



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 10:50 PM UTC

PDB ID : 7PZC / pdb_00007pzc
EMDB ID : EMD-13686
Title : Cryo-EM structure of the NLRP3 decamer bound to the inhibitor CRID3
Authors : Hochheiser, I.V.; Pilsl, M.; Hagelueken, G.; Engel, C.; Geyer, M.
Deposited on : 2021-10-12
Resolution : 3.90 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:

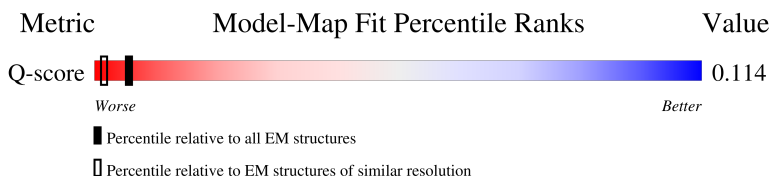
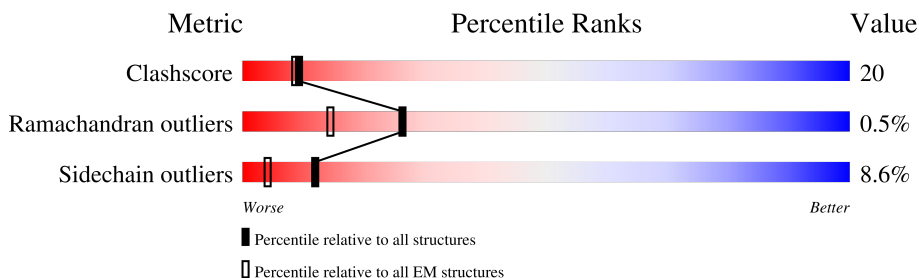
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.90 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	8855 (3.40 - 4.40)

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	35% 54% 39% 5%
1	B	1036	26% 46% 35% 15%
1	C	1036	29% 46% 35% 15%
1	D	1036	23% 46% 34% 15%

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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

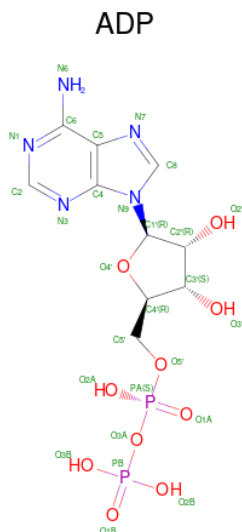
There are 3 unique types of molecules in this entry. The entry contains 72752 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

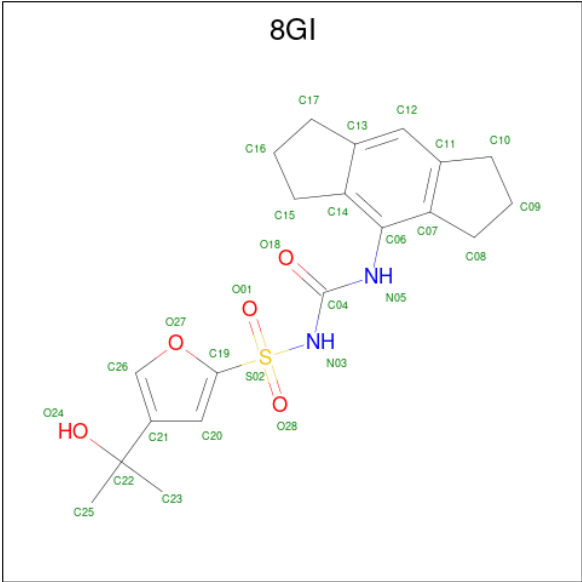
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1010	Total	C	N	O	S	0	0
			8065	5117	1377	1501	70		
1	B	880	Total	C	N	O	S	0	0
			7009	4450	1197	1302	60		
1	C	880	Total	C	N	O	S	0	0
			7009	4450	1197	1302	60		
1	D	880	Total	C	N	O	S	0	0
			7009	4450	1197	1302	60		
1	E	880	Total	C	N	O	S	0	0
			7009	4450	1197	1302	60		
1	F	880	Total	C	N	O	S	0	0
			7009	4450	1197	1302	60		
1	G	880	Total	C	N	O	S	0	0
			7009	4450	1197	1302	60		
1	H	1010	Total	C	N	O	S	0	0
			8065	5117	1377	1501	70		
1	I	880	Total	C	N	O	S	0	0
			7009	4450	1197	1302	60		
1	J	880	Total	C	N	O	S	0	0
			7009	4450	1197	1302	60		

- 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 1-(1,2,3,5,6,7-hexahydro-s-indacen-4-yl)-3-[4-(2-oxidanylpropan-2-yl)furan-2-yl]sulfonyl-urea (CCD ID: 8GI) (formula: $\text{C}_{20}\text{H}_{24}\text{N}_2\text{O}_5\text{S}$) (labeled as "Ligand of Interest" by depositor).

