



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 09:37 AM UTC

PDB ID : 6E11 / pdb_00006e11
EMDB ID : EMD-8952
Title : PTEX Core Complex in the Resetting (Compact) State
Authors : Ho, C.; Lai, M.; Zhou, Z.H.
Deposited on : 2018-07-08
Resolution : 4.23 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

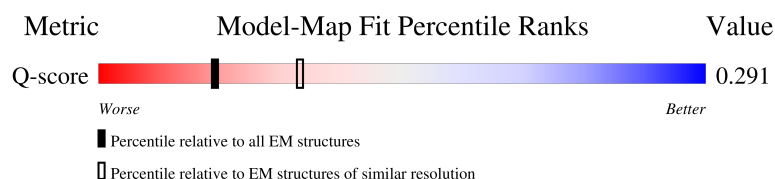
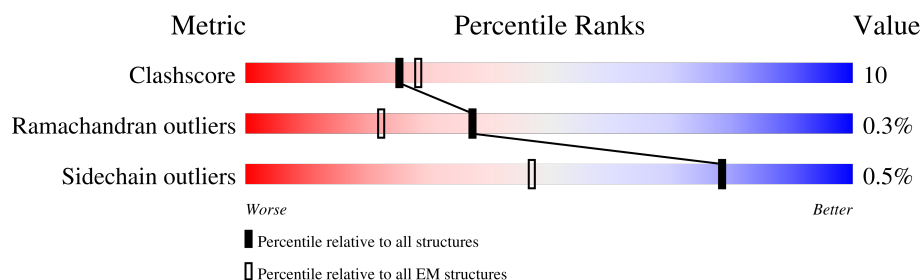
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.23 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.



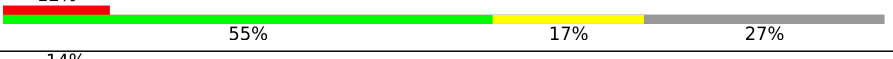
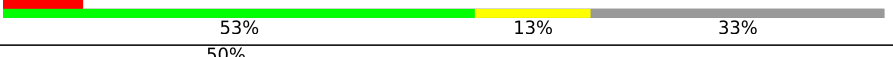
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4685 (3.74 - 4.73)

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	h	60	
1	i	60	
1	j	60	
1	k	60	

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Mol	Chain	Length	Quality of chain
1	l	60	
1	m	60	
1	n	60	
2	1	906	
2	2	906	
2	3	906	
2	4	906	
2	5	906	
2	6	906	
3	A	287	
3	B	287	
3	C	287	
3	D	287	
3	E	287	
3	F	287	
3	G	287	
4	0	6	
5	a	993	
5	b	993	
5	c	993	
5	d	993	
5	e	993	
5	f	993	
5	g	993	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	AGS	1	1003	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 57401 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 Unknown (Claw).

Mol	Chain	Residues	Atoms				AltConf	Trace
1	i	46	Total	C	N	O	0	0
			230	138	46	46		
1	j	55	Total	C	N	O	0	0
			275	165	55	55		
1	k	60	Total	C	N	O	0	0
			300	180	60	60		
1	n	36	Total	C	N	O	0	0
			180	108	36	36		
1	h	47	Total	C	N	O	0	0
			235	141	47	47		
1	l	53	Total	C	N	O	0	0
			265	159	53	53		
1	m	58	Total	C	N	O	0	0
			290	174	58	58		

- Molecule 2 is a protein called Heat shock protein 101.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	717	Total	C	N	O	S	0	0
			5752	3687	964	1086	15		
2	2	717	Total	C	N	O	S	0	0
			5752	3687	964	1086	15		
2	3	717	Total	C	N	O	S	0	0
			5752	3687	964	1086	15		
2	4	717	Total	C	N	O	S	0	0
			5752	3687	964	1086	15		
2	5	716	Total	C	N	O	S	0	0
			5744	3681	963	1085	15		
2	6	716	Total	C	N	O	S	0	0
			5744	3681	963	1085	15		

- Molecule 3 is a protein called Exported protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	209	Total	C	N	O	S	0	0
			1715	1107	293	309	6		
3	D	209	Total	C	N	O	S	0	0
			1715	1107	293	309	6		
3	E	210	Total	C	N	O	S	0	0
			1724	1112	294	312	6		
3	B	209	Total	C	N	O	S	0	0
			1715	1107	293	309	6		
3	A	191	Total	C	N	O	S	0	0
			1571	1019	271	275	6		
3	G	191	Total	C	N	O	S	0	0
			1571	1019	271	275	6		
3	F	209	Total	C	N	O	S	0	0
			1715	1107	293	309	6		

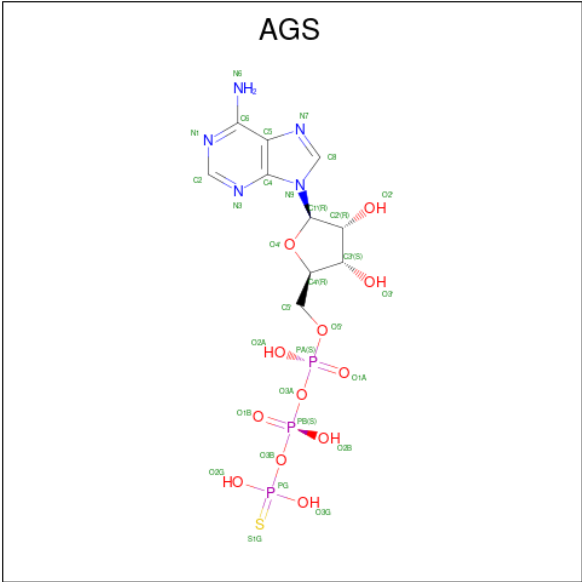
- Molecule 4 is a protein called Endogenous cargo polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	0	6	Total	C	N	O	0	0
			30	18	6	6		

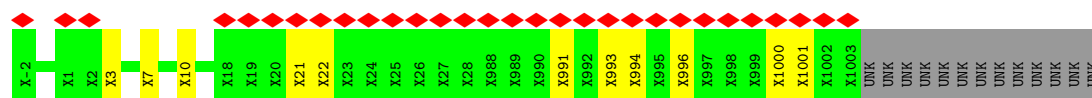
- Molecule 5 is a protein called Translocon component PTEX150.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	d	156	Total	C	N	O	S	0	0
			1286	809	203	273	1		
5	c	156	Total	C	N	O	S	0	0
			1286	809	203	273	1		
5	b	156	Total	C	N	O	S	0	0
			1286	809	203	273	1		
5	a	156	Total	C	N	O	S	0	0
			1286	809	203	273	1		
5	g	156	Total	C	N	O	S	0	0
			1286	809	203	273	1		
5	f	156	Total	C	N	O	S	0	0
			1286	809	203	273	1		
5	e	156	Total	C	N	O	S	0	0
			1286	809	203	273	1		

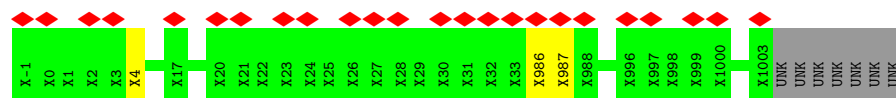
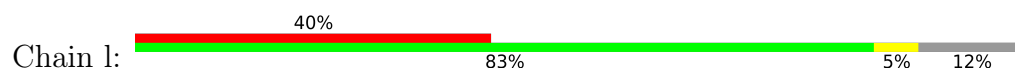
- Molecule 6 is PHOSPHOTHIPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



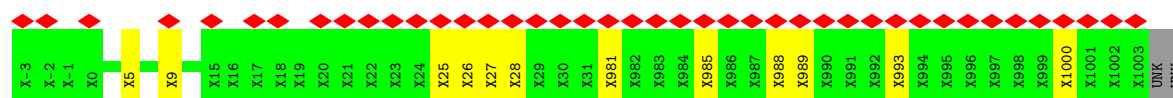
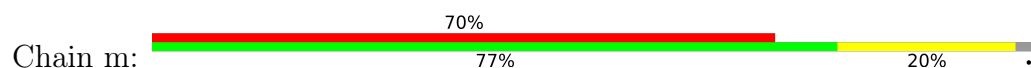
Mol	Chain	Residues	Atoms						AltConf
6	1	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
6	1	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
6	1	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
6	2	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
6	3	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
6	3	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
6	4	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
6	4	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
6	5	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
6	5	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
6	6	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
6	6	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	



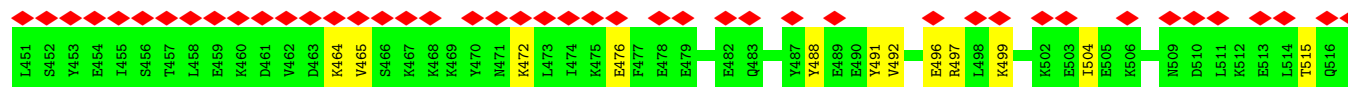
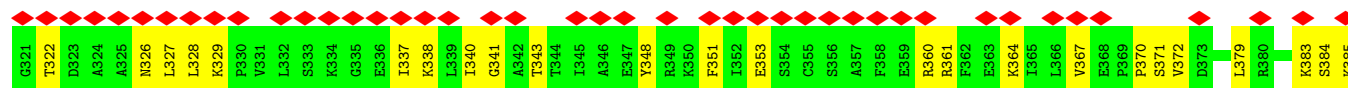
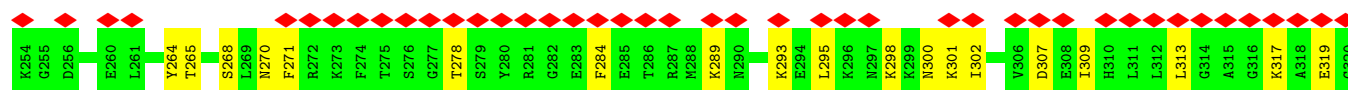
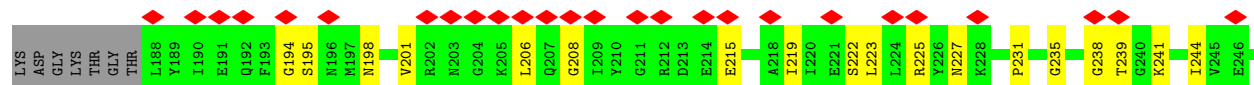
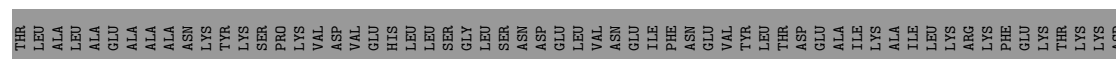
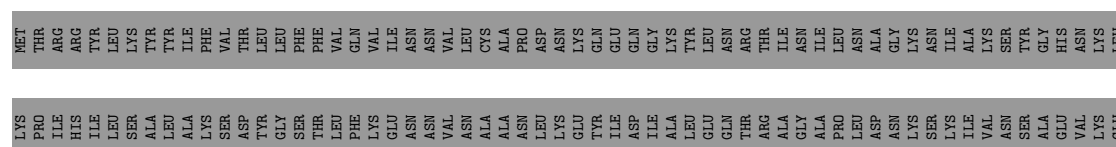
• Molecule 1: Unknown (Claw)

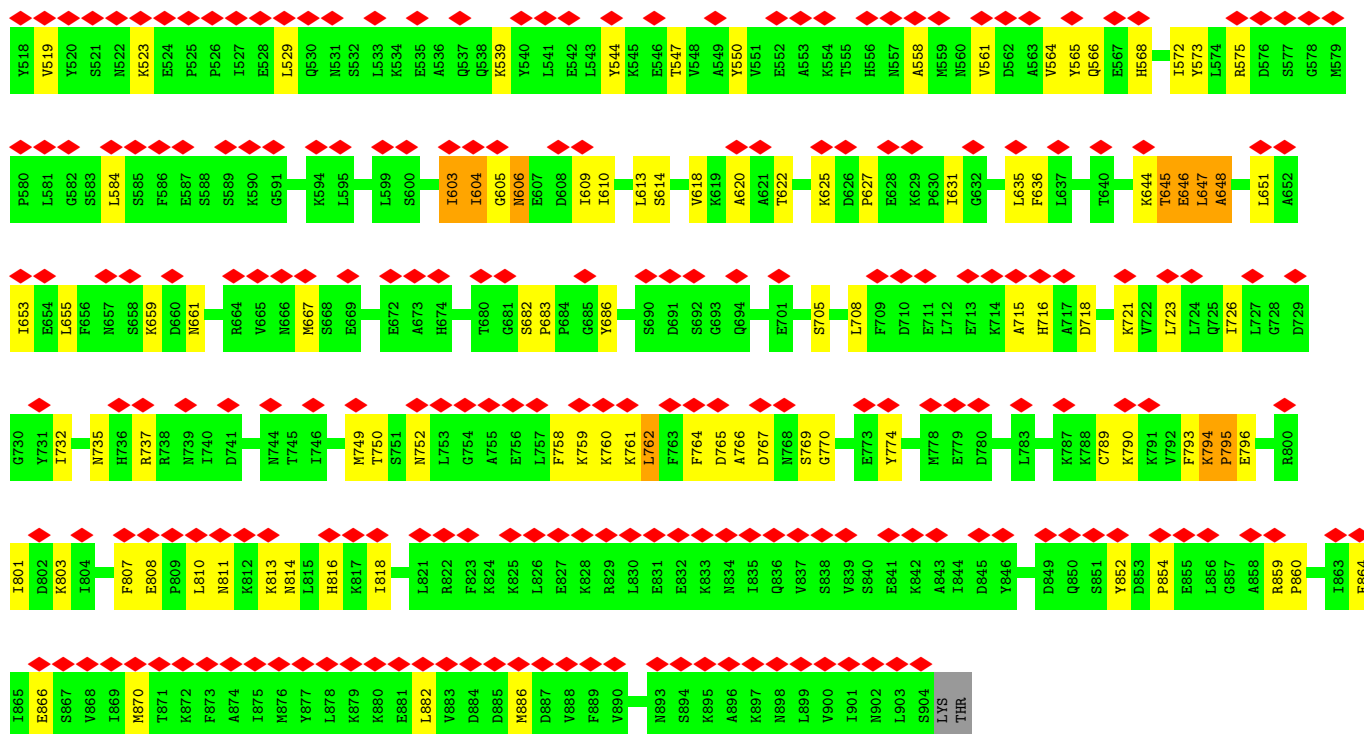


• Molecule 1: Unknown (Claw)

