



wwPDB EM Validation Summary Report ⓘ

Aug 30, 2026 – 12:27 am BST

PDB ID : 9Q8V / pdb_00009q8v
EMDB ID : EMD-52908
Title : Cryo-EM structure of the NLRP3 decamer bound to the inhibitor BAL-1516
Authors : Torp, J.; Wilhelmsen, K.; Hartman, G.; Hagelueken, G.; Geyer, M.
Deposited on : 2025-02-25
Resolution : 3.06 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:

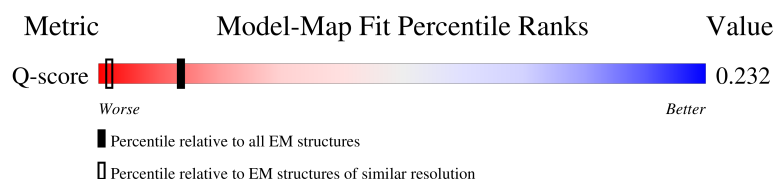
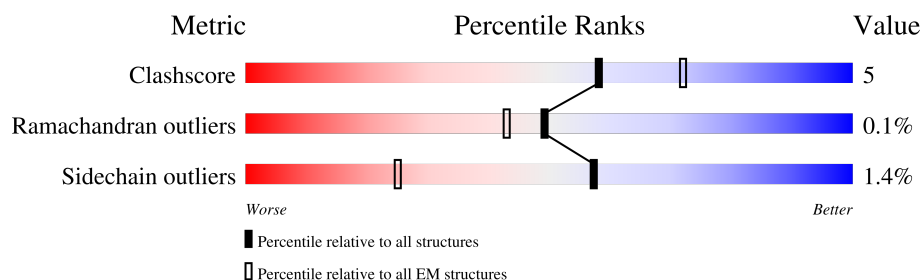
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance

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

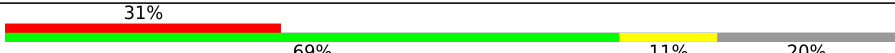
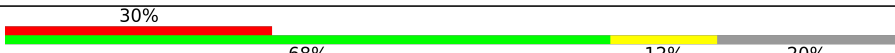
The reported resolution of this entry is 3.06 Å.

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.



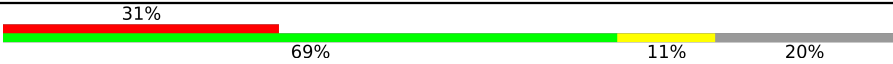
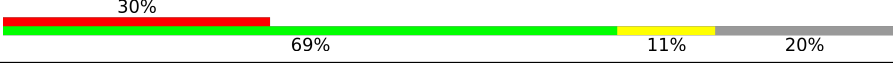
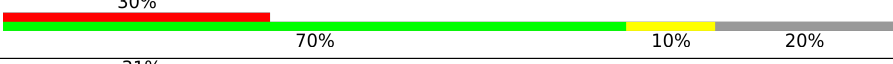
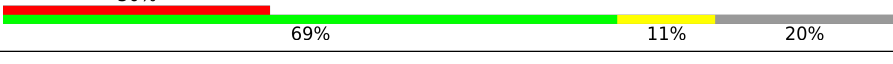
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13976 (2.56 - 3.56)

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	A	1036	
1	B	1036	
1	C	1036	
1	D	1036	

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Mol	Chain	Length	Quality of chain
1	E	1036	
1	F	1036	
1	G	1036	
1	H	1036	
1	I	1036	
1	J	1036	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 67130 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 NACHT, LRR and PYD domains-containing protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	833	Total	C	N	O	S	0	0
			6654	4239	1133	1226	56		
1	B	833	Total	C	N	O	S	0	0
			6654	4239	1133	1226	56		
1	C	833	Total	C	N	O	S	0	0
			6654	4239	1133	1226	56		
1	D	833	Total	C	N	O	S	0	0
			6654	4239	1133	1226	56		
1	E	833	Total	C	N	O	S	0	0
			6654	4239	1133	1226	56		
1	F	833	Total	C	N	O	S	0	0
			6654	4239	1133	1226	56		
1	G	833	Total	C	N	O	S	0	0
			6654	4239	1133	1226	56		
1	H	833	Total	C	N	O	S	0	0
			6654	4239	1133	1226	56		
1	I	833	Total	C	N	O	S	0	0
			6654	4239	1133	1226	56		
1	J	833	Total	C	N	O	S	0	0
			6654	4239	1133	1226	56		

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 27	C 10	N 5	O 10	P 2	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0
2	C	1	Total 27	C 10	N 5	O 10	P 2	0
2	D	1	Total 27	C 10	N 5	O 10	P 2	0
2	E	1	Total 27	C 10	N 5	O 10	P 2	0
2	F	1	Total 27	C 10	N 5	O 10	P 2	0
2	G	1	Total 27	C 10	N 5	O 10	P 2	0
2	H	1	Total 27	C 10	N 5	O 10	P 2	0
2	I	1	Total 27	C 10	N 5	O 10	P 2	0
2	J	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

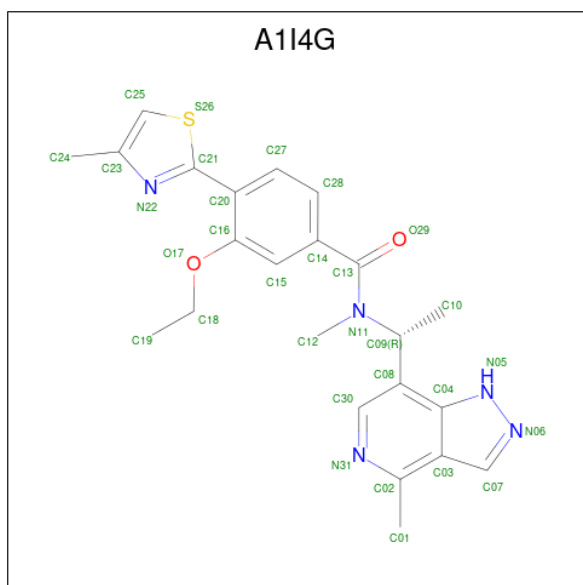
Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Mg 1 1	0
3	B	1	Total Mg 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
3	C	1	Total	Mg	0
			1	1	
3	D	1	Total	Mg	0
			1	1	
3	E	1	Total	Mg	0
			1	1	
3	F	1	Total	Mg	0
			1	1	
3	G	1	Total	Mg	0
			1	1	
3	H	1	Total	Mg	0
			1	1	
3	I	1	Total	Mg	0
			1	1	
3	J	1	Total	Mg	0
			1	1	

- Molecule 4 is 3-ethoxy- {N}-methyl- {N}-[(1 {R})-1-(4-methyl-1 {H}-pyrazolo[4,3-c]pyridin-7-yl)ethyl]-4-(4-methyl-1,3-thiazol-2-yl)benzamide (CCD ID: A1I4G) (formula: C₂₃H₂₅N₅O₂S).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	S	0
			31	23	5	2	1	
4	B	1	Total	C	N	O	S	0
			31	23	5	2	1	

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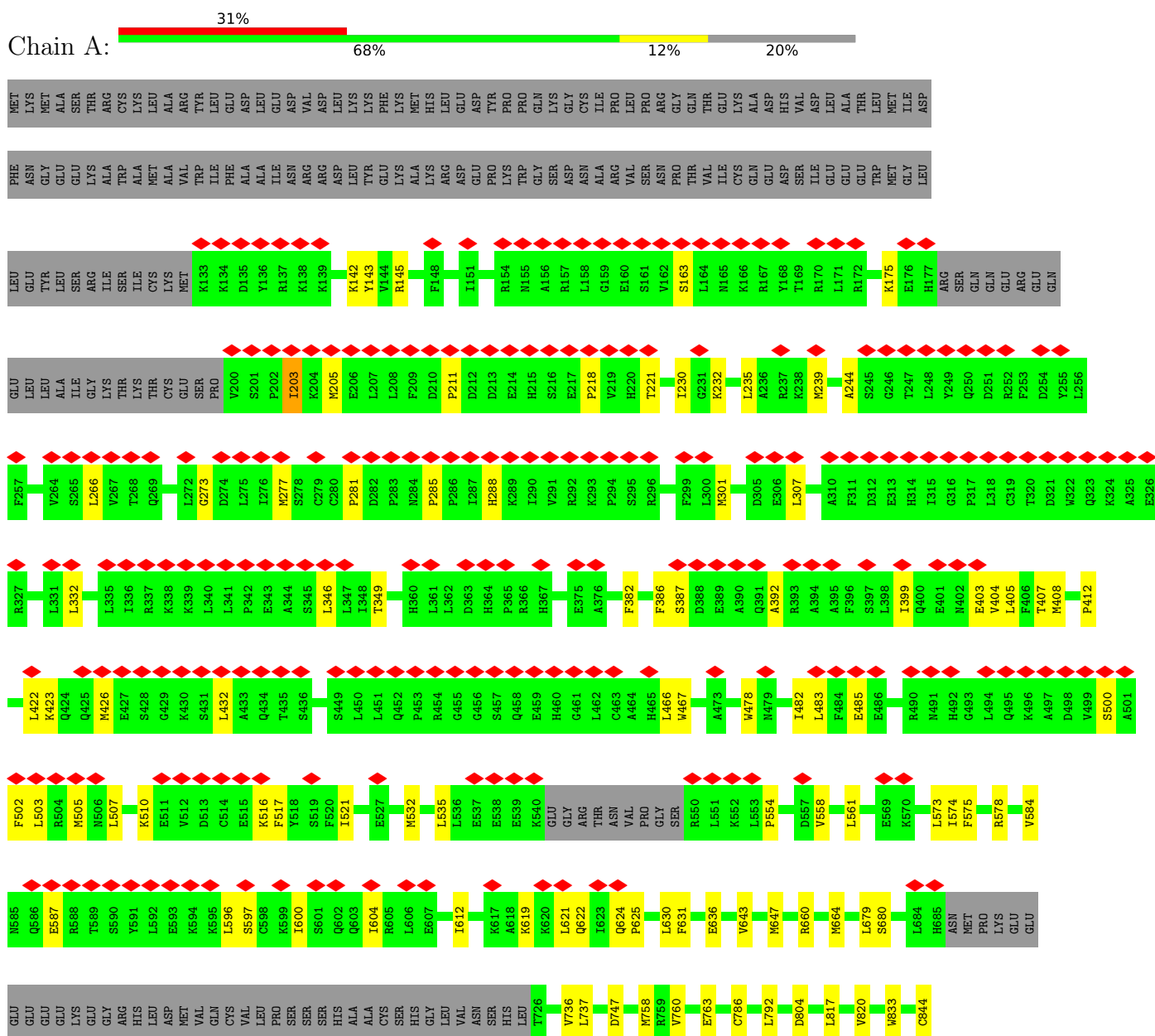
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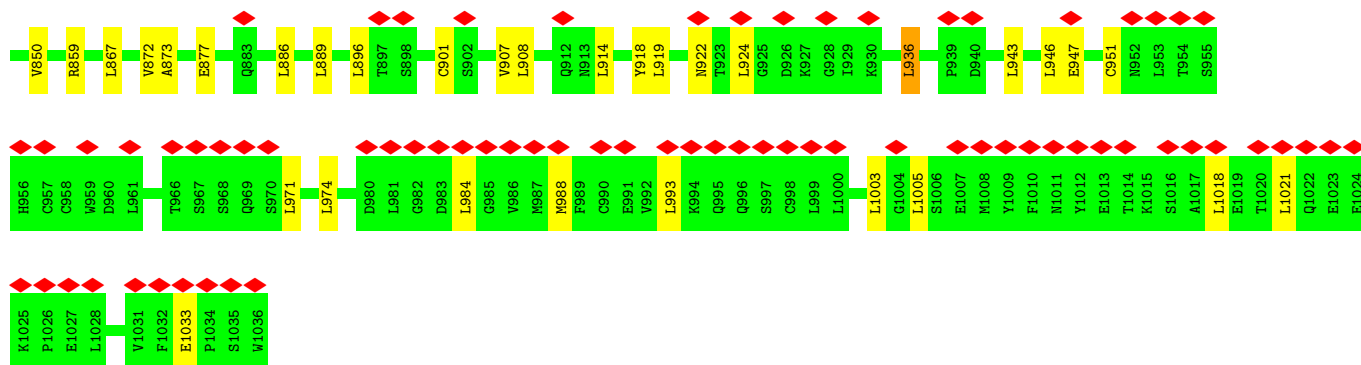
Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total 31	C 23	N 5	O 2	S 1	0
4	D	1	Total 31	C 23	N 5	O 2	S 1	0
4	E	1	Total 31	C 23	N 5	O 2	S 1	0
4	F	1	Total 31	C 23	N 5	O 2	S 1	0
4	G	1	Total 31	C 23	N 5	O 2	S 1	0
4	H	1	Total 31	C 23	N 5	O 2	S 1	0
4	I	1	Total 31	C 23	N 5	O 2	S 1	0
4	J	1	Total 31	C 23	N 5	O 2	S 1	0

3 Residue-property plots

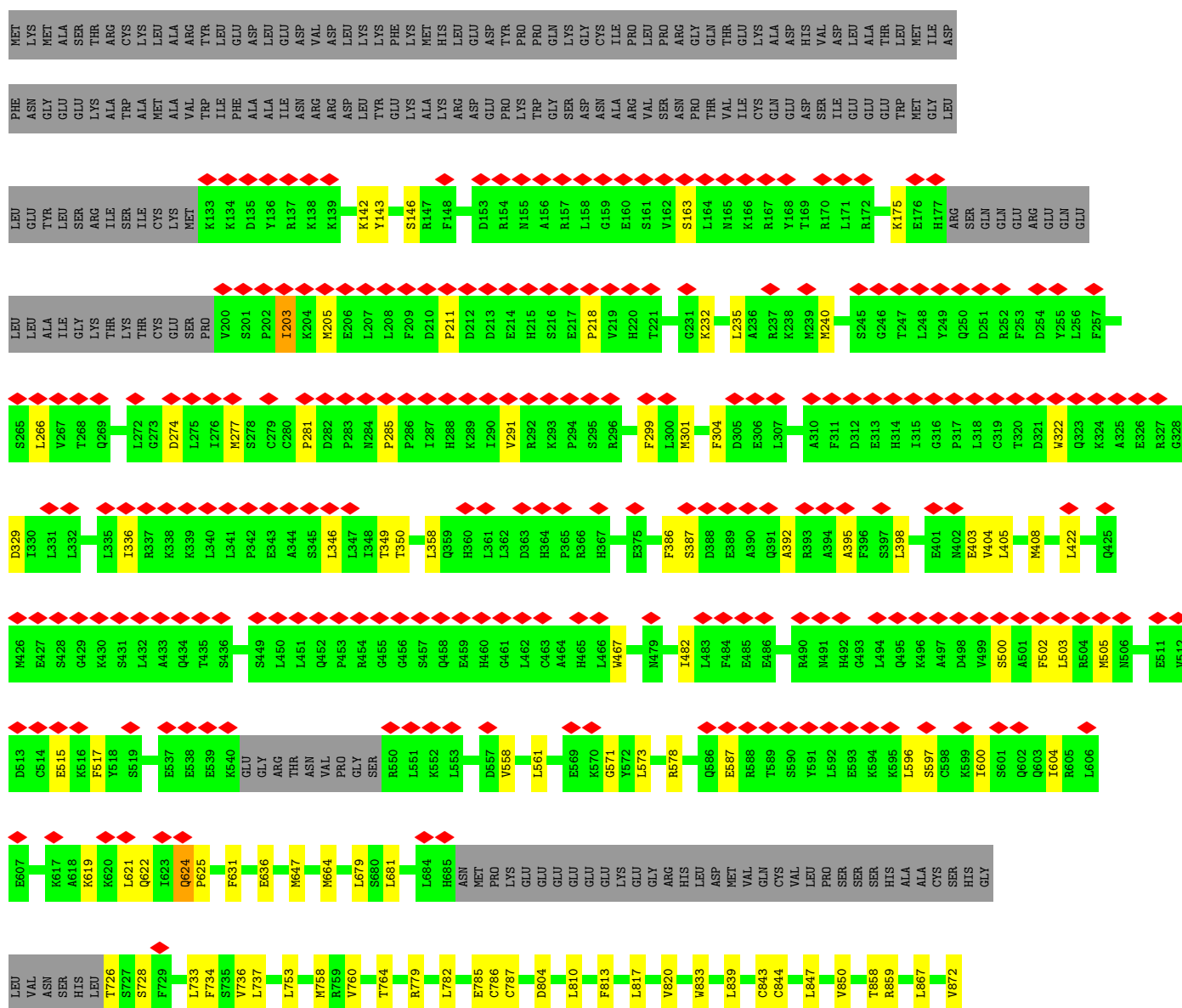
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

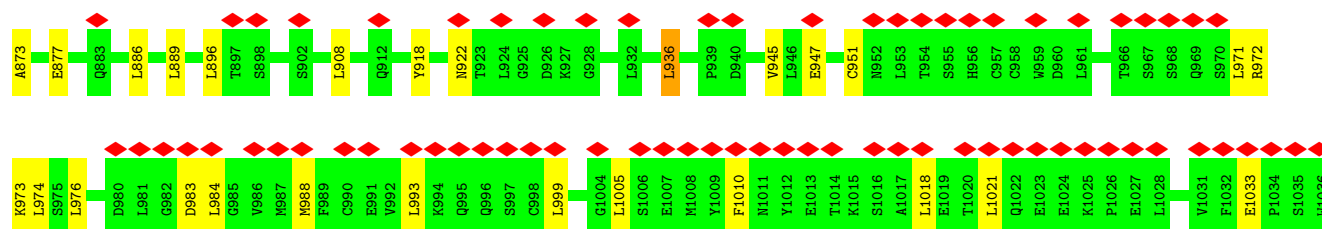
- Molecule 1: NACHT, LRR and PYD domains-containing protein 3