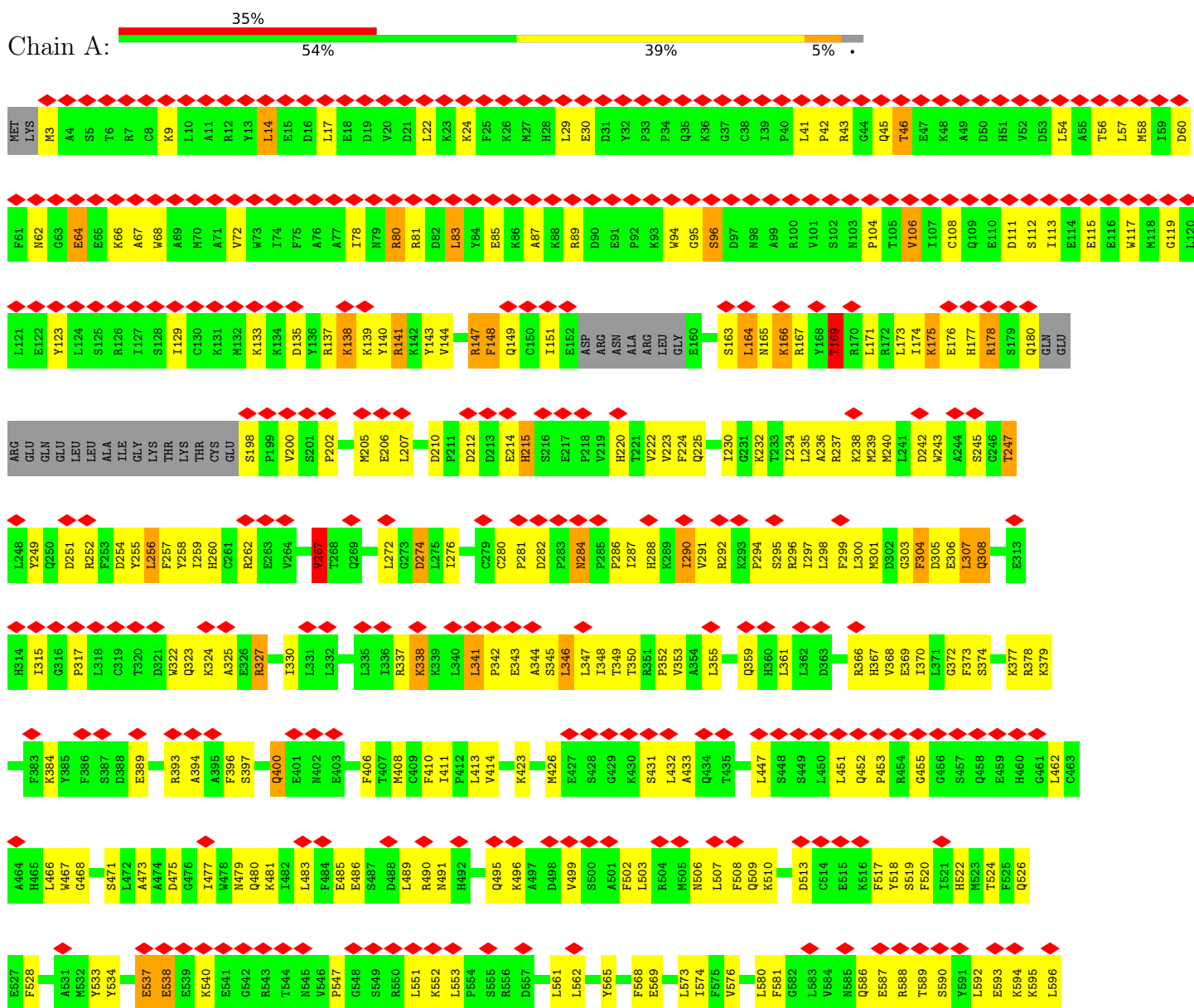


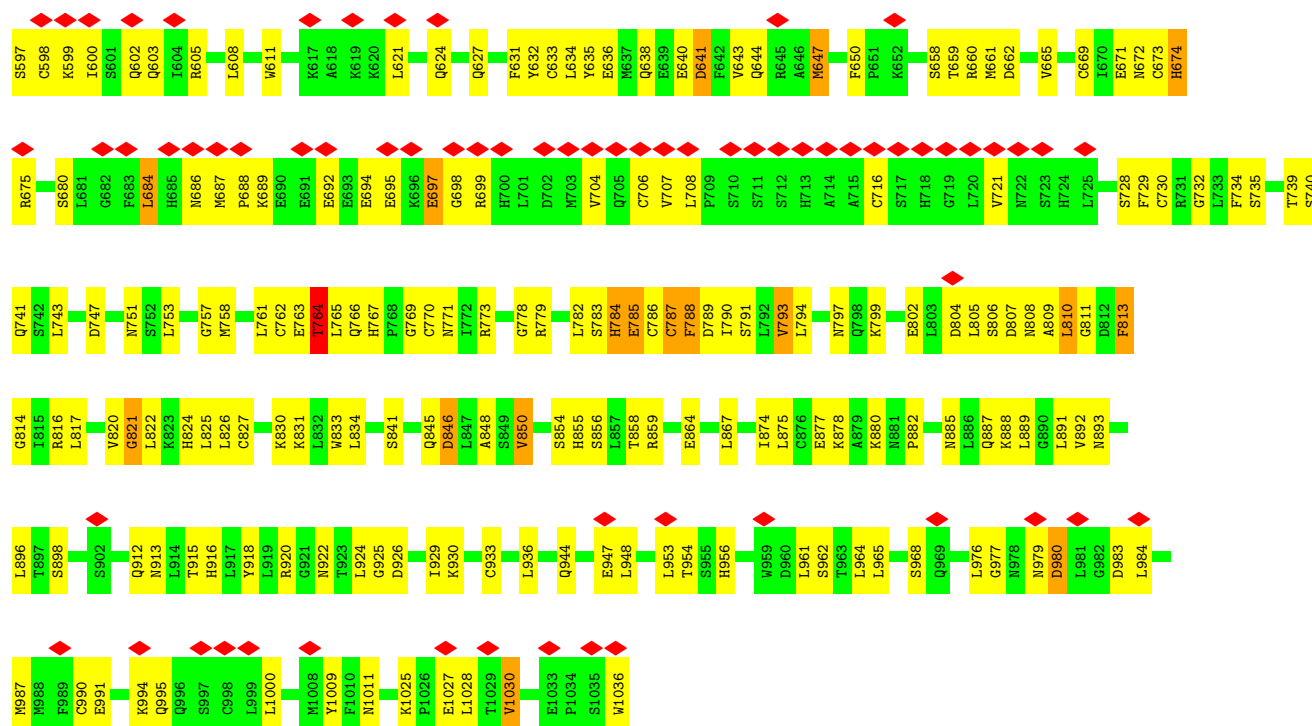
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	S	0
			28	20	2	5	1	
3	B	1	Total	C	N	O	S	0
			28	20	2	5	1	
3	C	1	Total	C	N	O	S	0
			28	20	2	5	1	
3	D	1	Total	C	N	O	S	0
			28	20	2	5	1	
3	E	1	Total	C	N	O	S	0
			28	20	2	5	1	
3	F	1	Total	C	N	O	S	0
			28	20	2	5	1	
3	G	1	Total	C	N	O	S	0
			28	20	2	5	1	
3	H	1	Total	C	N	O	S	0
			28	20	2	5	1	
3	I	1	Total	C	N	O	S	0
			28	20	2	5	1	
3	J	1	Total	C	N	O	S	0
			28	20	2	5	1	