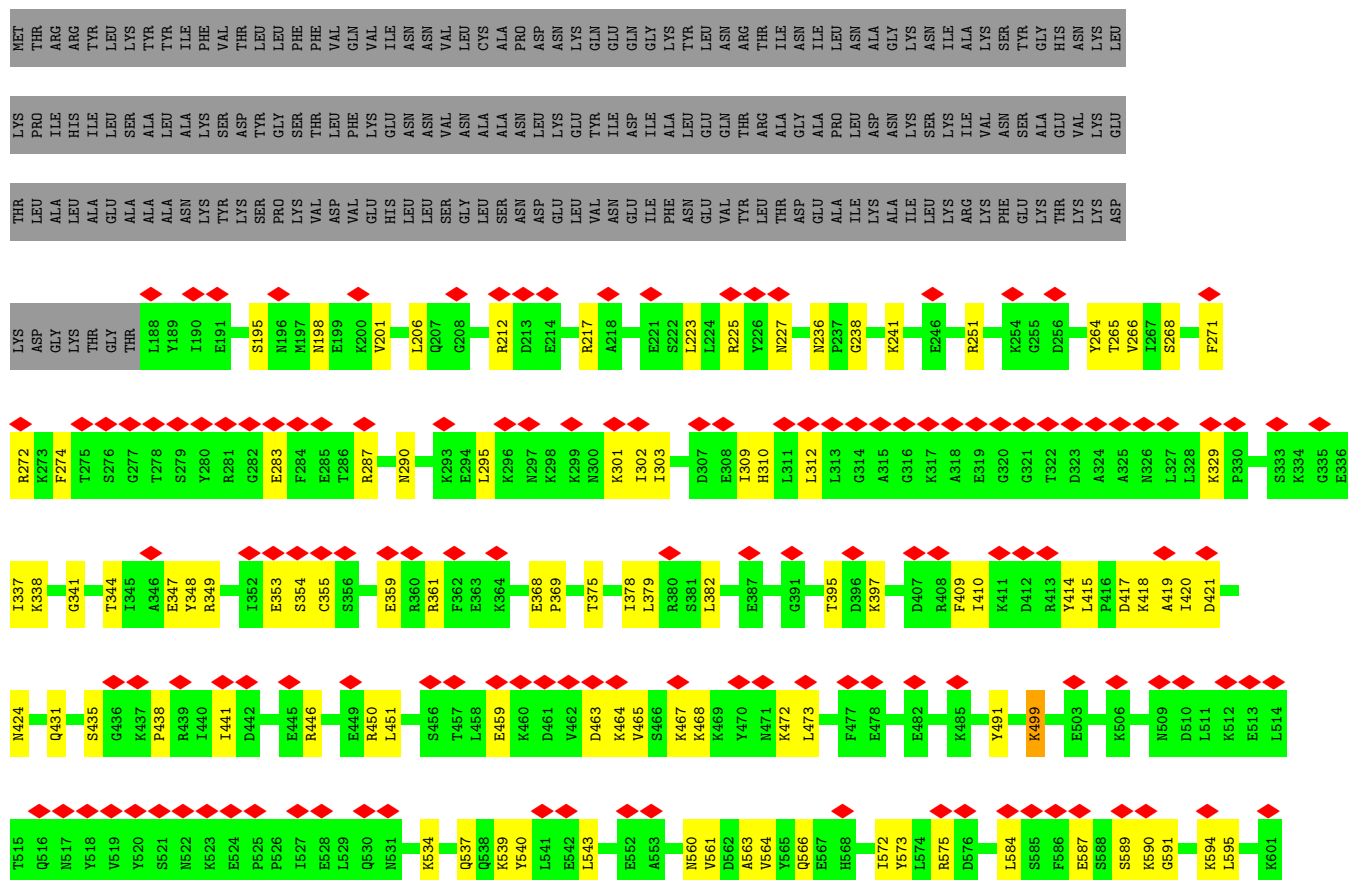


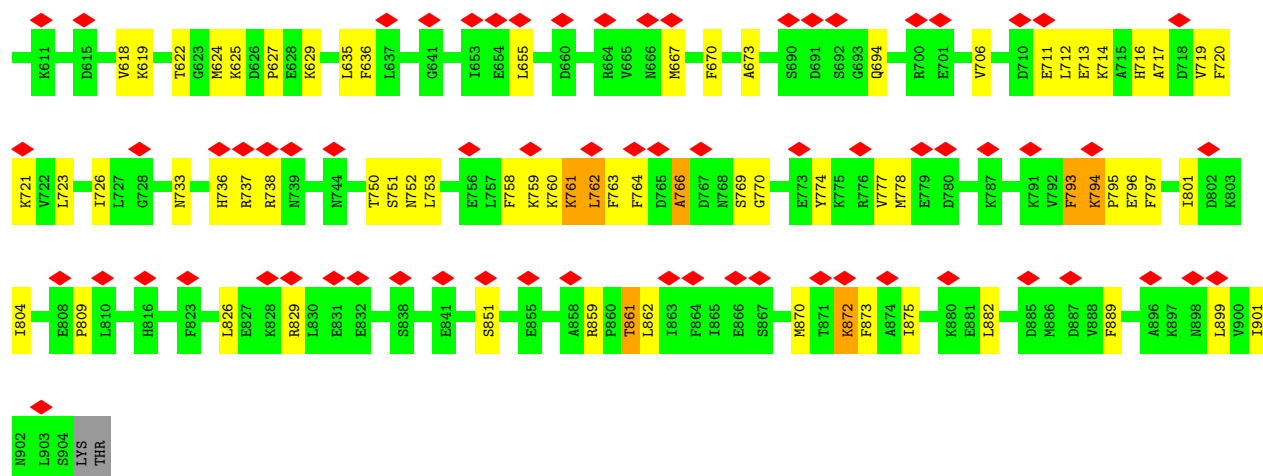
• Molecule 2: Heat shock protein 101



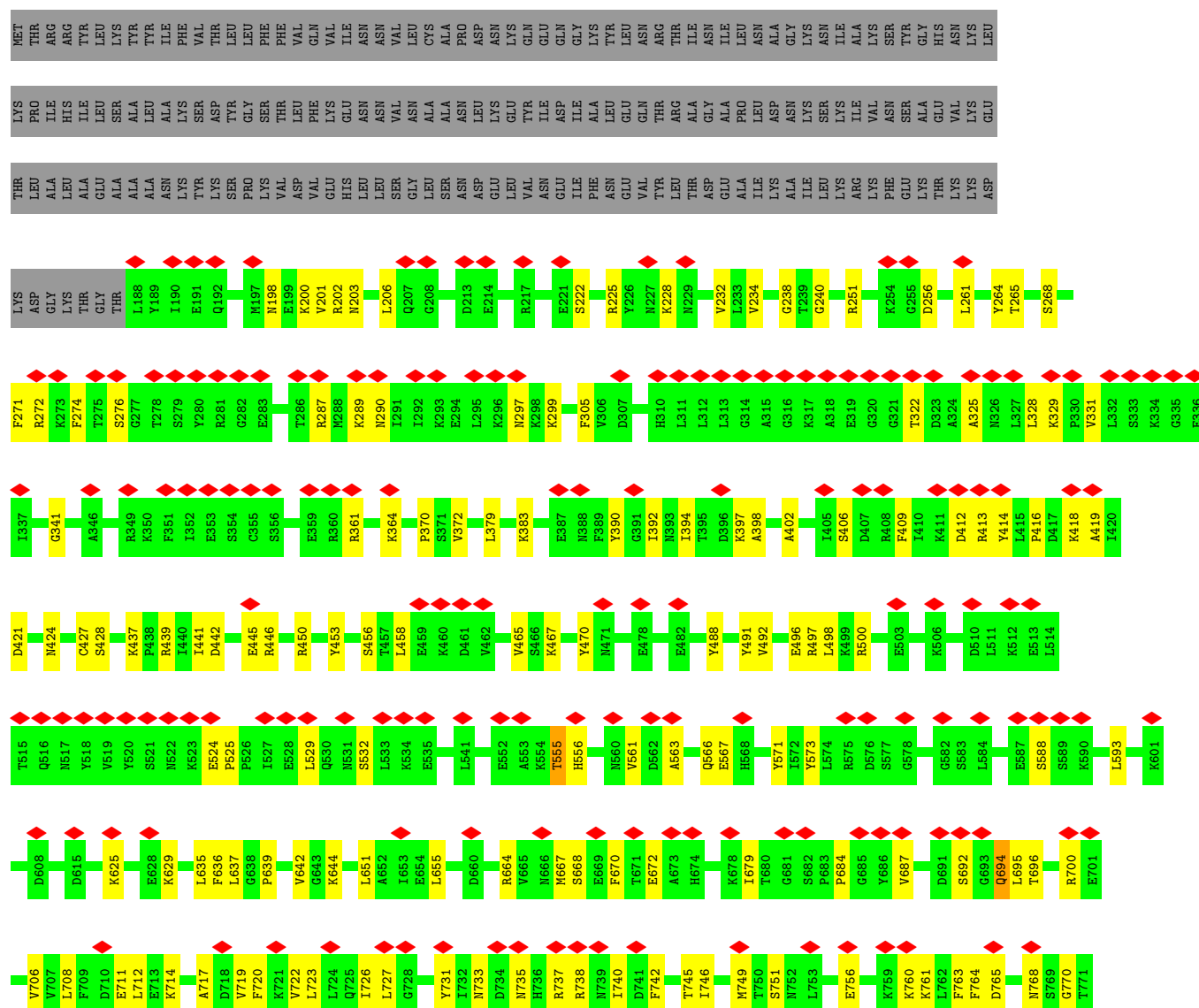


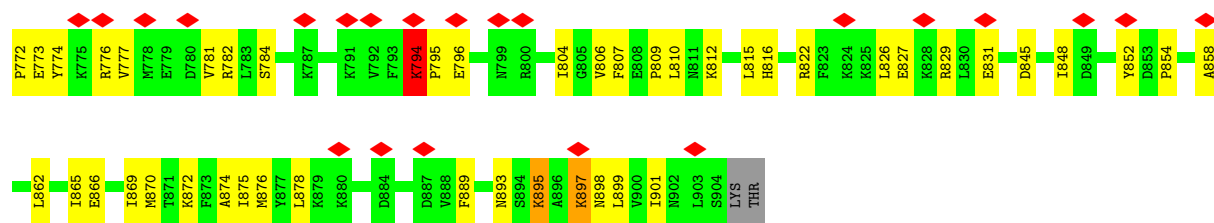
• Molecule 2: Heat shock protein 101



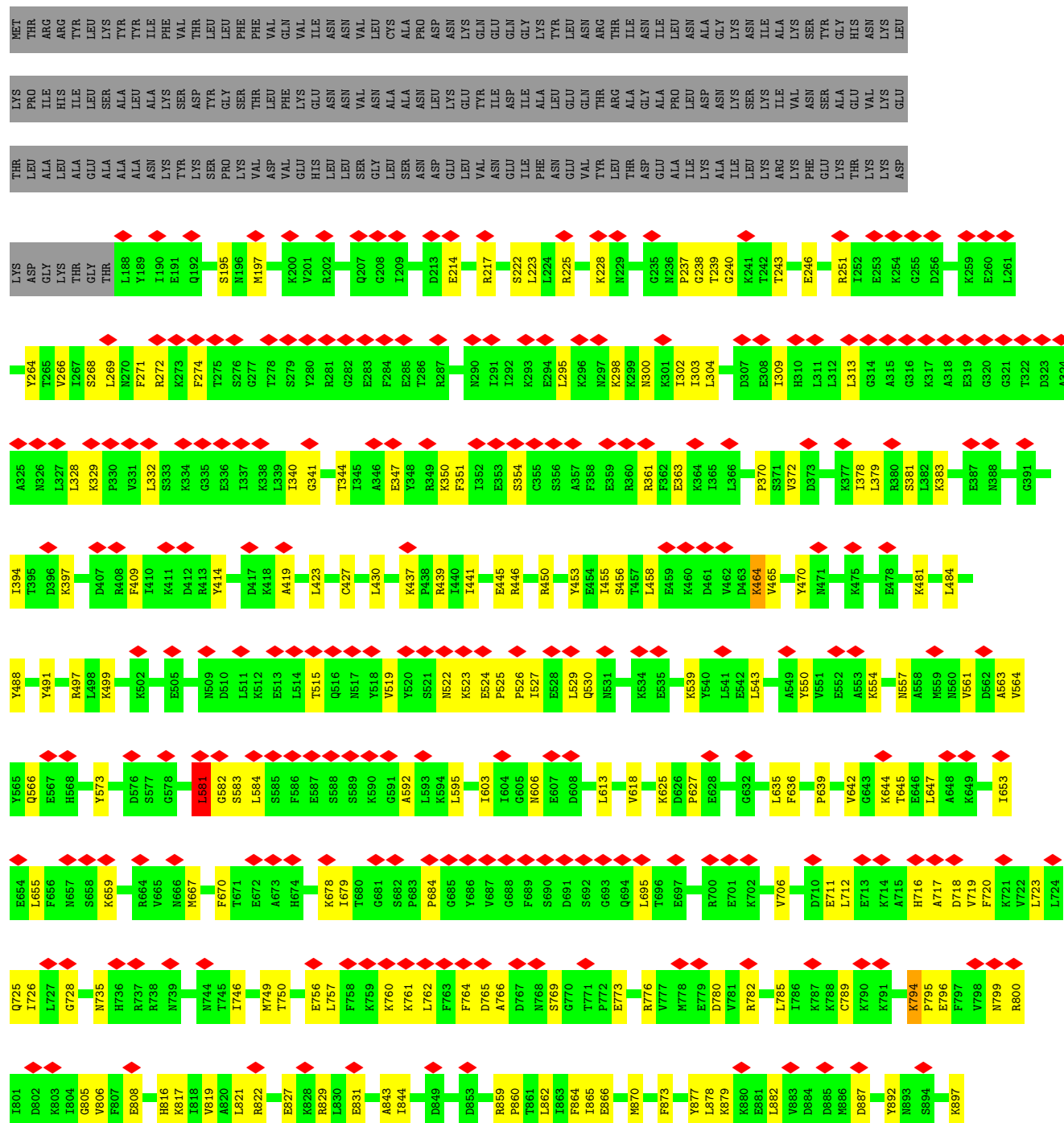


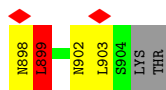
• Molecule 2: Heat shock protein 101



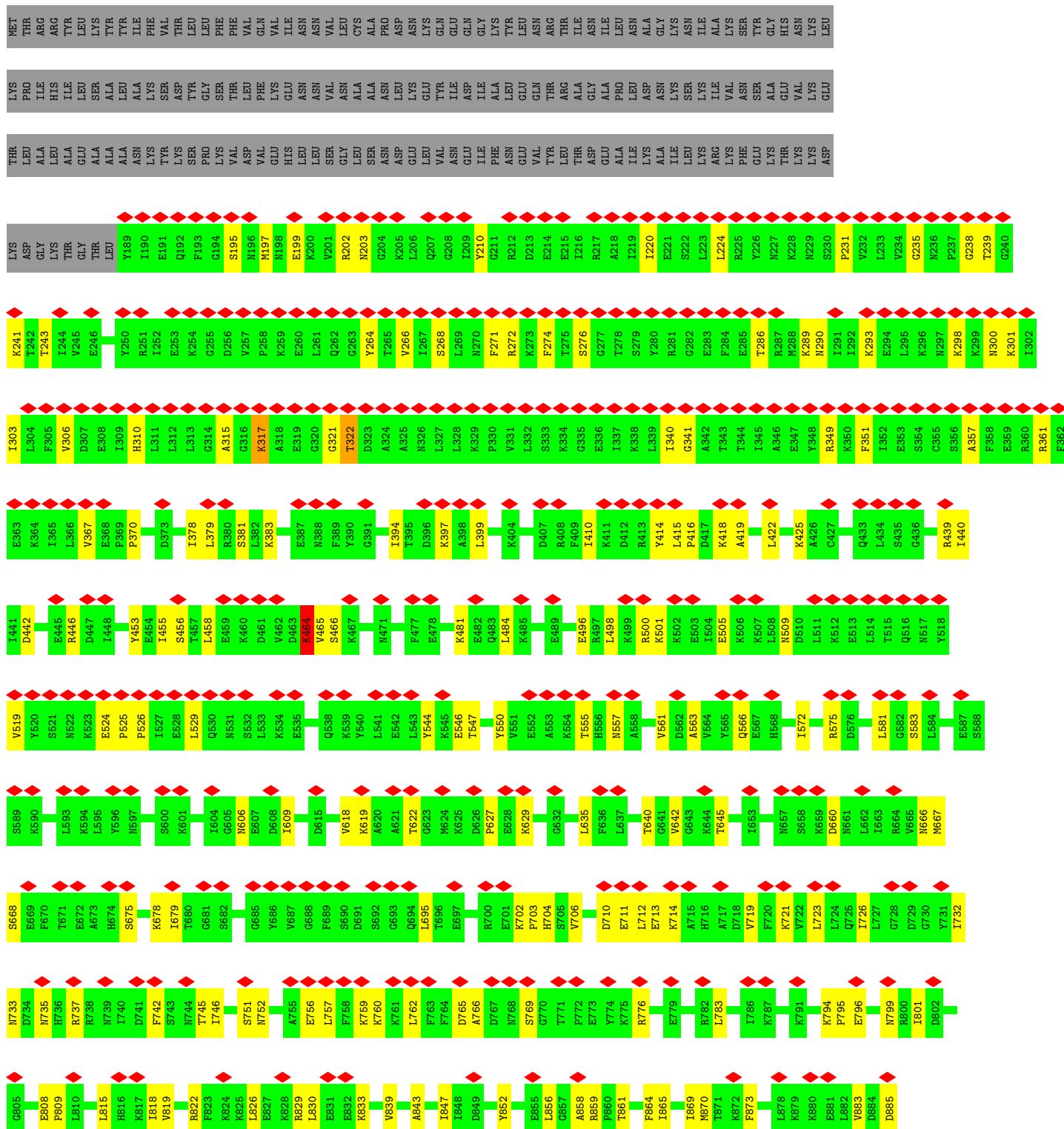
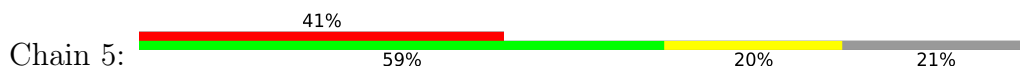


