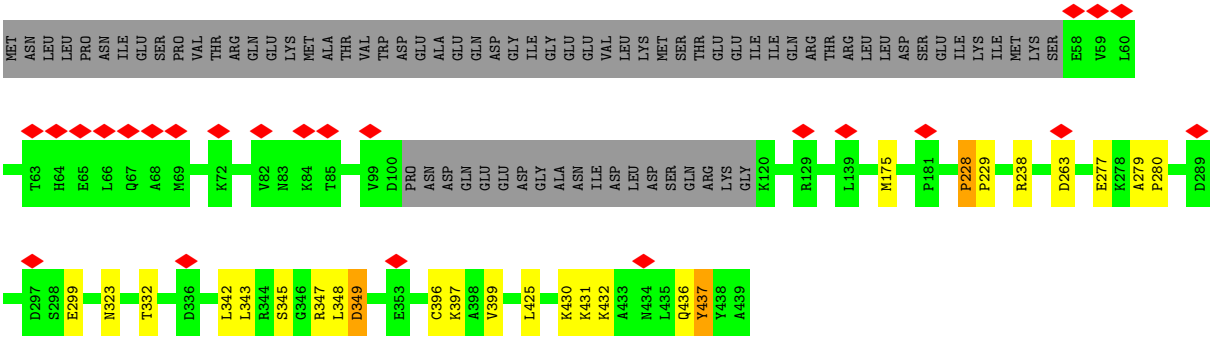


• Molecule 20: 26S protease regulatory subunit 10B

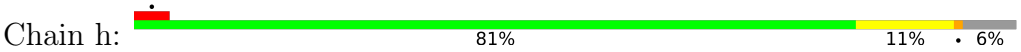


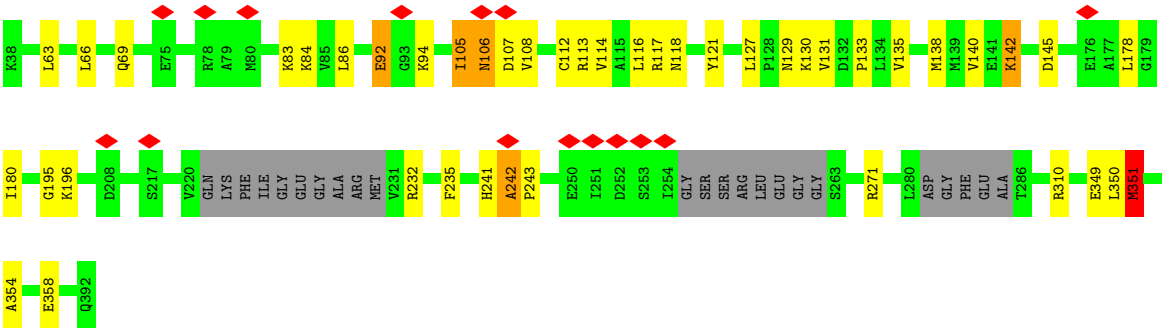
• Molecule 21: 26S protease regulatory subunit 6A



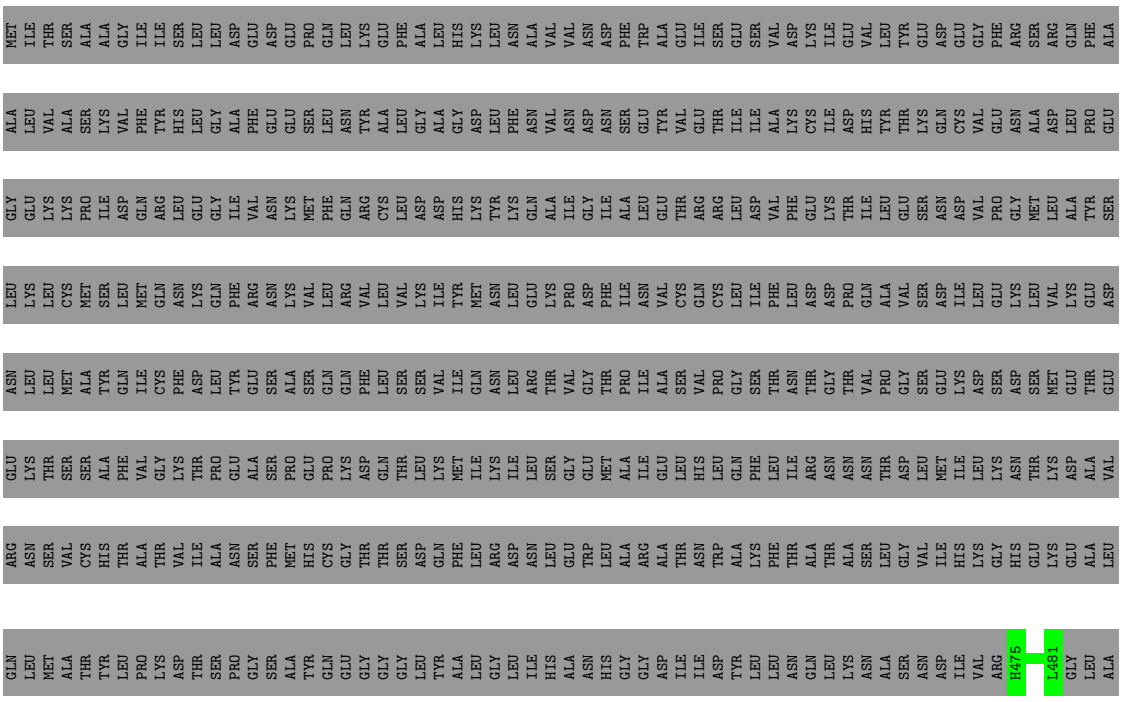


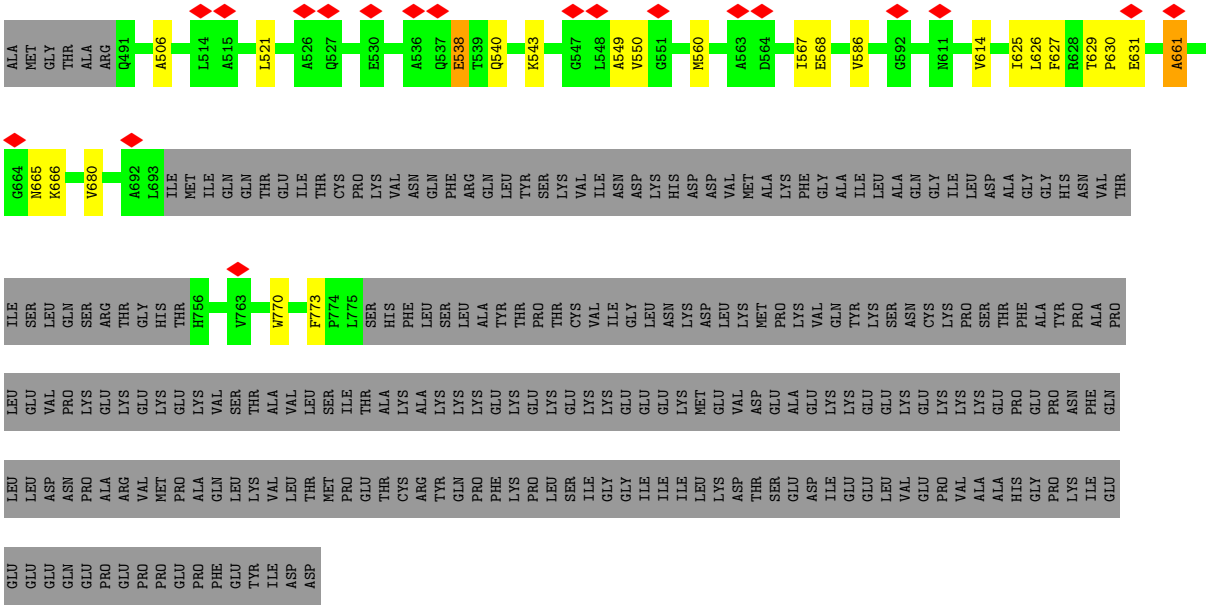
• Molecule 22: 26S protease regulatory subunit 8





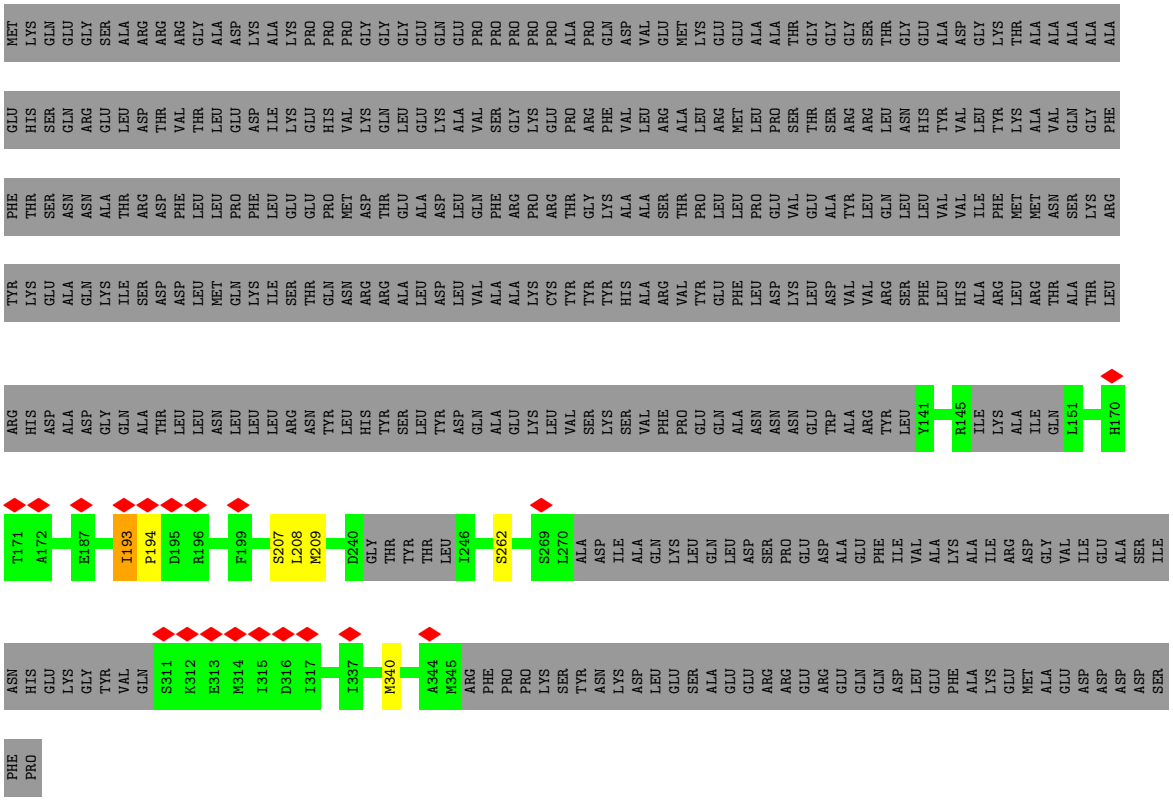
• Molecule 23: 26S proteasome non-ATPase regulatory subunit 1