3 Residue-property plots

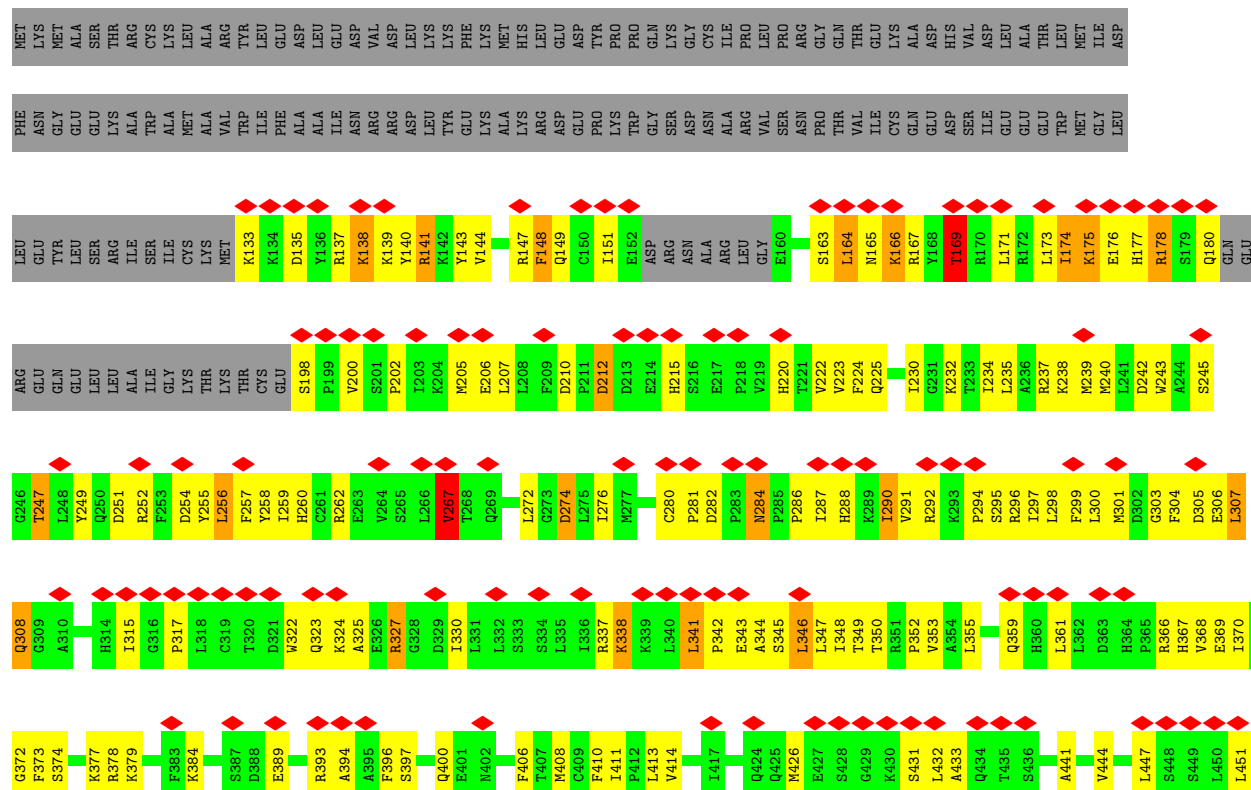
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

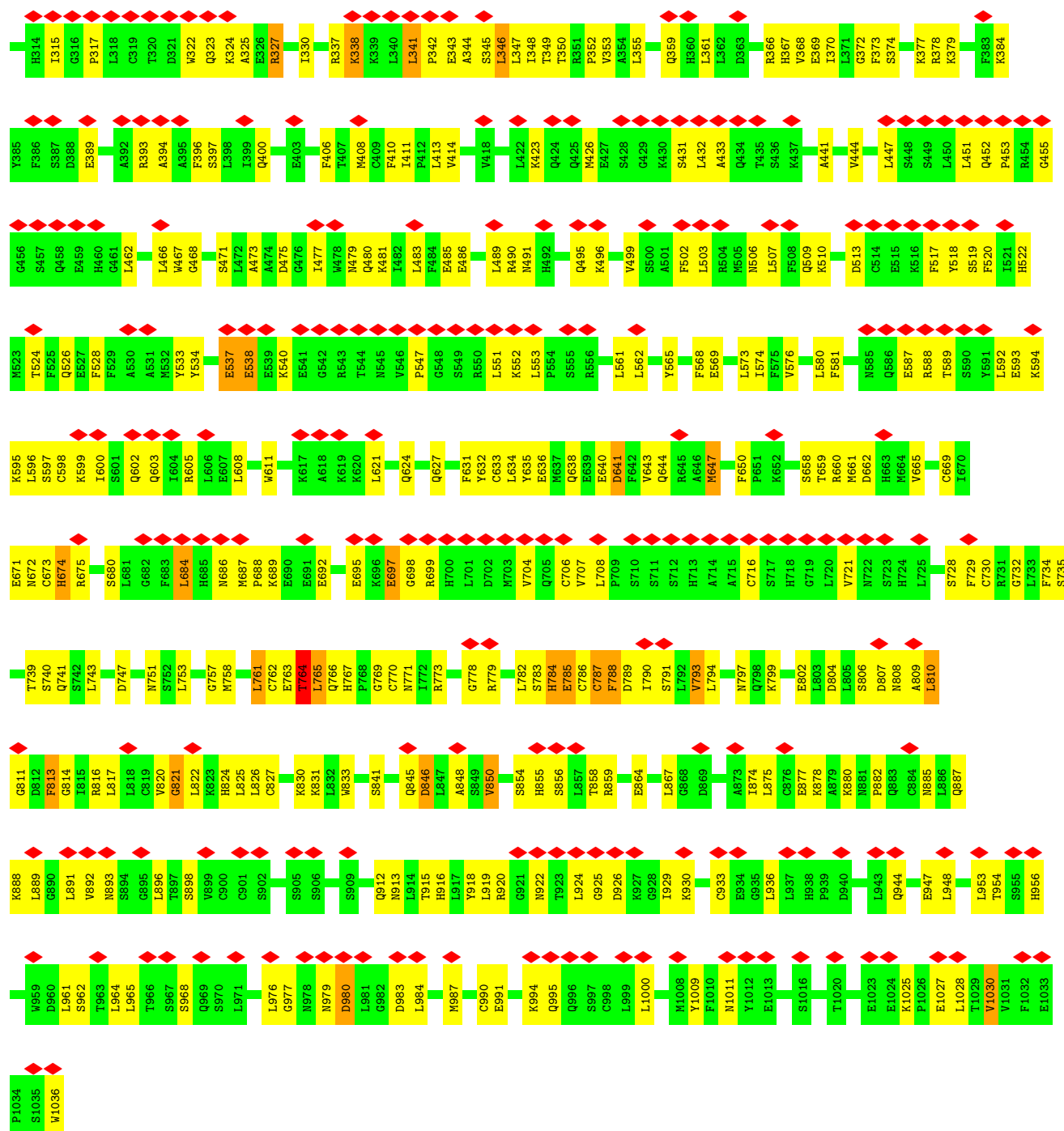
- Molecule 1: NACHT, LRR and PYD domains-containing protein 3