• Molecule 2: Heat shock protein 101



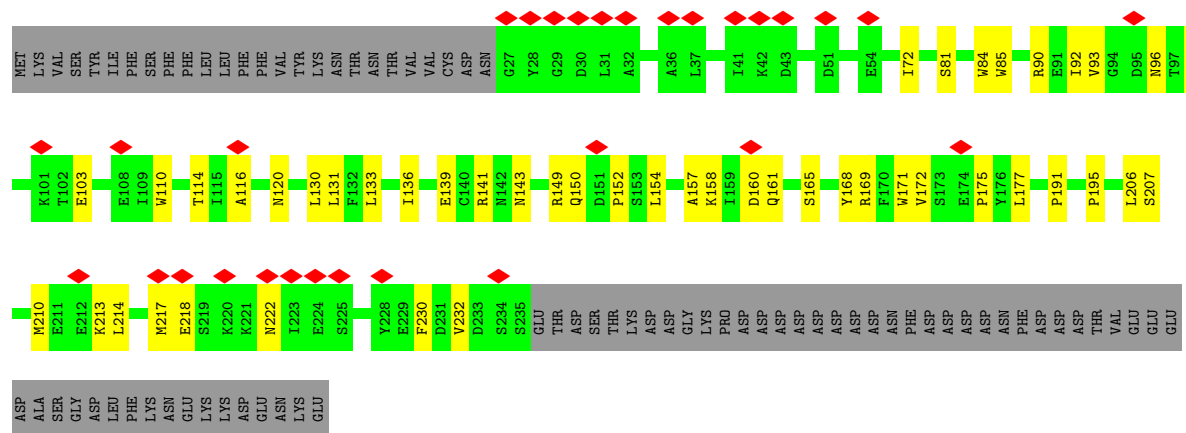


• Molecule 2: Heat shock protein 101

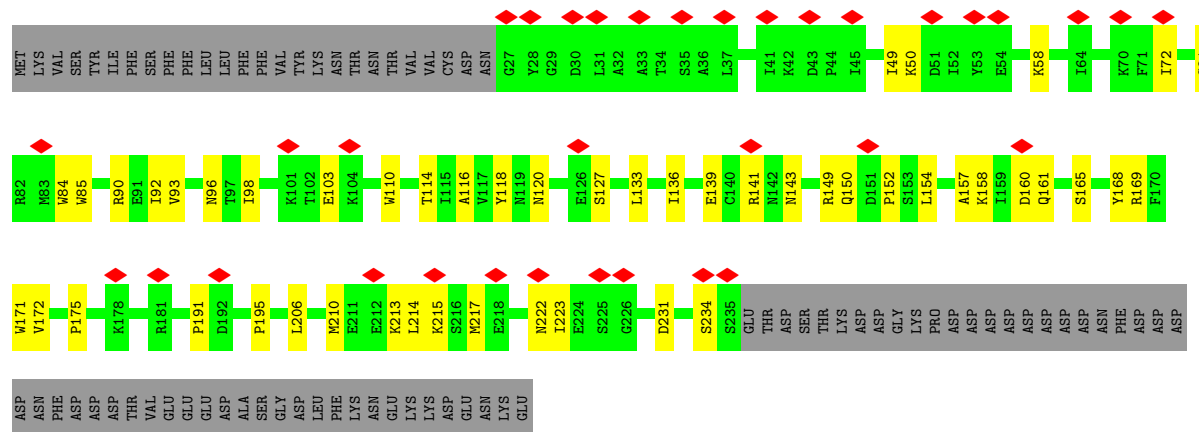




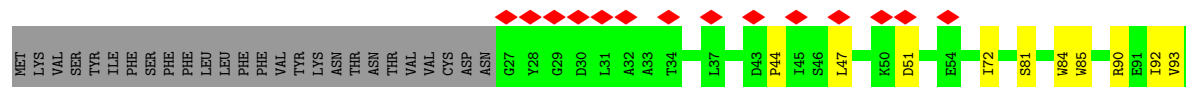
• Molecule 3: Exported protein 2



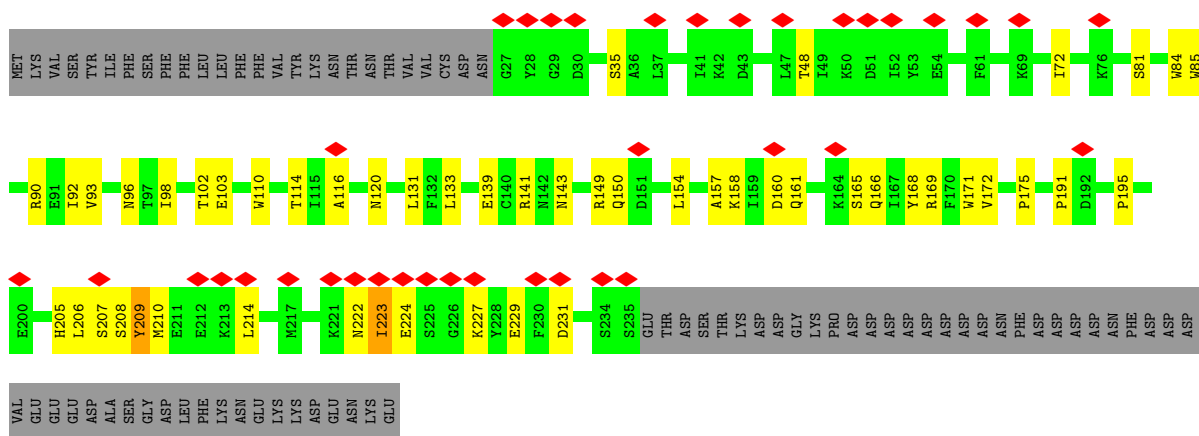
• Molecule 3: Exported protein 2



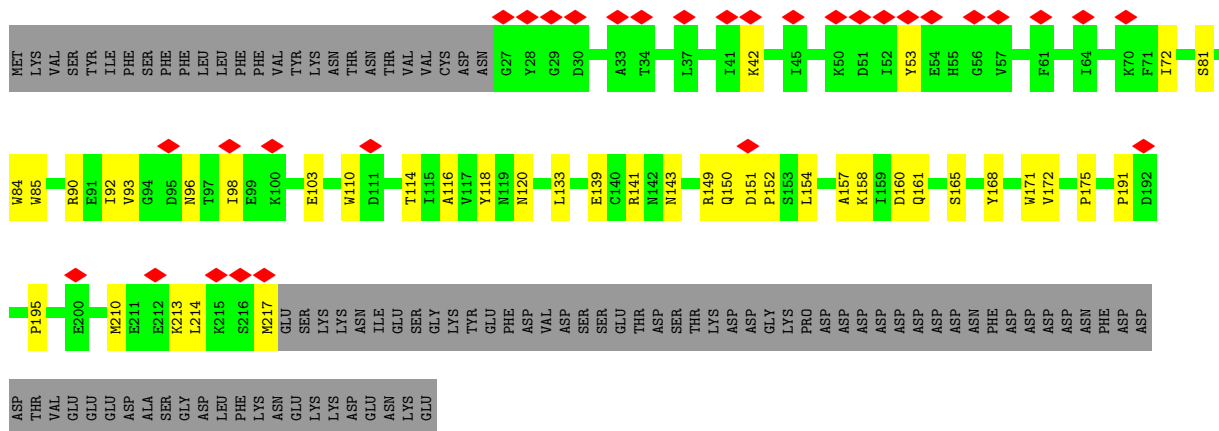
• Molecule 3: Exported protein 2



- Molecule 3: Exported protein 2

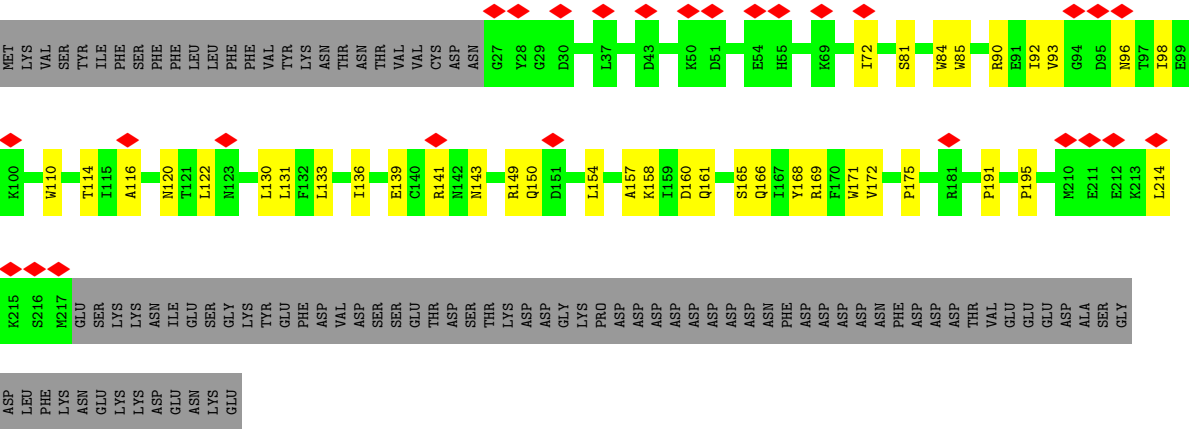


- Molecule 3: Exported protein 2

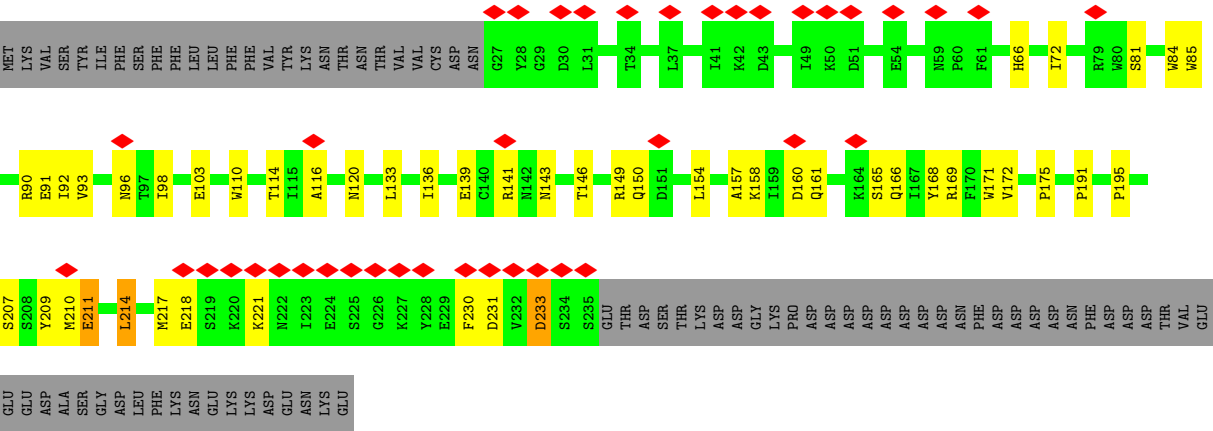


- Molecule 3: Exported protein 2

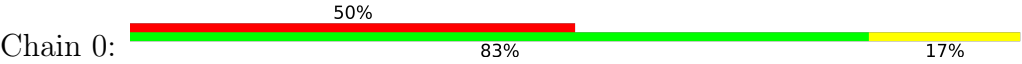




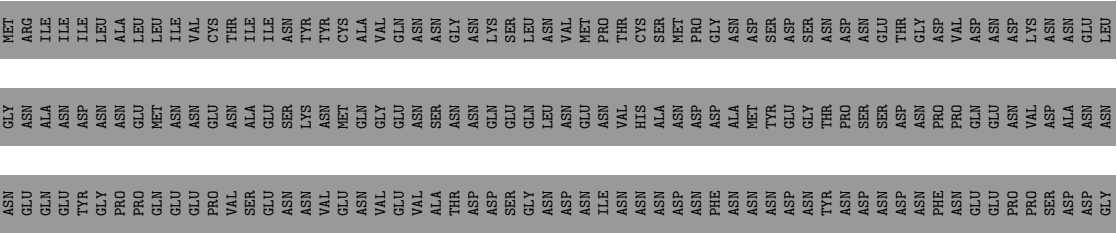
• Molecule 3: Exported protein 2



• Molecule 4: Endogenous cargo polypeptide

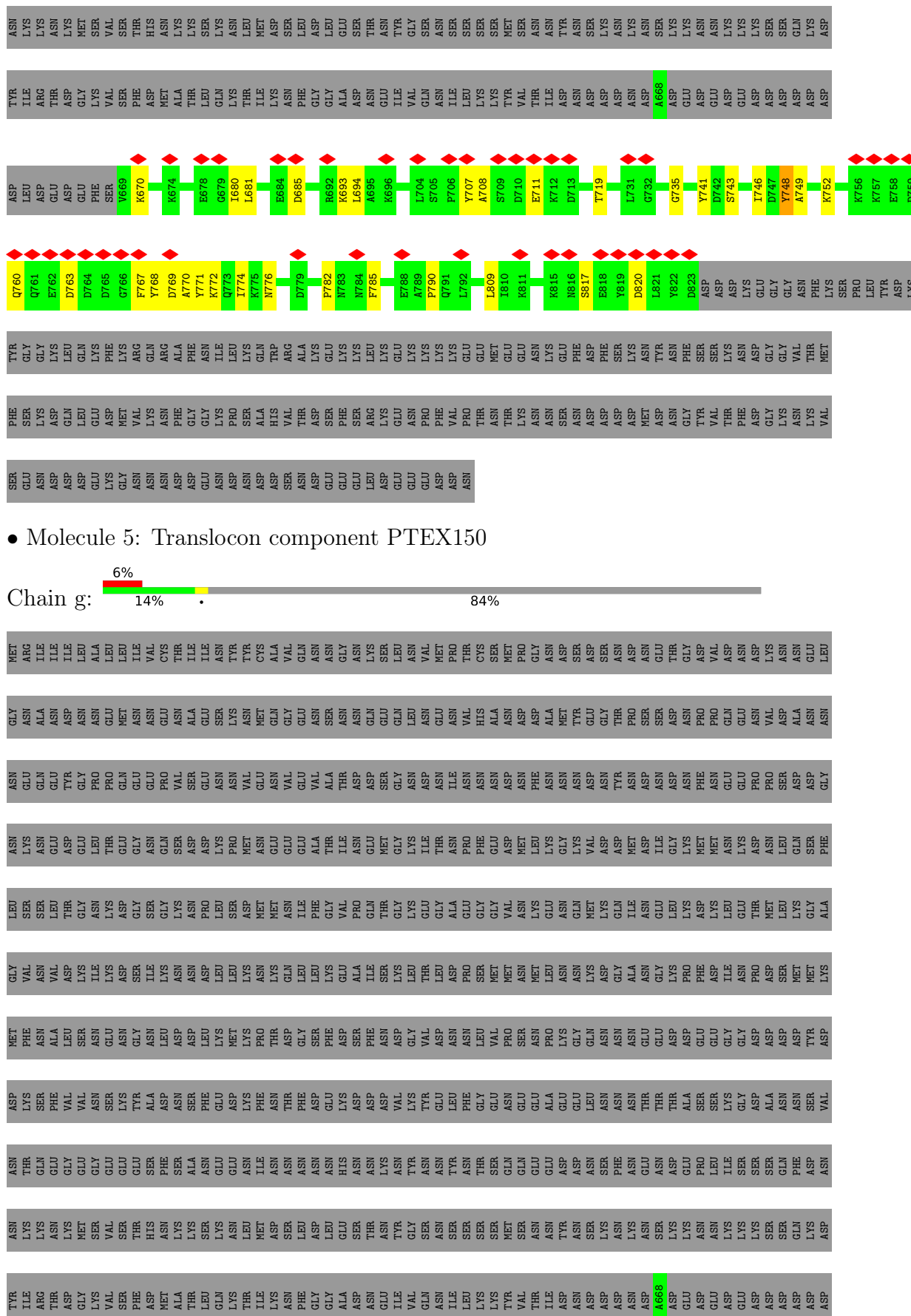


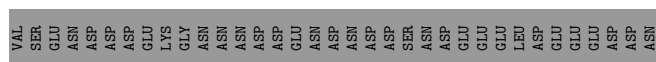
• Molecule 5: Translocon component PTEX150



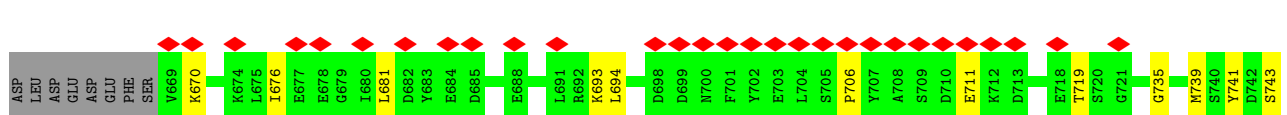
- Molecule 5: Translocon component PTEX150

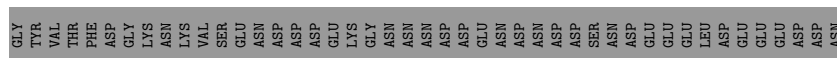
[illegible]



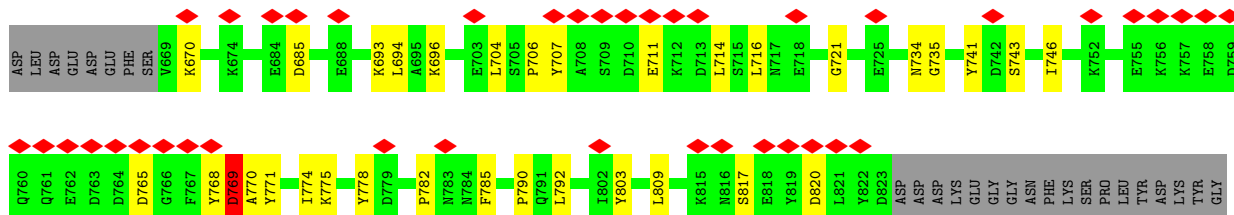
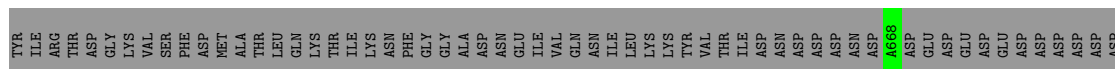


- Molecule 5: Translocon component PTEX150





Chain e: 12% 84%



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78499	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.131	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0405	Depositor
Map size (Å)	499.19998, 499.19998, 499.19998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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: AGS

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$
2	1	0.31	2/5843 (0.0%)	0.62	8/7848 (0.1%)
2	2	0.35	0/5843	0.66	2/7848 (0.0%)
2	3	0.37	0/5843	0.70	7/7848 (0.1%)
2	4	0.33	0/5843	0.63	5/7848 (0.1%)
2	5	0.31	1/5835 (0.0%)	0.62	3/7837 (0.0%)
2	6	0.27	0/5835	0.67	8/7837 (0.1%)
3	A	0.29	0/1607	0.69	0/2175
3	B	0.34	1/1753 (0.1%)	0.79	4/2369 (0.2%)
3	C	0.28	0/1753	0.70	1/2369 (0.0%)
3	D	0.29	0/1753	0.70	1/2369 (0.0%)
3	E	0.31	0/1762	0.74	2/2381 (0.1%)
3	F	0.31	0/1753	0.77	0/2369
3	G	0.28	0/1607	0.68	0/2175
5	a	0.24	0/1309	0.65	4/1760 (0.2%)
5	b	0.24	0/1309	0.66	3/1760 (0.2%)
5	c	0.24	0/1309	0.64	2/1760 (0.1%)
5	d	0.24	0/1309	0.62	2/1760 (0.1%)
5	e	0.24	0/1309	0.64	3/1760 (0.2%)
5	f	0.23	0/1309	0.63	2/1760 (0.1%)
5	g	0.24	0/1309	0.66	3/1760 (0.2%)
All	All	0.31	4/56193 (0.0%)	0.67	60/75593 (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	i	0	1
2	1	0	3
2	2	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	3	0	7
2	4	0	4
2	5	0	3
3	A	0	1
3	B	0	3
3	C	0	1
3	D	0	1
3	E	0	2
3	F	0	3
3	G	0	1
All	All	0	33

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	317	LYS	C-N	-6.50	1.24	1.33
3	B	209	TYR	CA-C	6.29	1.61	1.52
2	1	646	GLU	CA-C	6.11	1.60	1.52
2	1	647	LEU	CA-C	5.45	1.60	1.52

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6	763	PHE	N-CA-C	11.43	123.74	111.28
2	6	486	LYS	N-CA-C	10.92	122.94	111.14
3	B	208	SER	N-CA-C	-9.37	101.27	112.89
2	1	648	ALA	N-CA-C	9.07	122.31	111.33
3	C	218	GLU	N-CA-C	8.77	120.92	111.36

There are no chirality outliers.