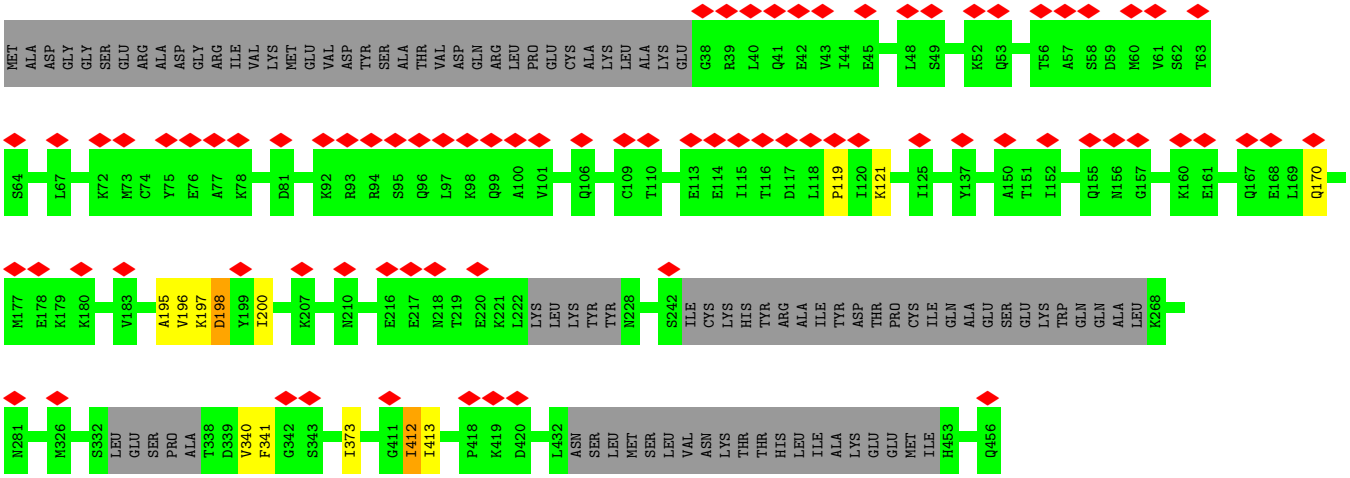
• Molecule 24: 26S proteasome non-ATPase regulatory subunit 3

Chain j:



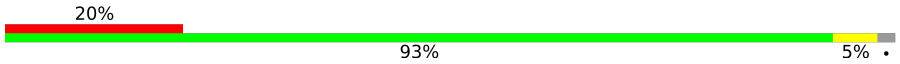
• Molecule 25: 26S proteasome non-ATPase regulatory subunit 12

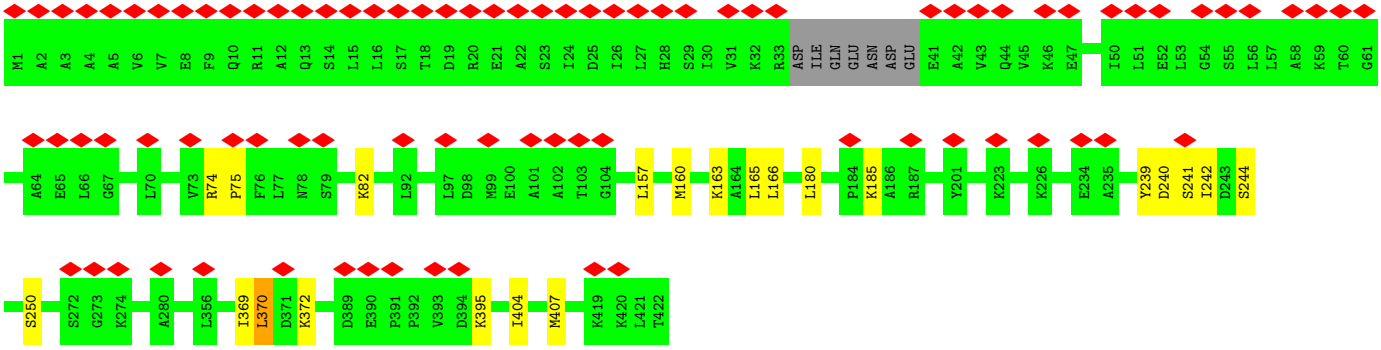
Chain k:



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

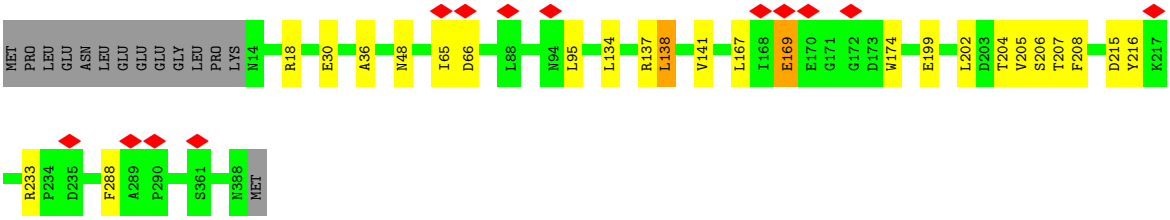
Chain l:





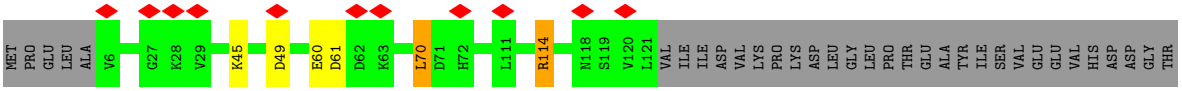
• Molecule 27: 26S proteasome non-ATPase regulatory subunit 6

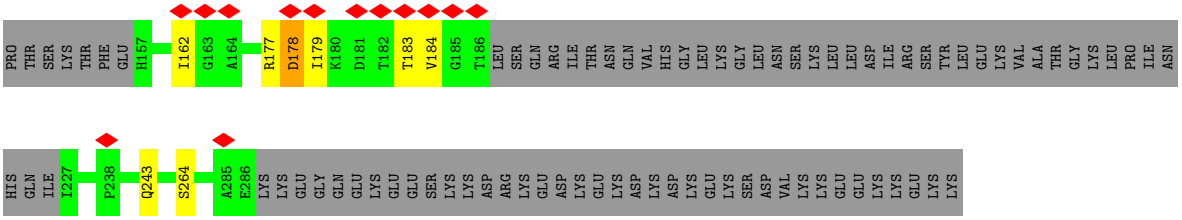
Chain m:



• Molecule 28: 26S proteasome non-ATPase regulatory subunit 7

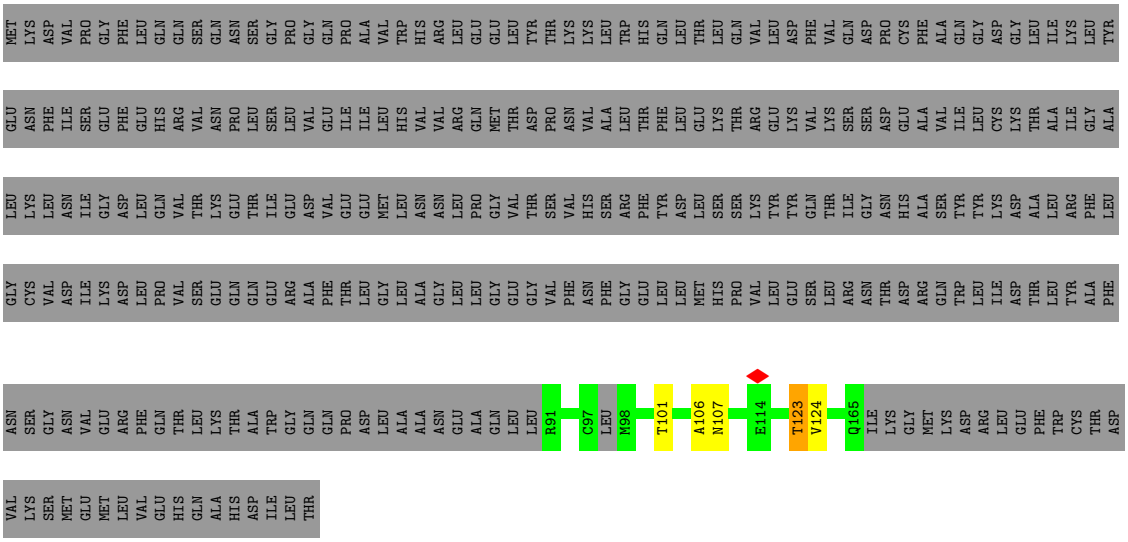
Chain n:





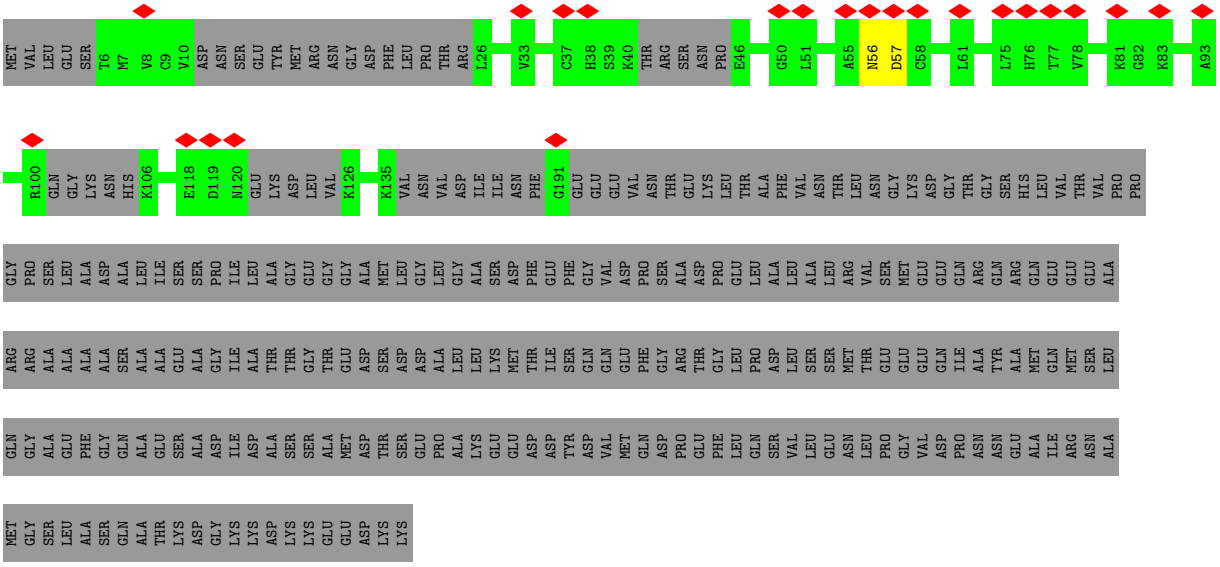
• Molecule 29: 26S proteasome non-ATPase regulatory subunit 13