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

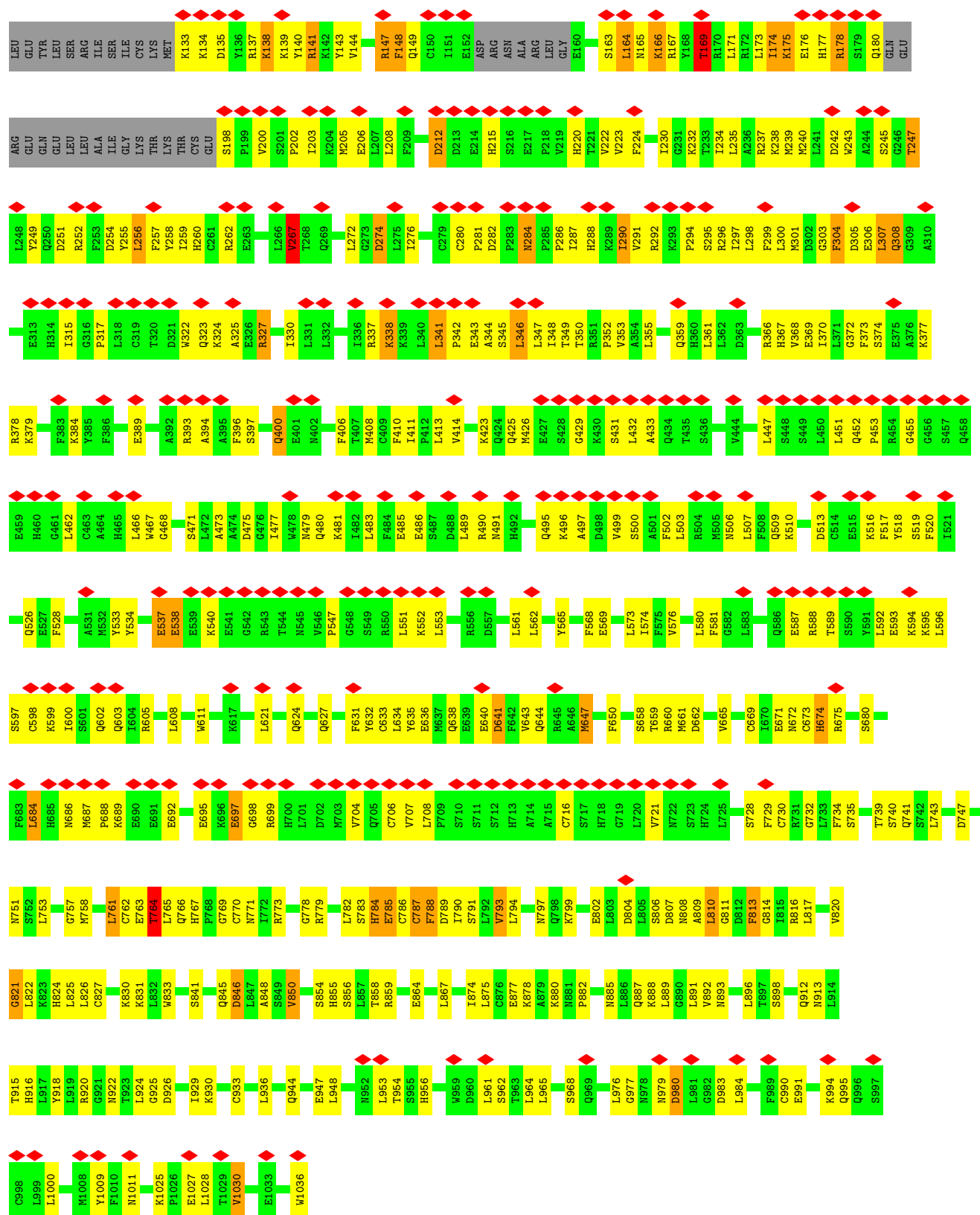




• Molecule 1: NACHT, LRR and PYD domains-containing protein 3



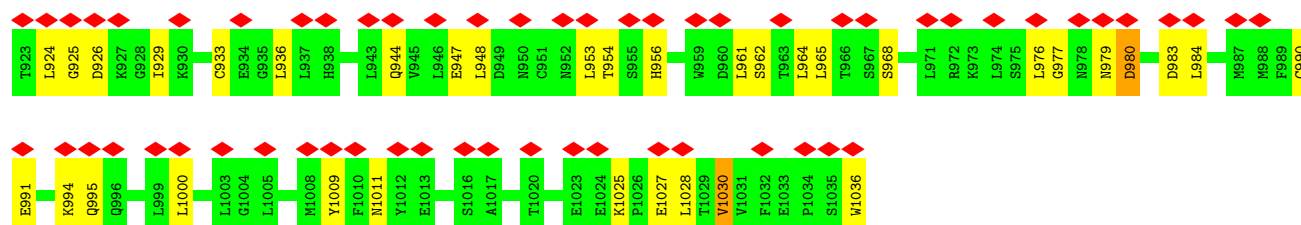
MET	PHE
LYS	ASN
MET	GLY
ALA	GLU
ALA	GLY
SER	GLY
THR	GLY
ARG	ALA
CYS	TRP
LYS	ALA
LEU	ALA
ALA	MET
ALA	TRP
ARG	ILE
TYR	PHE
LEU	ASP
GLU	ALA
LEU	ALA
ASP	ILE
ASN	ASN
VAL	ARG