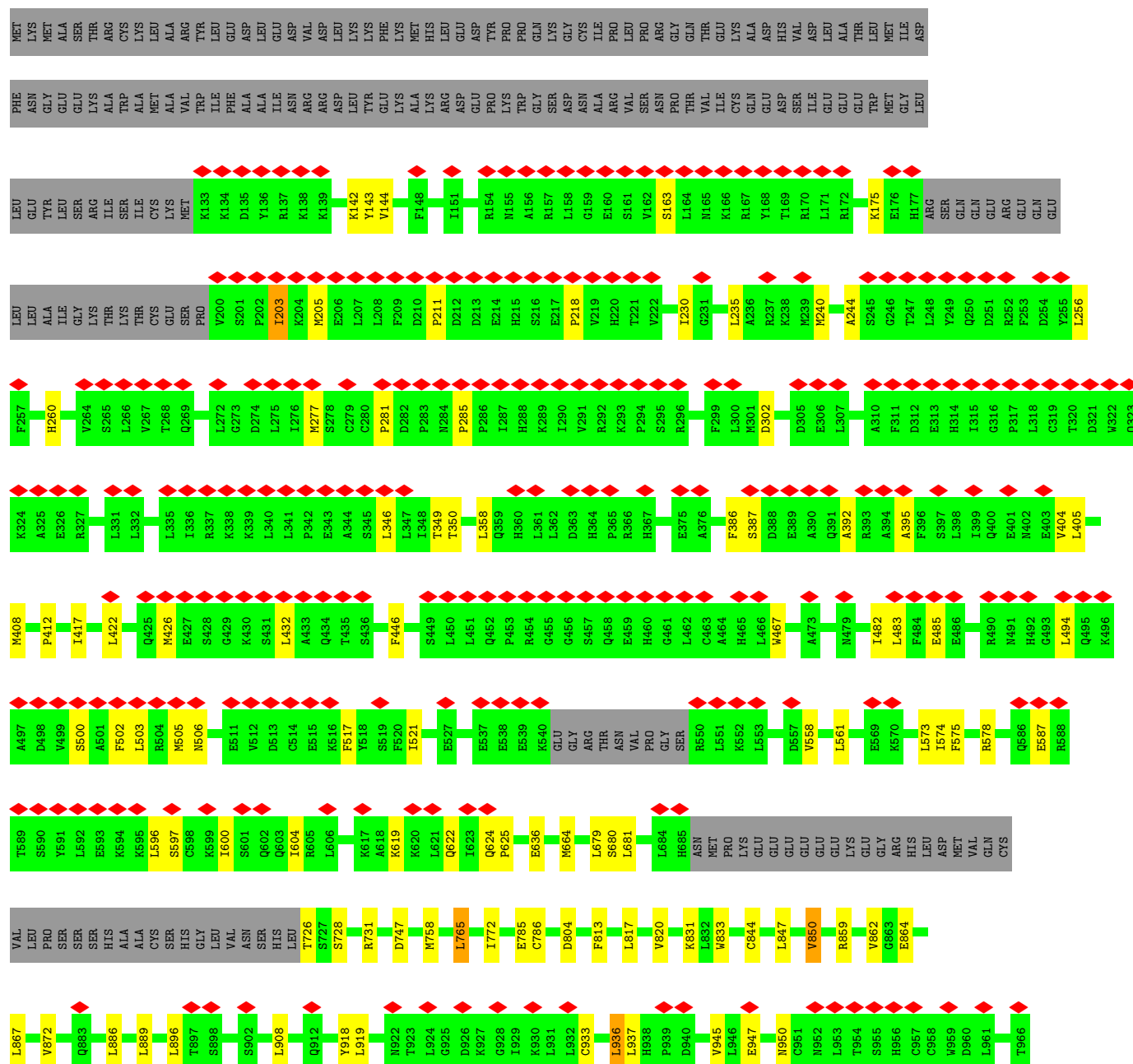


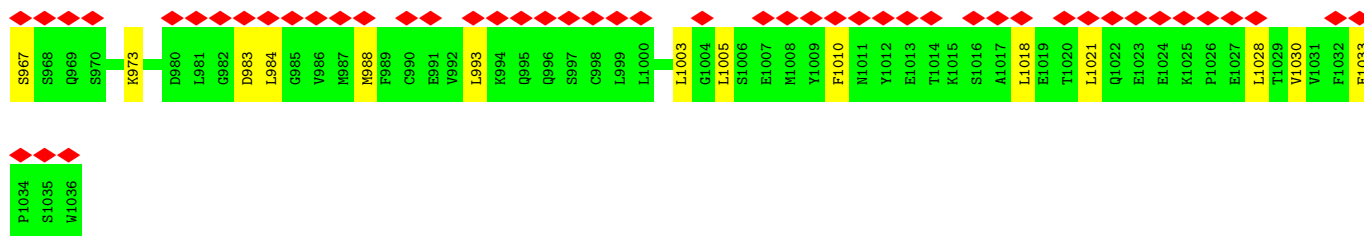
● Molecule 1: NACHT, LRR and PYD domains-containing protein 3



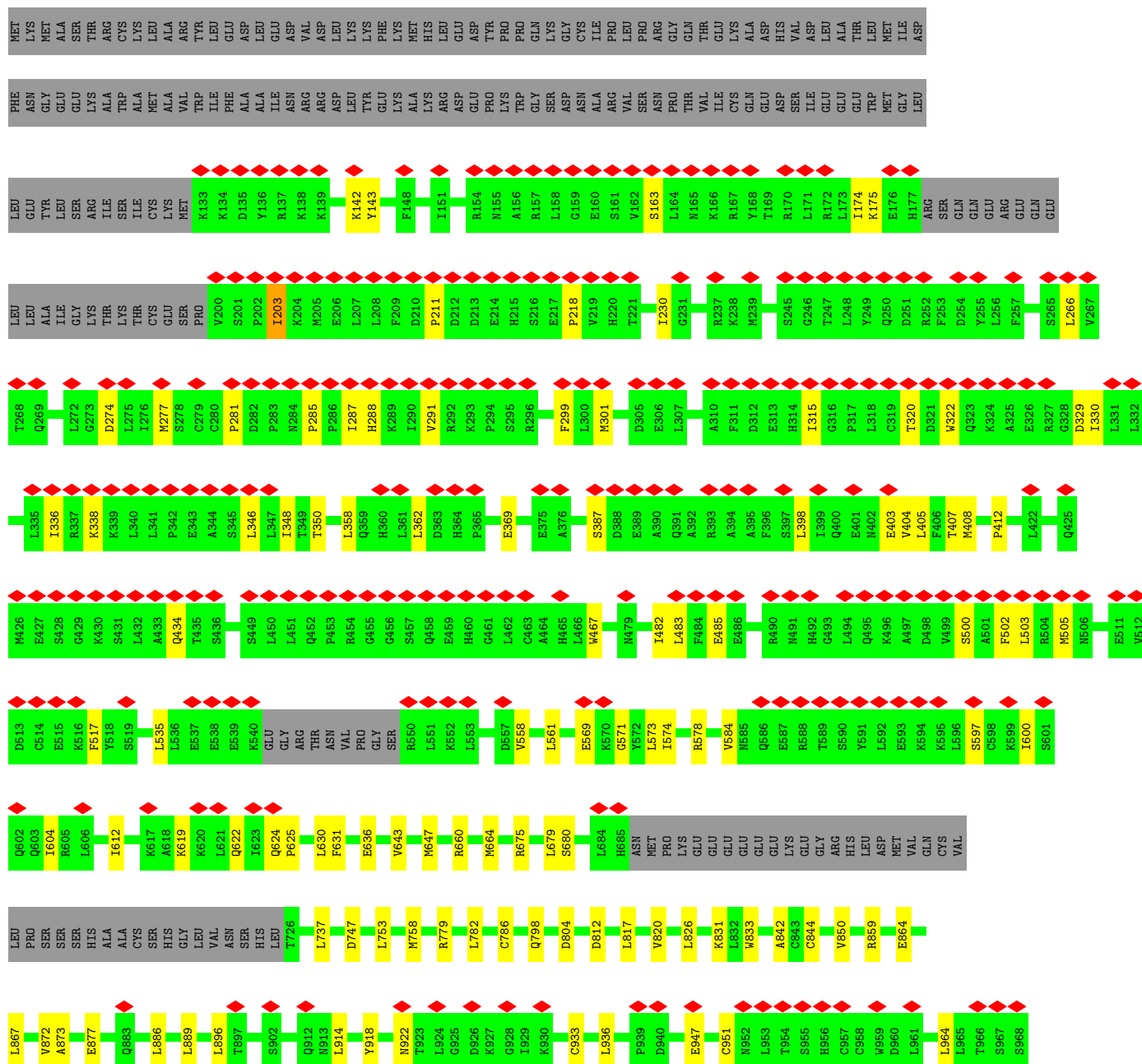


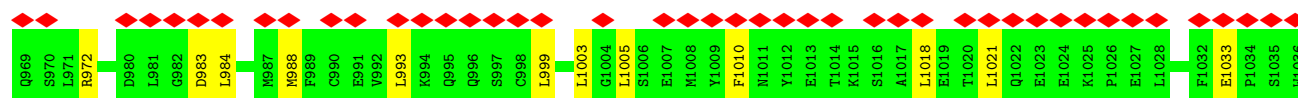
● Molecule 1: NACHT, LRR and PYD domains-containing protein 3



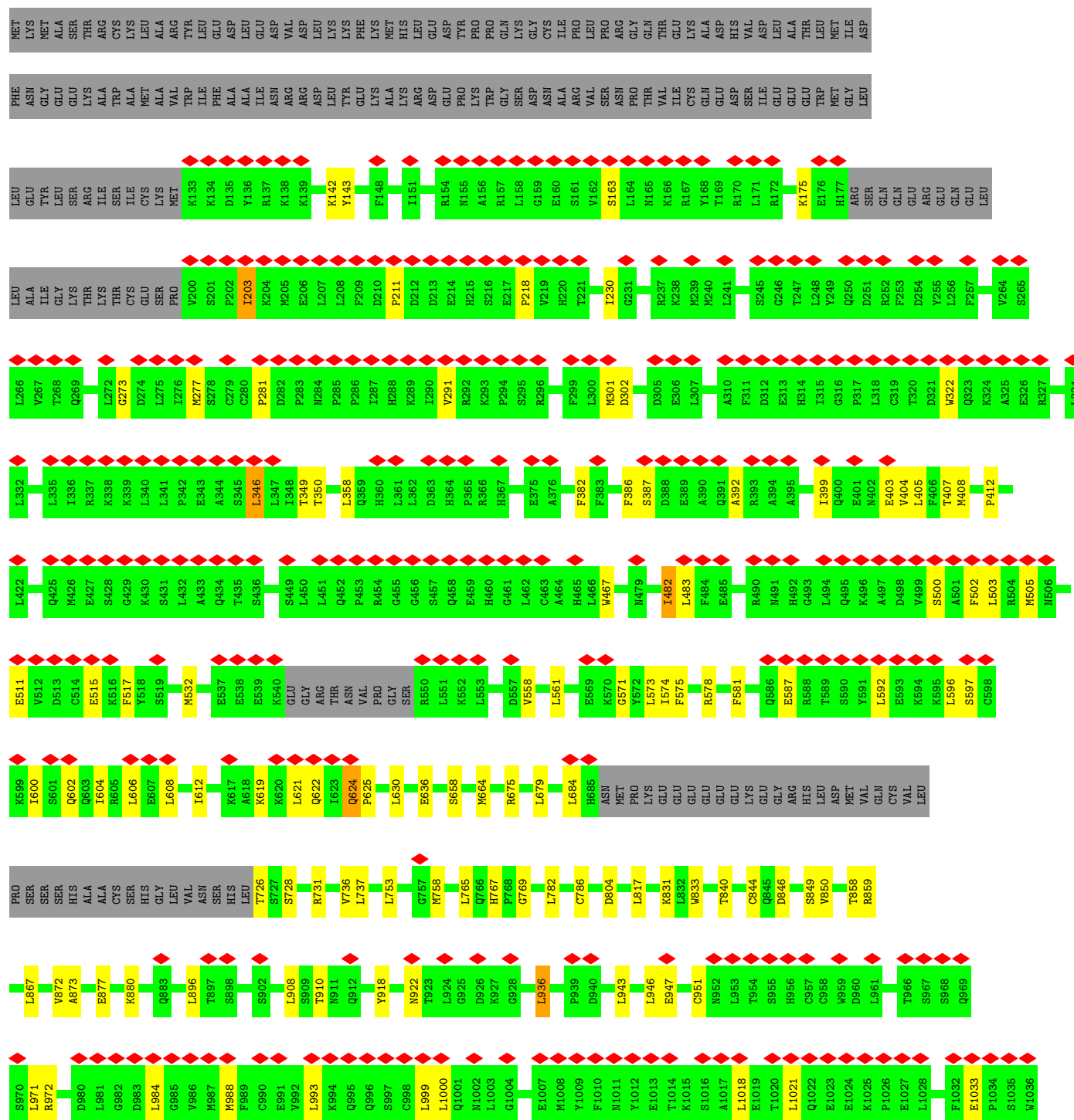


• Molecule 1: NACHT, LRR and PYD domains-containing protein 3

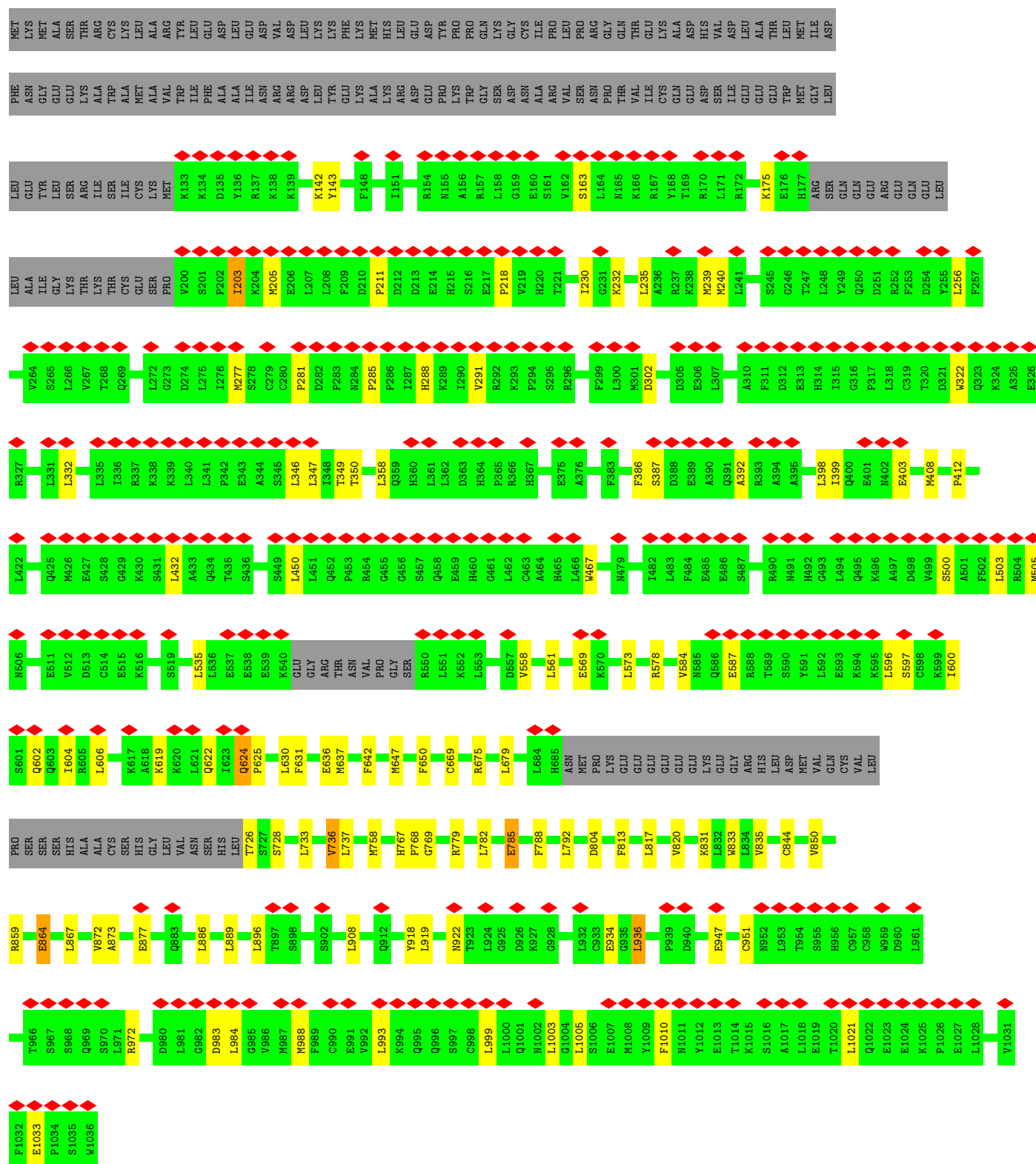




- Molecule 1: NACHT, LRR and PYD domains-containing protein 3



- Molecule 1: NACHT, LRR and PYD domains-containing protein 3



- Molecule 1: NACHT, LRR and PYD domains-containing protein 3



M987	M988	F989	C990	E991	V992	L993	K994	Q995	Q996	S997	C998	L999	L1003	G1004	L1005	S1006	E1007	M1008	F1009	F1010	N1011	Y1012	E1013	T1014	K1015	S1016	A1017	L1018	E1019	T1020	L1021	Q1022	E1023	E1024	K1025	P1026	E1027	L1028	F1032	E1033	P1034	S1035	W1036												
T897	S898	S902	Q912	N913	L914	Y918	L919	N922	T923	L924	G928	T929	R930	C933	L936	P939	P940	L943	L946	E947	C951	R952	L953	T954	S955	H956	C957	C958	W959	D960	L961	T966	S967	S968	Q969	L974	S975	L980	P980	L981	Q982	D983	L984	G985	V986										
PRO	SER	SER	SER	HIS	ALA	ALA	CYS	SER	HIS	GLY	LEU	VAL	ASN	SER	HIS	LEU	T726	S727	S728	F729	V736	L753	M758	L782	C786	Q798	D804	L826	W833	L847	V850	R859	V862	V872	A873	E877	K880	Q883	Q887	L896															
I600	S601	Q602	Q603	I604	R605	L606	E607	L608	I612	K617	A618	K619	K620	L621	Q622	L623	Q624	P625	L630	F631	E636	M647	R660	M664	R675	L684	H685	ASN	MET	PRO	LYS	GLU	GLU	GLU	GLU	LYS	GLY	ARG	HIS	LEU	ASP	MET	VAL	GLN	CYS	VAL	LEU								
N506	K510	E511	V512	D513	C514	E515	K516	F517	Y518	S519	E537	E538	E539	K540	GLU	GLY	ARG	THR	ASN	VAL	PRO	GLY	SER	R550	L551	K552	L553	D557	V558	L561	E569	K570	L573	I574	F575	R578	F579	L580	E587	R588	T589	S590	Y591	L592	E593	K594	K595	L596	S597	C598	K599				
L422	Q425	M426	E427	S428	G429	K430	S431	L432	A433	Q434	T435	S436	S449	L450	L451	Q452	P453	R454	G455	G456	S457	Q458	E459	H460	G461	L462	C463	A464	H465	L466	W467	M479	I482	L483	F484	E485	E486	R490	N491	H492	G493	L494	Q495	K496	A497	D498	V499	S500	A501	F502	L503	R504	M505		
T268	Q269	L272	G273	D274	L275	I276	M277	S278	C279	C280	P281	D282	P283	N284	P285	P286	I287	H288	K289	I290	V291	R292	K293	P294	S295	R296	F299	L300	M301	F304	D305	E306	L307	A310	F311	D312	E313	H314	I315	G316	P317	L318	C319	T320	D321	W322	Q323	K324	A325	E326	R327	L331	L332		
LEU	ALA	ILE	GLY	LYS	THR	LYS	THR	CYS	GLU	SER	PRO	V200	S201	P202	I203	K204	M205	E206	L207	L208	F209	D210	P211	D212	D213	E214	H215	S216	E217	P218	V219	H220	T221	L230	G231	K232	R237	K238	M239	S245	Q246	L247	L248	Y249	Q250	D251	R252	F253	D254	Y255	L256	F257	S265	L266	V267

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	765958	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.7	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	10.698	Depositor
Minimum map value	-6.587	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.177	Depositor
Recommended contour level	0.744	Depositor
Map size ($\text{\AA}$)	354.24002, 354.24002, 354.24002	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0933334, 1.0933334, 1.0933334	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, A1I4G, MG

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	0.11	0/6780	0.27	0/9138
1	B	0.11	0/6780	0.27	0/9138
1	C	0.11	0/6780	0.27	0/9138
1	D	0.11	0/6780	0.28	0/9138
1	E	0.11	0/6780	0.27	0/9138
1	F	0.11	0/6780	0.27	0/9138
1	G	0.11	0/6780	0.27	0/9138
1	H	0.11	0/6780	0.27	0/9138
1	I	0.11	0/6780	0.27	0/9138
1	J	0.11	0/6780	0.27	0/9138
All	All	0.11	0/67800	0.27	0/91380

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	6654	0	6709	70	0
1	B	6654	0	6709	75	0
1	C	6654	0	6709	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	6654	0	6709	67	0
1	E	6654	0	6709	65	0
1	F	6654	0	6709	67	0
1	G	6654	0	6709	61	0
1	H	6654	0	6709	58	0
1	I	6654	0	6709	64	0
1	J	6654	0	6709	64	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	E	27	0	12	0	0
2	F	27	0	12	0	0
2	G	27	0	12	0	0
2	H	27	0	12	0	0
2	I	27	0	12	0	0
2	J	27	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	A	31	0	0	0	0
4	B	31	0	0	0	0
4	C	31	0	0	0	0
4	D	31	0	0	0	0
4	E	31	0	0	0	0
4	F	31	0	0	0	0
4	G	31	0	0	0	0
4	H	31	0	0	0	0
4	I	31	0	0	0	0
4	J	31	0	0	0	0
All	All	67130	0	67210	630	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 5.