Chain o:



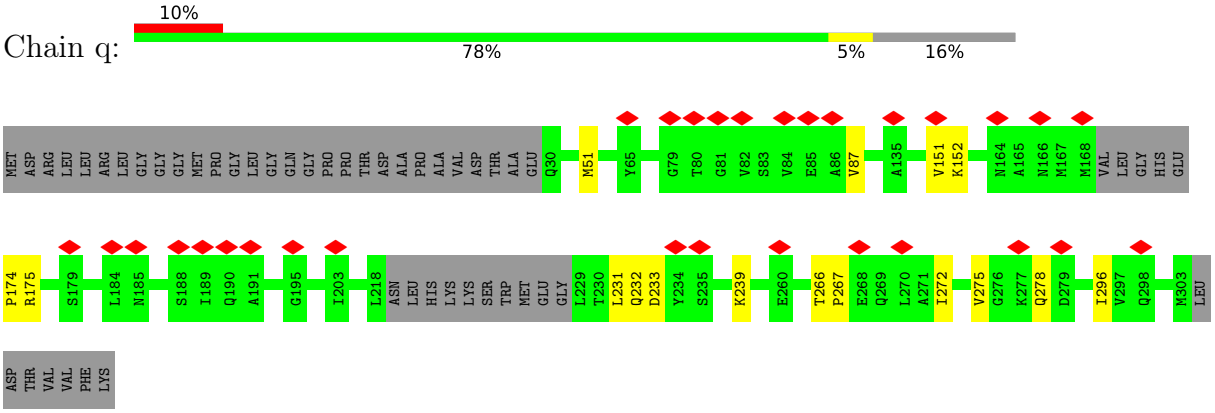
• Molecule 30: 26S proteasome non-ATPase regulatory subunit 4

Chain p:



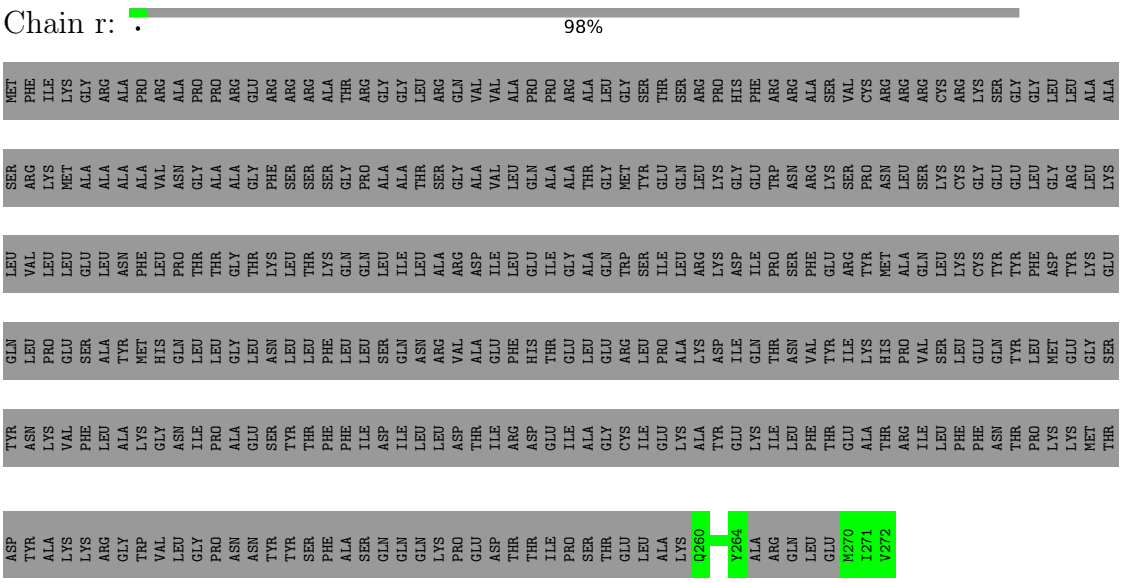
• Molecule 31: 26S proteasome non-ATPase regulatory subunit 14

Chain q:



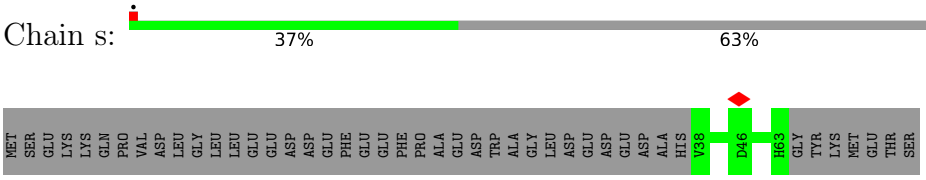
• Molecule 32: 26S proteasome non-ATPase regulatory subunit 8

Chain r:



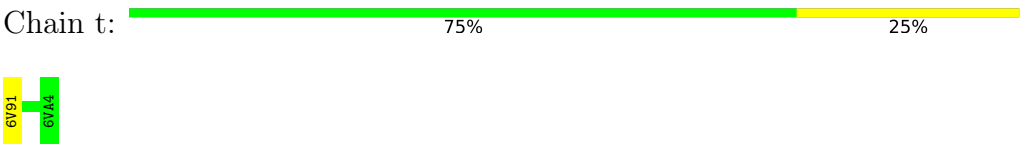
• Molecule 33: 26S proteasome complex subunit SEM1

Chain s:



• Molecule 34: bound Oprozomib

Chain t:



• Molecule 34: bound Oprozomib

Chain u:


6V91
6VA4

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	233000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	8400	Depositor
Magnification	110236	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.275	Depositor
Minimum map value	-0.131	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	426.72, 426.72, 426.72	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.27, 1.27, 1.27	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: ADP, 7C9, 6V9, 6VA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.40	0/1802	0.69	4/2446 (0.2%)
1	O	0.41	0/1802	0.70	5/2446 (0.2%)
2	B	0.37	0/1864	0.77	4/2513 (0.2%)
2	P	0.38	0/1904	0.83	7/2573 (0.3%)
3	C	0.41	0/1796	0.69	2/2438 (0.1%)
4	D	0.36	0/1784	0.68	1/2416 (0.0%)
4	R	0.36	0/1795	0.68	1/2424 (0.0%)
5	E	0.42	0/1839	0.84	8/2492 (0.3%)
6	F	0.44	0/1852	0.73	2/2494 (0.1%)
6	T	0.43	0/1912	0.74	3/2576 (0.1%)
7	G	0.39	0/1836	0.70	1/2481 (0.0%)
7	U	0.39	0/1875	0.67	1/2542 (0.0%)
8	H	0.42	0/1690	0.74	2/2289 (0.1%)
8	V	0.42	0/1657	0.73	2/2252 (0.1%)
9	I	0.40	0/1619	0.68	2/2184 (0.1%)
9	W	0.40	0/1614	0.68	2/2176 (0.1%)
10	J	0.39	0/1592	0.62	0/2153
10	X	0.39	0/1595	0.62	0/2157
11	K	0.44	0/1576	0.65	0/2131
11	Y	0.44	0/1590	0.65	0/2147
12	L	0.40	0/1670	0.73	4/2254 (0.2%)
12	Z	0.40	0/1672	0.73	4/2253 (0.2%)
13	M	0.42	0/1720	0.70	1/2328 (0.0%)
13	a	0.43	0/1712	0.68	0/2319
14	N	0.43	0/1539	0.62	0/2082
14	b	0.43	0/1546	0.69	2/2094 (0.1%)
15	Q	0.85	2/1810 (0.1%)	0.85	8/2456 (0.3%)
16	S	0.43	0/1868	0.85	8/2531 (0.3%)
17	c	0.37	0/2774	0.72	1/3739 (0.0%)
18	d	0.40	0/2597	1.00	14/3514 (0.4%)
19	e	0.36	0/2818	0.83	4/3812 (0.1%)
20	f	0.36	0/2734	0.70	4/3690 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
21	g	0.37	0/2815	0.79	2/3804 (0.1%)
22	h	0.35	0/2550	0.75	2/3442 (0.1%)
23	i	0.30	0/1150	0.74	2/1599 (0.1%)
24	j	0.32	0/780	0.72	0/1086
25	k	0.28	0/1819	0.66	2/2536 (0.1%)
26	l	0.33	0/2601	0.68	2/3569 (0.1%)
27	m	0.34	0/2450	0.74	4/3356 (0.1%)
28	n	0.30	0/1032	0.74	1/1438 (0.1%)
29	o	0.30	0/378	0.62	0/528
30	p	0.26	0/501	0.52	0/691
31	q	0.31	0/1318	0.78	2/1836 (0.1%)
32	r	0.26	0/38	0.60	0/50
33	s	0.33	0/129	0.69	0/179
All	All	0.40	2/77015 (0.0%)	0.73	114/104516 (0.1%)

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
1	A	0	2
1	O	0	1
2	B	0	4
2	P	0	10
3	C	0	1
4	D	0	1
4	R	0	1
5	E	0	4
6	F	0	3
6	T	0	3
7	G	0	3
7	U	0	2
8	H	0	1
8	V	0	1
9	I	0	2
9	W	0	2
10	J	0	1
10	X	0	1
13	a	0	1
14	b	0	2
15	Q	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	S	0	5
17	c	0	7
18	d	0	12
19	e	0	4
20	f	0	3
21	g	0	3
22	h	0	4
23	i	0	4
24	j	0	4
25	k	0	8
26	l	0	7
27	m	0	8
28	n	0	9
29	o	0	1
30	p	0	1
31	q	0	6
All	All	0	136

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Q	45	VAL	C-N	-30.59	0.63	1.34
15	Q	63	CYS	C-N	9.29	1.55	1.34

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	e	323	ARG	C-N-CD	-26.33	62.68	120.60
18	d	145	GLU	C-N-CD	-25.89	63.65	120.60
21	g	228	PRO	C-N-CD	-22.40	71.32	120.60
15	Q	63	CYS	O-C-N	-14.91	98.84	122.70
31	q	266	THR	C-N-CD	-14.89	87.84	120.60

There are no chirality outliers.