ASP	ARG
LEU	ASP
LEU	LEU
LYS	TYR
PHE	GLY
LYS	LYS
LYS	ALA
MET	LYS
HIS	ALA
LEU	ARG
GLU	GLY
ASP	ASP
TYR	PRO
PRO	LYS
PRO	GLY
GLN	GLY
THR	THR
ILE	VAL
GLU	ILE
LYS	CYS
ALA	GLN
ALA	GLY
ASP	ASP
HIS	SER
VAL	ILE
ASP	GLY
LEU	GLY
ALA	THR
LEU	LEU
LEU	TRP
MET	MET
ILE	GLY
ASP	LEU



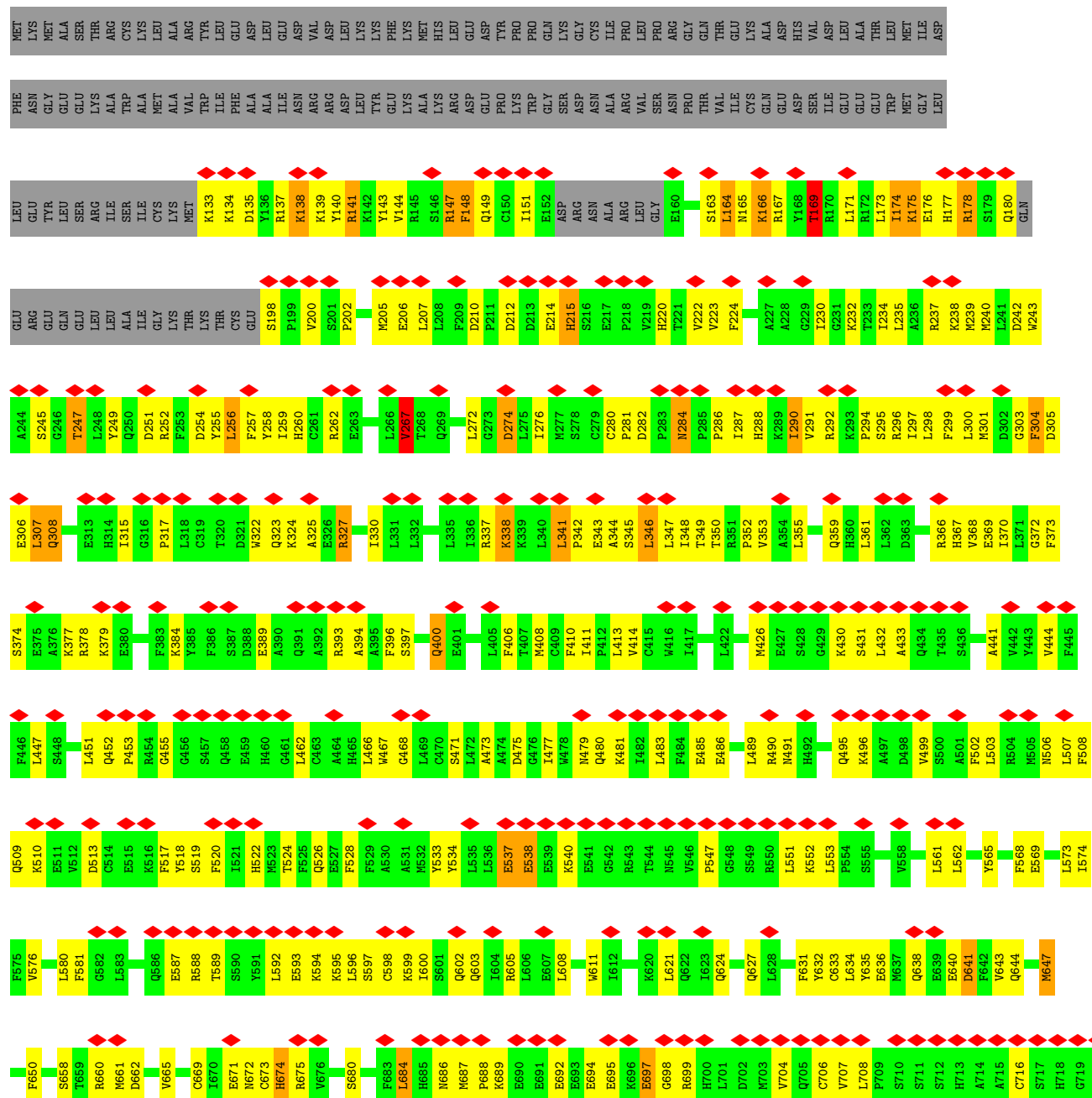
• Molecule 1: NACHT, LRR and PYD domains-containing protein 3