The worst 5 of 630 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)
1:J:304:PHE:HB3	1:J:350:THR:HG22	1.63	0.79
1:D:872:VAL:HG21	1:D:896:LEU:HD11	1.64	0.79
1:A:679:LEU:HD23	1:A:737:LEU:HD21	1.67	0.74
1:C:872:VAL:HG21	1:C:896:LEU:HD11	1.69	0.73
1:I:1033:GLU:HG2	1:J:1033:GLU:HG2	1.70	0.73

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	825/1036 (80%)	807 (98%)	17 (2%)	1 (0%)	48	75
1	B	825/1036 (80%)	807 (98%)	17 (2%)	1 (0%)	48	75
1	C	825/1036 (80%)	806 (98%)	18 (2%)	1 (0%)	48	75
1	D	825/1036 (80%)	808 (98%)	16 (2%)	1 (0%)	48	75
1	E	825/1036 (80%)	809 (98%)	15 (2%)	1 (0%)	48	75
1	F	825/1036 (80%)	808 (98%)	16 (2%)	1 (0%)	48	75
1	G	825/1036 (80%)	807 (98%)	17 (2%)	1 (0%)	48	75
1	H	825/1036 (80%)	806 (98%)	18 (2%)	1 (0%)	48	75
1	I	825/1036 (80%)	806 (98%)	18 (2%)	1 (0%)	48	75
1	J	825/1036 (80%)	808 (98%)	16 (2%)	1 (0%)	48	75
All	All	8250/10360 (80%)	8072 (98%)	168 (2%)	10 (0%)	49	75

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	624	GLN
1	B	624	GLN
1	C	624	GLN

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Mol	Chain	Res	Type
1	D	624	GLN
1	E	624	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	754/933 (81%)	743 (98%)	11 (2%)	57	73
1	B	754/933 (81%)	743 (98%)	11 (2%)	57	73
1	C	754/933 (81%)	742 (98%)	12 (2%)	55	72
1	D	754/933 (81%)	744 (99%)	10 (1%)	61	74
1	E	754/933 (81%)	743 (98%)	11 (2%)	57	73
1	F	754/933 (81%)	739 (98%)	15 (2%)	48	69
1	G	754/933 (81%)	745 (99%)	9 (1%)	63	75
1	H	754/933 (81%)	744 (99%)	10 (1%)	61	74
1	I	754/933 (81%)	745 (99%)	9 (1%)	63	75
1	J	754/933 (81%)	744 (99%)	10 (1%)	61	74
All	All	7540/9330 (81%)	7432 (99%)	108 (1%)	57	73

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	288	HIS
1	G	346	LEU
1	J	288	HIS
1	F	346	LEU
1	F	850	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	672	ASN

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Mol	Chain	Res	Type
1	I	672	ASN
1	H	674	HIS
1	I	359	GLN
1	I	1022	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 10 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A1I4G	B	1103	-	34,34,34	2.08	8 (23%)	41,49,49	4.05	13 (31%)
2	ADP	B	1101	3	27,29,29	1.34	4 (14%)	42,45,45	1.96	10 (23%)
2	ADP	G	1101	3	27,29,29	1.34	4 (14%)	42,45,45	1.97	9 (21%)
2	ADP	J	1101	3	27,29,29	1.34	4 (14%)	42,45,45	1.98	9 (21%)
2	ADP	A	1101	3	27,29,29	1.34	4 (14%)	42,45,45	1.98	9 (21%)
4	A1I4G	D	1103	-	34,34,34	2.10	8 (23%)	41,49,49	4.04	13 (31%)
2	ADP	F	1101	3	27,29,29	1.35	4 (14%)	42,45,45	1.98	10 (23%)
2	ADP	H	1101	3	27,29,29	1.34	4 (14%)	42,45,45	1.97	10 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A1I4G	E	1103	-	34,34,34	2.09	8 (23%)	41,49,49	4.00	13 (31%)
2	ADP	D	1101	3	27,29,29	1.35	4 (14%)	42,45,45	1.98	9 (21%)
4	A1I4G	H	1103	-	34,34,34	2.09	8 (23%)	41,49,49	4.02	13 (31%)
2	ADP	C	1101	3	27,29,29	1.33	4 (14%)	42,45,45	1.98	9 (21%)
4	A1I4G	A	1103	-	34,34,34	2.11	8 (23%)	41,49,49	4.06	13 (31%)
2	ADP	I	1101	3	27,29,29	1.35	4 (14%)	42,45,45	1.96	10 (23%)
4	A1I4G	G	1103	-	34,34,34	2.09	7 (20%)	41,49,49	3.99	13 (31%)
4	A1I4G	J	1103	-	34,34,34	2.10	8 (23%)	41,49,49	4.02	13 (31%)
2	ADP	E	1101	3	27,29,29	1.34	4 (14%)	42,45,45	1.97	9 (21%)
4	A1I4G	C	1103	-	34,34,34	2.08	7 (20%)	41,49,49	4.01	13 (31%)
4	A1I4G	F	1103	-	34,34,34	2.09	7 (20%)	41,49,49	3.99	12 (29%)
4	A1I4G	I	1103	-	34,34,34	2.10	8 (23%)	41,49,49	4.06	13 (31%)

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
4	A1I4G	B	1103	-	-	3/23/23/23	0/4/4/4
2	ADP	B	1101	3	-	4/16/32/32	0/3/3/3
2	ADP	G	1101	3	-	4/16/32/32	0/3/3/3
2	ADP	J	1101	3	-	2/16/32/32	0/3/3/3
2	ADP	A	1101	3	-	4/16/32/32	0/3/3/3
4	A1I4G	D	1103	-	-	3/23/23/23	0/4/4/4
2	ADP	F	1101	3	-	4/16/32/32	0/3/3/3
2	ADP	H	1101	3	-	4/16/32/32	0/3/3/3
4	A1I4G	E	1103	-	-	3/23/23/23	0/4/4/4
2	ADP	D	1101	3	-	3/16/32/32	0/3/3/3
4	A1I4G	H	1103	-	-	3/23/23/23	0/4/4/4
2	ADP	C	1101	3	-	4/16/32/32	0/3/3/3
4	A1I4G	A	1103	-	-	2/23/23/23	0/4/4/4
2	ADP	I	1101	3	-	4/16/32/32	0/3/3/3
4	A1I4G	G	1103	-	-	3/23/23/23	0/4/4/4
4	A1I4G	J	1103	-	-	3/23/23/23	0/4/4/4
2	ADP	E	1101	3	-	4/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1I4G	C	1103	-	-	3/23/23/23	0/4/4/4
4	A1I4G	F	1103	-	-	3/23/23/23	0/4/4/4
4	A1I4G	I	1103	-	-	3/23/23/23	0/4/4/4

The worst 5 of 117 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1103	A1I4G	C13-N11	6.48	1.47	1.34
4	A	1103	A1I4G	C13-N11	6.46	1.47	1.34
4	I	1103	A1I4G	C13-N11	6.46	1.47	1.34
4	J	1103	A1I4G	C13-N11	6.44	1.47	1.34
4	F	1103	A1I4G	C13-N11	6.43	1.47	1.34

The worst 5 of 223 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1103	A1I4G	C03-C07-N06	-12.87	107.32	111.41
4	A	1103	A1I4G	C03-C07-N06	-12.87	107.32	111.41
4	B	1103	A1I4G	C03-C07-N06	-12.76	107.36	111.41
4	J	1103	A1I4G	C03-C07-N06	-12.76	107.36	111.41
4	D	1103	A1I4G	C03-C07-N06	-12.70	107.38	111.41

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

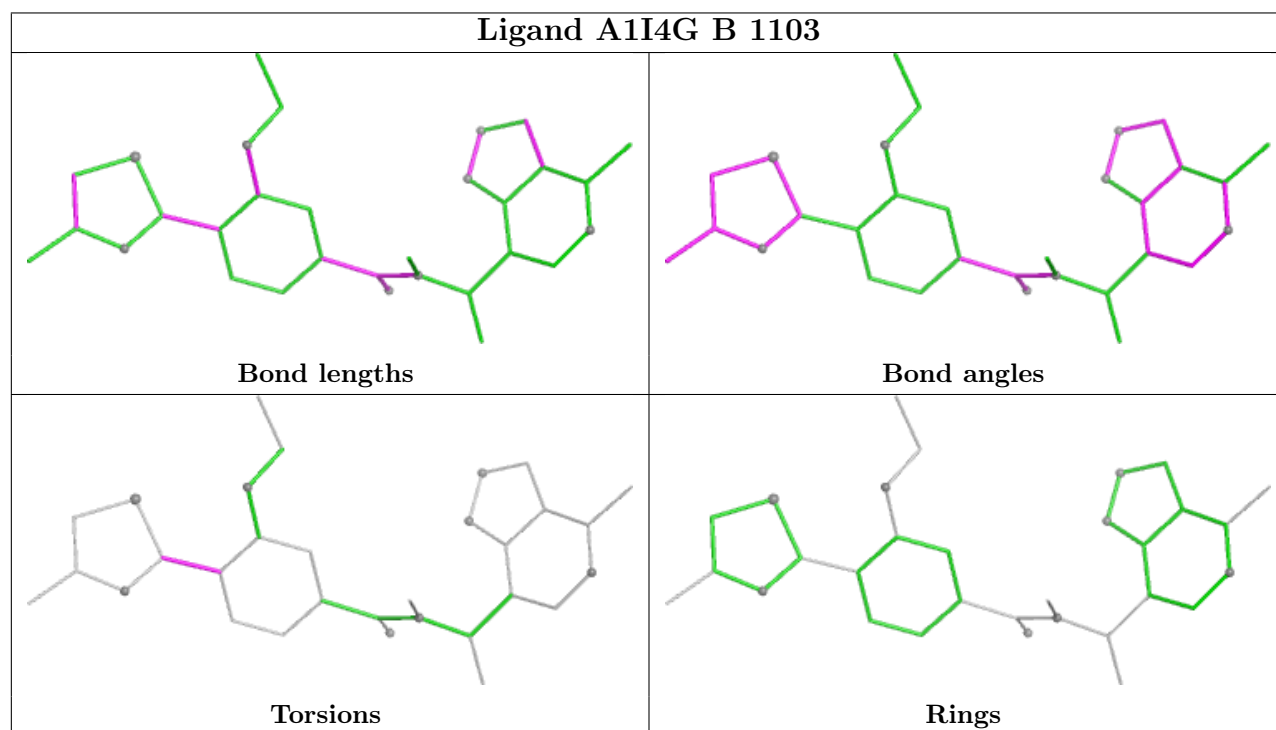
Mol	Chain	Res	Type	Atoms
2	A	1101	ADP	C5'-O5'-PA-O3A
2	B	1101	ADP	C5'-O5'-PA-O3A
2	C	1101	ADP	C5'-O5'-PA-O3A
2	D	1101	ADP	C5'-O5'-PA-O1A
2	D	1101	ADP	C5'-O5'-PA-O3A

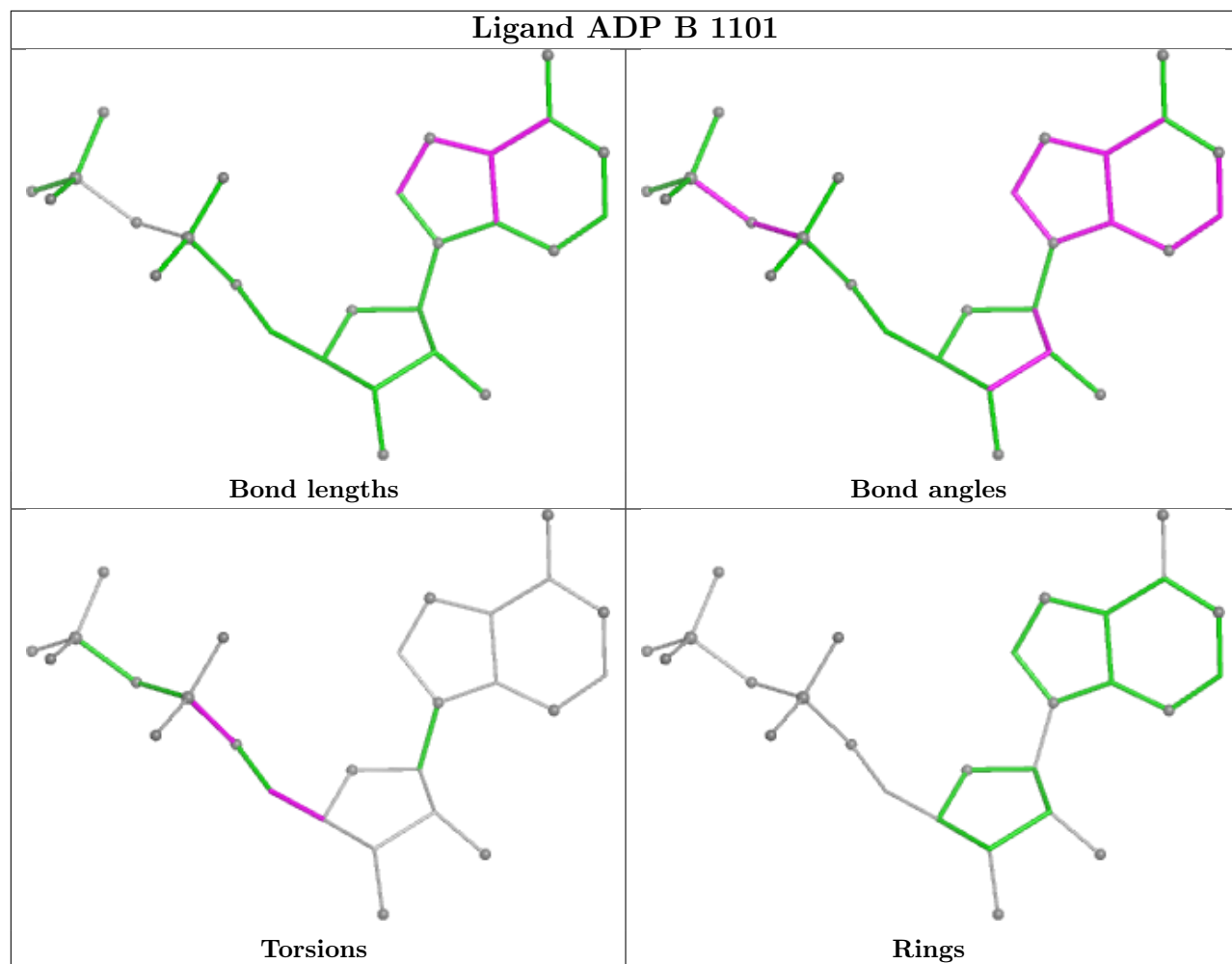
There are no ring outliers.

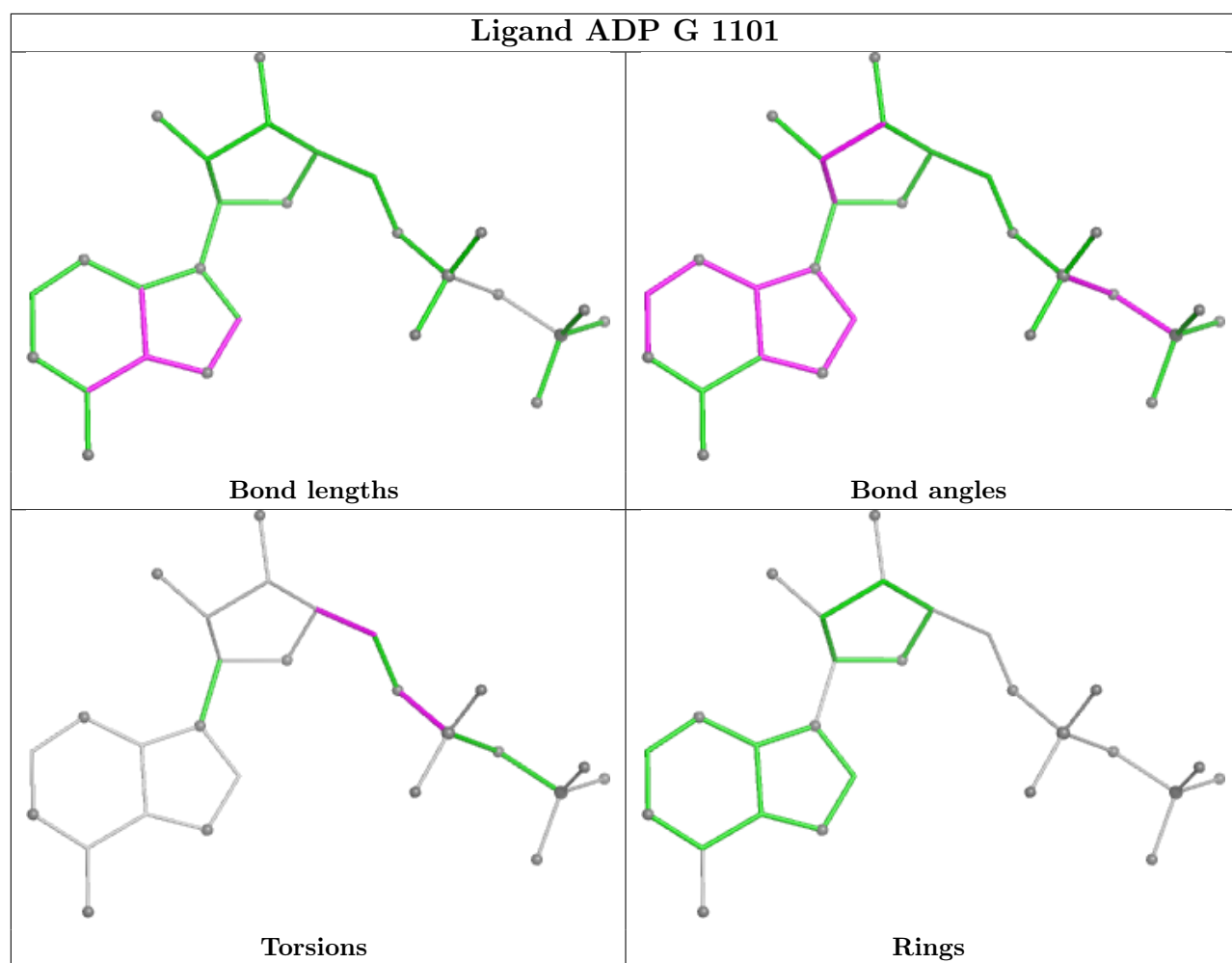
No monomer is involved in short contacts.