5 of 136 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	TRP	Peptide
1	A	139	ASN	Peptide
2	B	229	LYS	Peptide
2	B	54	LYS	Peptide

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Mol	Chain	Res	Type	Group
2	B	60	PHE	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	A	228/234 (97%)	197 (86%)	31 (14%)	0	100	100
1	O	228/234 (97%)	197 (86%)	31 (14%)	0	100	100
2	B	228/261 (87%)	195 (86%)	30 (13%)	3 (1%)	12	48
2	P	242/261 (93%)	203 (84%)	35 (14%)	4 (2%)	9	43
3	C	232/234 (99%)	191 (82%)	38 (16%)	3 (1%)	12	48
4	D	231/241 (96%)	199 (86%)	32 (14%)	0	100	100
4	R	231/241 (96%)	199 (86%)	32 (14%)	0	100	100
5	E	232/234 (99%)	190 (82%)	41 (18%)	1 (0%)	34	70
6	F	228/255 (89%)	195 (86%)	31 (14%)	2 (1%)	17	54
6	T	238/255 (93%)	202 (85%)	34 (14%)	2 (1%)	19	57
7	G	229/246 (93%)	206 (90%)	21 (9%)	2 (1%)	17	54
7	U	239/246 (97%)	213 (89%)	25 (10%)	1 (0%)	34	70
8	H	219/277 (79%)	208 (95%)	11 (5%)	0	100	100
8	V	219/277 (79%)	208 (95%)	11 (5%)	0	100	100
9	I	202/205 (98%)	182 (90%)	18 (9%)	2 (1%)	15	52
9	W	202/205 (98%)	182 (90%)	18 (9%)	2 (1%)	15	52
10	J	194/196 (99%)	175 (90%)	19 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	X	194/196 (99%)	175 (90%)	19 (10%)	0	100	100
11	K	198/204 (97%)	174 (88%)	24 (12%)	0	100	100
11	Y	199/204 (98%)	175 (88%)	24 (12%)	0	100	100
12	L	212/241 (88%)	184 (87%)	28 (13%)	0	100	100
12	Z	211/241 (88%)	184 (87%)	27 (13%)	0	100	100
13	M	214/264 (81%)	192 (90%)	21 (10%)	1 (0%)	29	66
13	a	214/264 (81%)	192 (90%)	21 (10%)	1 (0%)	29	66
14	N	199/239 (83%)	179 (90%)	20 (10%)	0	100	100
14	b	201/239 (84%)	179 (89%)	21 (10%)	1 (0%)	29	66
15	Q	233/235 (99%)	186 (80%)	38 (16%)	9 (4%)	3	28
16	S	236/238 (99%)	195 (83%)	39 (16%)	2 (1%)	19	57
17	c	343/433 (79%)	256 (75%)	74 (22%)	13 (4%)	3	29
18	d	329/428 (77%)	251 (76%)	59 (18%)	19 (6%)	1	21
19	e	355/418 (85%)	279 (79%)	63 (18%)	13 (4%)	3	29
20	f	346/379 (91%)	285 (82%)	51 (15%)	10 (3%)	4	34
21	g	359/439 (82%)	292 (81%)	60 (17%)	7 (2%)	8	42
22	h	324/355 (91%)	248 (76%)	59 (18%)	17 (5%)	2	23
23	i	224/953 (24%)	173 (77%)	31 (14%)	20 (9%)	1	12
24	j	147/534 (28%)	111 (76%)	32 (22%)	4 (3%)	5	35
25	k	354/456 (78%)	272 (77%)	77 (22%)	5 (1%)	11	46
26	l	411/422 (97%)	341 (83%)	62 (15%)	8 (2%)	8	42
27	m	373/389 (96%)	318 (85%)	51 (14%)	4 (1%)	14	51
28	n	200/324 (62%)	147 (74%)	46 (23%)	7 (4%)	3	31
29	o	73/376 (19%)	56 (77%)	12 (16%)	5 (7%)	1	18
30	p	90/377 (24%)	78 (87%)	11 (12%)	1 (1%)	14	51
31	q	253/310 (82%)	191 (76%)	54 (21%)	8 (3%)	4	32
32	r	4/350 (1%)	4 (100%)	0	0	100	100
33	s	24/70 (34%)	19 (79%)	5 (21%)	0	100	100
All	All	10342/13680 (76%)	8678 (84%)	1487 (14%)	177 (2%)	13	43

5 of 177 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	69	HIS
6	F	227	VAL
6	F	228	PRO
7	G	69	LEU
13	M	79	ASP

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	A	181/191 (95%)	178 (98%)	3 (2%)	60	78
1	O	181/191 (95%)	178 (98%)	3 (2%)	60	78
2	B	195/221 (88%)	183 (94%)	12 (6%)	18	49
2	P	194/221 (88%)	184 (95%)	10 (5%)	23	54
3	C	179/197 (91%)	169 (94%)	10 (6%)	21	52
4	D	189/203 (93%)	182 (96%)	7 (4%)	34	62
4	R	192/203 (95%)	186 (97%)	6 (3%)	40	65
5	E	192/200 (96%)	188 (98%)	4 (2%)	53	74
6	F	190/212 (90%)	188 (99%)	2 (1%)	73	85
6	T	197/212 (93%)	195 (99%)	2 (1%)	76	86
7	G	197/210 (94%)	194 (98%)	3 (2%)	65	81
7	U	196/210 (93%)	191 (97%)	5 (3%)	46	69
8	H	181/228 (79%)	178 (98%)	3 (2%)	60	78
8	V	173/228 (76%)	171 (99%)	2 (1%)	71	84
9	I	173/174 (99%)	172 (99%)	1 (1%)	86	92
9	W	172/174 (99%)	171 (99%)	1 (1%)	86	92
10	J	163/166 (98%)	161 (99%)	2 (1%)	71	84
10	X	164/166 (99%)	162 (99%)	2 (1%)	71	84
11	K	154/159 (97%)	150 (97%)	4 (3%)	46	69
11	Y	156/159 (98%)	152 (97%)	4 (3%)	46	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	L	175/199 (88%)	173 (99%)	2 (1%)	73 85
12	Z	175/199 (88%)	173 (99%)	2 (1%)	73 85
13	M	179/215 (83%)	174 (97%)	5 (3%)	43 68
13	a	177/215 (82%)	172 (97%)	5 (3%)	43 68
14	N	157/181 (87%)	156 (99%)	1 (1%)	86 92
14	b	157/181 (87%)	156 (99%)	1 (1%)	86 92
15	Q	182/199 (92%)	169 (93%)	13 (7%)	14 45
16	S	194/202 (96%)	190 (98%)	4 (2%)	53 74
17	c	297/372 (80%)	279 (94%)	18 (6%)	18 50
18	d	281/375 (75%)	256 (91%)	25 (9%)	9 38
19	e	289/366 (79%)	268 (93%)	21 (7%)	14 45
20	f	287/331 (87%)	273 (95%)	14 (5%)	25 55
21	g	291/379 (77%)	274 (94%)	17 (6%)	20 51
22	h	266/307 (87%)	237 (89%)	29 (11%)	6 29
23	i	8/816 (1%)	8 (100%)	0	100 100
24	j	5/460 (1%)	5 (100%)	0	100 100
25	k	5/416 (1%)	5 (100%)	0	100 100
26	l	148/362 (41%)	142 (96%)	6 (4%)	30 59
27	m	154/344 (45%)	143 (93%)	11 (7%)	14 45
28	n	5/295 (2%)	5 (100%)	0	100 100
29	o	2/336 (1%)	2 (100%)	0	100 100
30	p	3/312 (1%)	3 (100%)	0	100 100
31	q	14/268 (5%)	14 (100%)	0	100 100
32	r	1/294 (0%)	1 (100%)	0	100 100
All	All	7071/11549 (61%)	6811 (96%)	260 (4%)	37 62

5 of 260 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	h	145	ASP
22	h	271	ARG
7	U	43	ARG
16	S	157	ARG
26	l	157	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
17	c	293	ASN
26	l	170	GLN
18	d	153	ASN
21	g	130	GLN
10	J	71	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)

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
34	7C9	u	3	34	5,6,7	0.56	0	2,6,8	0.31	0
34	6V9	t	1	34	6,8,9	0.74	0	3,10,12	4.62	3 (100%)
34	7C9	t	3	34	5,6,7	0.54	0	2,6,8	0.32	0
34	7C9	u	2	34	5,6,7	0.58	0	2,6,8	0.25	0
34	6V9	u	1	34	6,8,9	0.64	0	3,10,12	4.49	3 (100%)
34	7C9	t	2	34	5,6,7	0.51	0	2,6,8	0.40	0

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
34	7C9	u	3	34	-	0/3/5/7	-
34	6V9	t	1	34	-	0/0/2/4	0/1/1/1
34	7C9	t	3	34	-	0/3/5/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	7C9	u	2	34	-	2/3/5/7	-
34	6V9	u	1	34	-	0/0/2/4	0/1/1/1
34	7C9	t	2	34	-	2/3/5/7	-

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	t	1	6V9	O1-C4-C3	-5.79	118.73	124.22
34	u	1	6V9	O1-C4-C3	-5.49	119.02	124.22
34	t	1	6V9	C2-C1-N1	4.44	133.54	121.87
34	u	1	6V9	C2-C1-N1	4.39	133.42	121.87
34	u	1	6V9	C2-C1-S	-3.30	115.67	120.12

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	t	2	7C9	N03-C04-C19-O20
34	u	2	7C9	N03-C04-C19-O20
34	t	2	7C9	C05-C04-C19-O20
34	u	2	7C9	C05-C04-C19-O20

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
35	ADP	g	502	-	24,29,29	0.91	1 (4%)	29,45,45	1.58	4 (13%)
35	ADP	d	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.49	4 (13%)
35	ADP	e	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.50	4 (13%)
35	ADP	g	501	-	24,29,29	0.91	1 (4%)	29,45,45	1.61	4 (13%)
35	ADP	h	401	-	24,29,29	0.90	1 (4%)	29,45,45	1.54	4 (13%)
35	ADP	c	501	-	24,29,29	0.94	1 (4%)	29,45,45	1.50	4 (13%)

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
35	ADP	g	502	-	-	2/12/32/32	0/3/3/3
35	ADP	d	501	-	-	2/12/32/32	0/3/3/3
35	ADP	e	501	-	-	5/12/32/32	0/3/3/3
35	ADP	g	501	-	-	3/12/32/32	0/3/3/3
35	ADP	h	401	-	-	1/12/32/32	0/3/3/3
35	ADP	c	501	-	-	4/12/32/32	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	e	501	ADP	C5-C4	2.49	1.47	1.40
35	d	501	ADP	C5-C4	2.31	1.47	1.40
35	g	501	ADP	C5-C4	2.28	1.47	1.40
35	h	401	ADP	C5-C4	2.24	1.46	1.40
35	c	501	ADP	C5-C4	2.17	1.46	1.40

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	g	502	ADP	PA-O3A-PB	-5.29	114.66	132.83
35	g	501	ADP	PA-O3A-PB	-5.01	115.64	132.83
35	h	401	ADP	PA-O3A-PB	-4.63	116.94	132.83
35	c	501	ADP	PA-O3A-PB	-4.32	118.01	132.83
35	d	501	ADP	PA-O3A-PB	-4.16	118.54	132.83