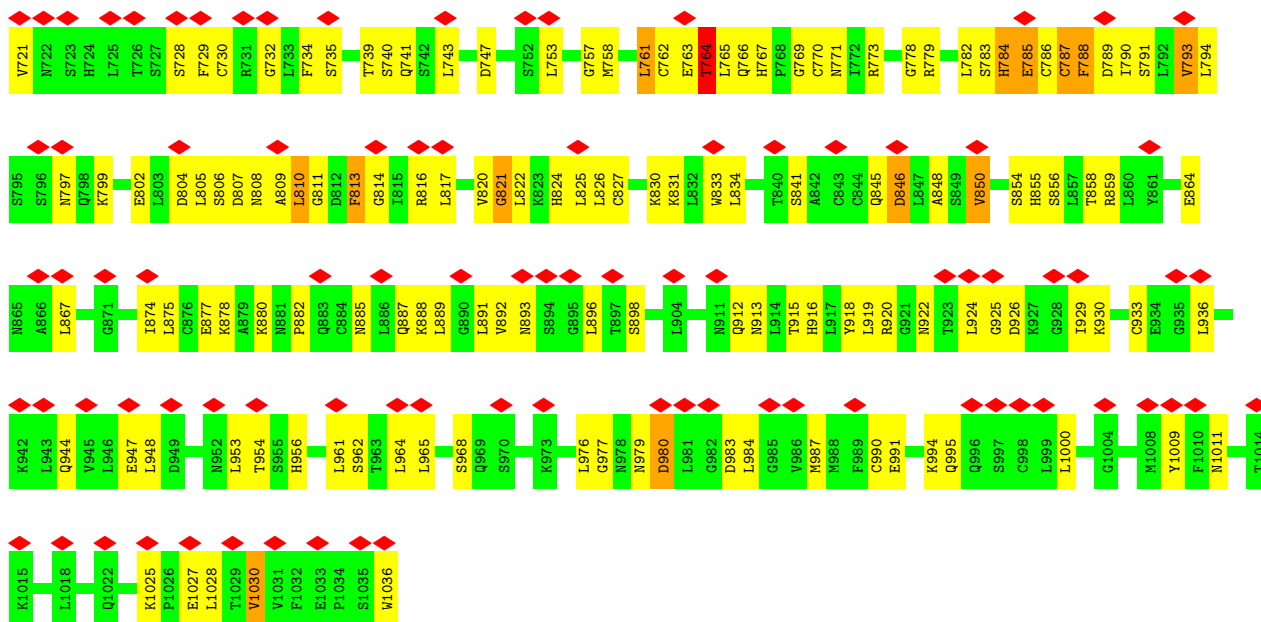


L860	Y861	Y862	G863	E864	R865	A866	L867	G868	D869	S870	A873	L874	L875	C876	F877	K878	A879	K880	N881	P882	Q883	C884	N885	Q887	H888	L889	G890	L891	V892	N893	S894	G895	L896	T897	S898	V899	C900	S902	S905	S906	V907	L908	S909	Q912	N913	L914	T915	H916	L917	L918	L919	R920	G921	N922			
LEU	GLU	TYR	LEU	SER	ARG	ALA	ILE	SER	ILE	CYS	MET	K133	K134	D135	Y136	R137	K138	K139	Y140	R141	K142	Y143	V144	R147	F148	Q149	C150	I151	E152	ASP	ARG	ASN	ALA	ARG	LEU	GLY	E160	S163	L164	N165	K166	R167	Y168	T169	R170	L171	R172	L173	I174	K175	E176	H177	R178	S179	Q180	GLN	GLU
ARG	GLU	GLN	GLU	LEU	LEU	ALA	ILE	GLY	LYS	THR	THR	GLU	S198	P199	V200	S201	P202	I203	M205	E206	L207	L208	D212	D213	E214	H215	S216	E217	P218	V219	H220	T221	V222	V223	F224	Q225	I230	G231	K232	T233	I234	L235	A236	R237	K238	M239	D240	L241	V243	A244	S245	L307	Q308	G309	A310		
E313	H314	I315	G316	P317	L318	C319	T320	C323	W322	K324	A325	E326	R327	I330	R337	K338	K339	L340	L341	P342	E343	A344	S345	L346	I347	I348	T349	T350	R351	P352	V353	A354	L355	Q359	H360	L361	L362	D363	H364	P365	R366	H367	V368	E369	I370	G372	F373	S374	K377	R378	K379						
F383	K384	S387	D388	A389	Q390	Q391	A392	R393	A394	F396	S397	Q400	E403	F406	T407	M408	C409	F410	I411	P412	L413	V414	T420	K423	Q424	Q425	M426	E427	S428	G429	K430	S431	L432	A433	Q434	T435	S436	K437	A441	V444	F445	F446	L447	S448	S449	L450	L451	Q452	P453	R454							
G455	G456	S457	Q458	H459	H460	G461	C463	A464	H465	A467	G468	S471	L472	A473	D475	G476	W478	Q479	M480	F481	L482	L483	F484	A485	E486	S487	D488	L489	Q490	K491	H492	Q495	K496	V499	S500	A501	F502	L503	R504	N506	L507	F508	Q509	K510	D513	C514	E515	F517	Y518								
S519	F520	H522	N523	T524	F525	Q526	E527	F528	F529	A530	A531	W532	Y533	Y534	L535	S536	E537	E538	E539	K540	E541	G542	R543	T544	N545	V546	P547	G548	S549	R550	L551	K552	L553	P554	S555	R556	L561	L562	E563	N564	Y565	G566	K567	F568	E569	L573	I574	F575	V576	R578	F579	F581	N585				
Q586	E587	R588	T589	S590	Y591	L592	E593	K594	K595	L596	S597	C598	K599	I600	S601	Q602	Q603	T604	R605	L606	E607	L608	W611	K617	A618	K619	G620	L621	Q622	I623	Q624	Q627	L628	F631	Y632	C633	L634	Y635	E636	N637	Q638	E639	E640	D641	F642	V643	Q644	R645	M647	F650	P651	K652	L653				
E654	S658	T659	R660	H661	D662	H663	H664	V665	S666	C669	L670	E671	L672	H673	H674	R675	V676	E677	S680	F683	L684	H685	N686	H687	P688	K689	E692	E695	K696	E697	G698	R699	H700	L701	D702	M703	V704	Q705	C706	V707	L708	S711	S712	H713	A714	A715	C716	S717	H718	G719	V721						
M722	S723	H724	L725	S728	F729	C730	R731	G732	L733	F734	S735	V736	L737	S738	T739	S740	O741	S742	L743	D747	L753	G757	M758	L761	C762	E763	T764	L765	L766	H767	P768	G769	C770	M771	L772	R773	G778	R779	C780	G781	L782	S783	H784	E785	L847	S849	V850	L851	S852	T853	S854	H855	S856	T858	R859		
N797	Q798	K799	E802	L803	D804	L805	S806	D807	N808	A809	L810	C811	D812	F813	C814	T815	R816	A879	K880	N881	P882	Q883	C884	N885	Q887	H888	L889	C827	K830	L831	L832	W833	G769	L834	V835	S836	C837	C838	S841	G844	Q845	D846	L847	S848	V850	L851	S852	T853	S854	H855	S856	T858	R859				
L860	Y861	Y862	G863	E864	R865	A866	L867	G868	D869	S870	A873	L874	L875	C876	F877	K878	A879	K880	N881	P882	Q883	C884	N885	Q887	H888	L889	G890	L891	V892	N893	S894	G895	L896	T897	S898	V899	C900	S902	S905	S906	V907	L908	S909	Q912	N913	L914	T915	H916	L917	L918	L919	R920	G921	N922			