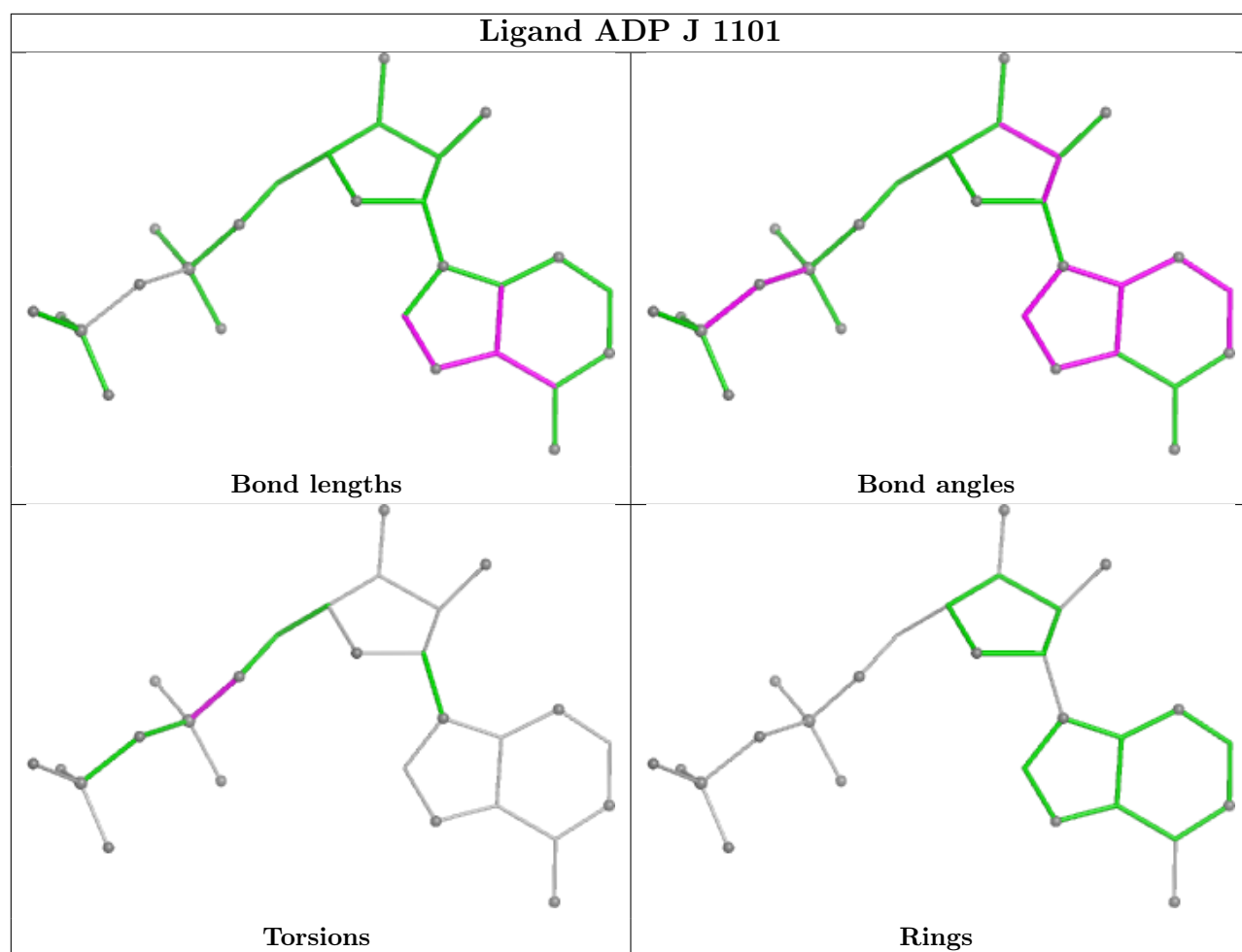
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