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

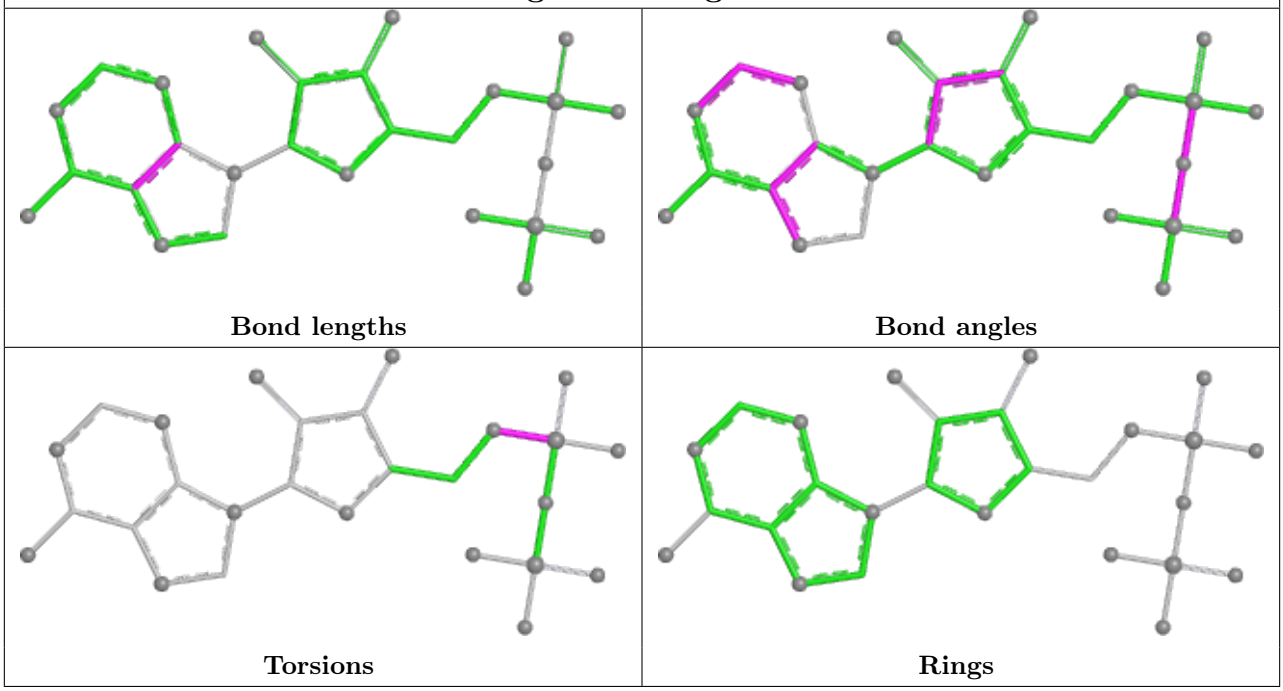
Mol	Chain	Res	Type	Atoms
35	c	501	ADP	C5'-O5'-PA-O1A
35	c	501	ADP	C3'-C4'-C5'-O5'
35	d	501	ADP	C4'-C5'-O5'-PA
35	e	501	ADP	C5'-O5'-PA-O1A
35	e	501	ADP	C5'-O5'-PA-O2A

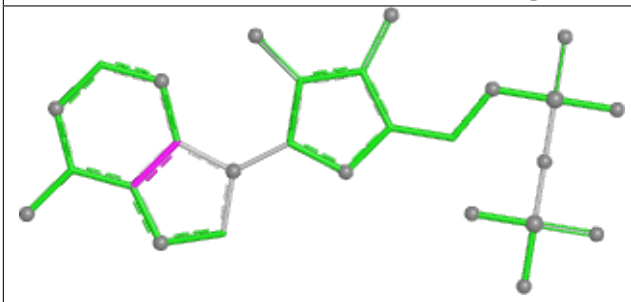
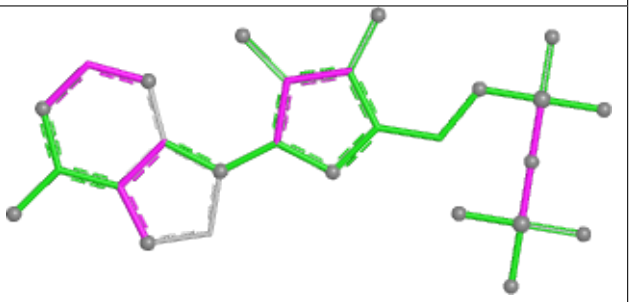
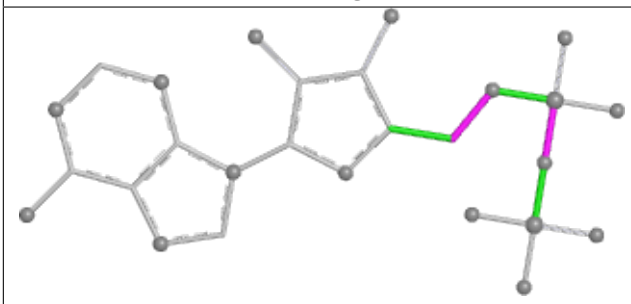
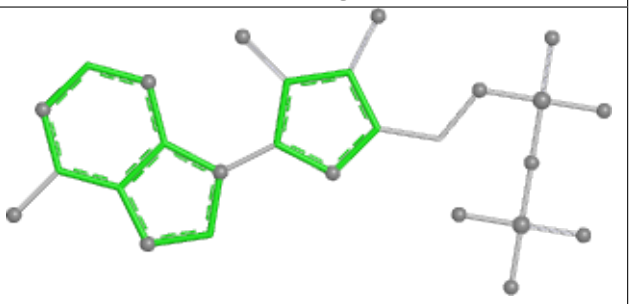
There are no ring outliers.

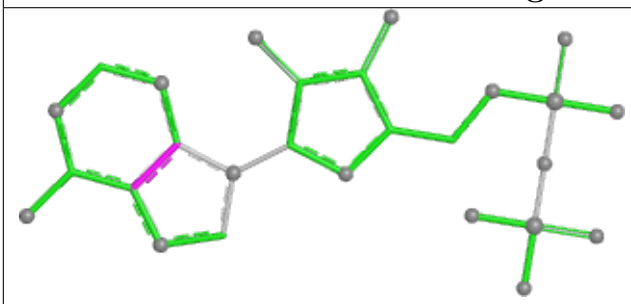
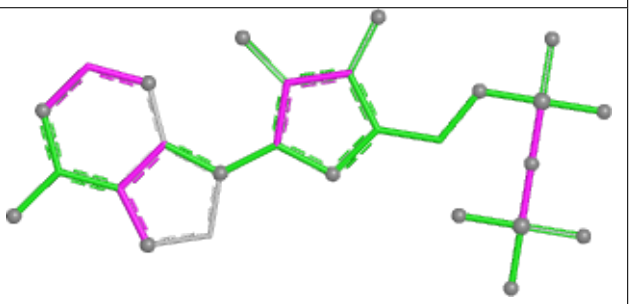
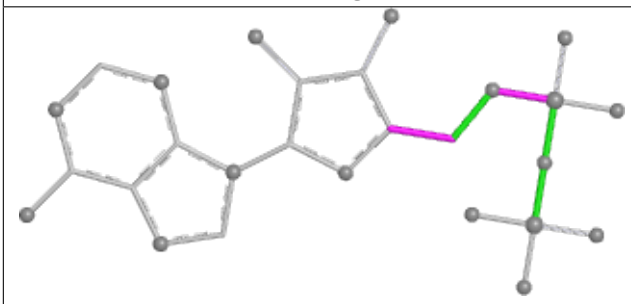
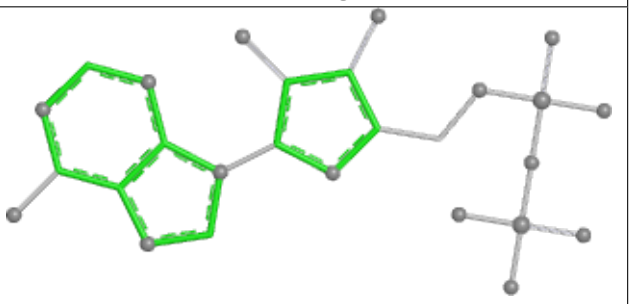
No monomer is involved in short contacts.

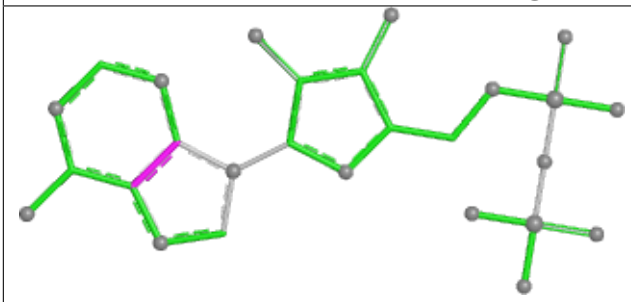
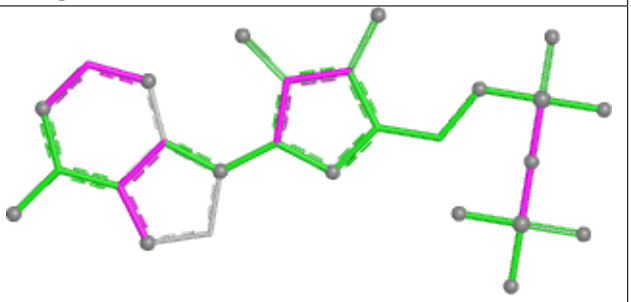
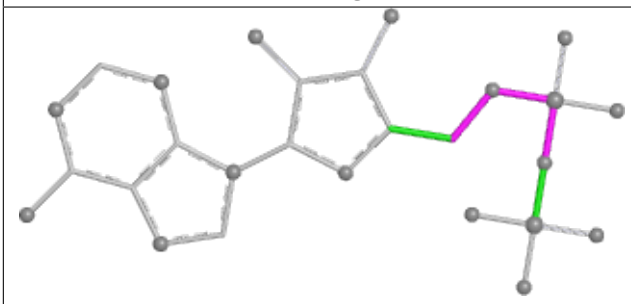
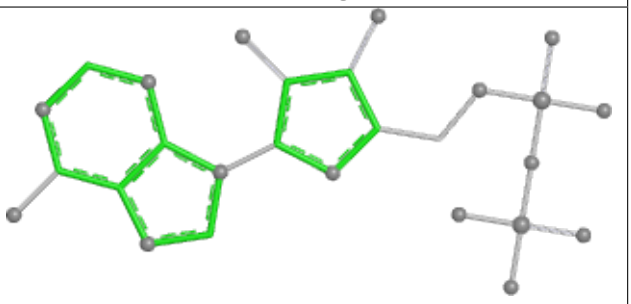
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