5 of 33 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	464	LYS	Peptide
2	1	758	PHE	Peptide
2	1	794	LYS	Peptide
2	2	793	PHE	Peptide
1	i	22	UNK	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	h	235	0	53	17	0
1	i	230	0	50	4	0
1	j	275	0	63	14	0
1	k	300	0	67	34	0
1	l	265	0	57	7	0
1	m	290	0	62	15	0
1	n	180	0	38	0	0
2	1	5752	0	5955	150	0
2	2	5752	0	5956	142	0
2	3	5752	0	5957	160	0
2	4	5752	0	5957	172	0
2	5	5744	0	5945	143	0
2	6	5744	0	5946	106	0
3	A	1571	0	1635	36	0
3	B	1715	0	1767	51	0
3	C	1715	0	1767	50	0
3	D	1715	0	1767	51	0
3	E	1724	0	1773	51	0
3	F	1715	0	1767	46	0
3	G	1571	0	1635	35	0
4	0	30	0	9	1	0
5	a	1286	0	1212	41	0
5	b	1286	0	1212	44	0
5	c	1286	0	1212	35	0
5	d	1286	0	1212	52	0
5	e	1286	0	1212	48	0
5	f	1286	0	1212	33	0
5	g	1286	0	1212	19	0
6	1	93	0	36	16	0
6	2	31	0	12	1	0
6	3	62	0	24	2	0
6	4	62	0	24	8	0
6	5	62	0	24	7	0
6	6	62	0	24	4	0
All	All	57401	0	56854	1190	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 1190 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:214:LEU:CD2	5:f:768:TYR:CD1	2.10	1.34
1:k:1001:UNK:HA	2:4:499:LYS:NZ	1.38	1.33
3:F:161:GLN:NE2	5:e:770:ALA:HB3	1.39	1.33
1:k:1001:UNK:CA	2:4:499:LYS:HZ1	1.48	1.25
3:G:214:LEU:CD2	5:f:768:TYR:HD1	1.47	1.25

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	715/906 (79%)	650 (91%)	61 (8%)	4 (1%)	21	58
2	2	715/906 (79%)	644 (90%)	69 (10%)	2 (0%)	36	71
2	3	715/906 (79%)	640 (90%)	71 (10%)	4 (1%)	21	58
2	4	715/906 (79%)	635 (89%)	75 (10%)	5 (1%)	18	55
2	5	714/906 (79%)	648 (91%)	63 (9%)	3 (0%)	30	66
2	6	714/906 (79%)	639 (90%)	71 (10%)	4 (1%)	21	58
3	A	189/287 (66%)	184 (97%)	5 (3%)	0	100	100
3	B	207/287 (72%)	200 (97%)	7 (3%)	0	100	100
3	C	207/287 (72%)	199 (96%)	8 (4%)	0	100	100
3	D	207/287 (72%)	201 (97%)	6 (3%)	0	100	100
3	E	208/287 (72%)	200 (96%)	8 (4%)	0	100	100
3	F	207/287 (72%)	196 (95%)	11 (5%)	0	100	100
3	G	189/287 (66%)	183 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	a	153/993 (15%)	143 (94%)	10 (6%)	0	100	100
5	b	153/993 (15%)	143 (94%)	10 (6%)	0	100	100
5	c	153/993 (15%)	141 (92%)	12 (8%)	0	100	100
5	d	153/993 (15%)	143 (94%)	10 (6%)	0	100	100
5	e	153/993 (15%)	143 (94%)	10 (6%)	0	100	100
5	f	153/993 (15%)	143 (94%)	10 (6%)	0	100	100
5	g	153/993 (15%)	142 (93%)	11 (7%)	0	100	100
All	All	6773/14396 (47%)	6217 (92%)	534 (8%)	22 (0%)	37	71

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	5	465	VAL
2	6	465	VAL
2	1	606	ASN
2	4	465	VAL
2	1	465	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1	641/804 (80%)	638 (100%)	3 (0%)	81	81
2	2	641/804 (80%)	637 (99%)	4 (1%)	78	80
2	3	641/804 (80%)	641 (100%)	0	100	100
2	4	641/804 (80%)	640 (100%)	1 (0%)	87	85
2	5	640/804 (80%)	638 (100%)	2 (0%)	86	84
2	6	640/804 (80%)	633 (99%)	7 (1%)	65	73
3	A	176/268 (66%)	175 (99%)	1 (1%)	78	80
3	B	193/268 (72%)	192 (100%)	1 (0%)	81	81
3	C	193/268 (72%)	192 (100%)	1 (0%)	81	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	193/268 (72%)	192 (100%)	1 (0%)	81	81
3	E	194/268 (72%)	193 (100%)	1 (0%)	81	81
3	F	193/268 (72%)	189 (98%)	4 (2%)	47	65
3	G	176/268 (66%)	175 (99%)	1 (1%)	78	80
5	a	143/906 (16%)	143 (100%)	0	100	100
5	b	143/906 (16%)	143 (100%)	0	100	100
5	c	143/906 (16%)	141 (99%)	2 (1%)	59	71
5	d	143/906 (16%)	143 (100%)	0	100	100
5	e	143/906 (16%)	142 (99%)	1 (1%)	76	78
5	f	143/906 (16%)	143 (100%)	0	100	100
5	g	143/906 (16%)	143 (100%)	0	100	100
All	All	6163/13042 (47%)	6133 (100%)	30 (0%)	78	81

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	6	493	ILE
3	F	214	LEU
2	6	761	LYS
5	e	769	ASP
3	G	72	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
5	c	724	ASN
5	b	776	ASN
3	G	161	GLN
2	3	566	GLN
2	3	326	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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$
6	AGS	6	1002	-	32,33,33	0.88	3 (9%)	45,52,52	1.01	2 (4%)
6	AGS	6	1001	-	32,33,33	0.81	2 (6%)	45,52,52	1.00	2 (4%)
6	AGS	3	1002	-	32,33,33	0.89	3 (9%)	45,52,52	1.06	2 (4%)
6	AGS	1	1001	-	32,33,33	1.25	2 (6%)	45,52,52	1.05	2 (4%)
6	AGS	2	1001	-	32,33,33	0.89	3 (9%)	45,52,52	1.06	2 (4%)
6	AGS	5	1001	-	32,33,33	1.10	3 (9%)	45,52,52	0.98	2 (4%)
6	AGS	1	1002	-	32,33,33	1.26	2 (6%)	45,52,52	1.05	2 (4%)
6	AGS	5	1002	-	32,33,33	0.77	3 (9%)	45,52,52	1.04	3 (6%)
6	AGS	4	1002	-	32,33,33	0.89	3 (9%)	45,52,52	1.06	2 (4%)
6	AGS	4	1001	-	32,33,33	1.27	2 (6%)	45,52,52	1.05	2 (4%)
6	AGS	3	1001	-	32,33,33	1.27	2 (6%)	45,52,52	1.05	2 (4%)
6	AGS	1	1003	-	32,33,33	2.04	6 (18%)	45,52,52	1.89	10 (22%)

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
6	AGS	6	1002	-	-	7/21/38/38	0/3/3/3
6	AGS	6	1001	-	-	3/21/38/38	0/3/3/3
6	AGS	3	1002	-	-	2/21/38/38	0/3/3/3
6	AGS	1	1001	-	-	2/21/38/38	0/3/3/3
6	AGS	2	1001	-	-	2/21/38/38	0/3/3/3
6	AGS	5	1001	-	-	3/21/38/38	0/3/3/3
6	AGS	1	1002	-	-	2/21/38/38	0/3/3/3
6	AGS	5	1002	-	-	7/21/38/38	0/3/3/3
6	AGS	4	1002	-	-	2/21/38/38	0/3/3/3
6	AGS	4	1001	-	-	2/21/38/38	0/3/3/3
6	AGS	3	1001	-	-	2/21/38/38	0/3/3/3
6	AGS	1	1003	-	-	7/21/38/38	0/3/3/3

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1	1003	AGS	PG-S1G	7.97	2.08	1.90
6	4	1001	AGS	PA-O3A	-4.87	1.54	1.59
6	3	1001	AGS	PA-O3A	-4.80	1.54	1.59
6	1	1002	AGS	PA-O3A	-4.79	1.54	1.59
6	1	1001	AGS	PA-O3A	-4.74	1.54	1.59

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1	1003	AGS	C5-C4-N3	-5.89	118.61	126.72
6	4	1001	AGS	PB-O3B-PG	-5.74	112.18	133.17
6	1	1002	AGS	PB-O3B-PG	-5.73	112.19	133.17
6	1	1001	AGS	PB-O3B-PG	-5.73	112.20	133.17
6	3	1001	AGS	PB-O3B-PG	-5.73	112.21	133.17

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

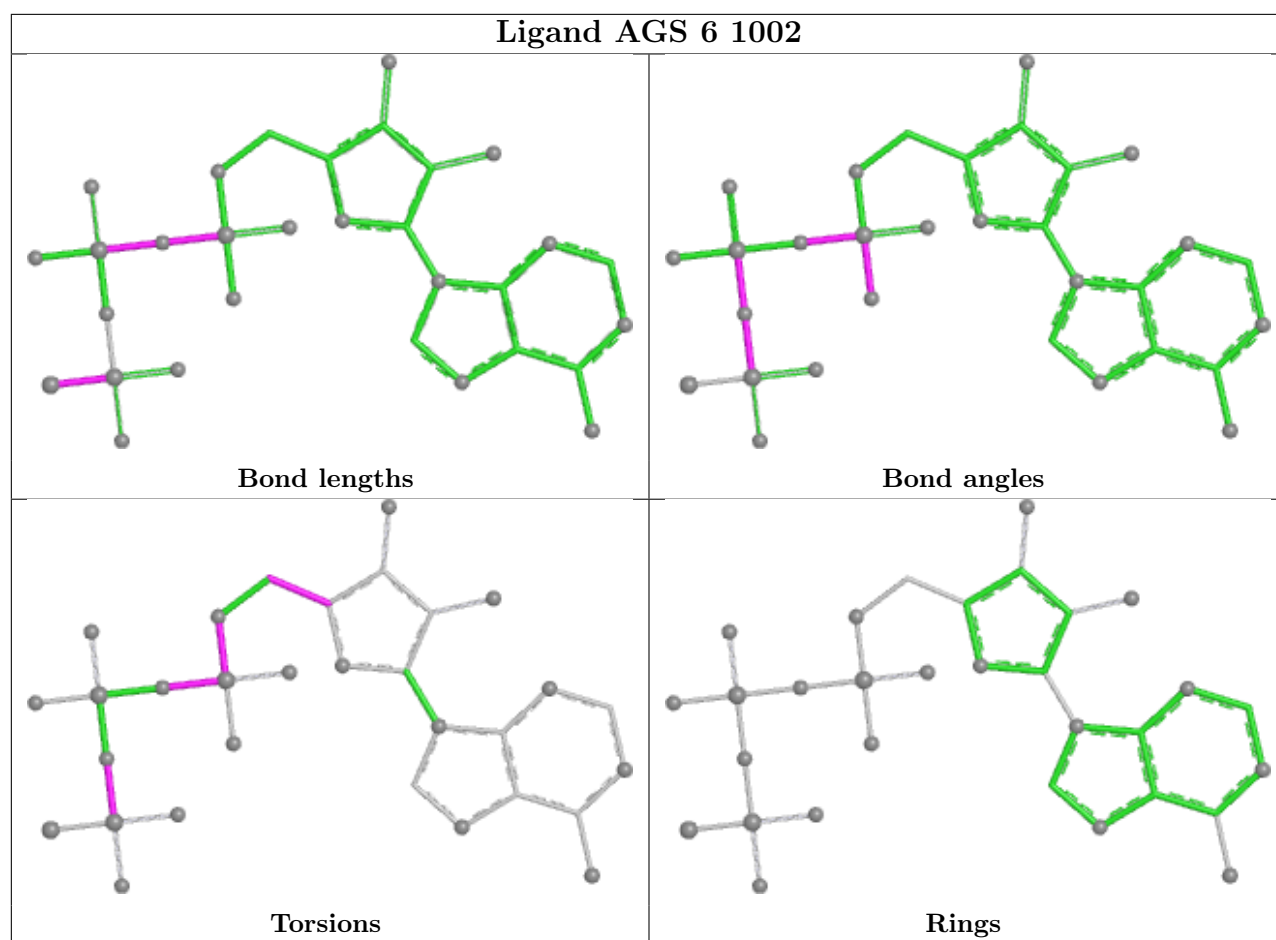
Mol	Chain	Res	Type	Atoms
6	6	1002	AGS	PB-O3B-PG-O2G
6	6	1002	AGS	C5'-O5'-PA-O1A
6	6	1002	AGS	C5'-O5'-PA-O2A
6	6	1002	AGS	C5'-O5'-PA-O3A
6	6	1002	AGS	C3'-C4'-C5'-O5'

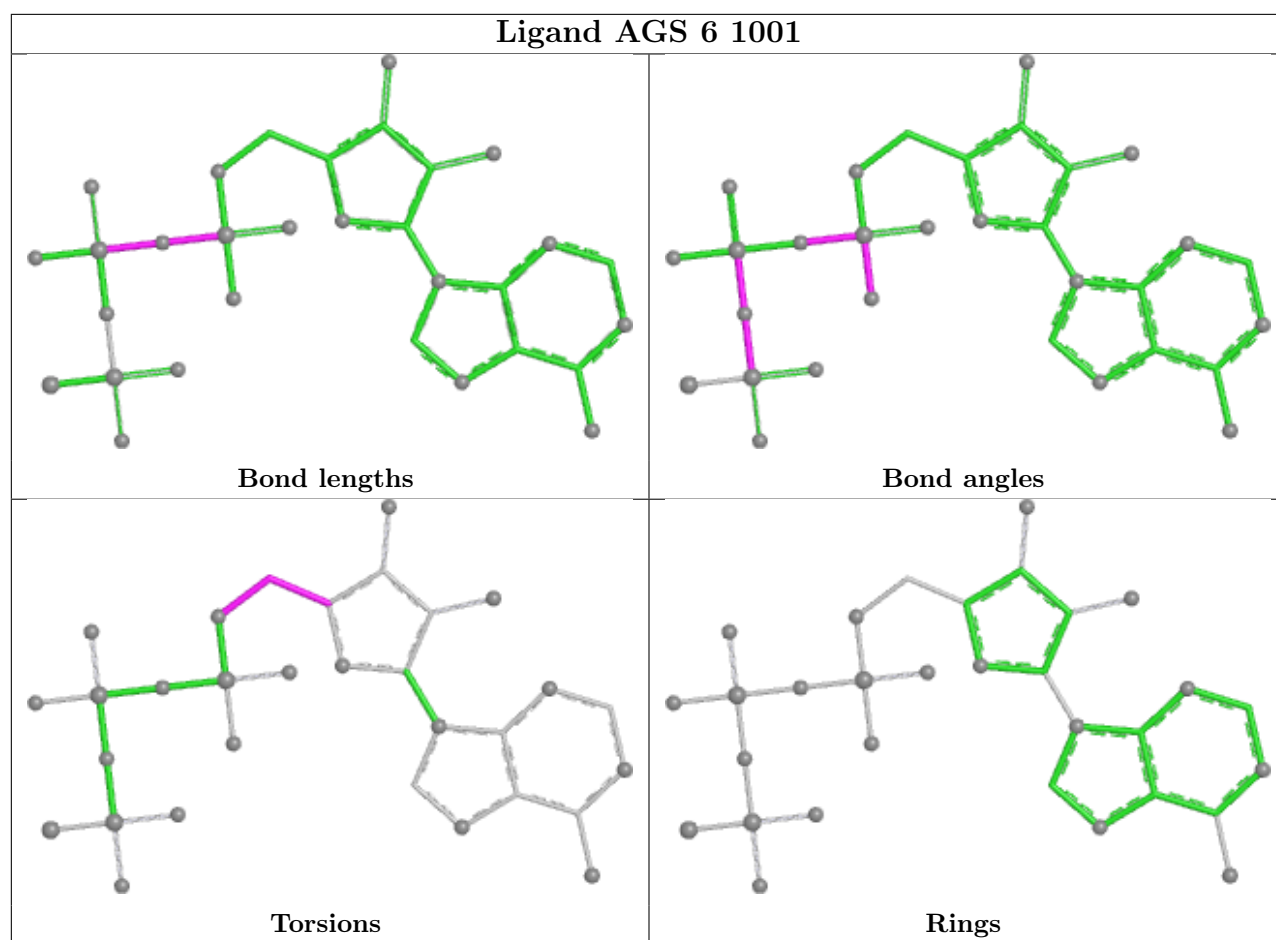
There are no ring outliers.