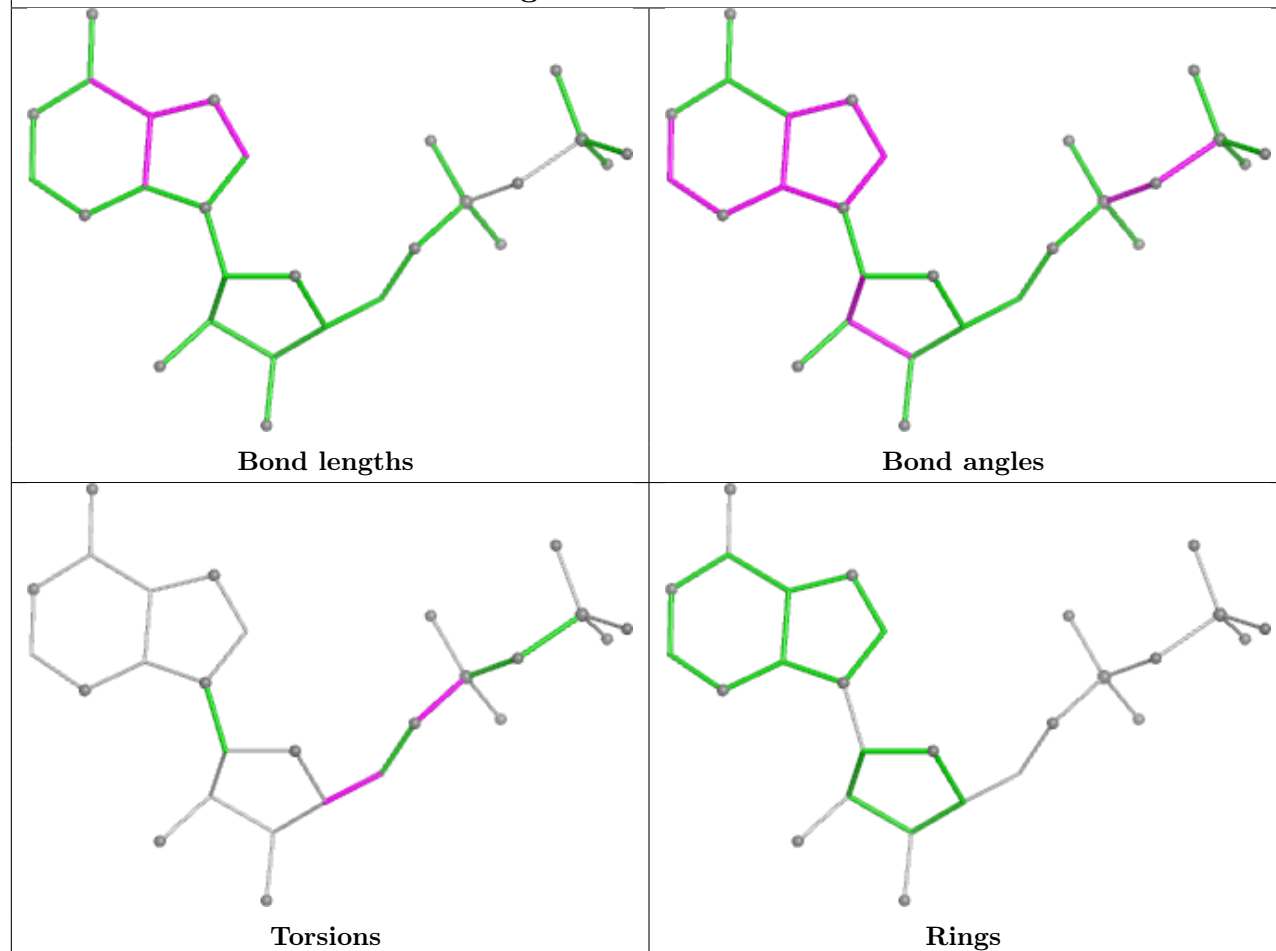




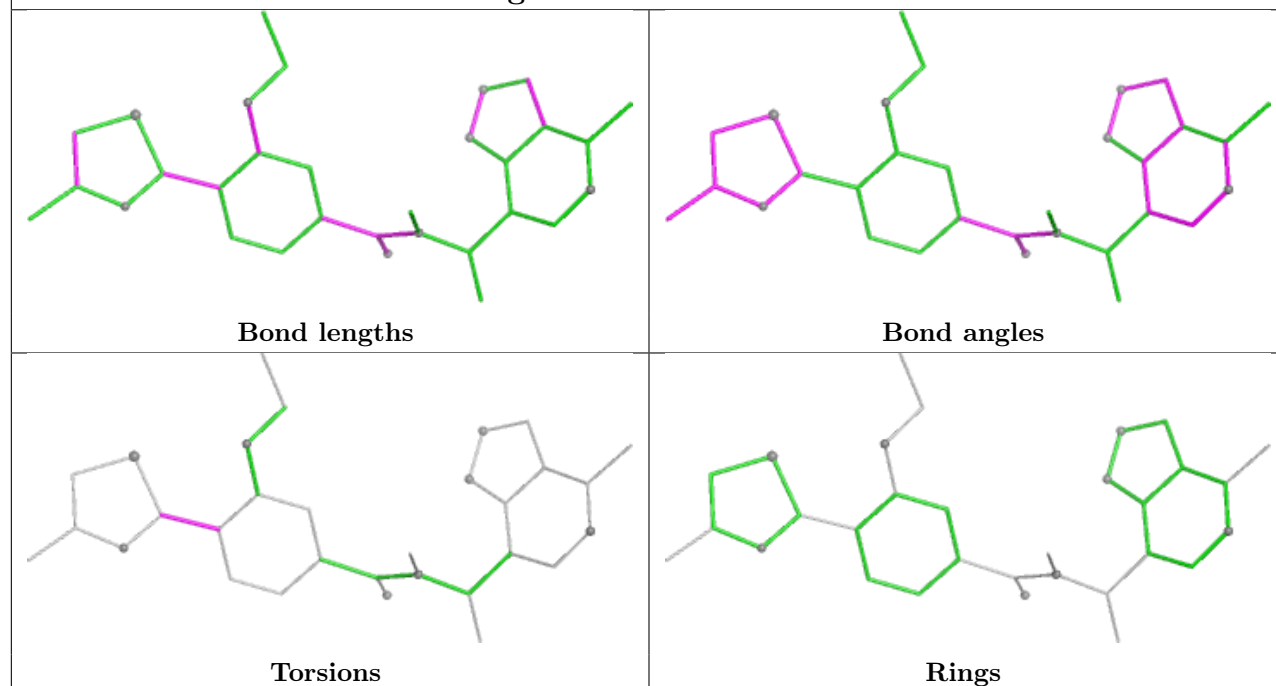


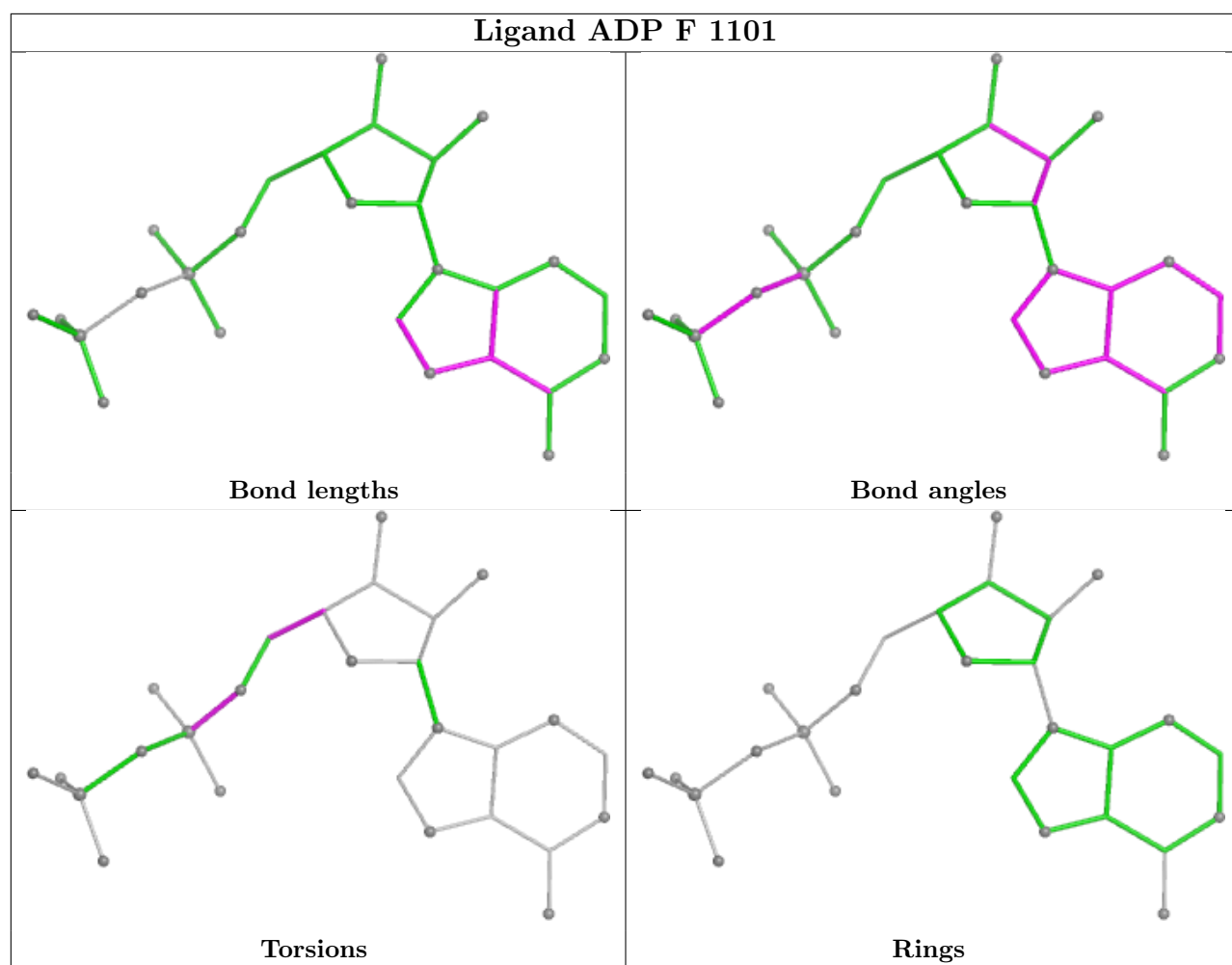


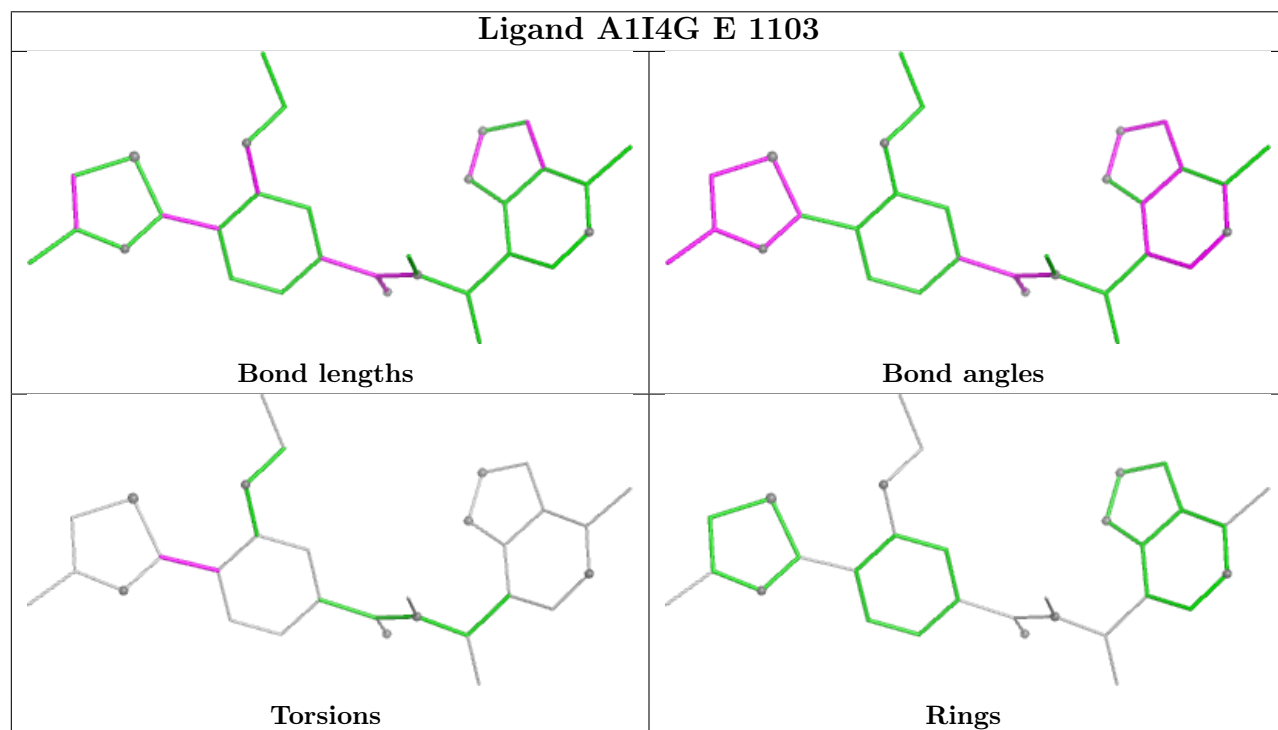
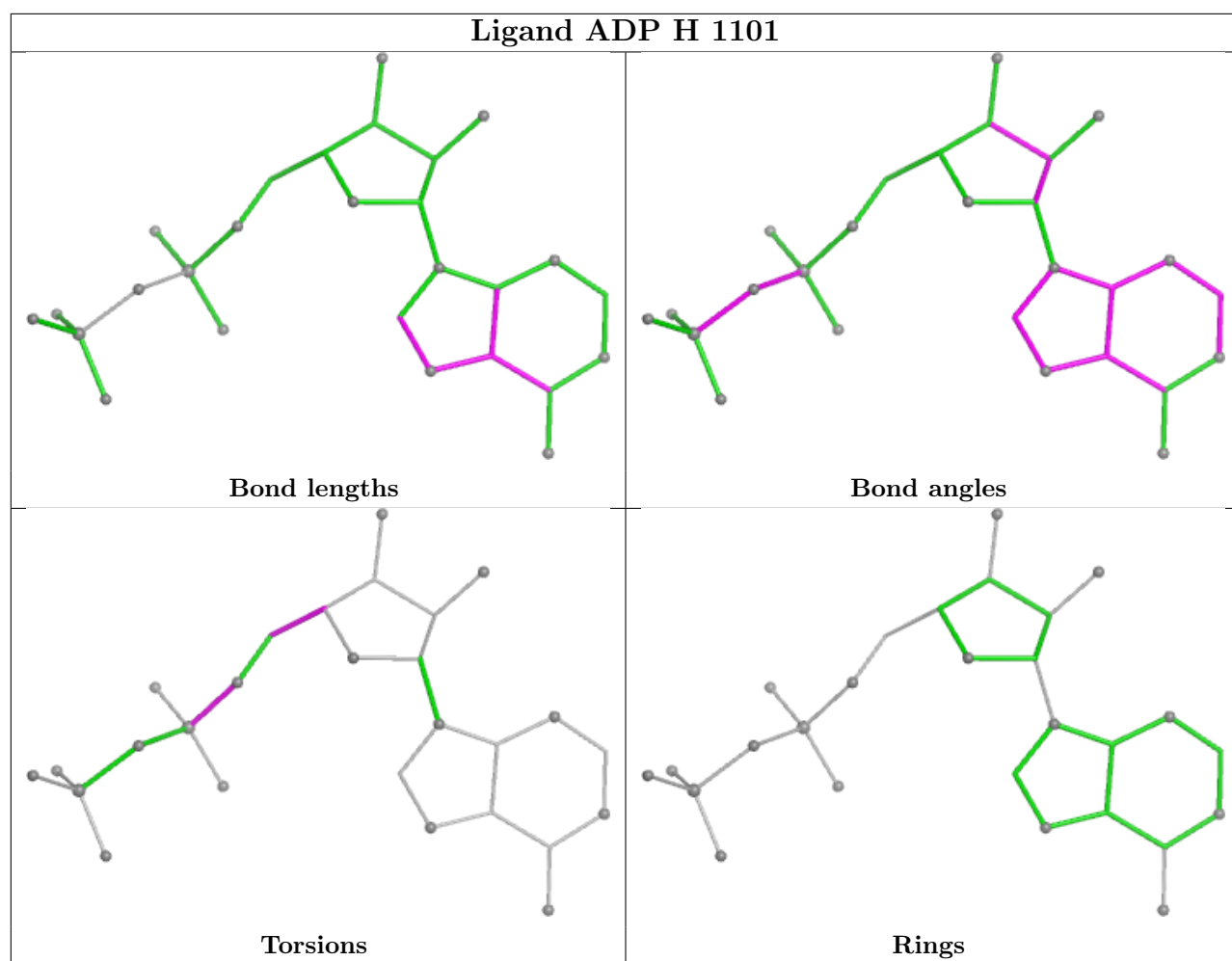
Ligand ADP A 1101

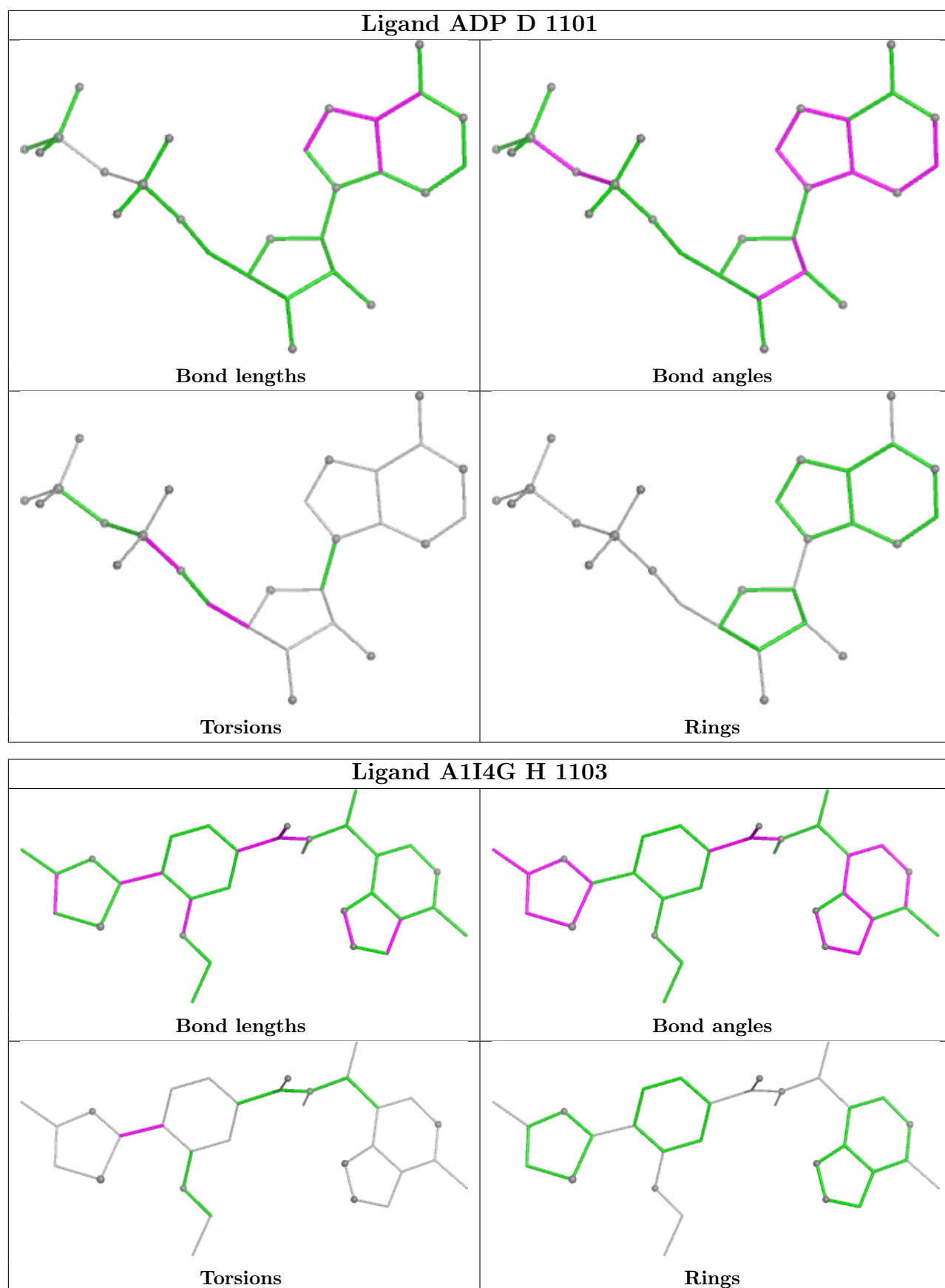


Ligand A1I4G D 1103

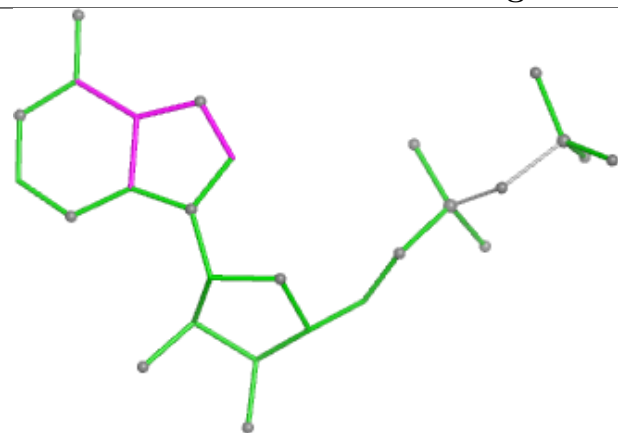




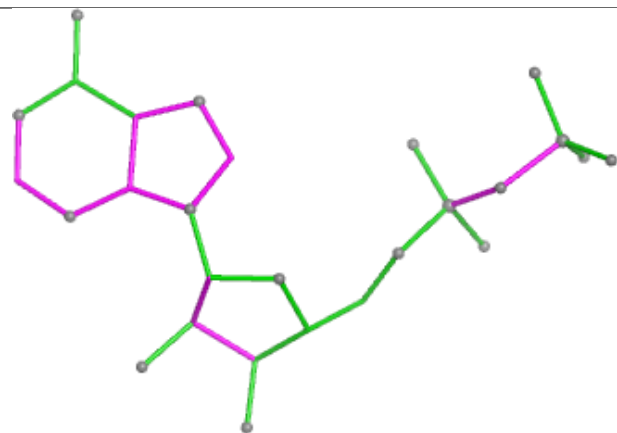




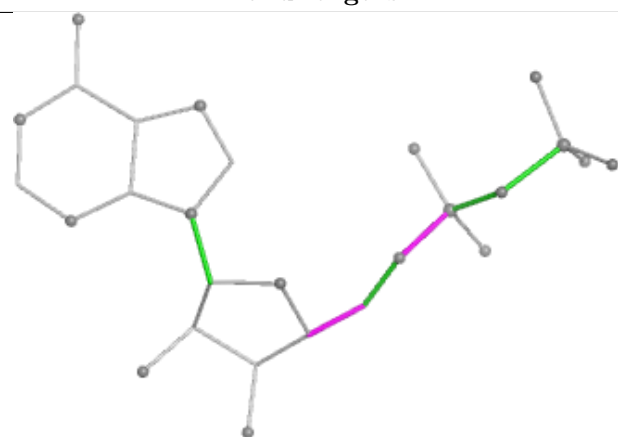
Ligand ADP C 1101



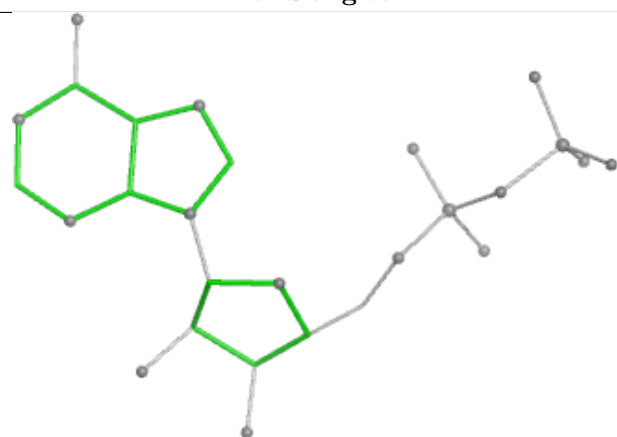
Bond lengths



Bond angles

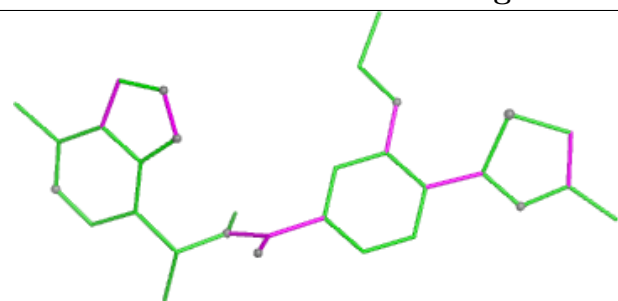


Torsions

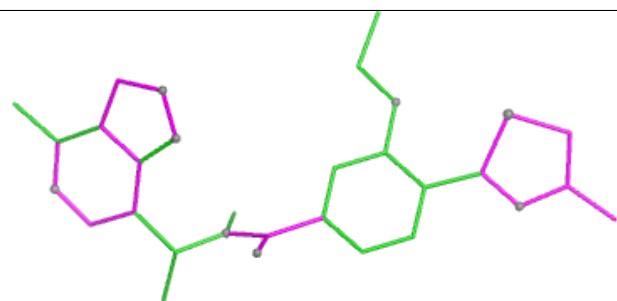


Rings

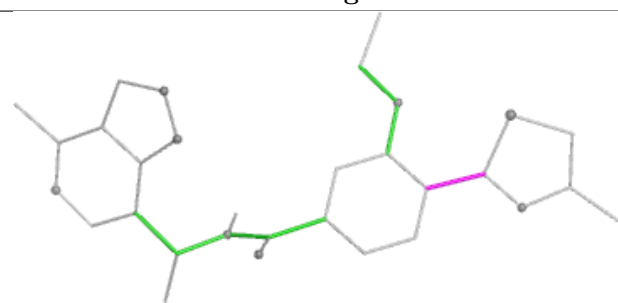
Ligand A1I4G A 1103



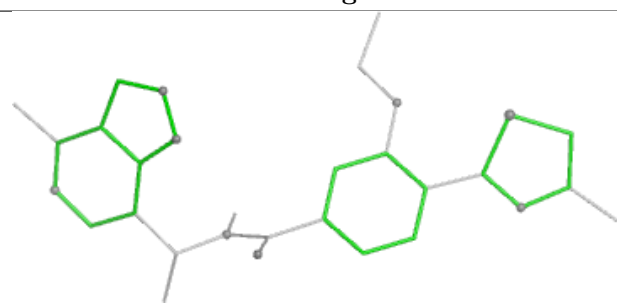
Bond lengths



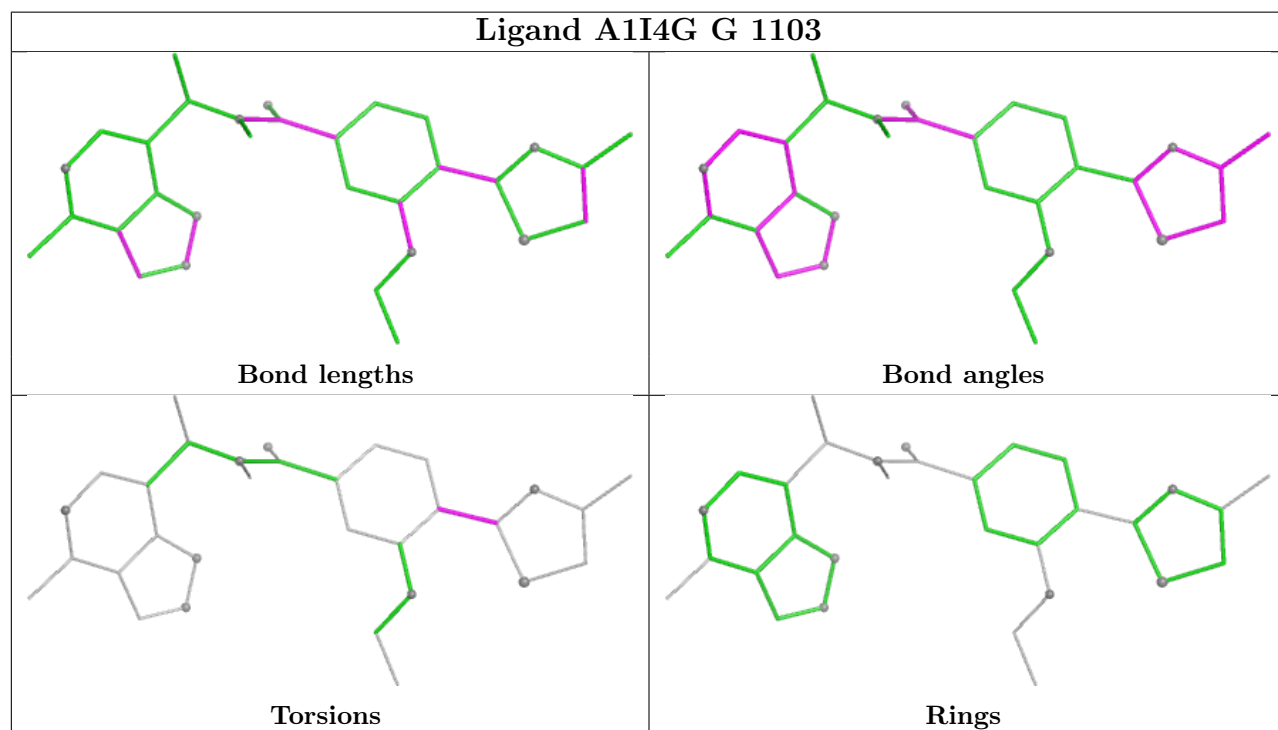
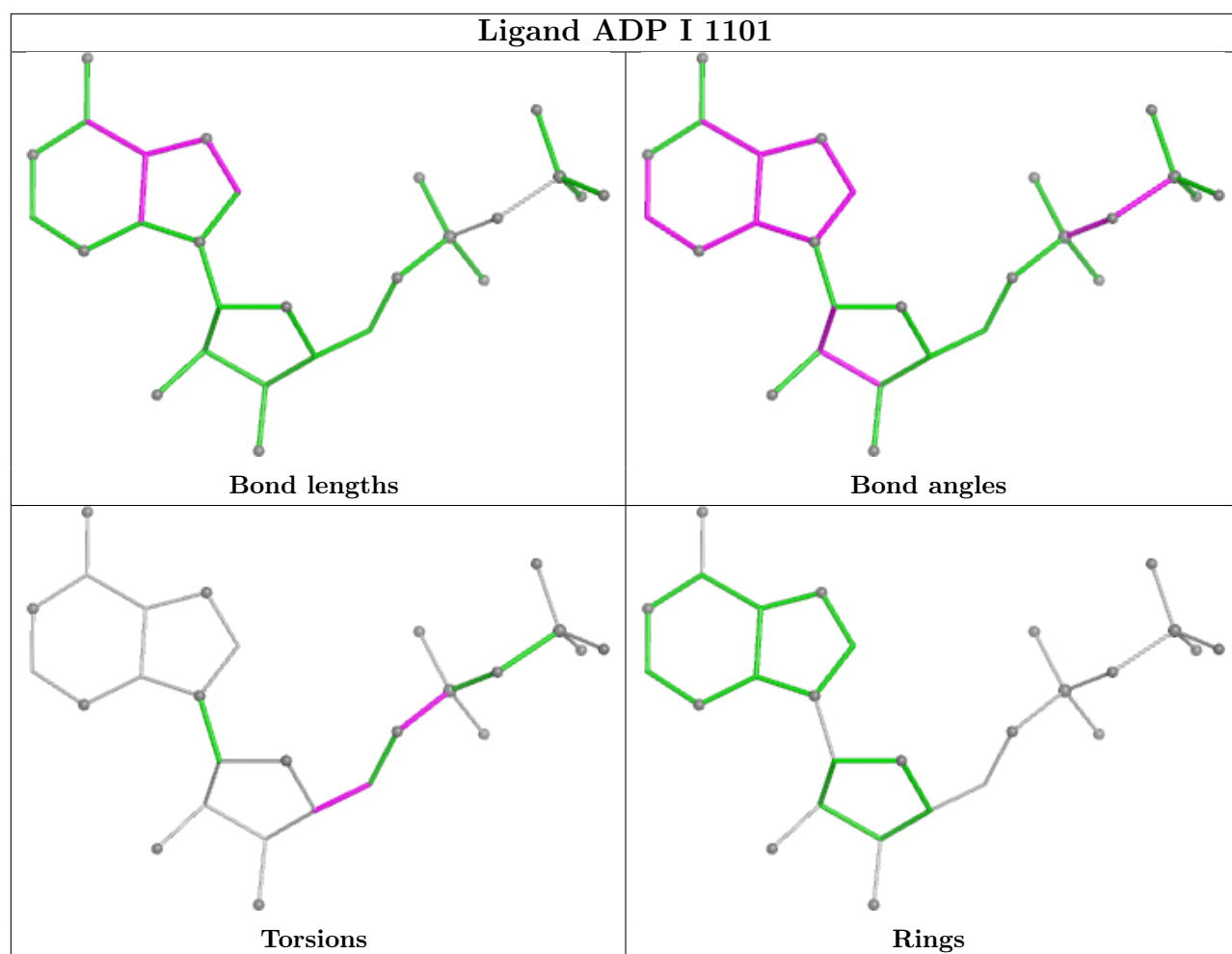
Bond angles