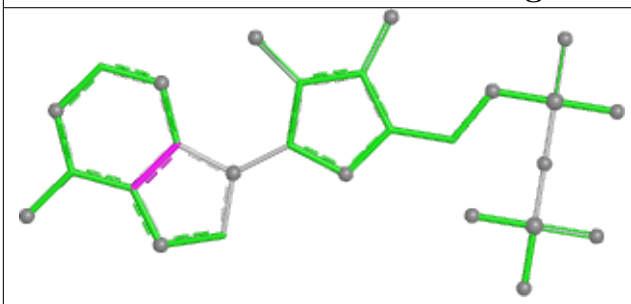
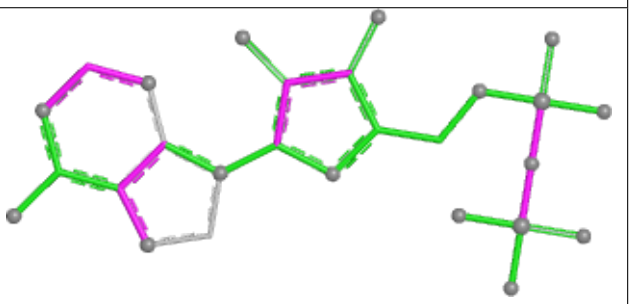
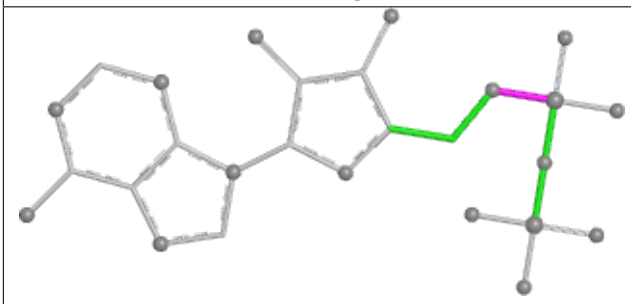
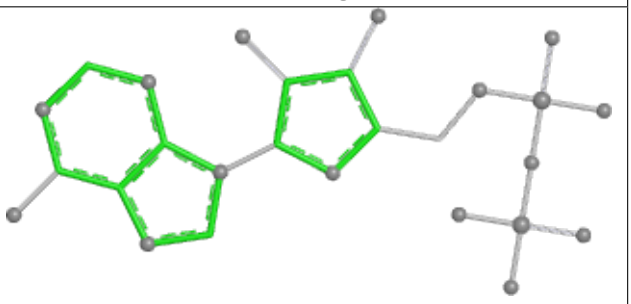
Ligand ADP g 502

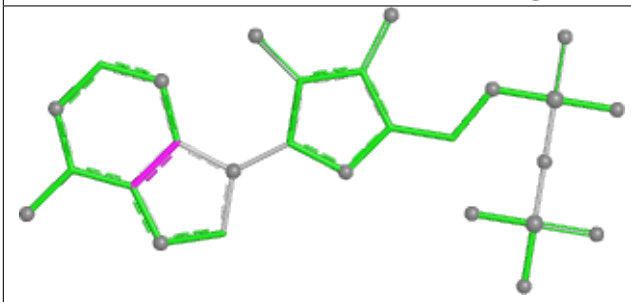
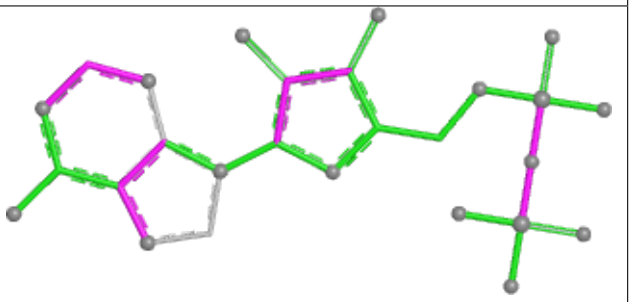
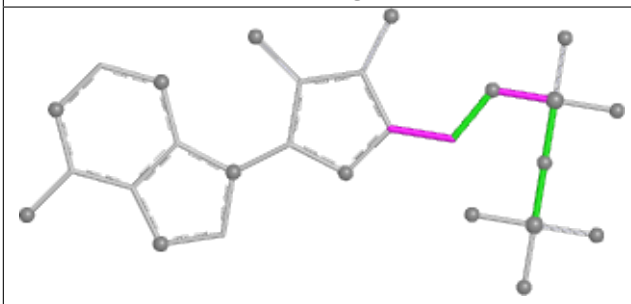
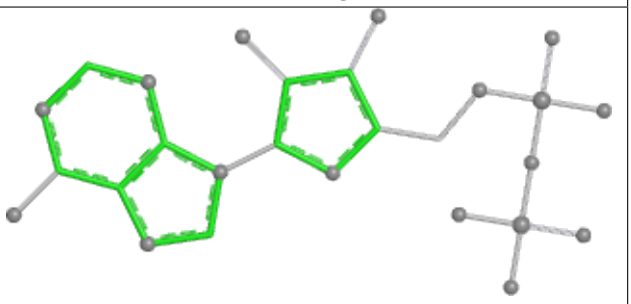


Ligand ADP d 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP e 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP g 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP h 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP c 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
19	e	1
15	Q	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	e	414:HIS	C	415:GLU	N	4.11
1	Q	45:VAL	C	46:GLU	N	0.63

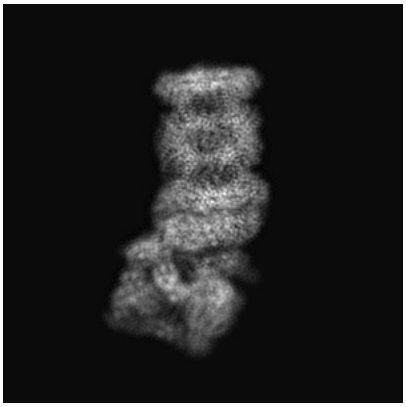
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4146. These allow visual inspection of the internal detail of the map and identification of artifacts.

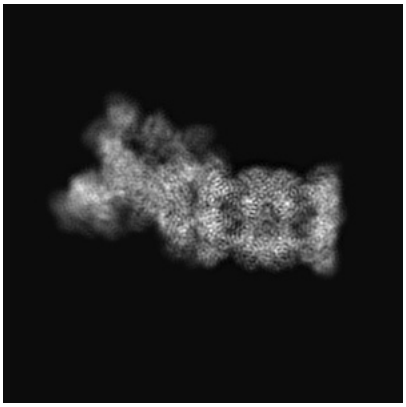
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

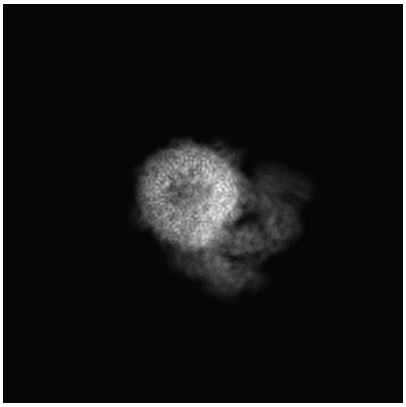
6.1.1 Primary map



X



Y

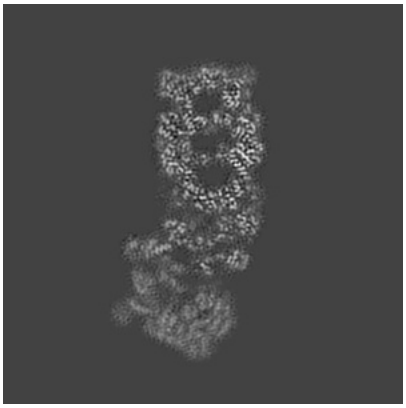


Z

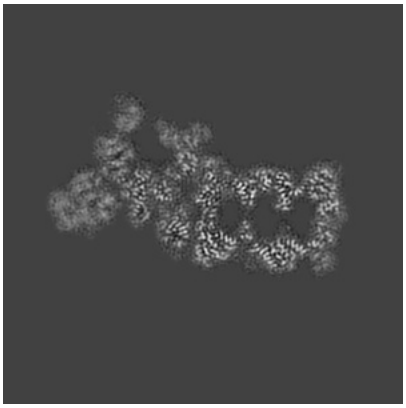
The images above show the map projected in three orthogonal directions.

6.2 Central slices

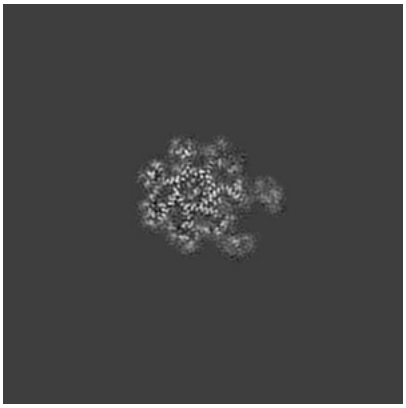
6.2.1 Primary map



X Index: 168



Y Index: 168

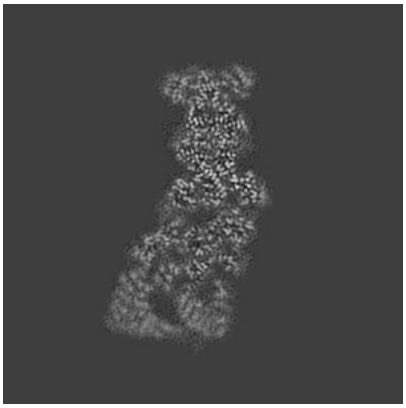


Z Index: 168

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

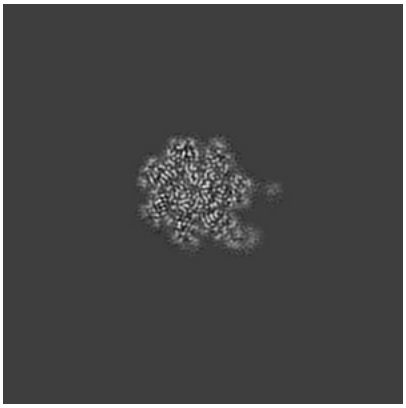
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 181

Y Index: 186



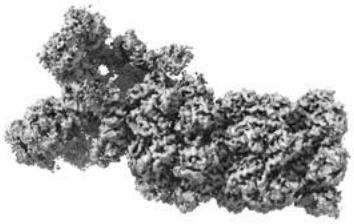
Z Index: 176

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

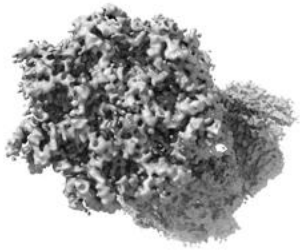
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