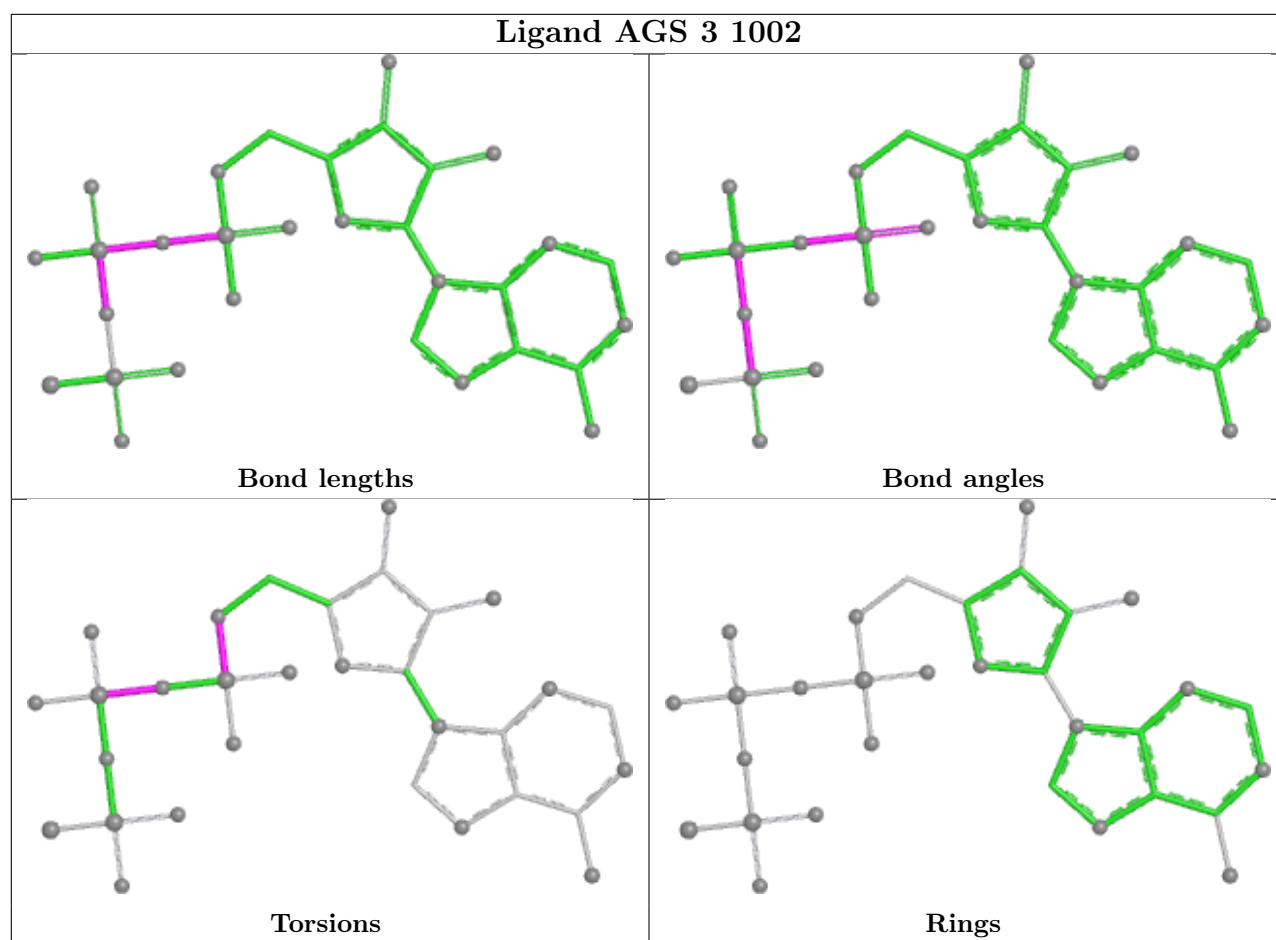
10 monomers are involved in 38 short contacts:

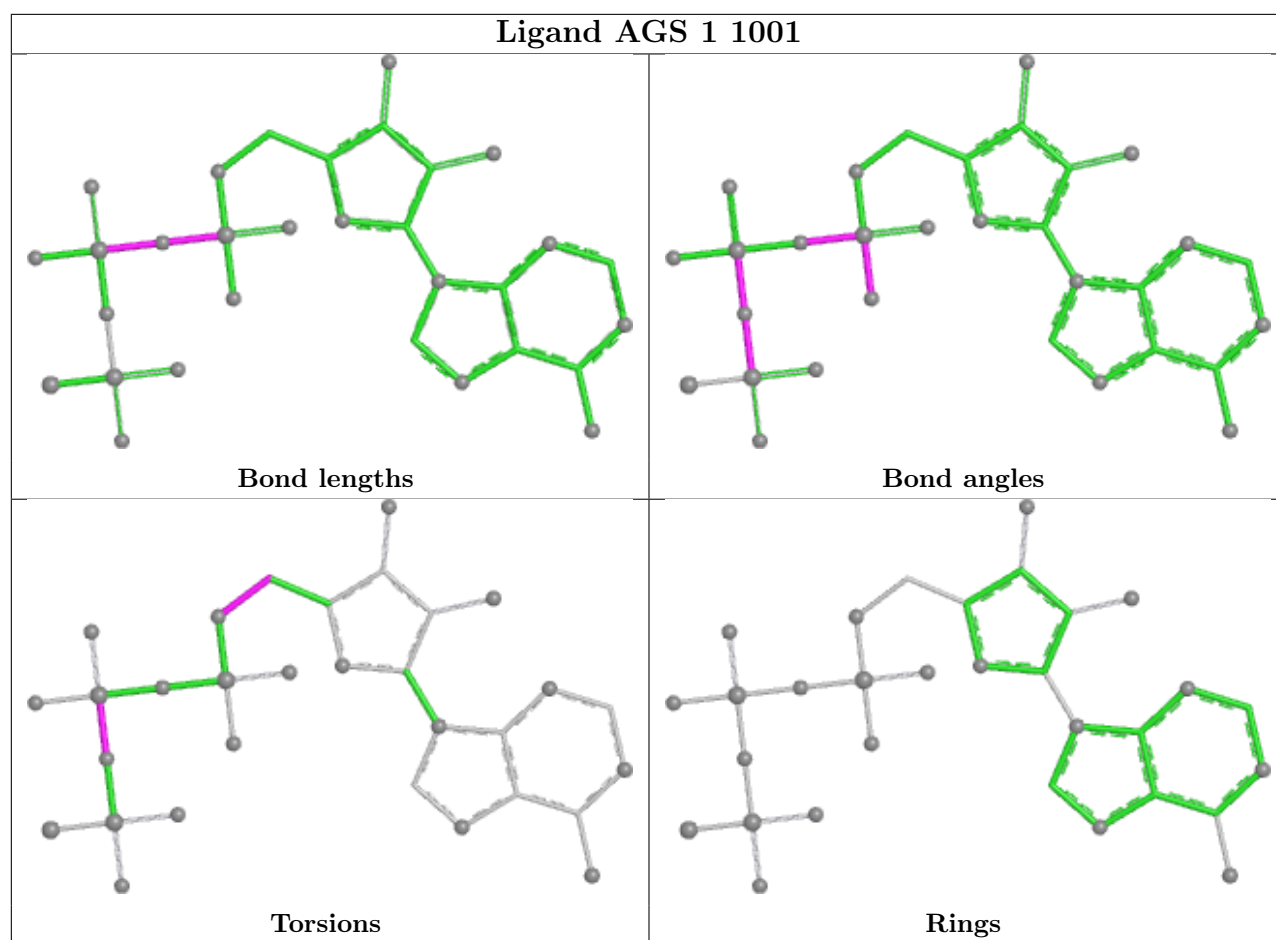
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	6	1002	AGS	3	0
6	6	1001	AGS	1	0
6	3	1002	AGS	2	0
6	1	1001	AGS	2	0
6	2	1001	AGS	1	0
6	5	1001	AGS	5	0
6	5	1002	AGS	2	0
6	4	1002	AGS	6	0
6	4	1001	AGS	2	0
6	1	1003	AGS	14	0

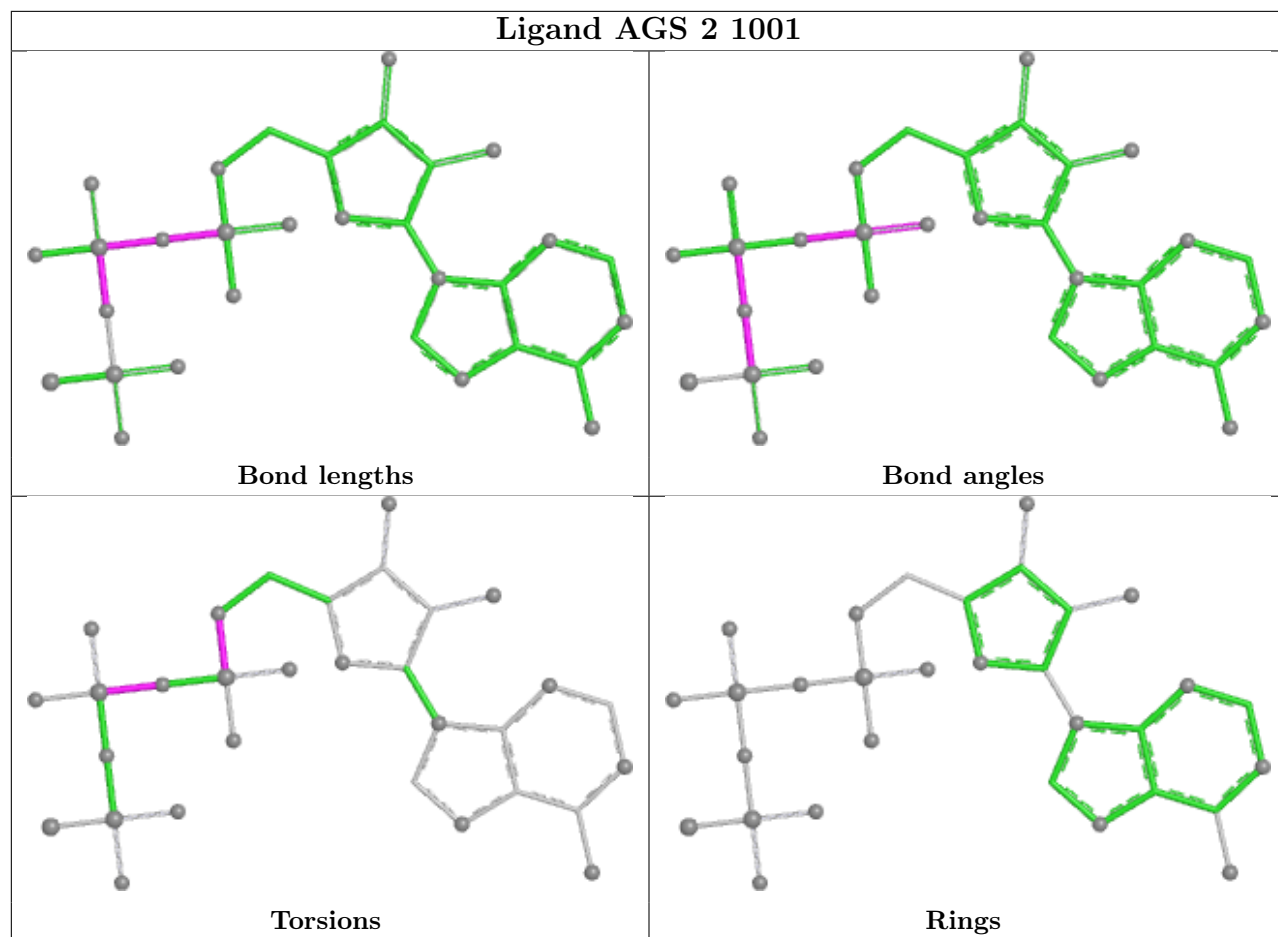
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