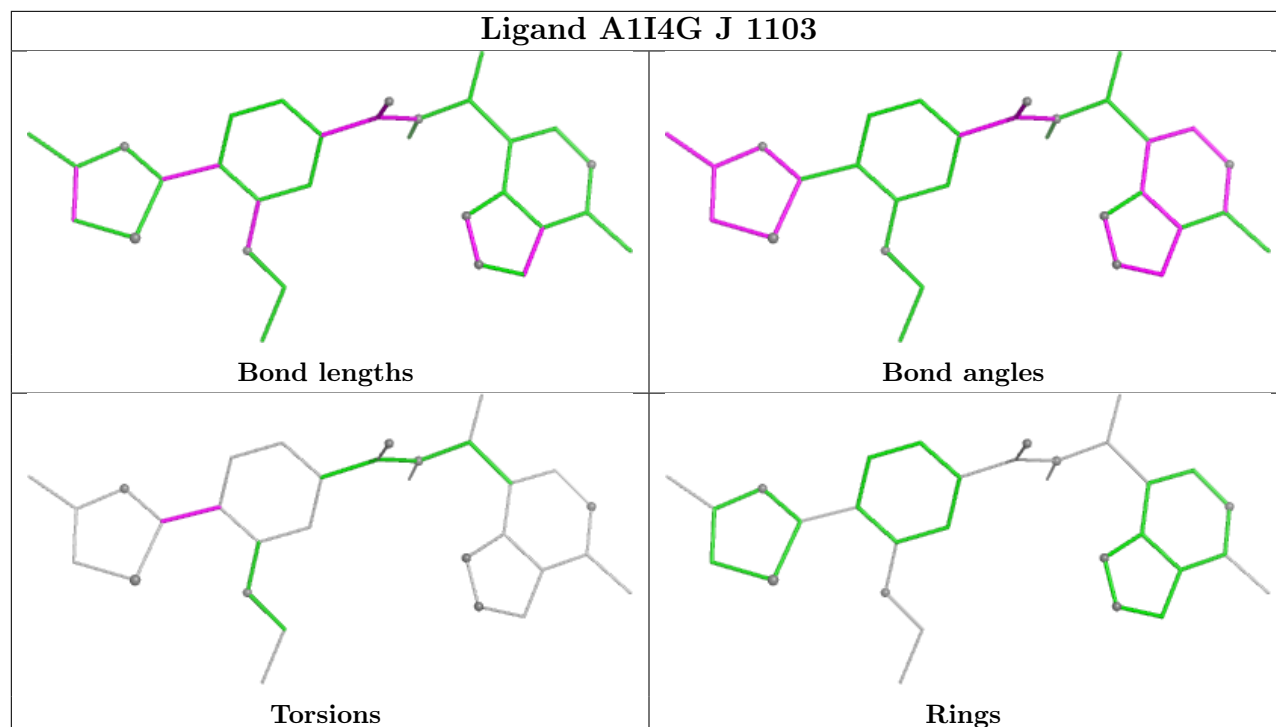
Torsions



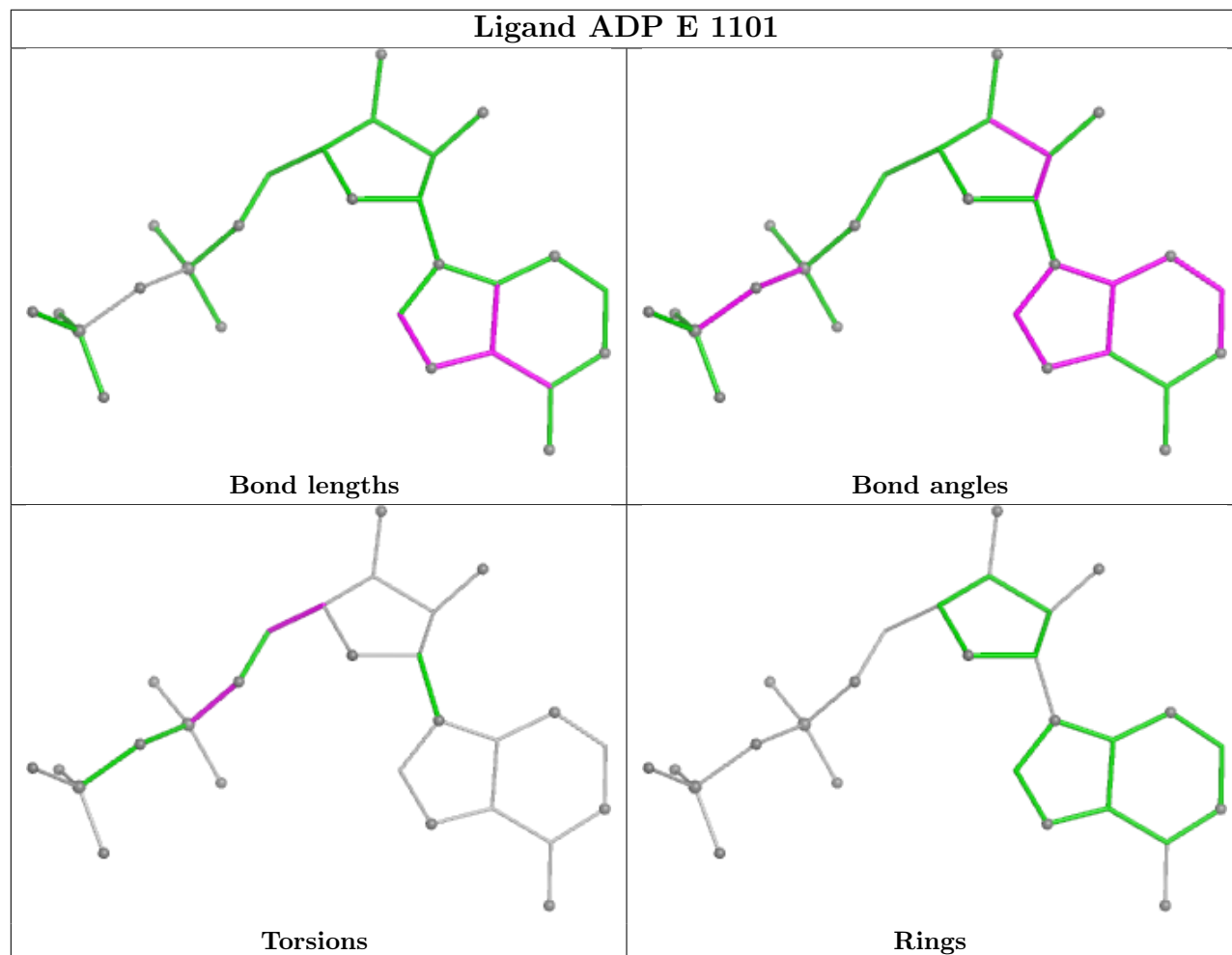
Rings



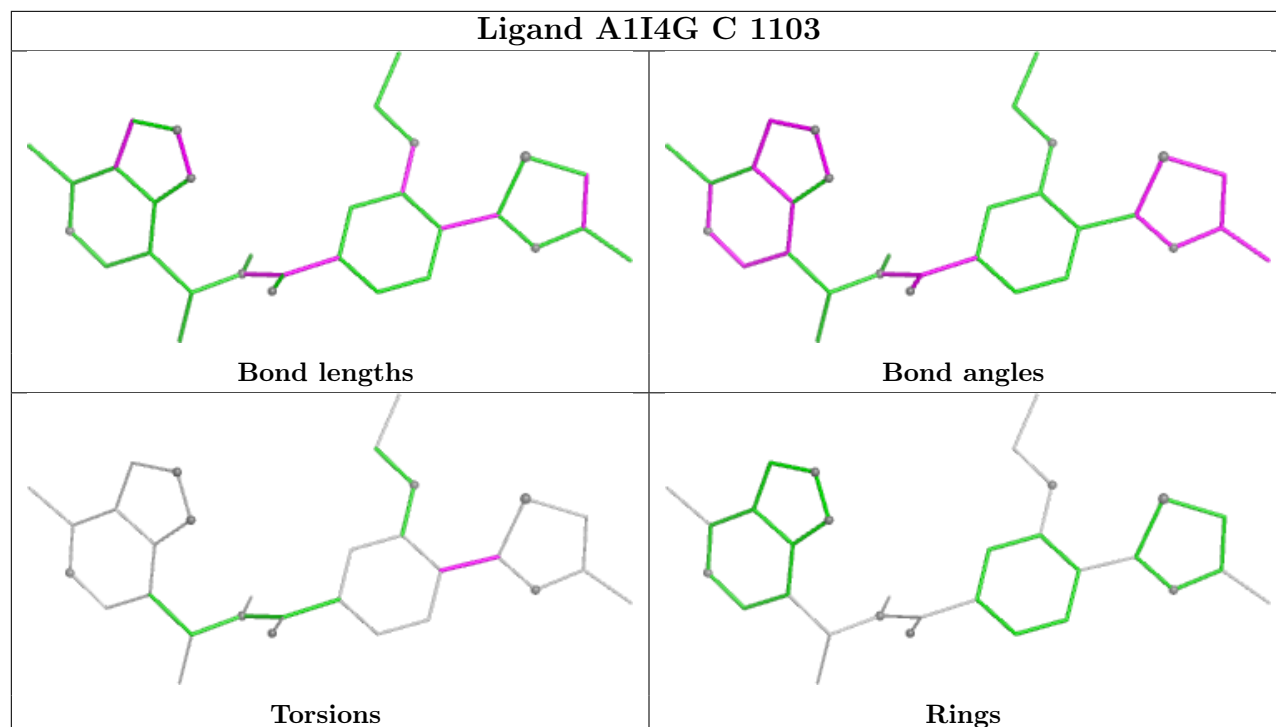
Ligand A1I4G J 1103



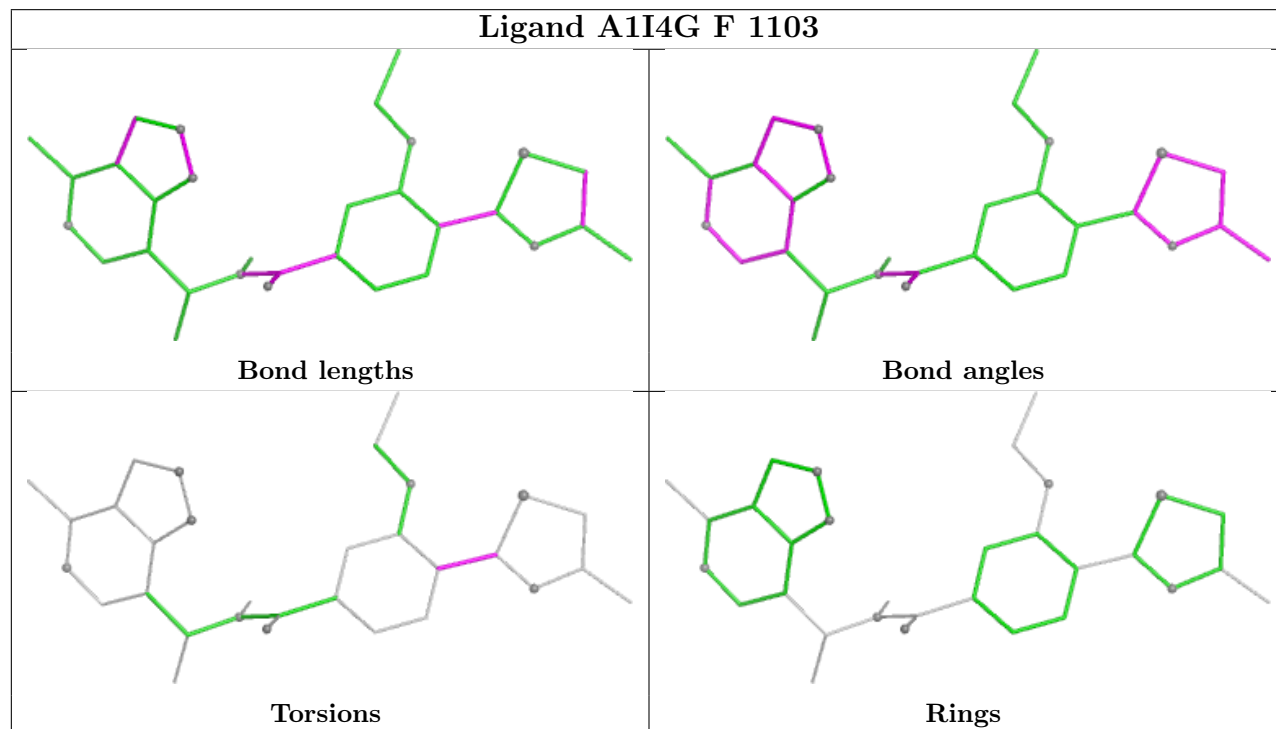
Ligand ADP E 1101

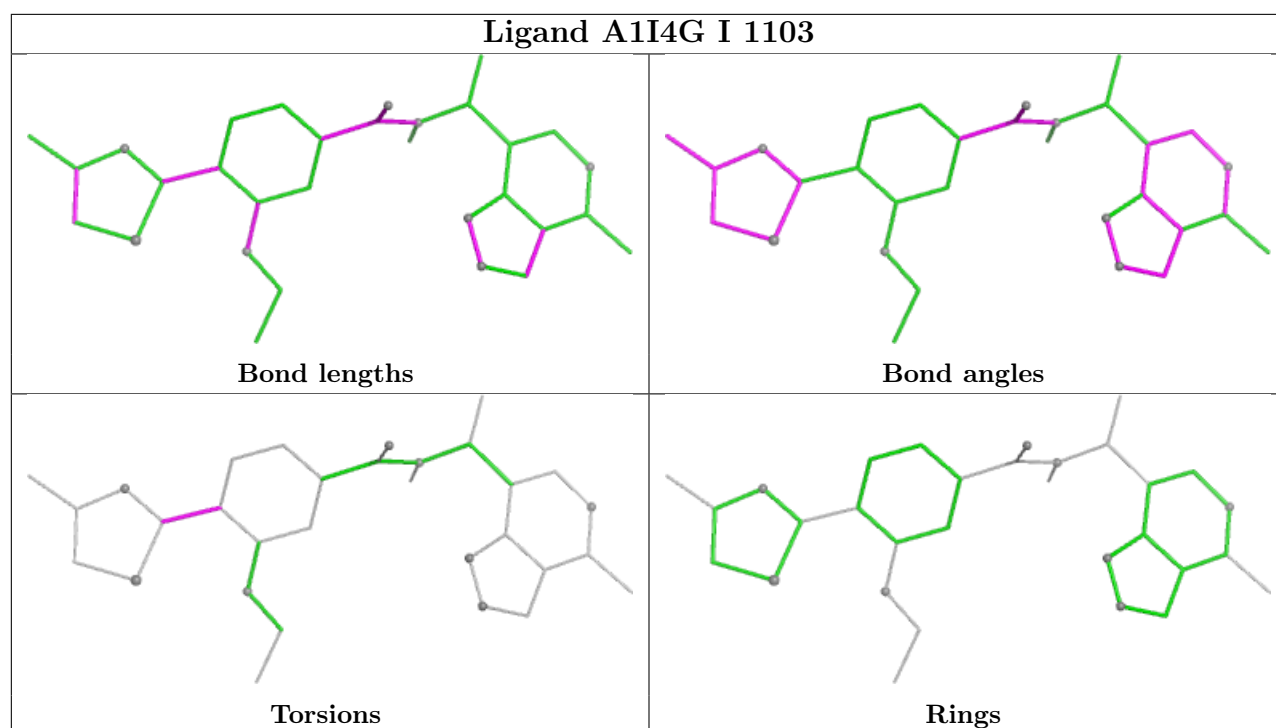


Ligand A1I4G C 1103



Ligand A1I4G F 1103





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

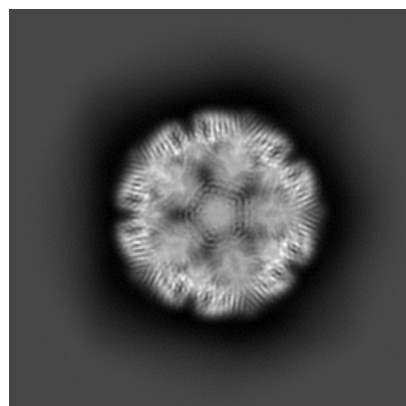
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52908. These allow visual inspection of the internal detail of the map and identification of artifacts.