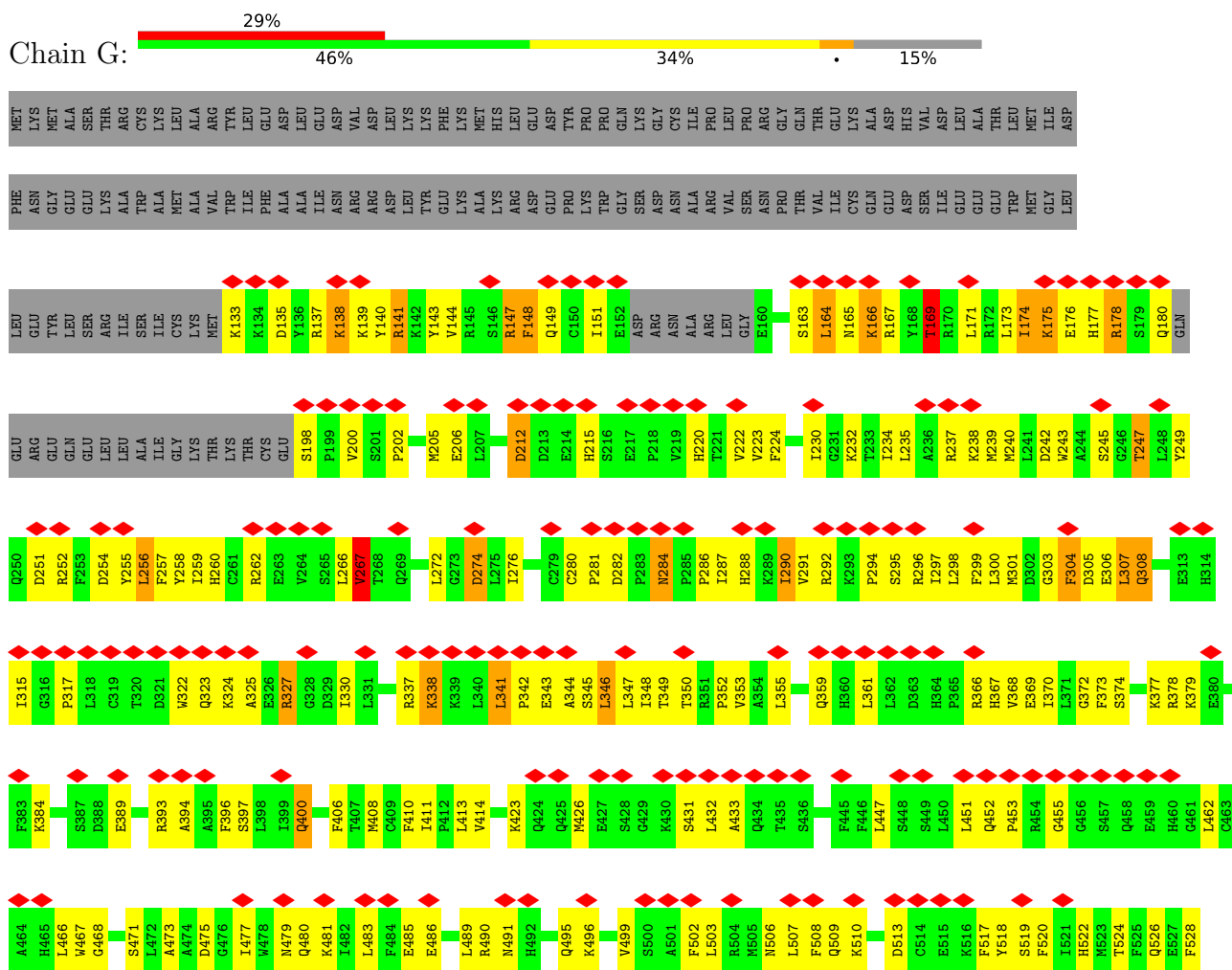


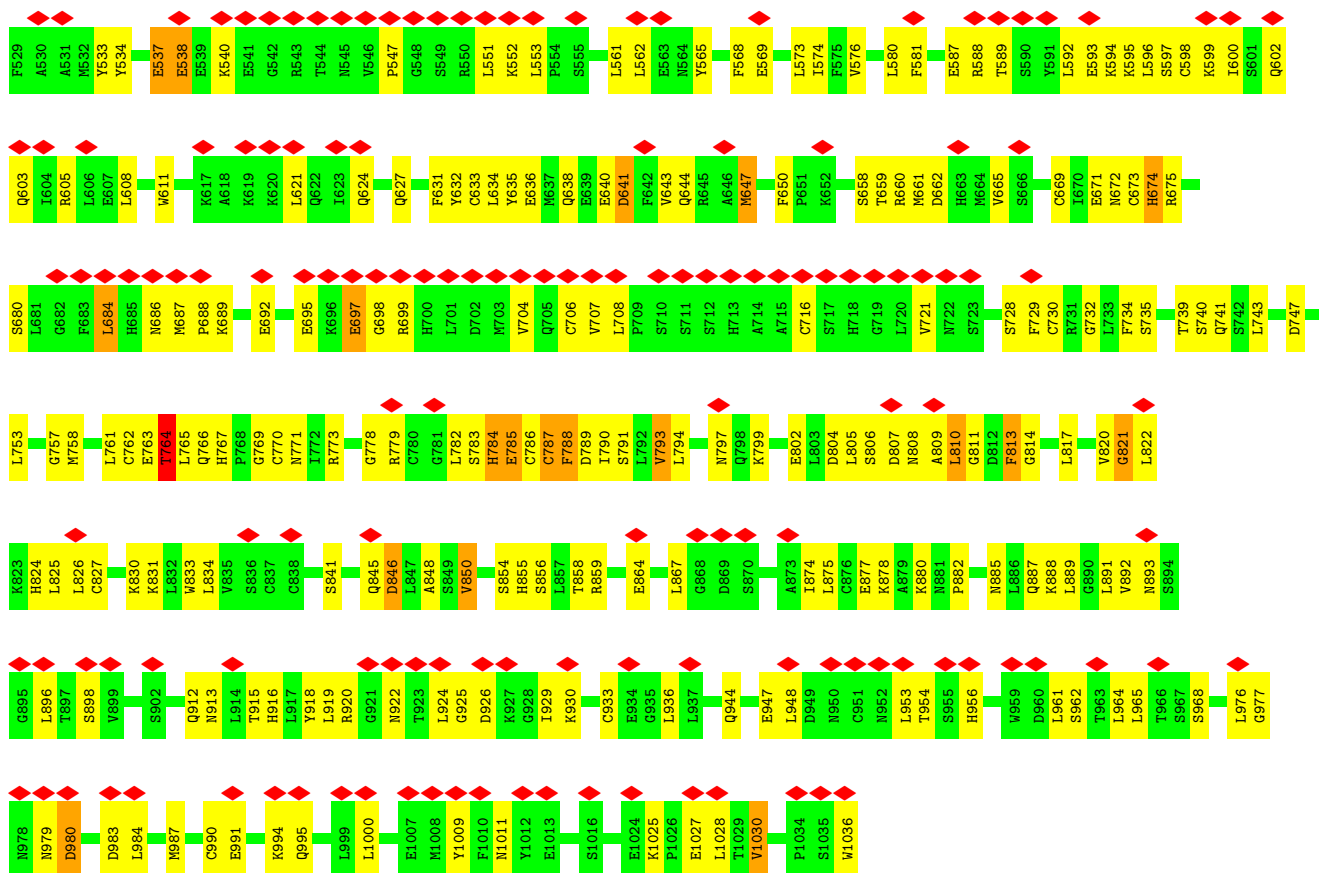