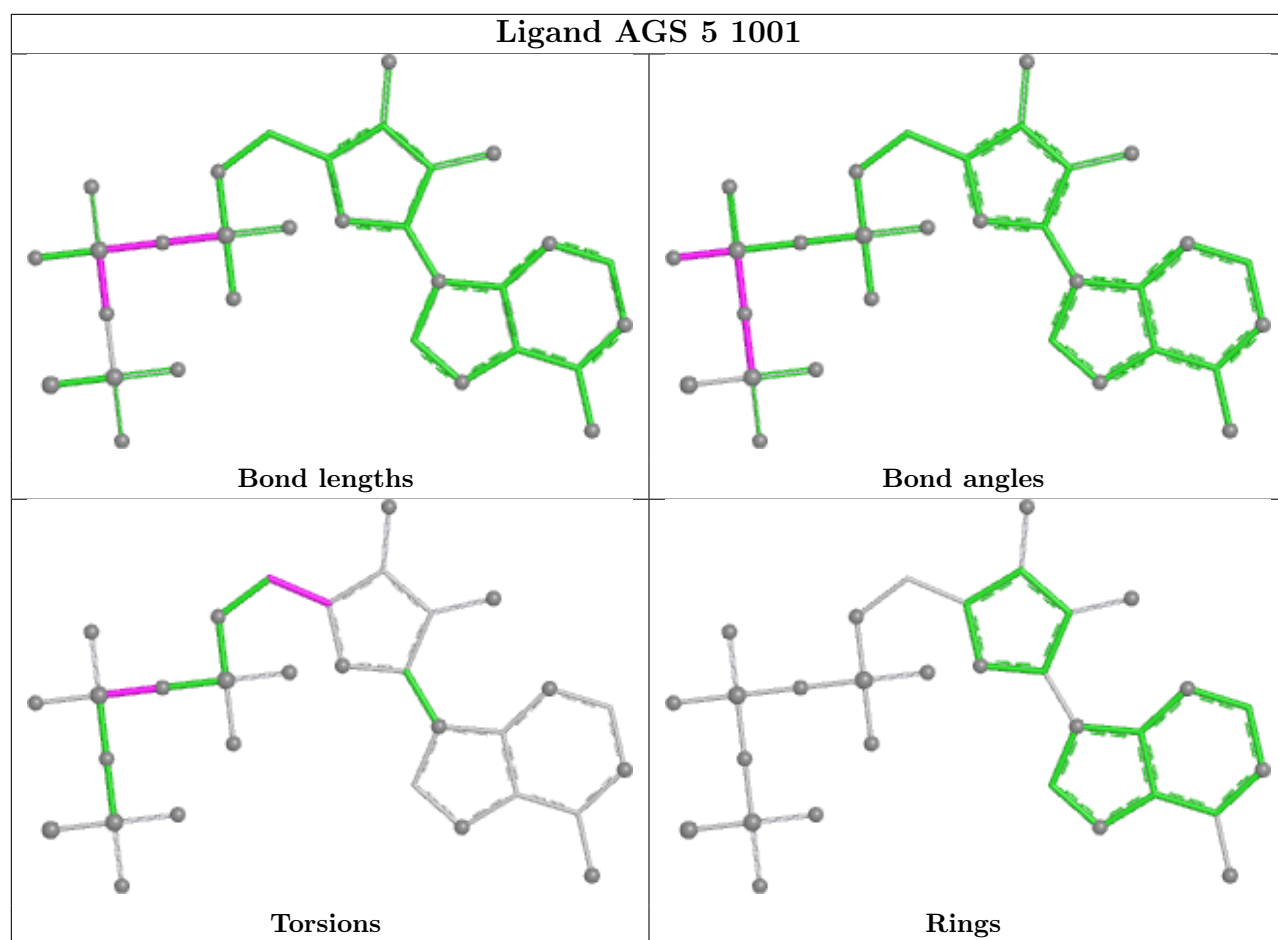


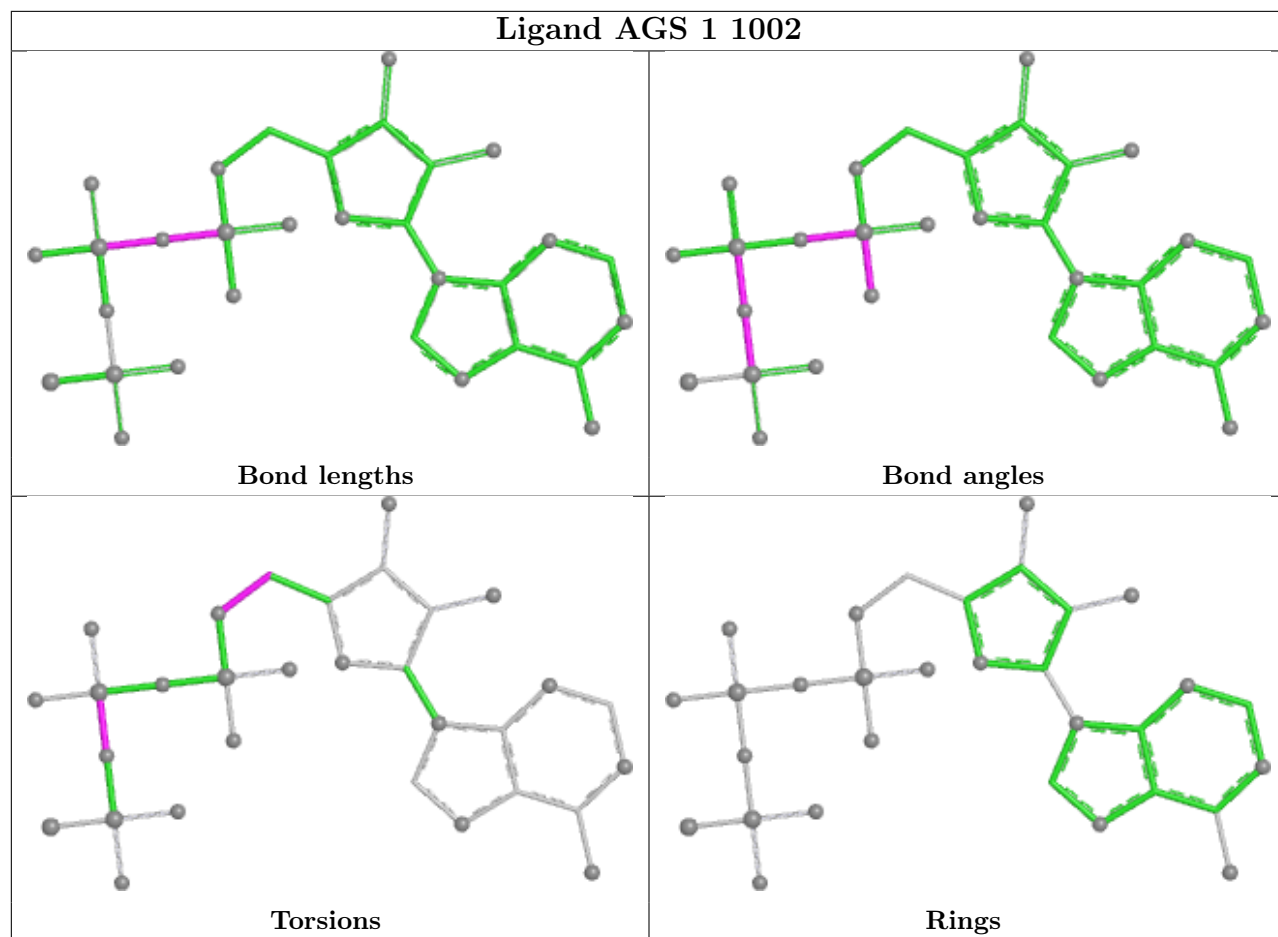


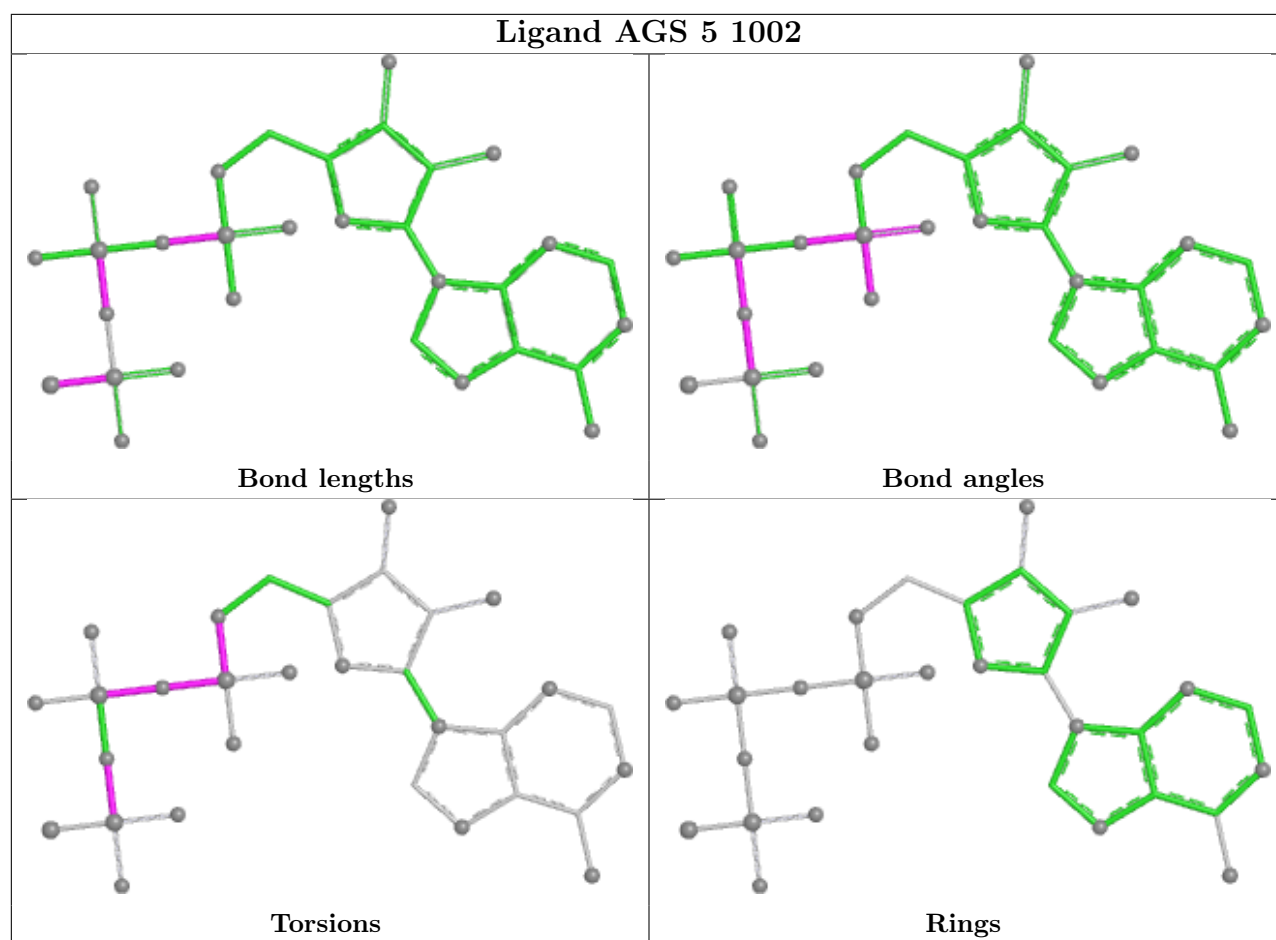


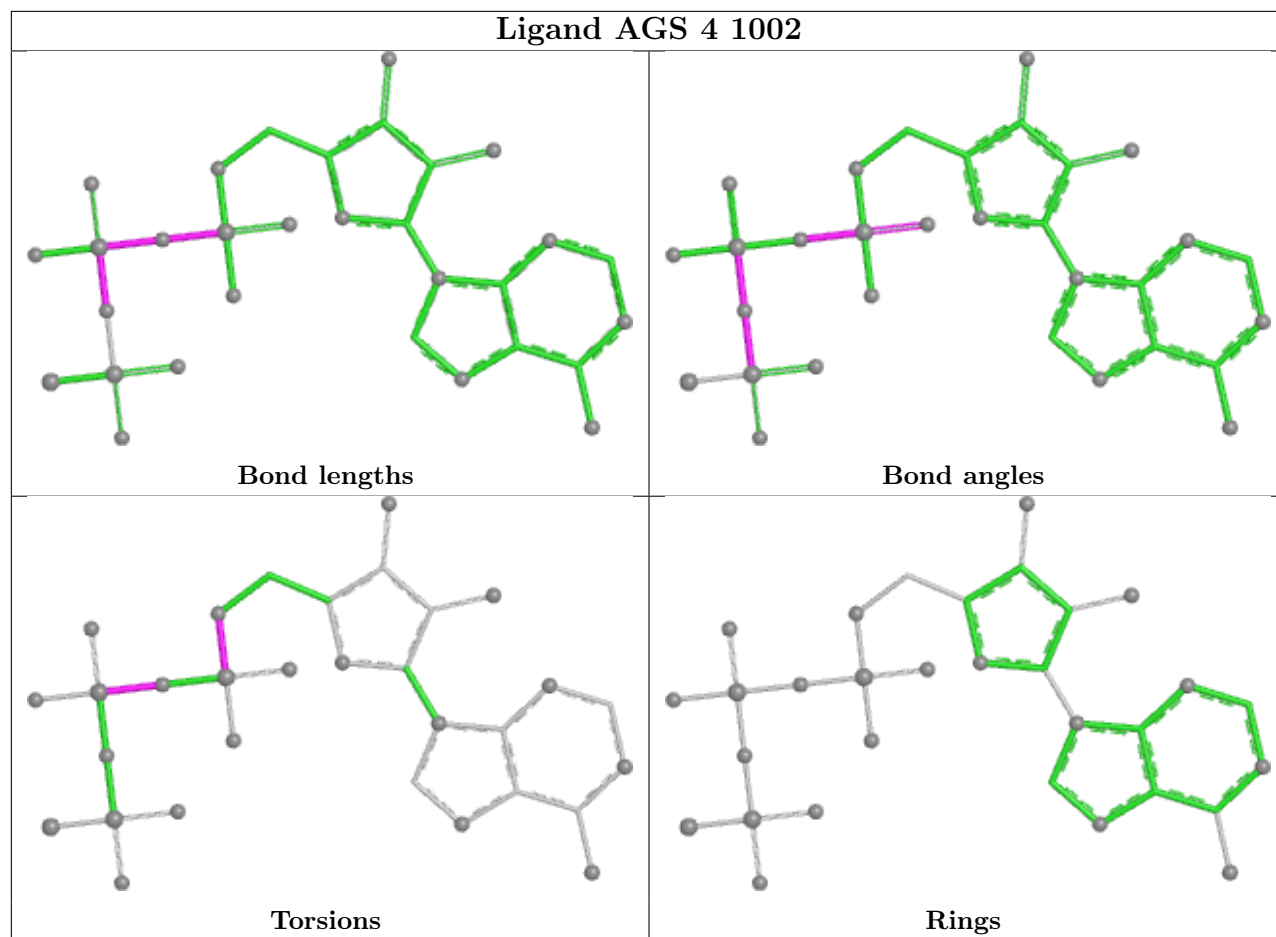


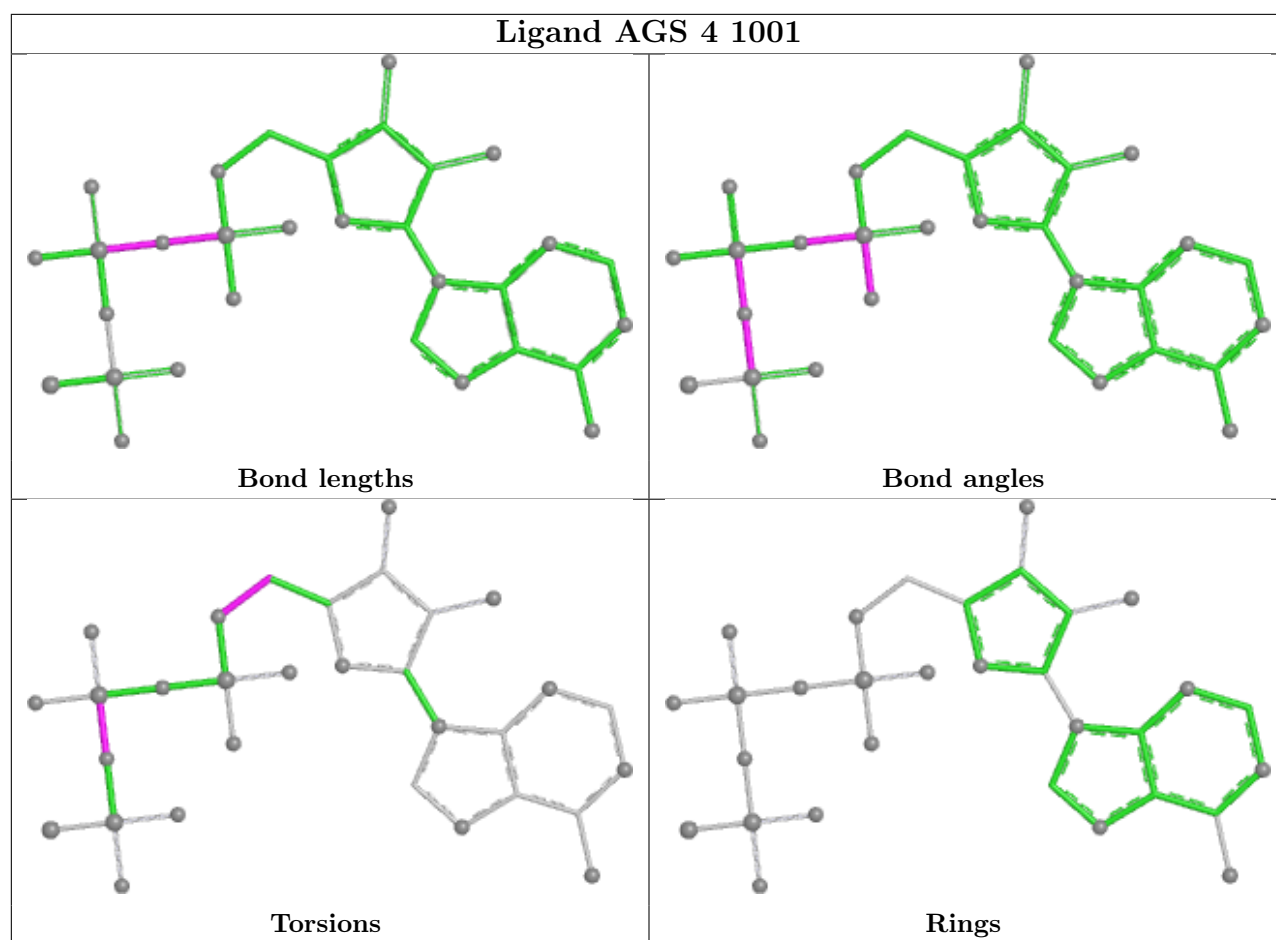


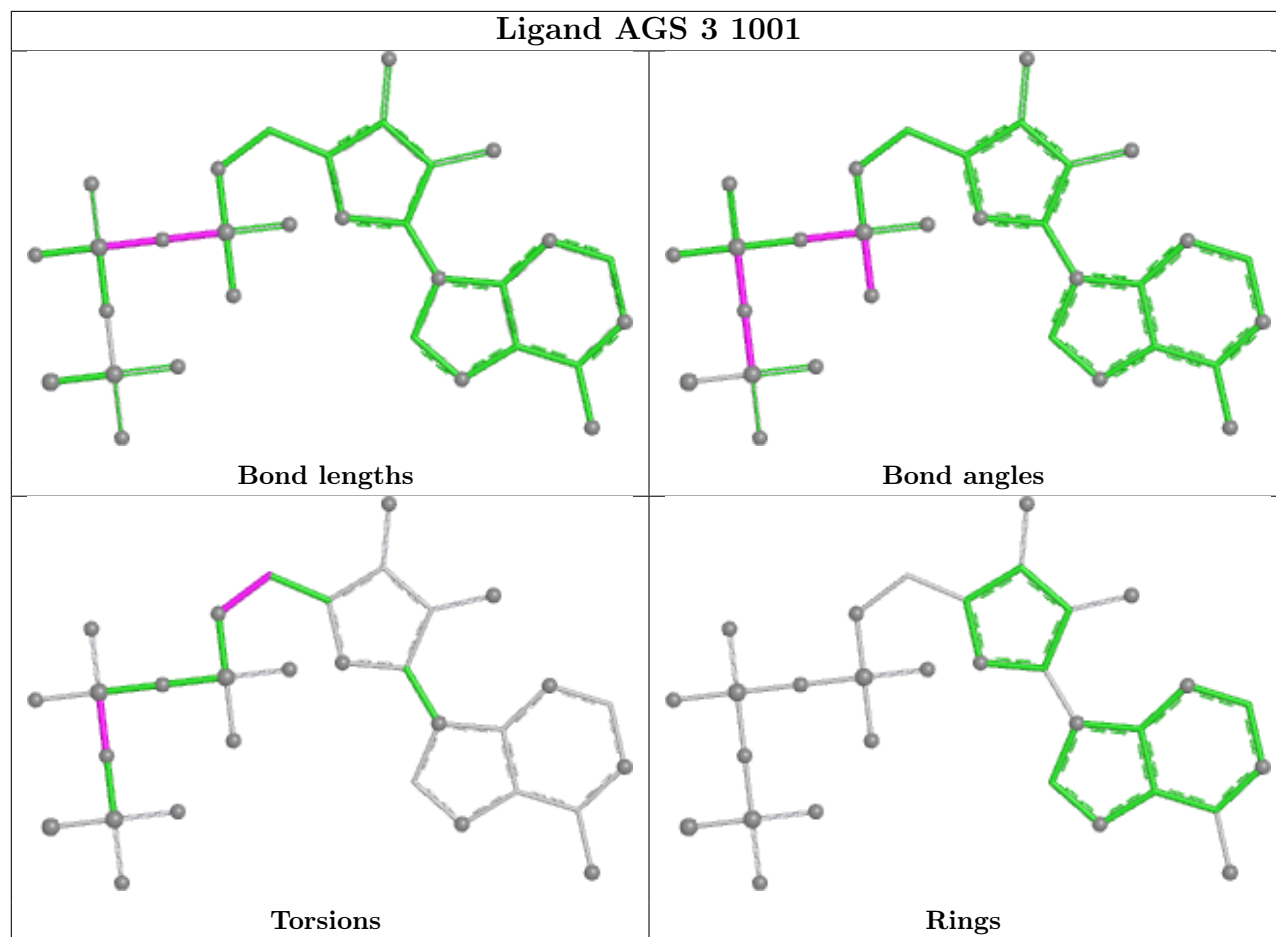


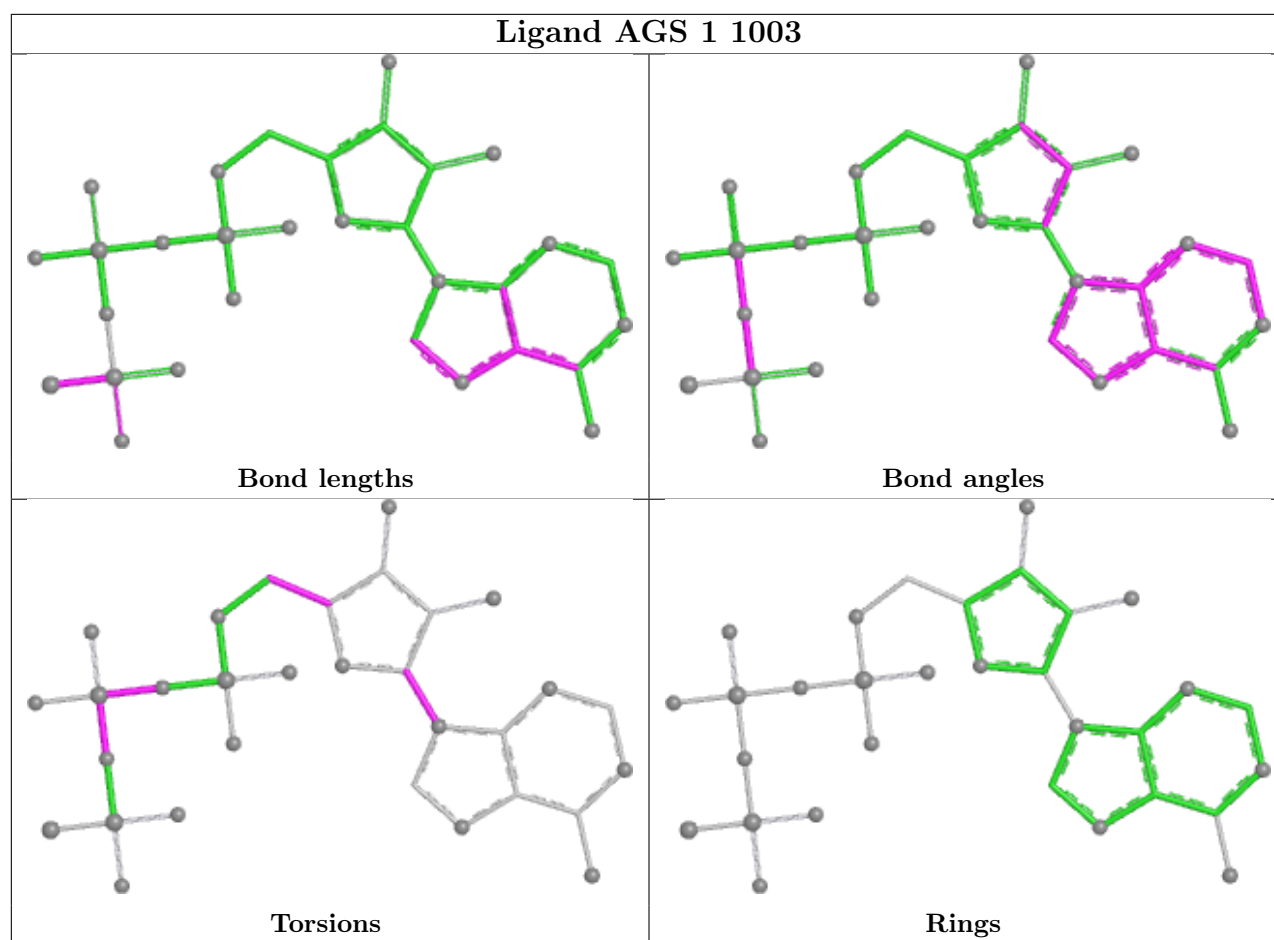












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	h	1
1	i	1
1	l	1
1	j	1
1	k	1
1	m	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	h	28:UNK	C	988:UNK	N	44.65
1	i	29:UNK	C	988:UNK	N	43.96
1	l	33:UNK	C	986:UNK	N	33.84
1	j	32:UNK	C	981:UNK	N	24.35
1	k	33:UNK	C	980:UNK	N	19.33

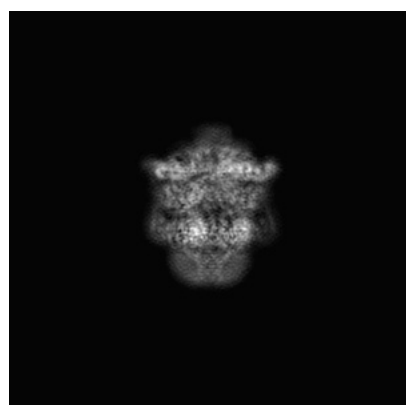
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8952. These allow visual inspection of the internal detail of the map and identification of artifacts.

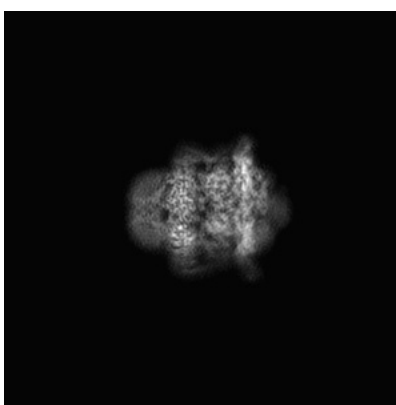
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

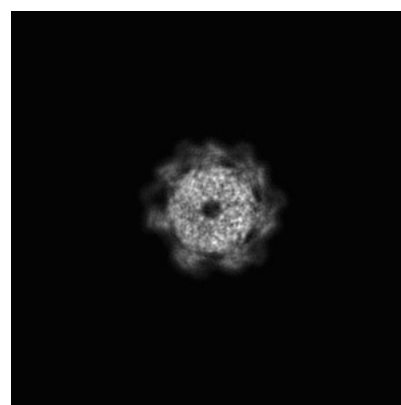