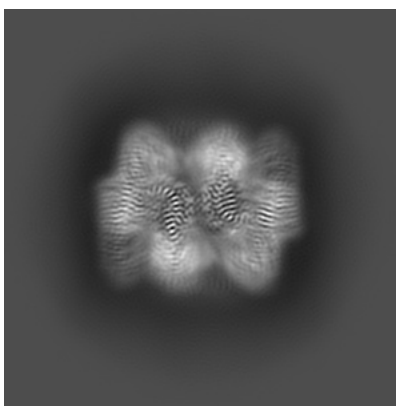
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

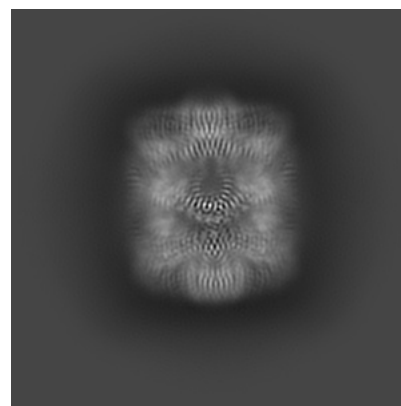
6.1.1 Primary map



X

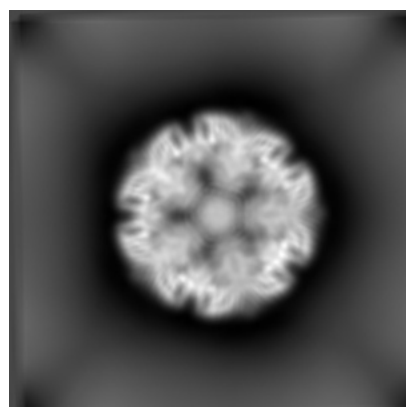


Y

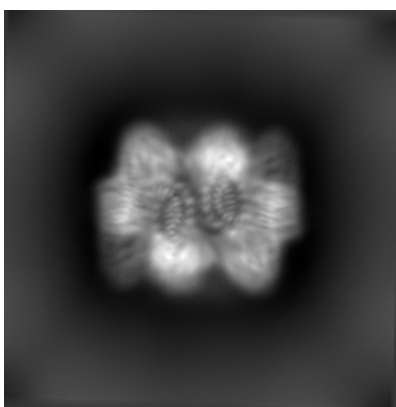


Z

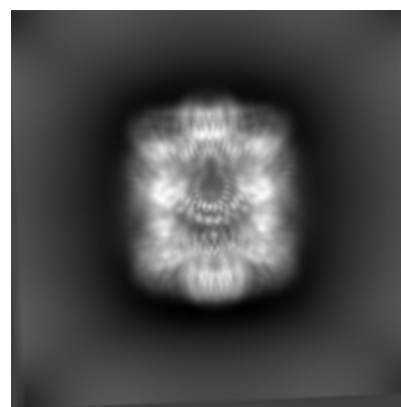
6.1.2 Raw map



X



Y

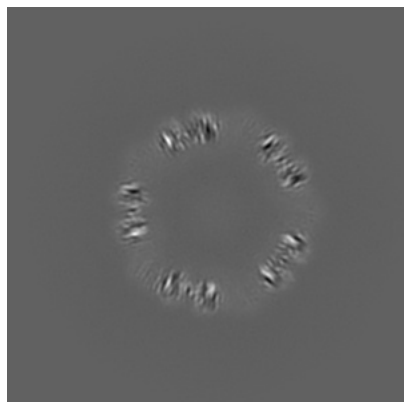


Z

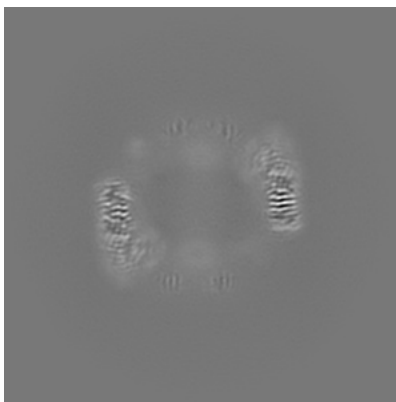
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

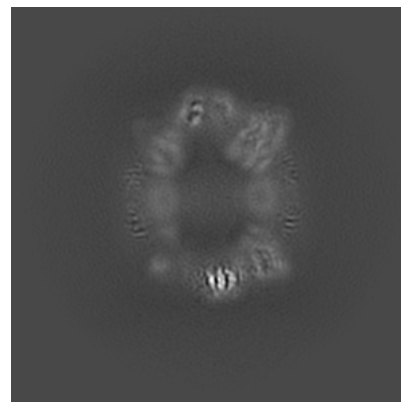
6.2.1 Primary map



X Index: 162

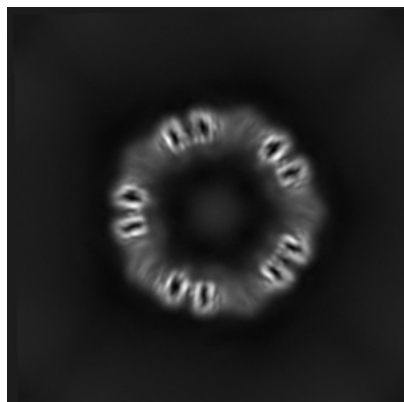


Y Index: 162

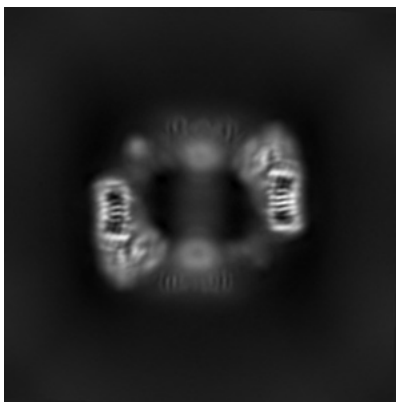


Z Index: 162

6.2.2 Raw map



X Index: 162



Y Index: 162

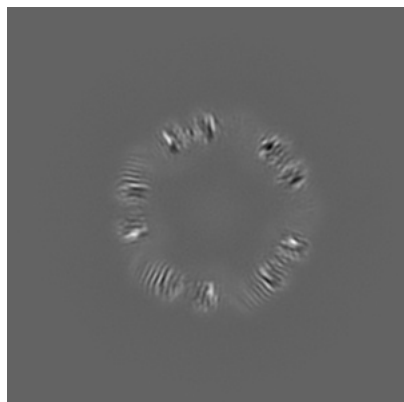


Z Index: 162

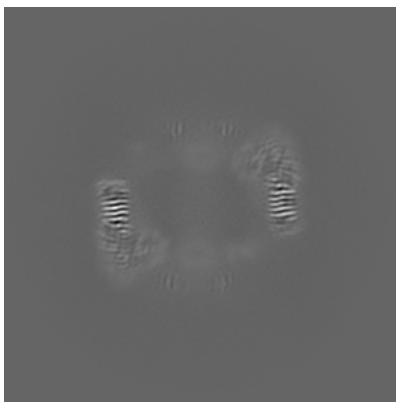
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

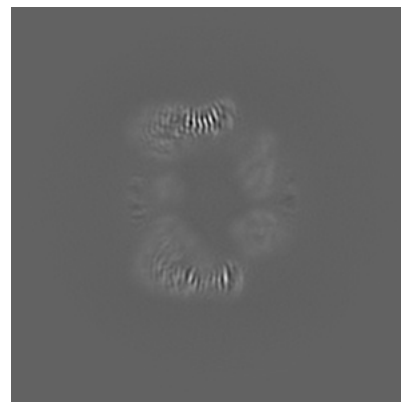
6.3.1 Primary map



X Index: 157

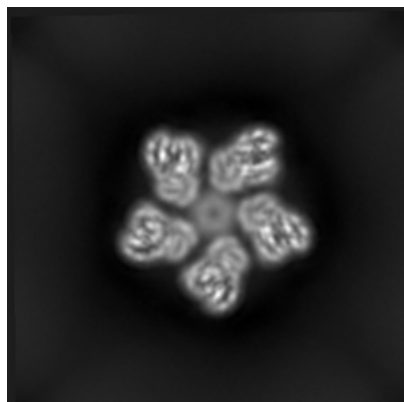


Y Index: 165



Z Index: 134

6.3.2 Raw map



X Index: 123



Y Index: 211

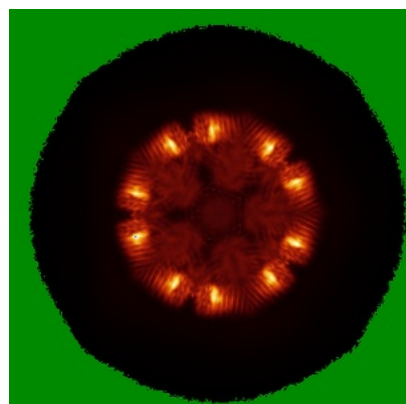


Z Index: 134

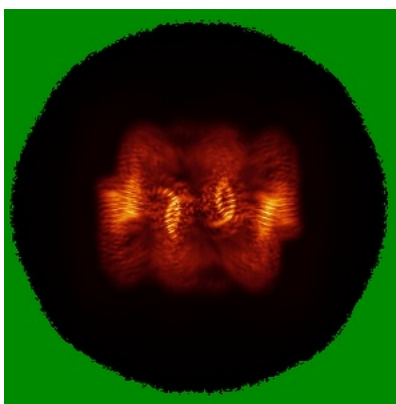
The images above show the largest variance slices of the map in three orthogonal directions.

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

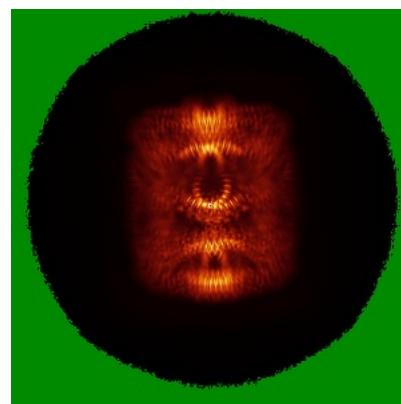
6.4.1 Primary map



X

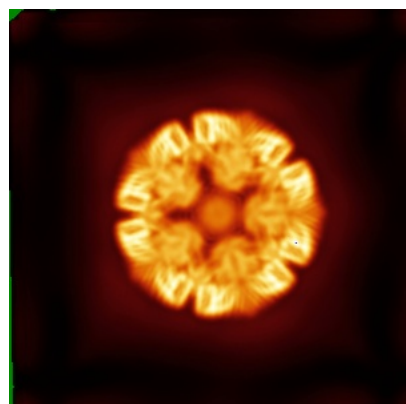


Y

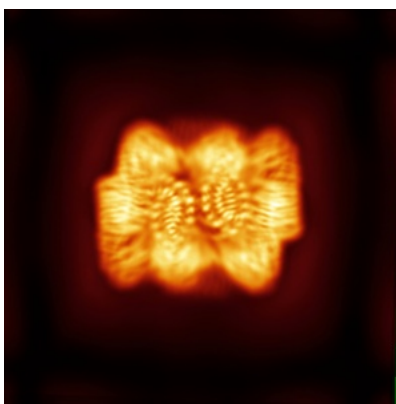


Z

6.4.2 Raw map



X



Y

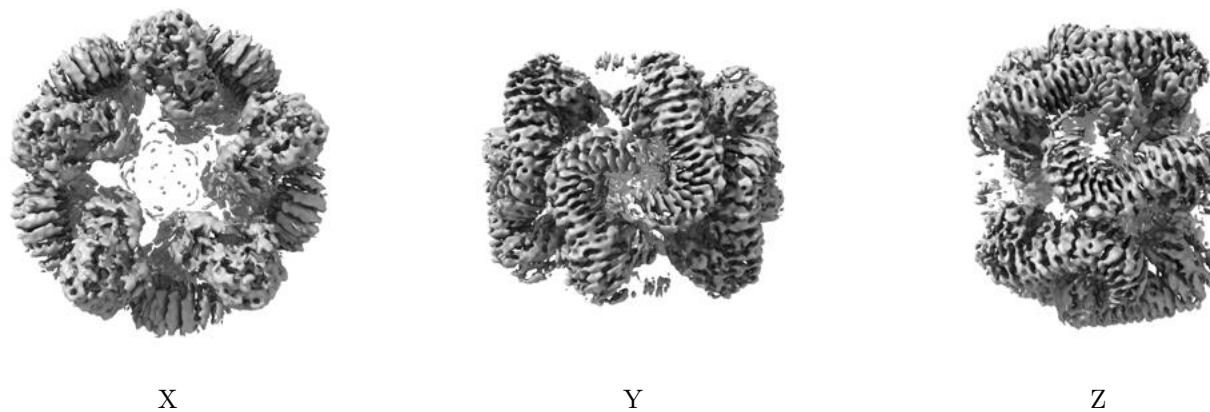


Z

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.

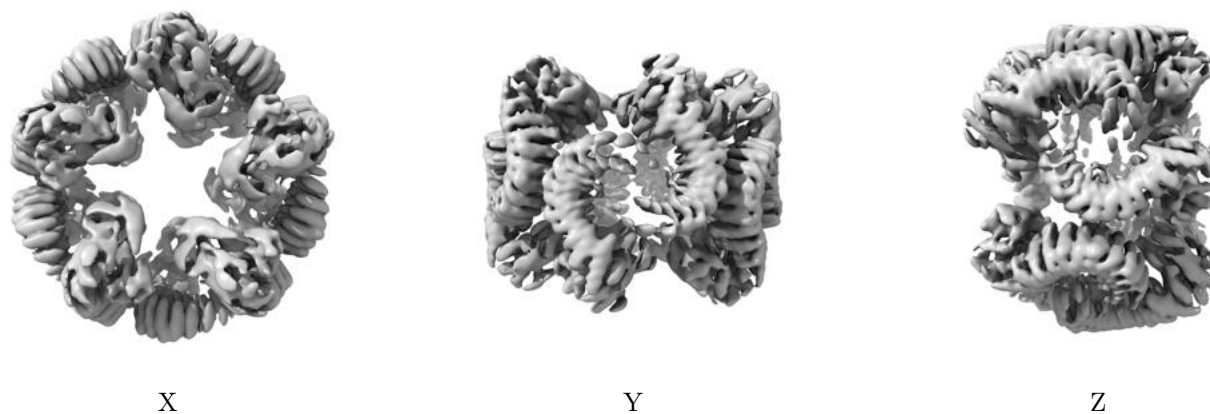
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.744. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

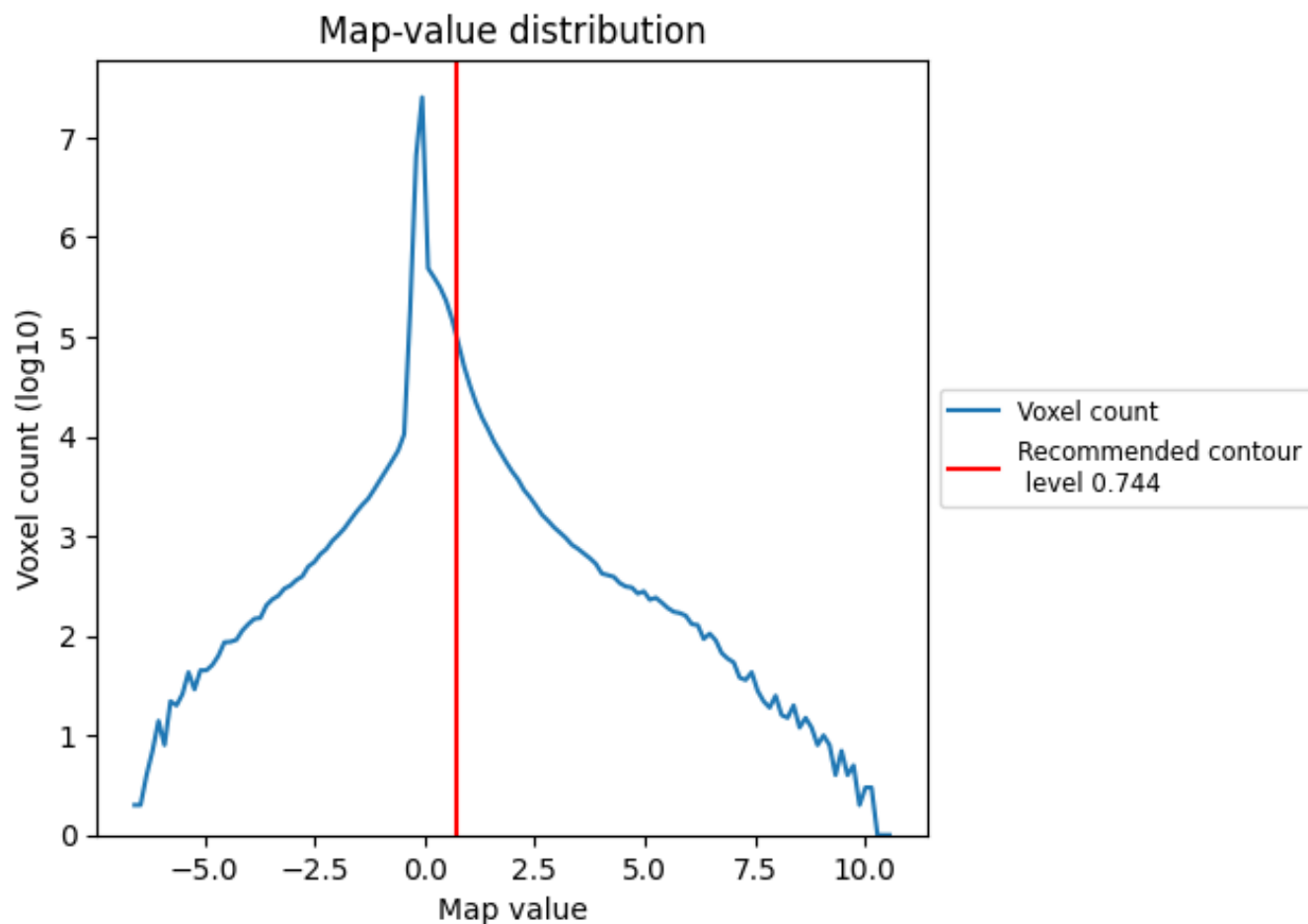
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

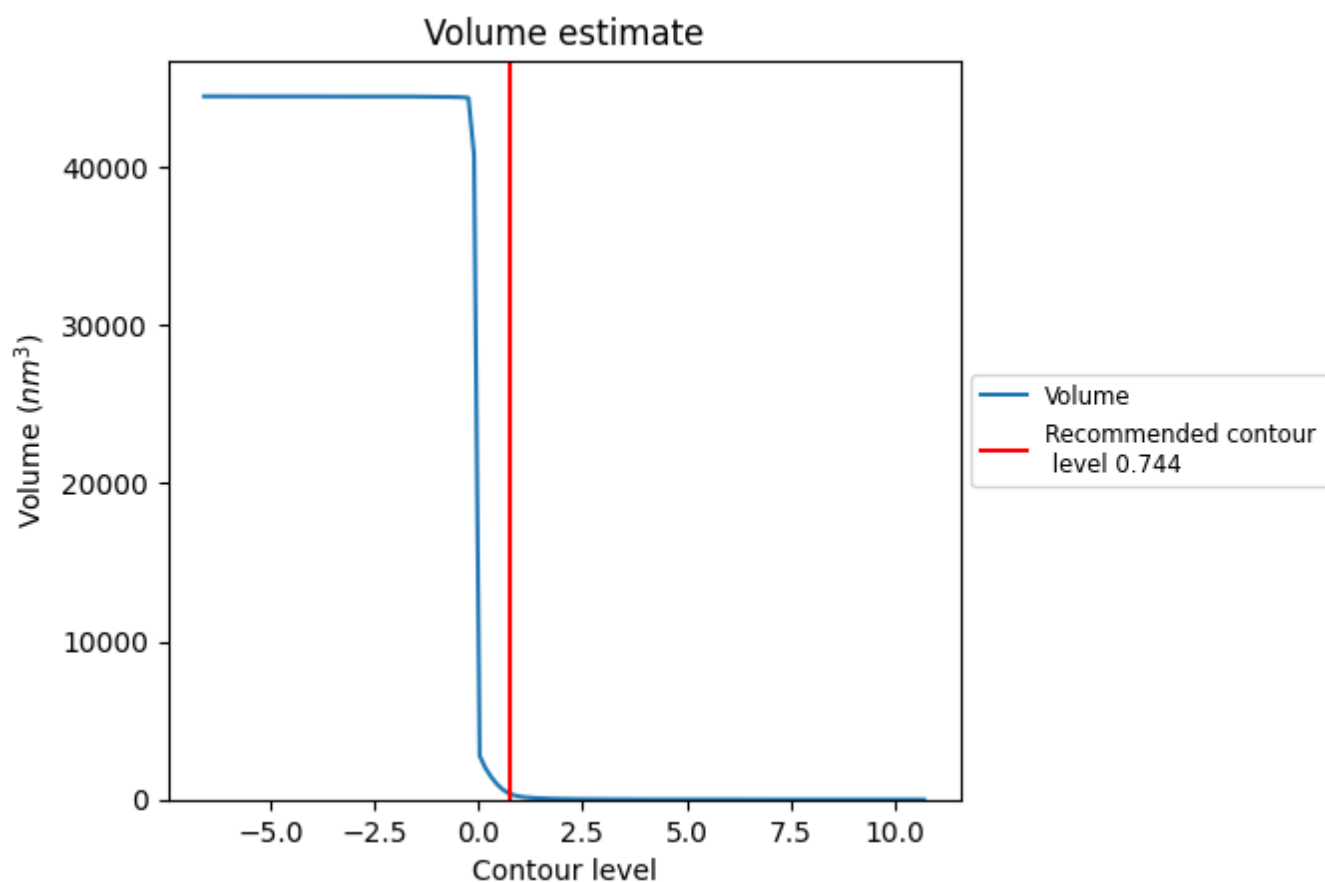
This section contains the results of statistical analysis of the map.