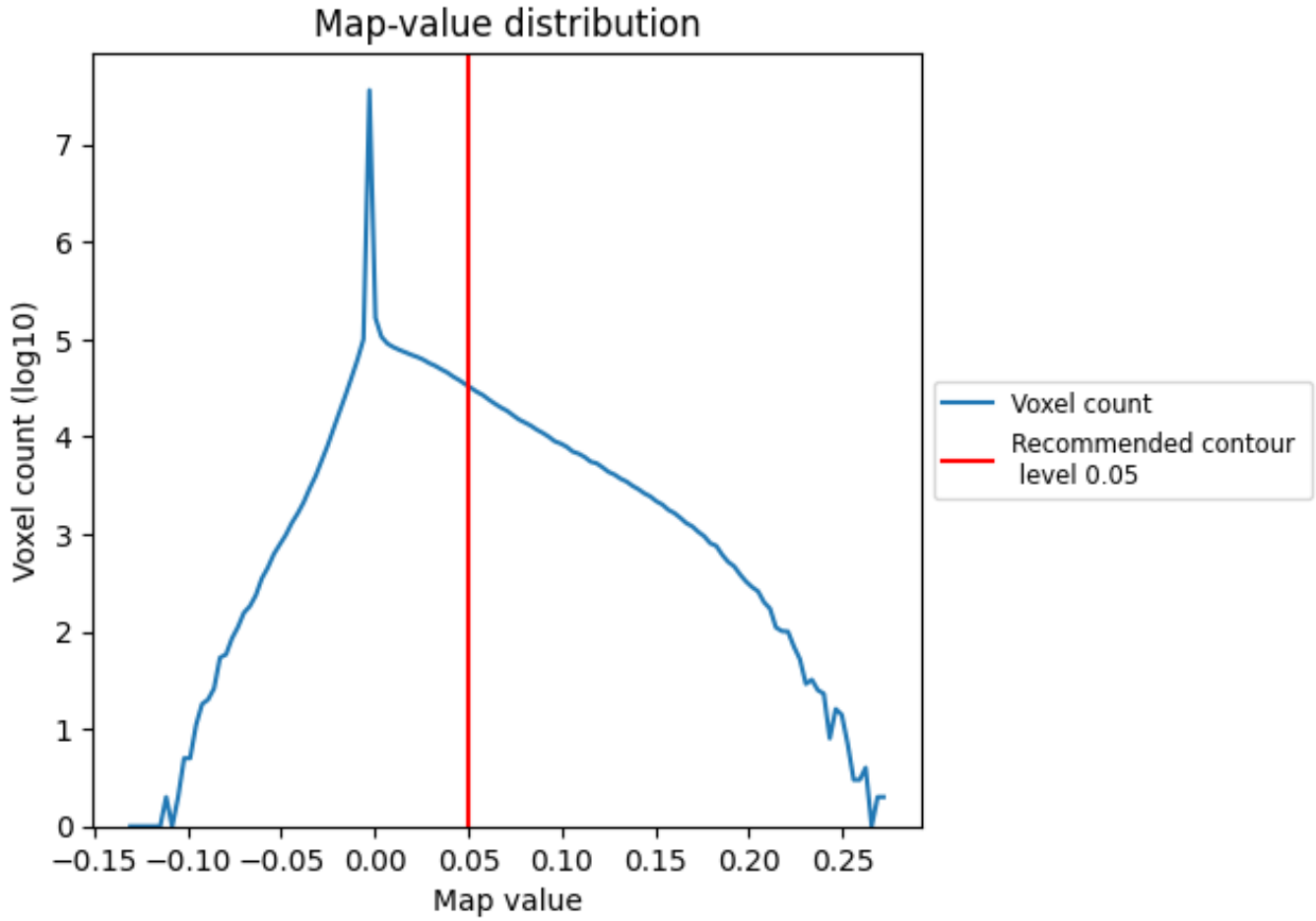
6.5 Mask visualisation (i)

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

7 Map analysis

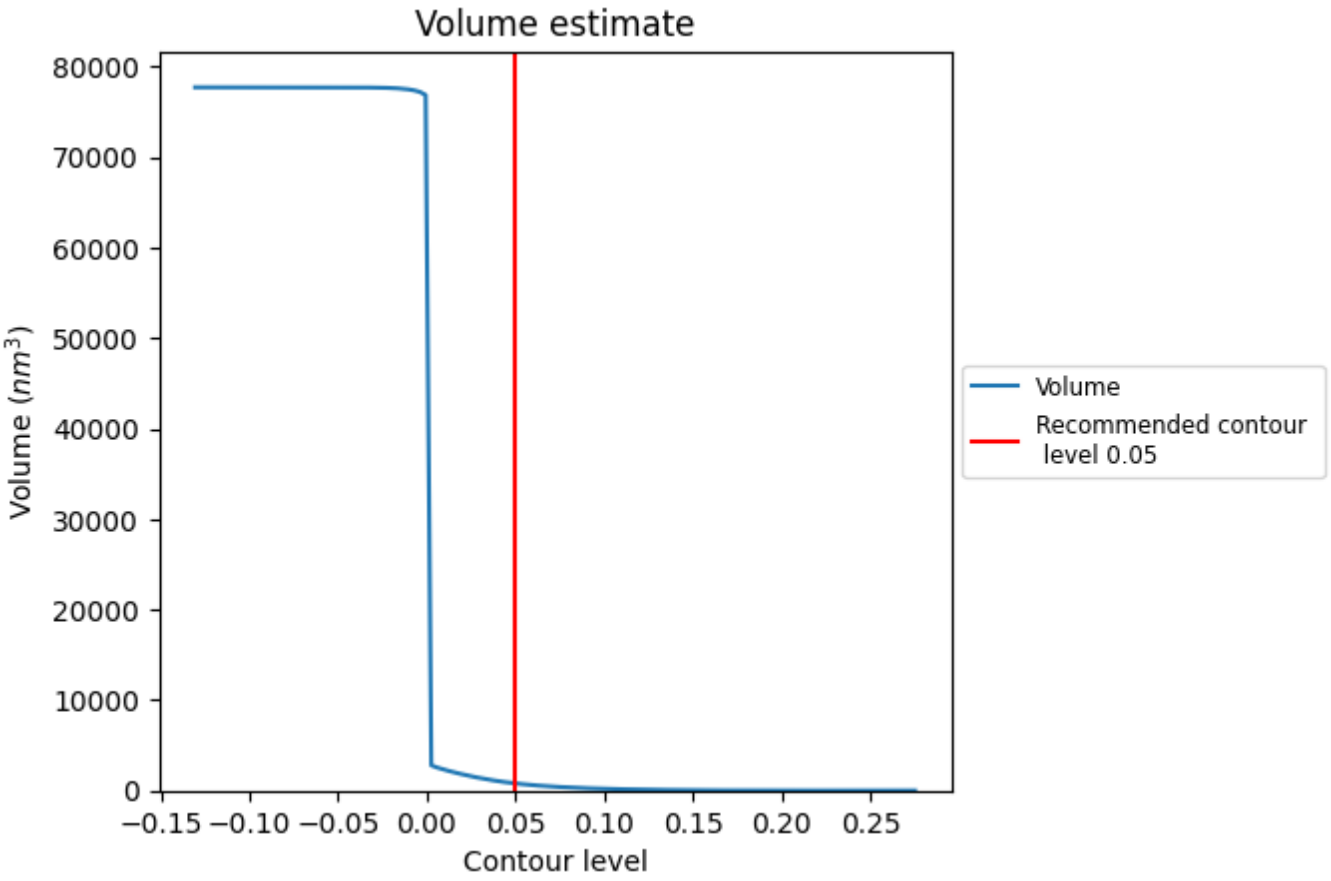
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

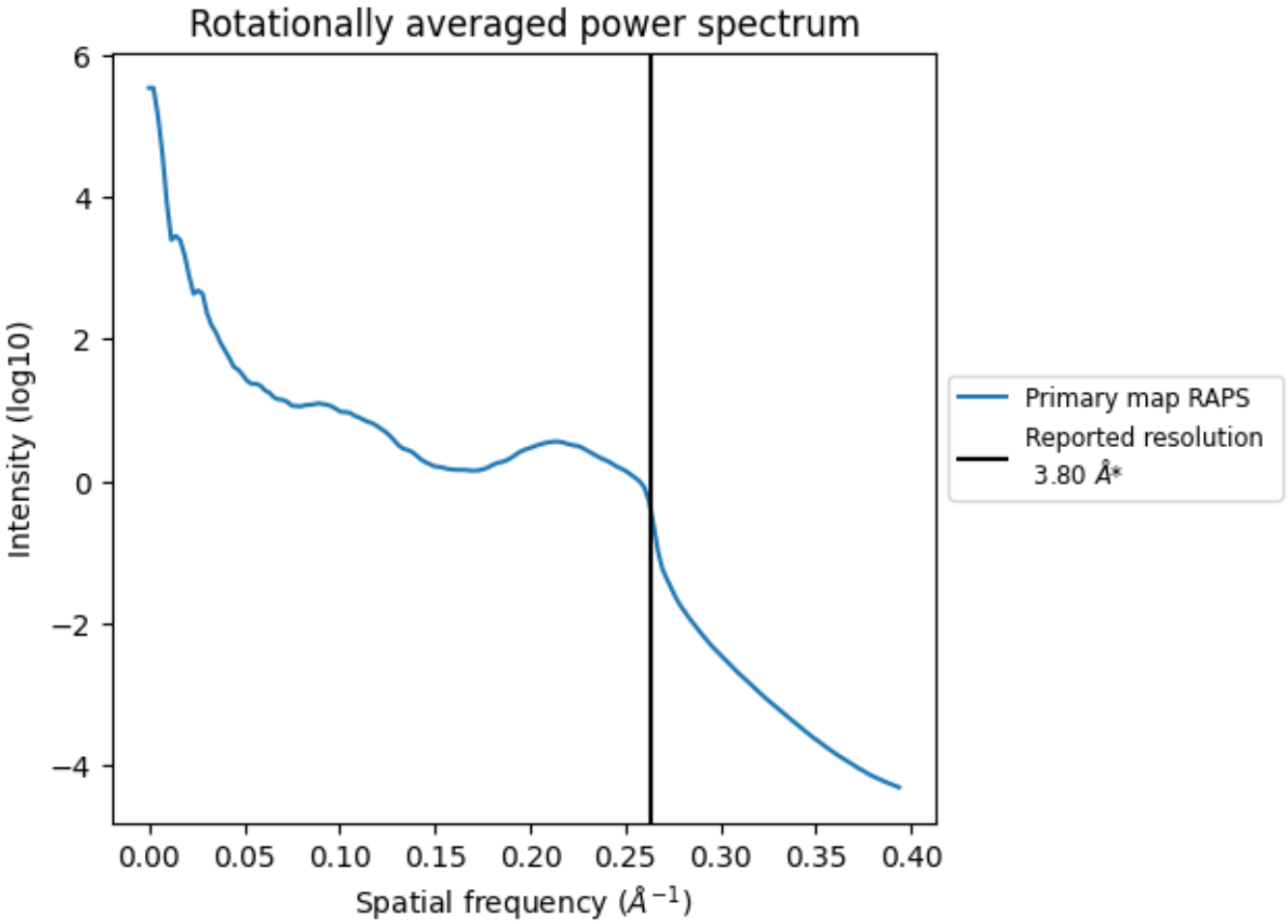
7.2 Volume estimate (i)