6.1.1 Primary map



X



Y

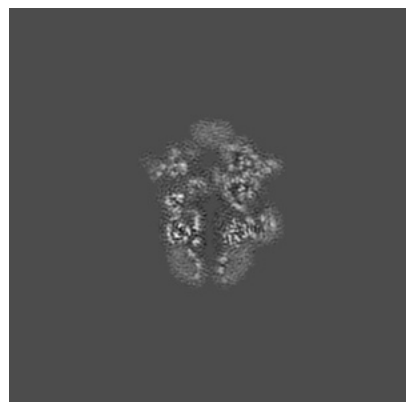


Z

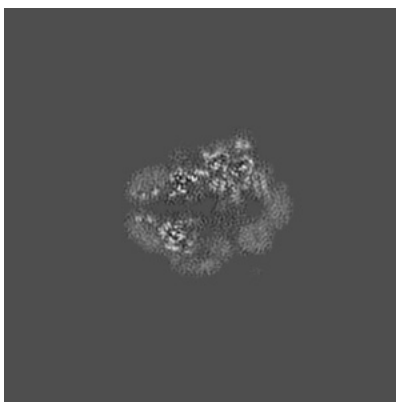
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

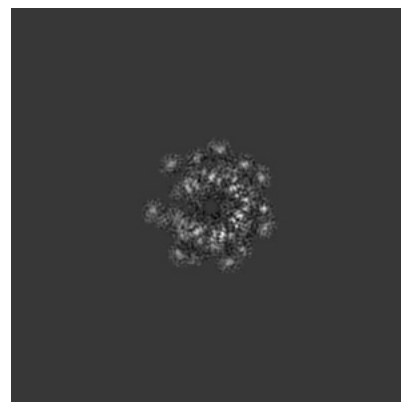
6.2.1 Primary map



X Index: 240



Y Index: 240

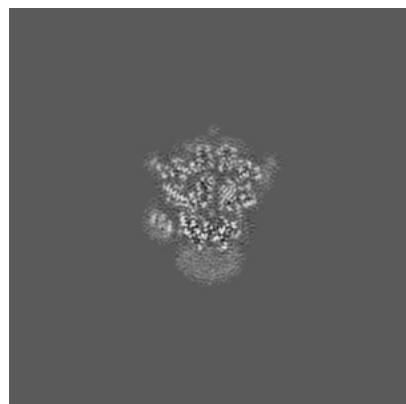


Z Index: 240

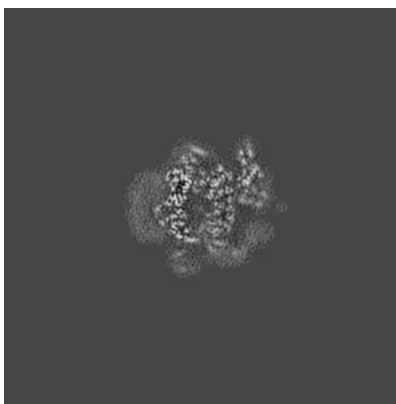
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 269



Y Index: 219

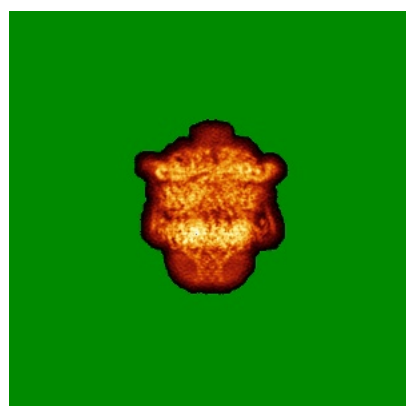


Z Index: 212

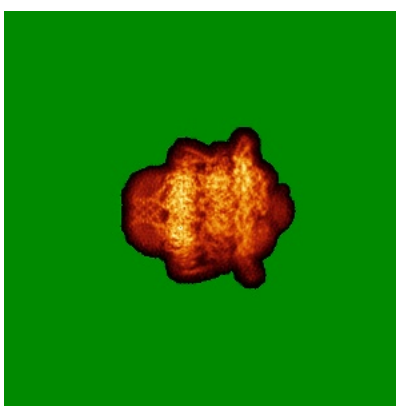
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

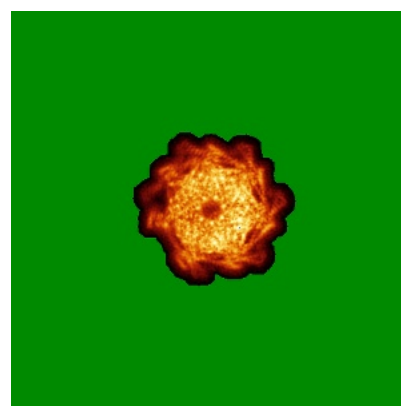
6.4.1 Primary map



X



Y

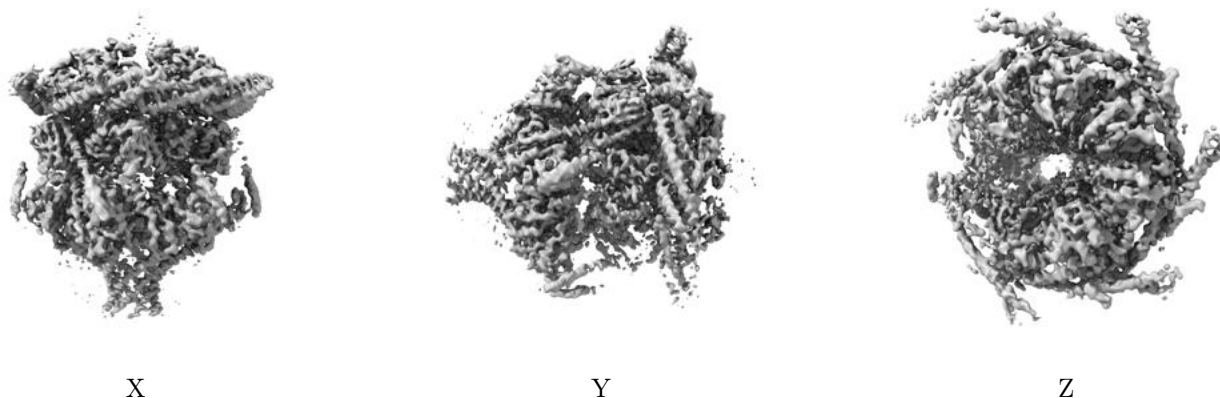


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0405. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

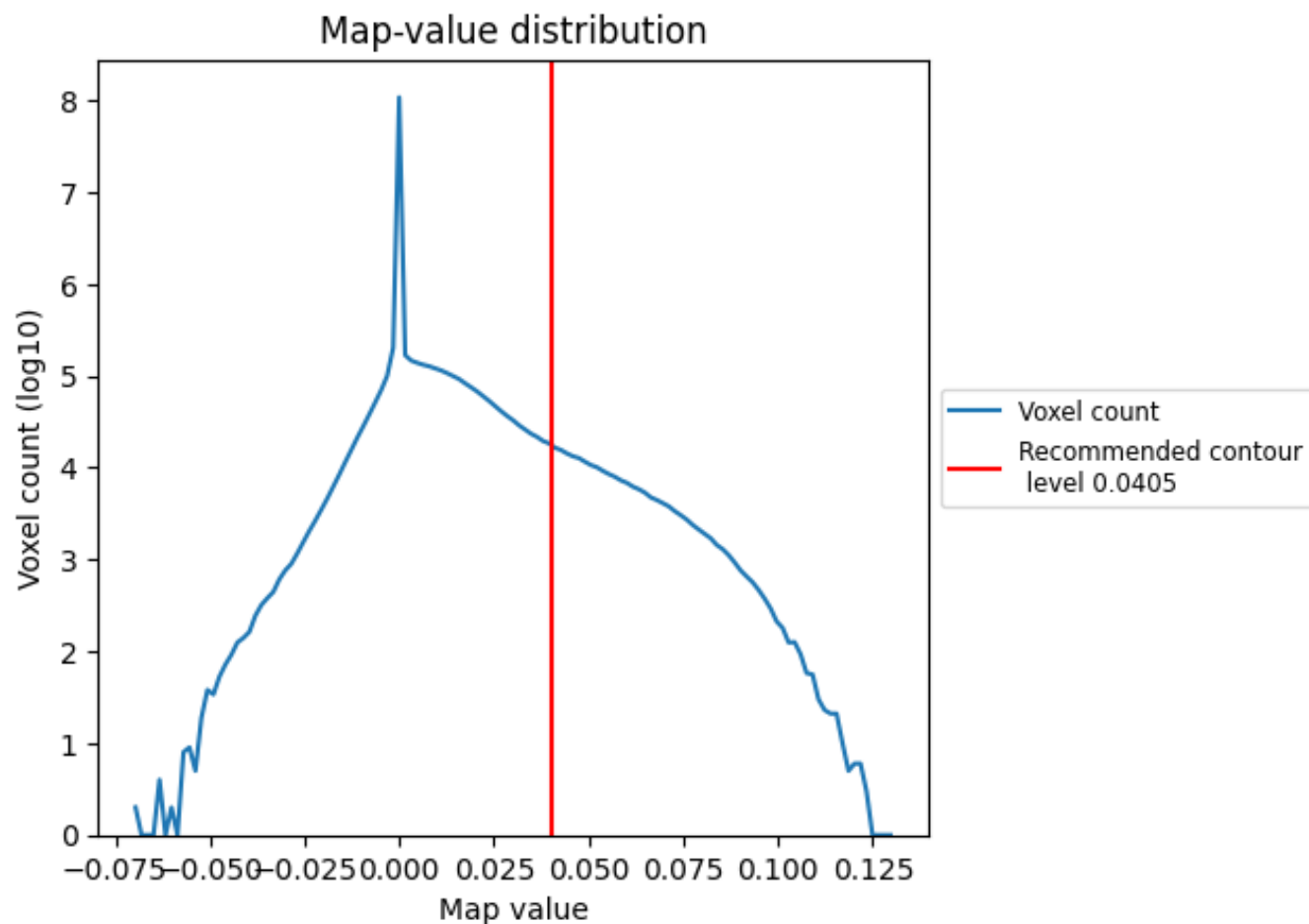
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