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.

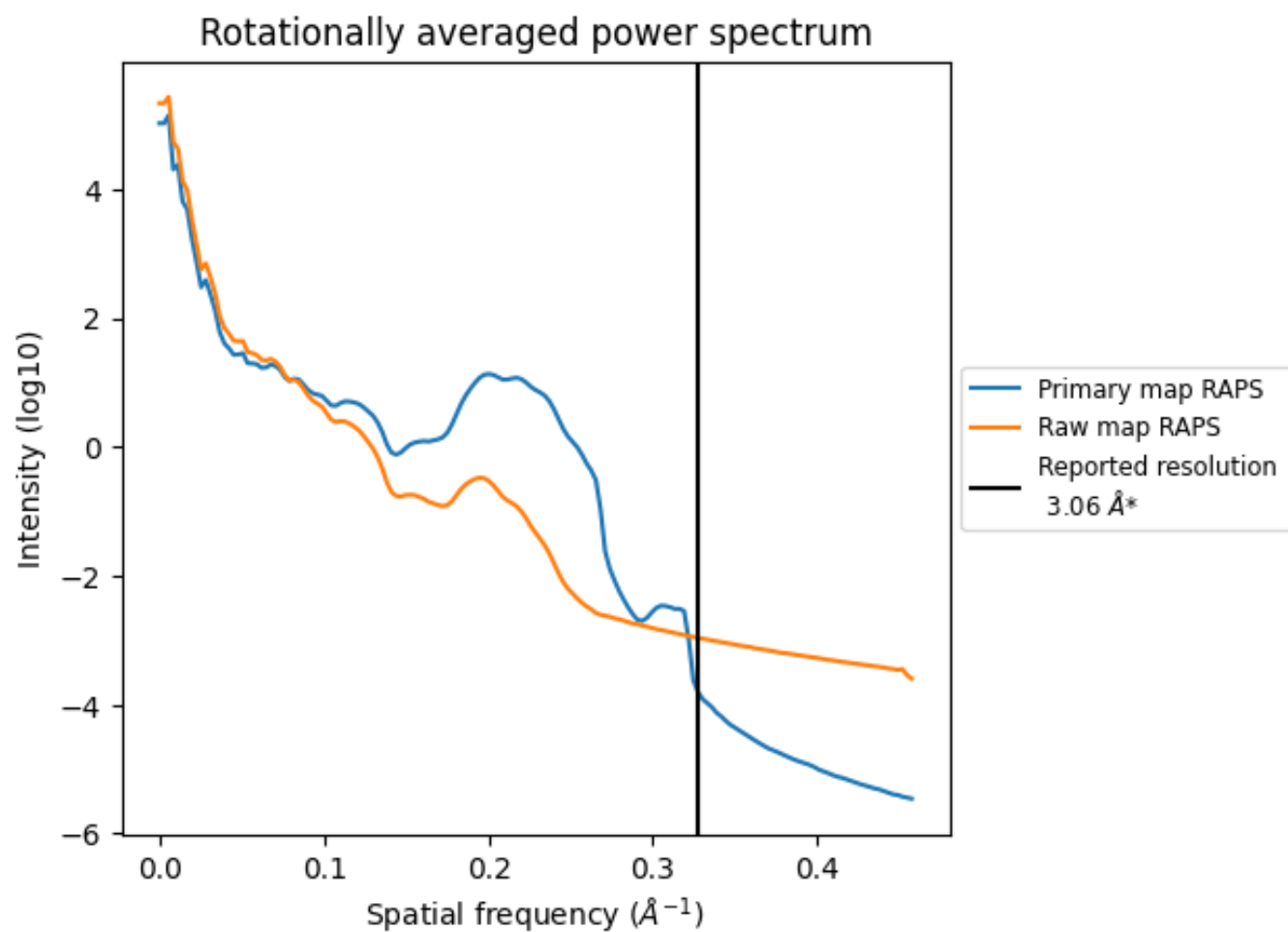
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 384 nm³; this corresponds to an approximate mass of 347 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 ⓘ

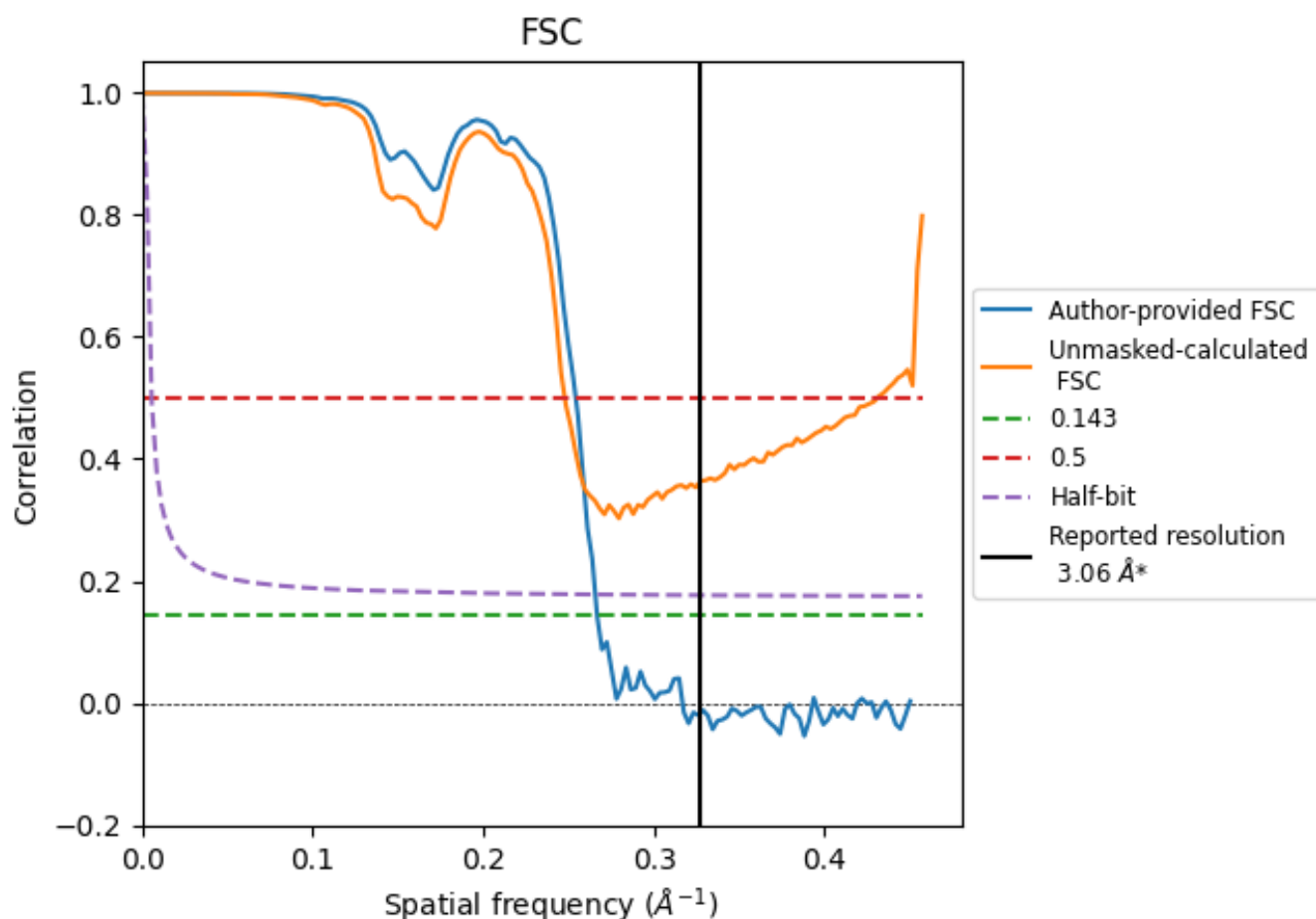


*Reported resolution corresponds to spatial frequency of 0.327 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.327 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

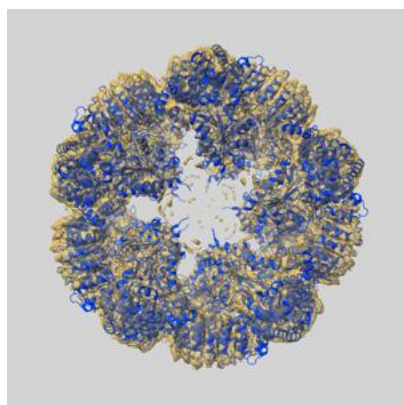
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	3.75	3.93	3.76
Unmasked-calculated*	-	4.04	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.75 differs from the reported value 3.06 by more than 10 %

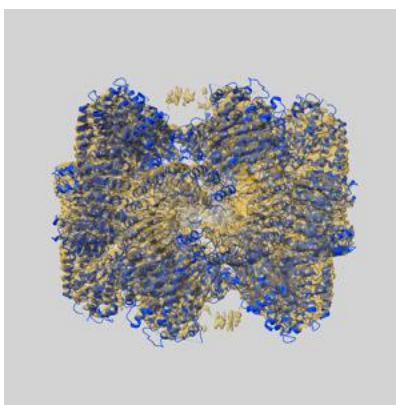
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52908 and PDB model 9Q8V. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

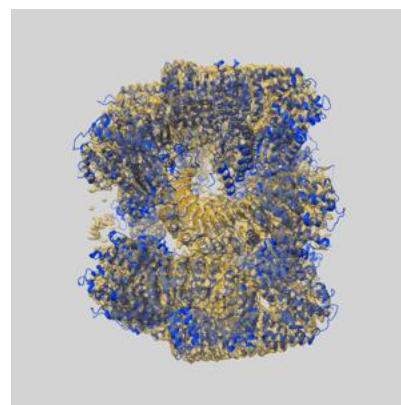
9.1 Map-model overlay [i](#)



X



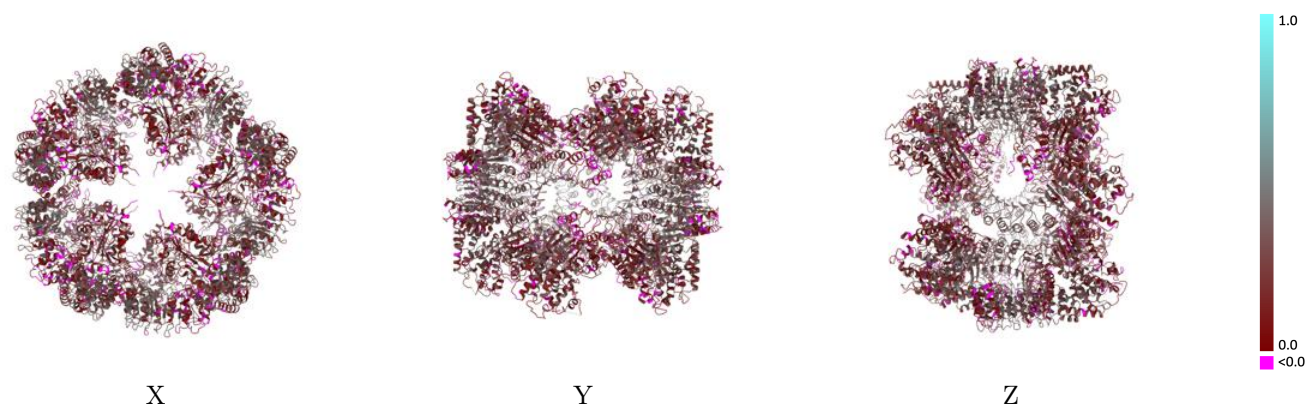
Y



Z

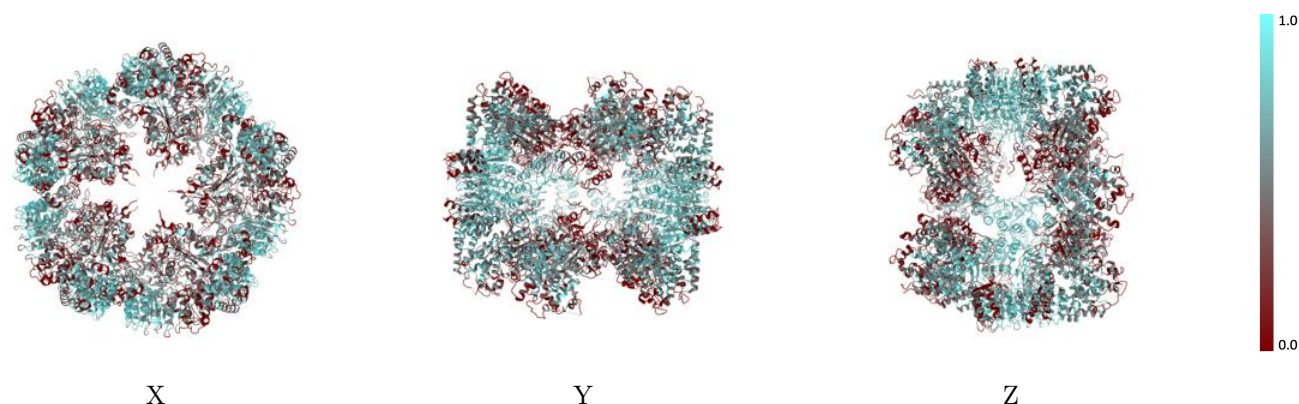
The images above show the 3D surface view of the map at the recommended contour level 0.744 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



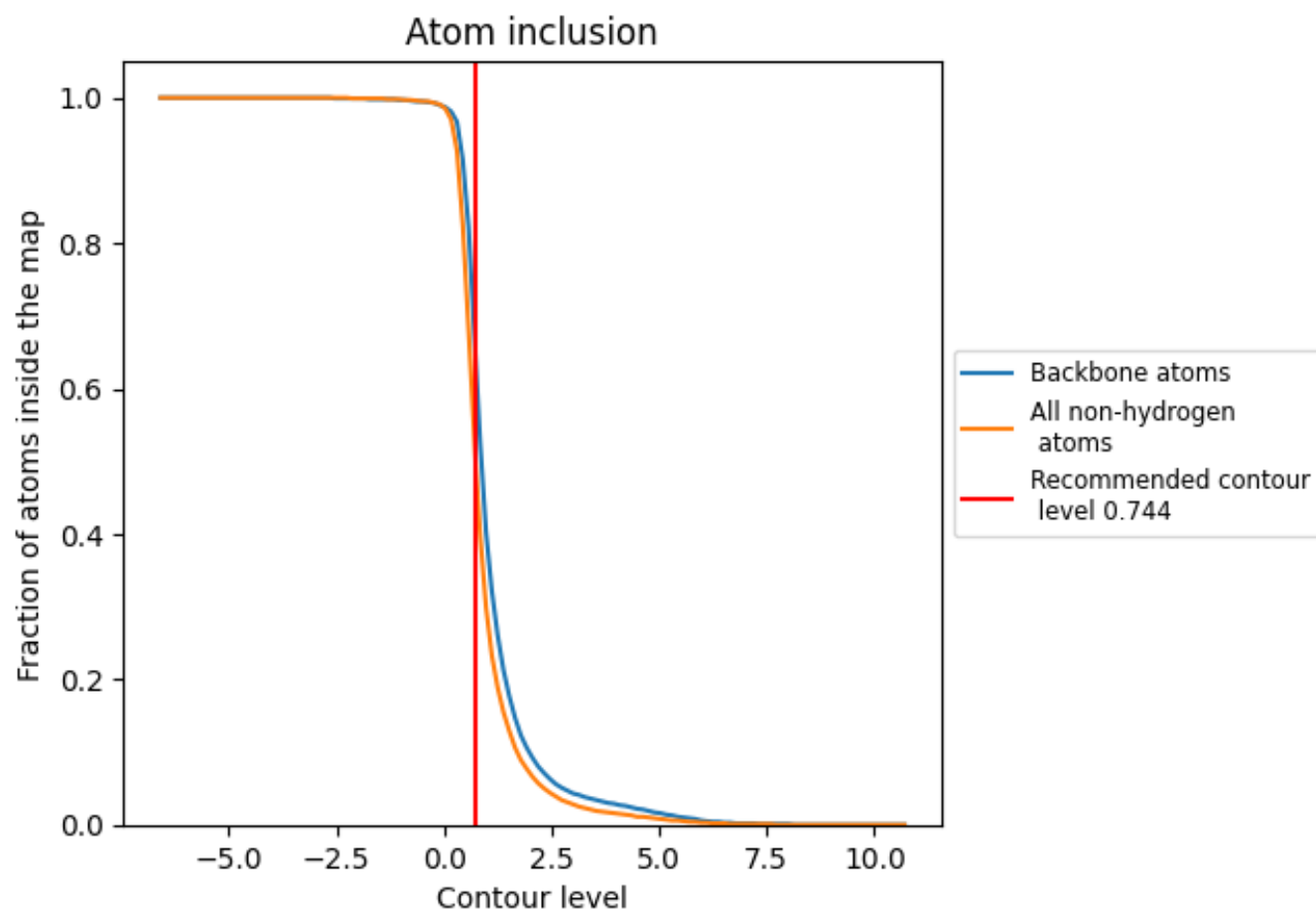
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.744).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 49% 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 (0.744) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4860	0.2320
A	0.4880	0.2320
B	0.4850	0.2340
C	0.4850	0.2340
D	0.4900	0.2320
E	0.4850	0.2300
F	0.4850	0.2320
G	0.4860	0.2330
H	0.4880	0.2320
I	0.4830	0.2320
J	0.4860	0.2300

1.0

0.0

<0.0