The volume at the recommended contour level is 790 nm^3; this corresponds to an approximate mass of 714 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 0.263 Å^{-1}

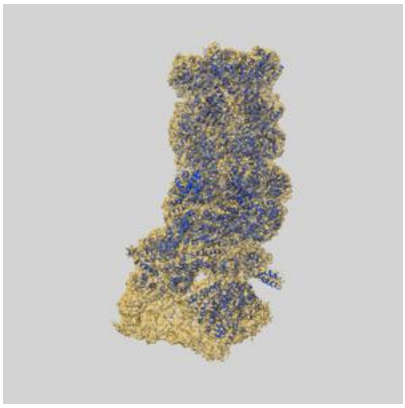
8 Fourier-Shell correlation

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

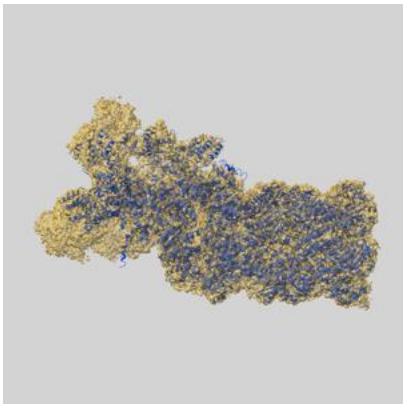
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4146 and PDB model 5M32. Per-residue inclusion information can be found in section 3 on page 13.

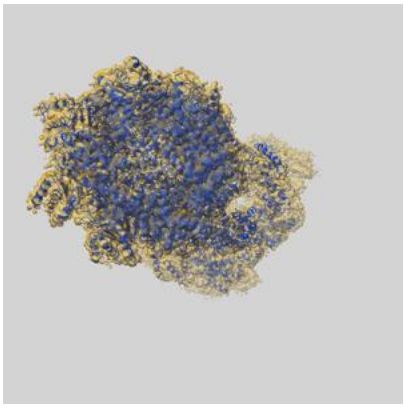
9.1 Map-model overlay



X



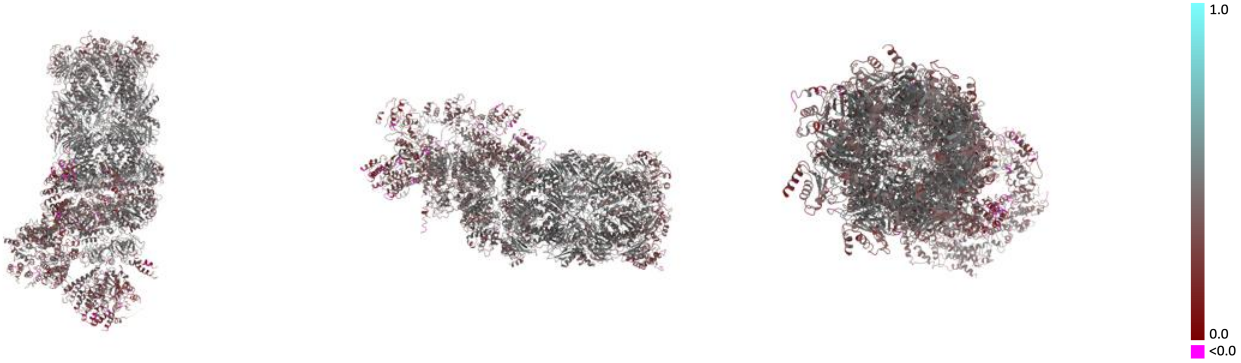
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

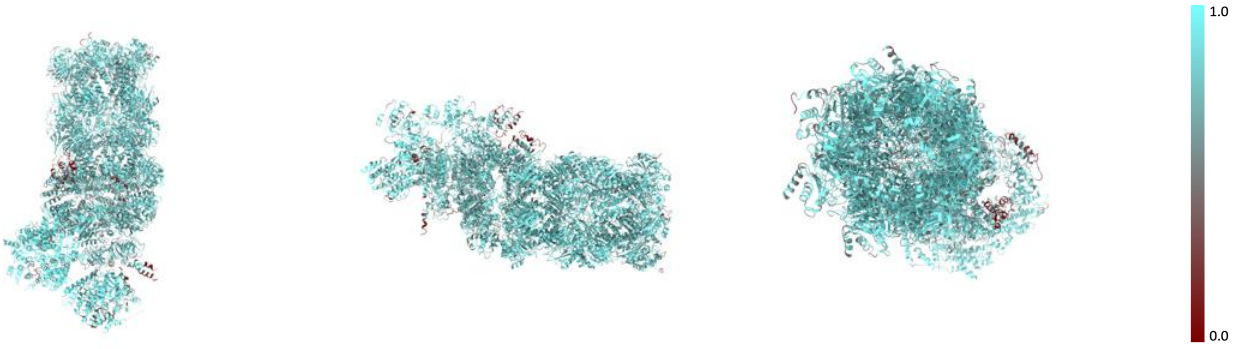
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

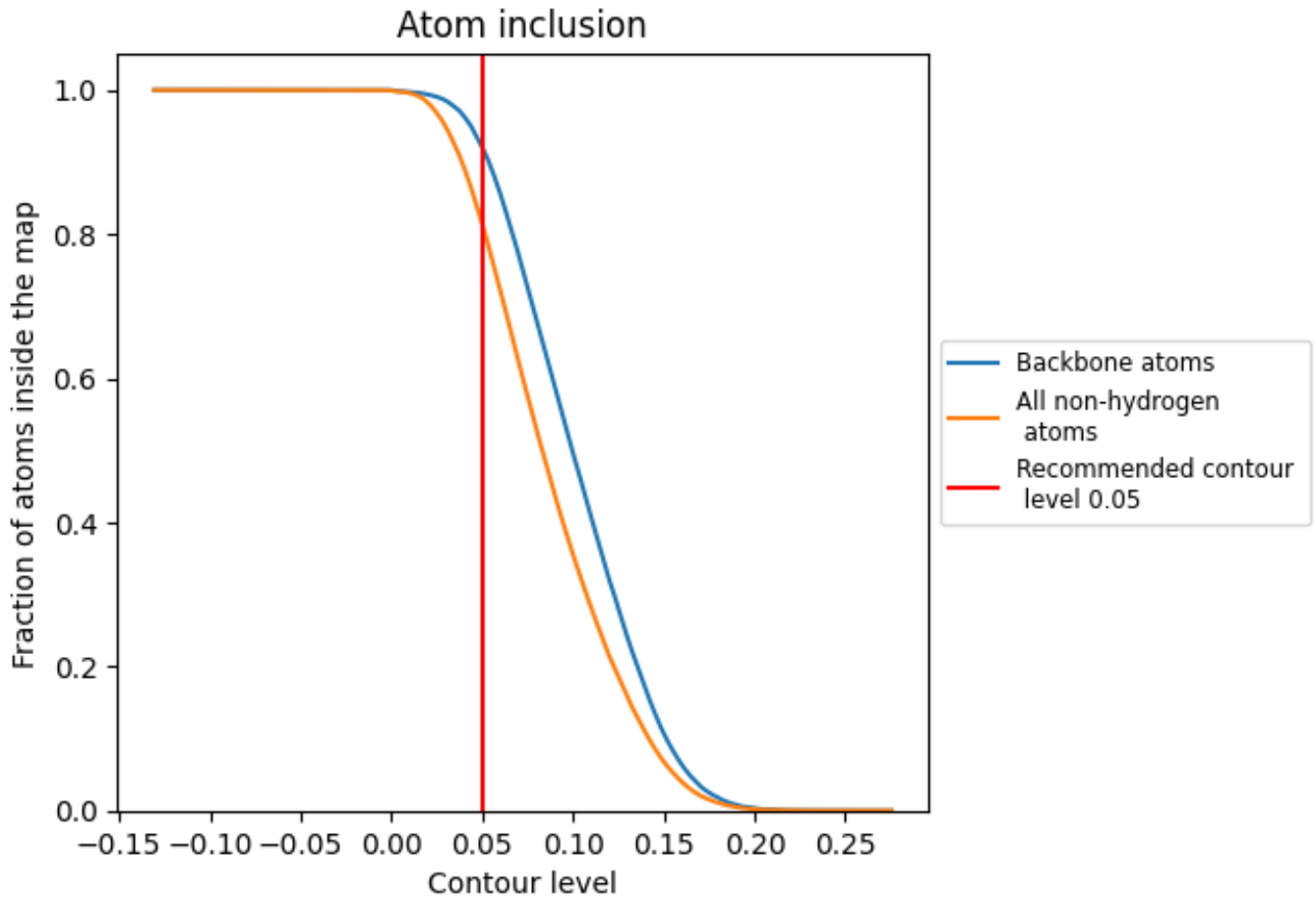
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 92% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8140	0.4040
A	0.8357	0.4360
B	0.8039	0.4240
C	0.8327	0.4260
D	0.8185	0.4310
E	0.8494	0.4320
F	0.8402	0.4380
G	0.8199	0.4210
H	0.8550	0.4440
I	0.8559	0.4560
J	0.8726	0.4530
K	0.8858	0.4500
L	0.8639	0.4550
M	0.8647	0.4590
N	0.8589	0.4520
O	0.8176	0.3950
P	0.7781	0.3820
Q	0.7961	0.3800
R	0.7808	0.3900
S	0.8349	0.4070
T	0.7963	0.3880
U	0.7982	0.3840
V	0.8491	0.4340
W	0.8459	0.4430
X	0.8644	0.4460
Y	0.8820	0.4530
Z	0.8408	0.4300
a	0.8641	0.4650
b	0.8393	0.4450
c	0.7786	0.4160
d	0.7214	0.3660
e	0.7748	0.4090
f	0.7914	0.4050
g	0.7688	0.4060
h	0.7602	0.4060

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.8498	0.2720
j	0.8331	0.2660
k	0.7493	0.2950
l	0.7084	0.3020
m	0.8323	0.3480
n	0.8301	0.3410
o	0.9257	0.3300
p	0.7063	0.2470
q	0.8215	0.3410
r	0.9750	0.3750
s	0.8923	0.3180
t	0.8649	0.4950
u	0.8649	0.5210