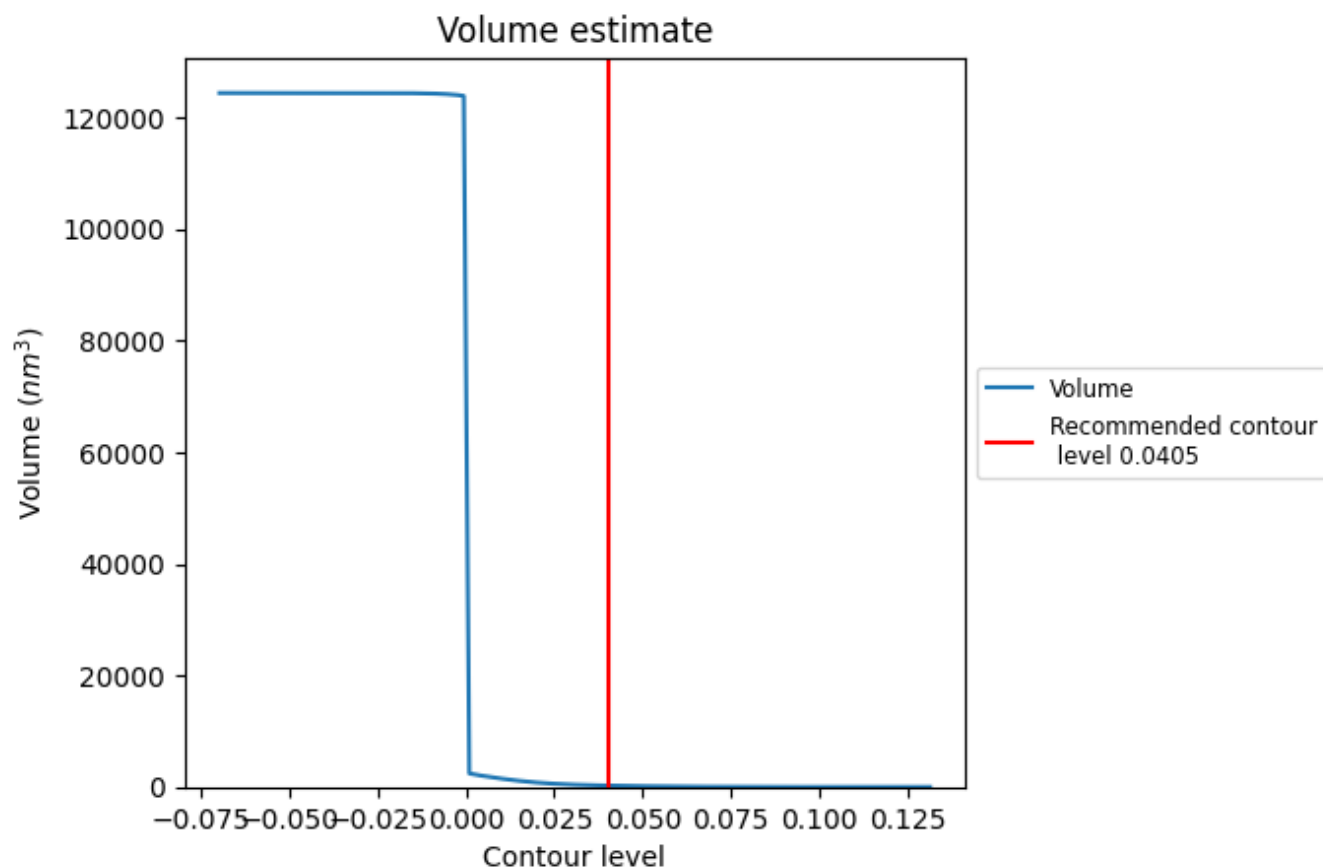
This section contains the results of statistical analysis of the map.

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.

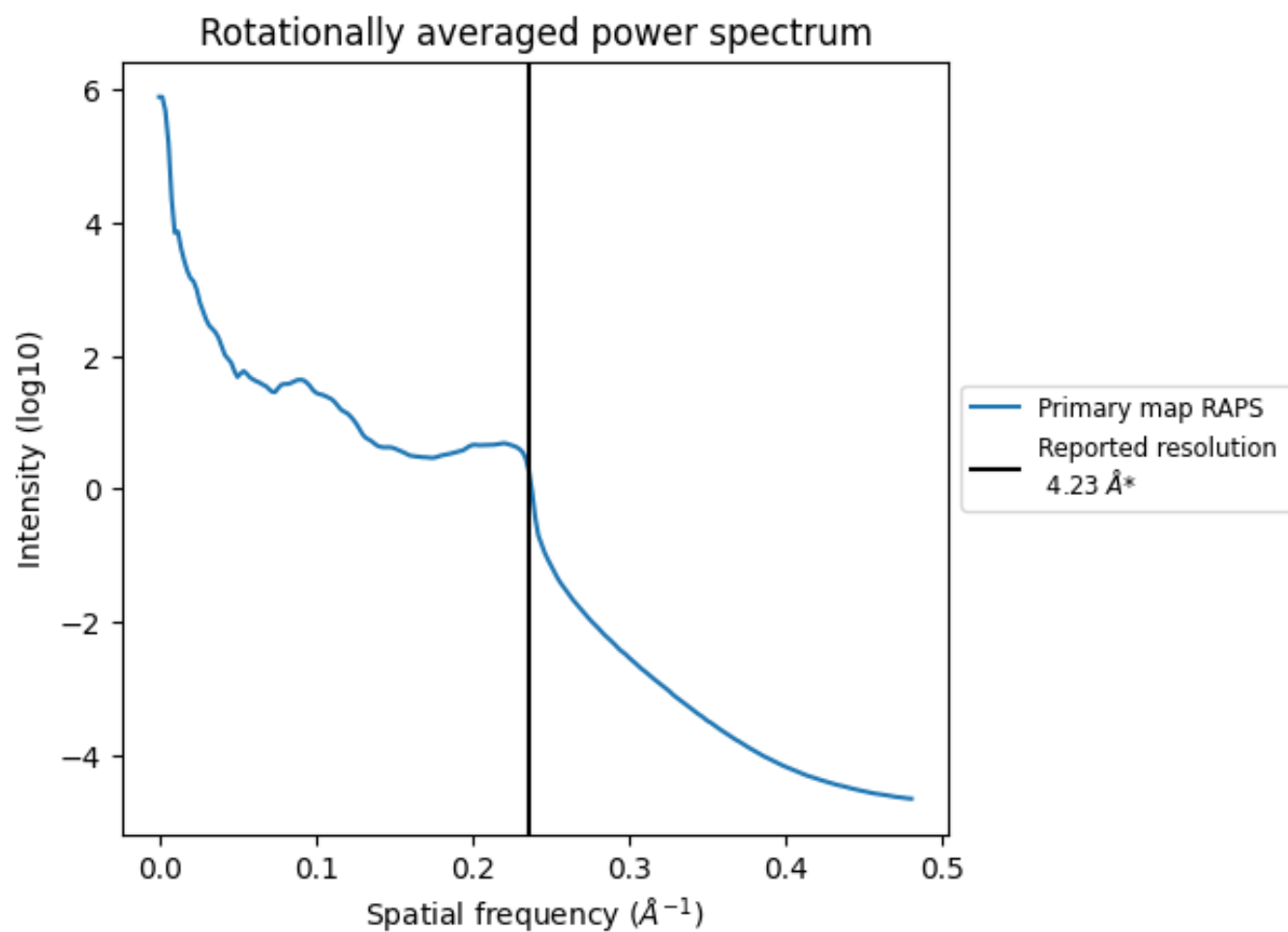
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 239 nm^3 ; this corresponds to an approximate mass of 216 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.236 $\text{\AA}^{-1}$

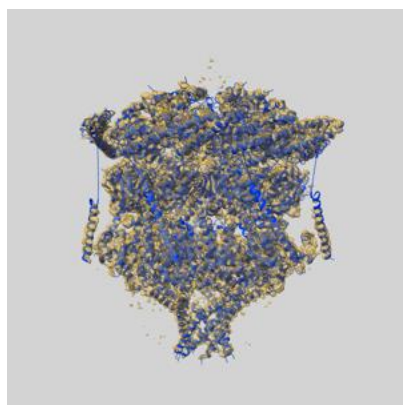
8 Fourier-Shell correlation

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

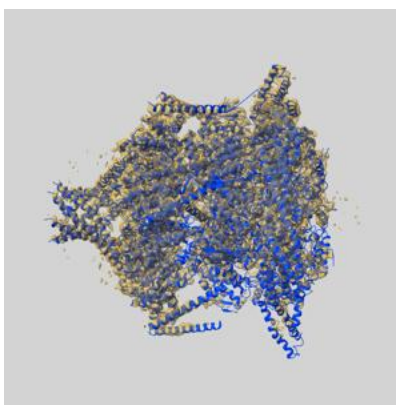
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8952 and PDB model 6E11. Per-residue inclusion information can be found in section 3 on page 8.

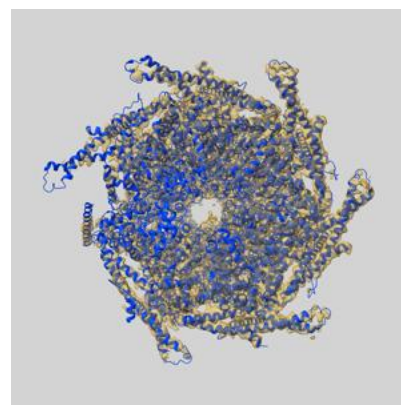
9.1 Map-model overlay [i](#)



X



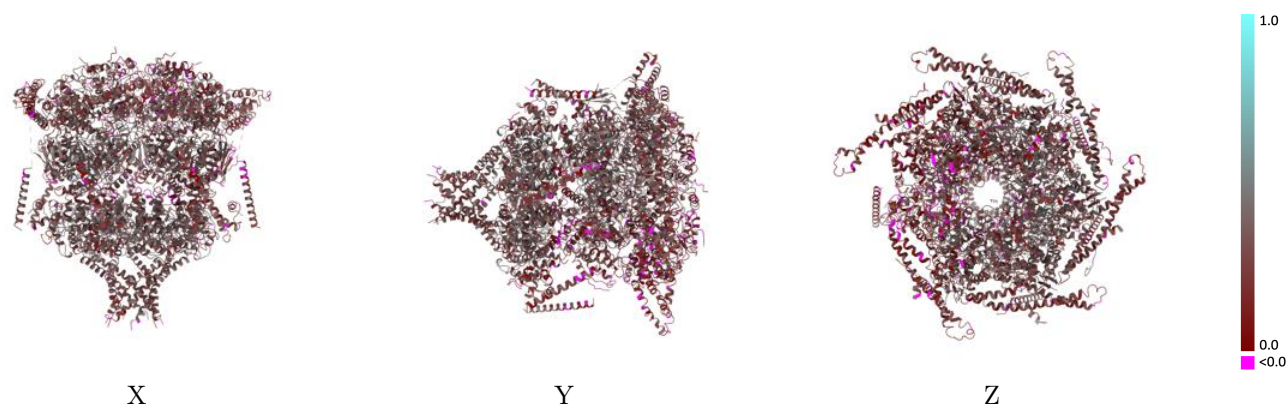
Y



Z

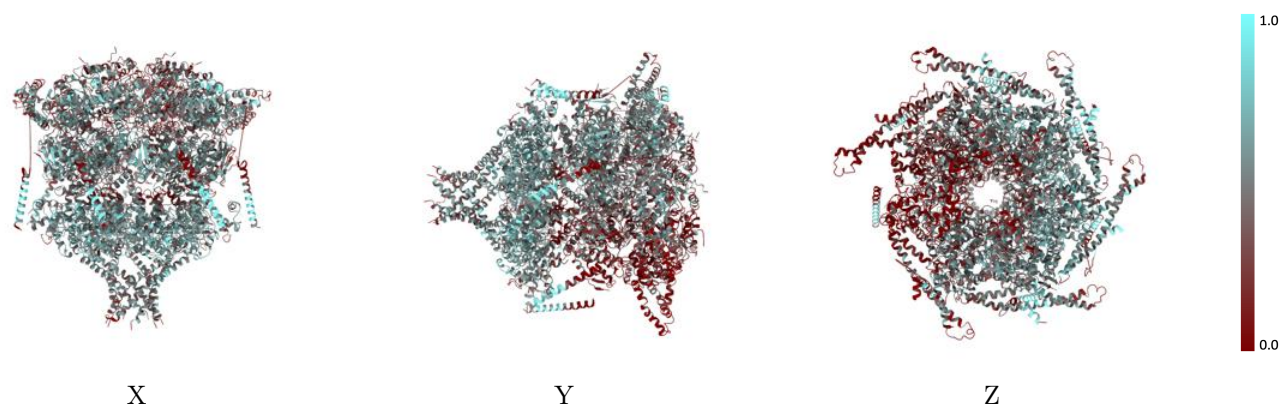
The images above show the 3D surface view of the map at the recommended contour level 0.0405 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



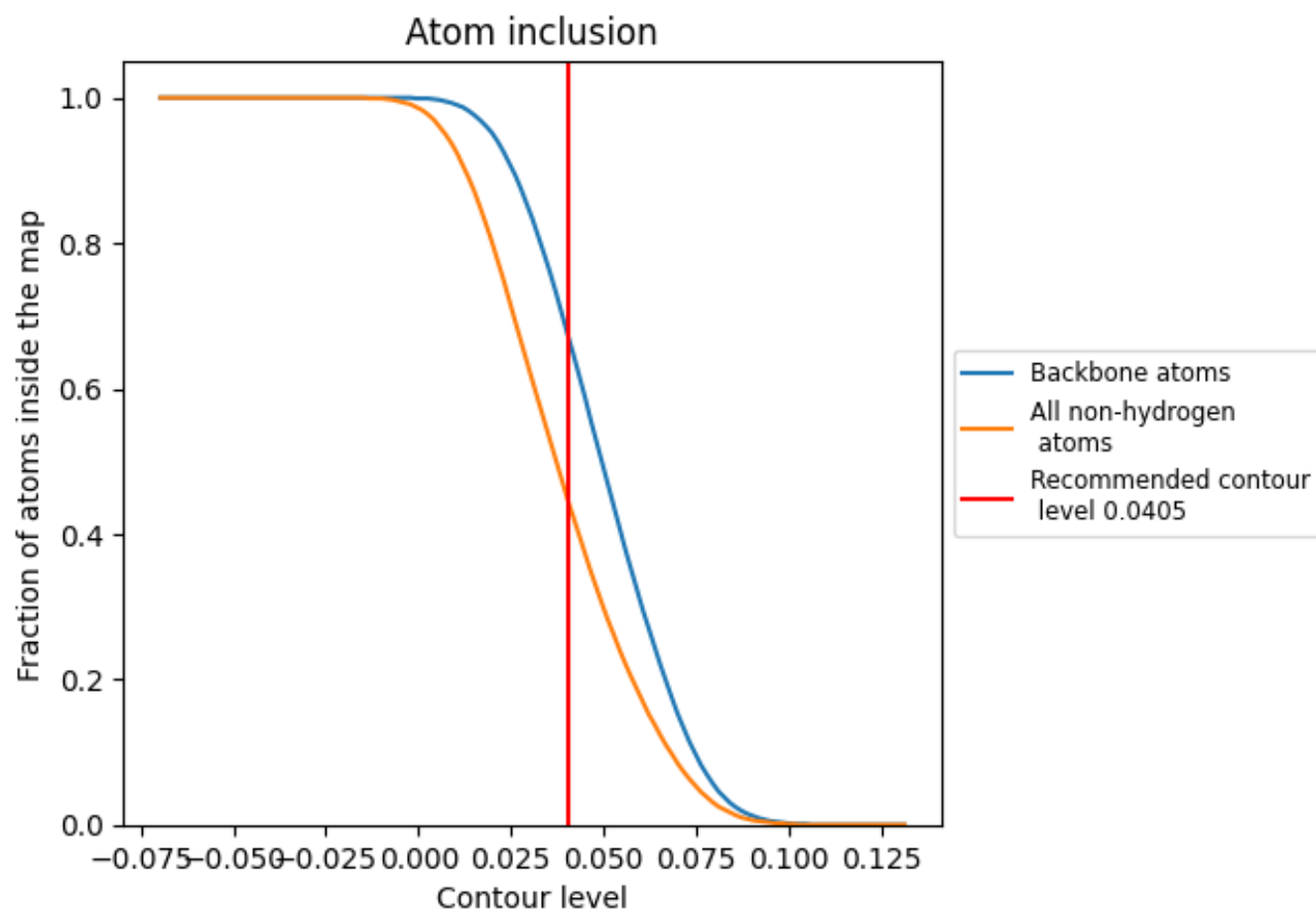
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0405).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 44% 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 (0.0405) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4440	 0.2910
0	 0.3670	 0.3690
1	 0.3430	 0.2560
2	 0.4990	 0.3100
3	 0.5110	 0.3230
4	 0.4810	 0.3120
5	 0.3820	 0.2800
6	 0.1580	 0.1980
A	 0.5660	 0.3100
B	 0.5540	 0.3270
C	 0.5840	 0.3440
D	 0.5670	 0.3380
E	 0.5500	 0.3350
F	 0.5440	 0.3340
G	 0.5610	 0.3190
a	 0.4810	 0.2880
b	 0.5050	 0.3100
c	 0.5180	 0.3210
d	 0.5010	 0.3050
e	 0.4860	 0.3080
f	 0.4460	 0.2620
g	 0.4330	 0.2720
h	 0.3230	 0.1980
i	 0.5650	 0.2920
j	 0.4840	 0.2560
k	 0.4830	 0.2190
l	 0.5090	 0.2530
m	 0.2930	 0.1960
n	 0.4500	 0.2350