• Molecule 1: NACHT, LRR and PYD domains-containing protein 3



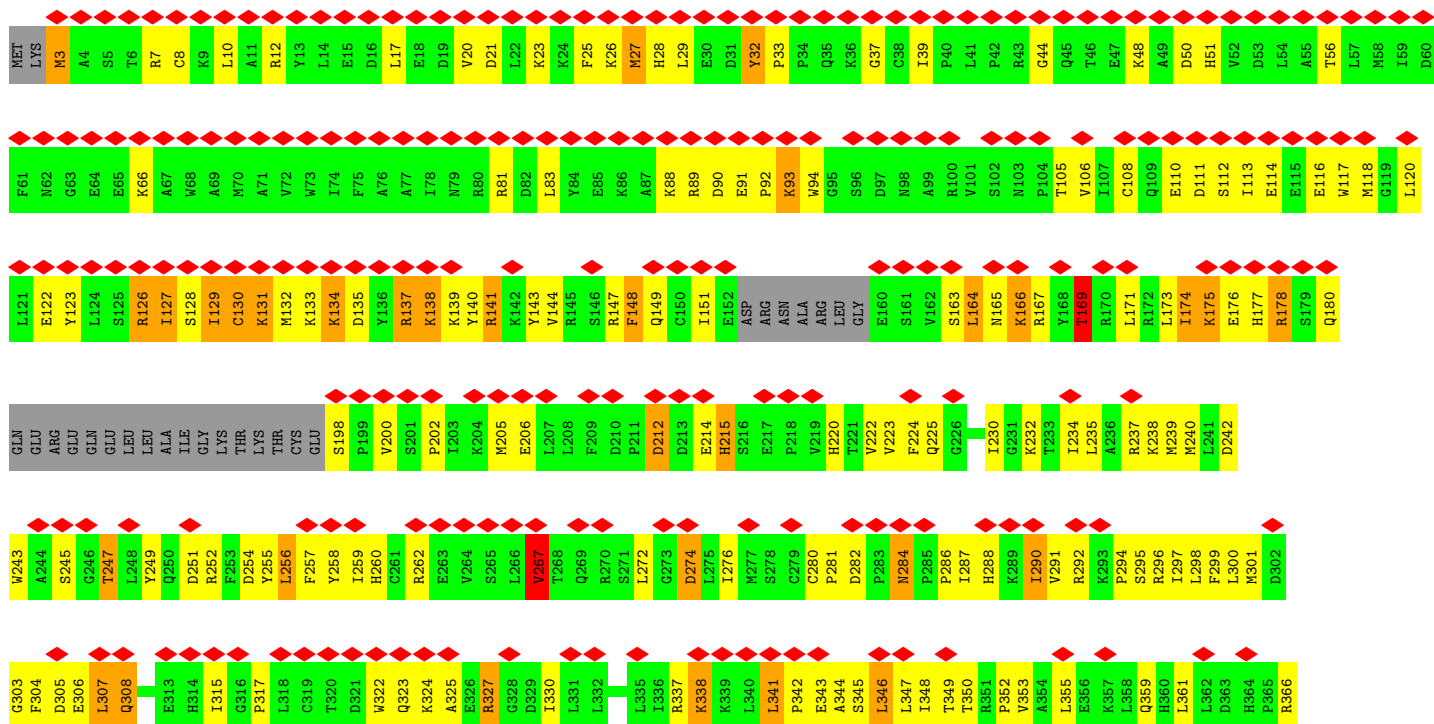


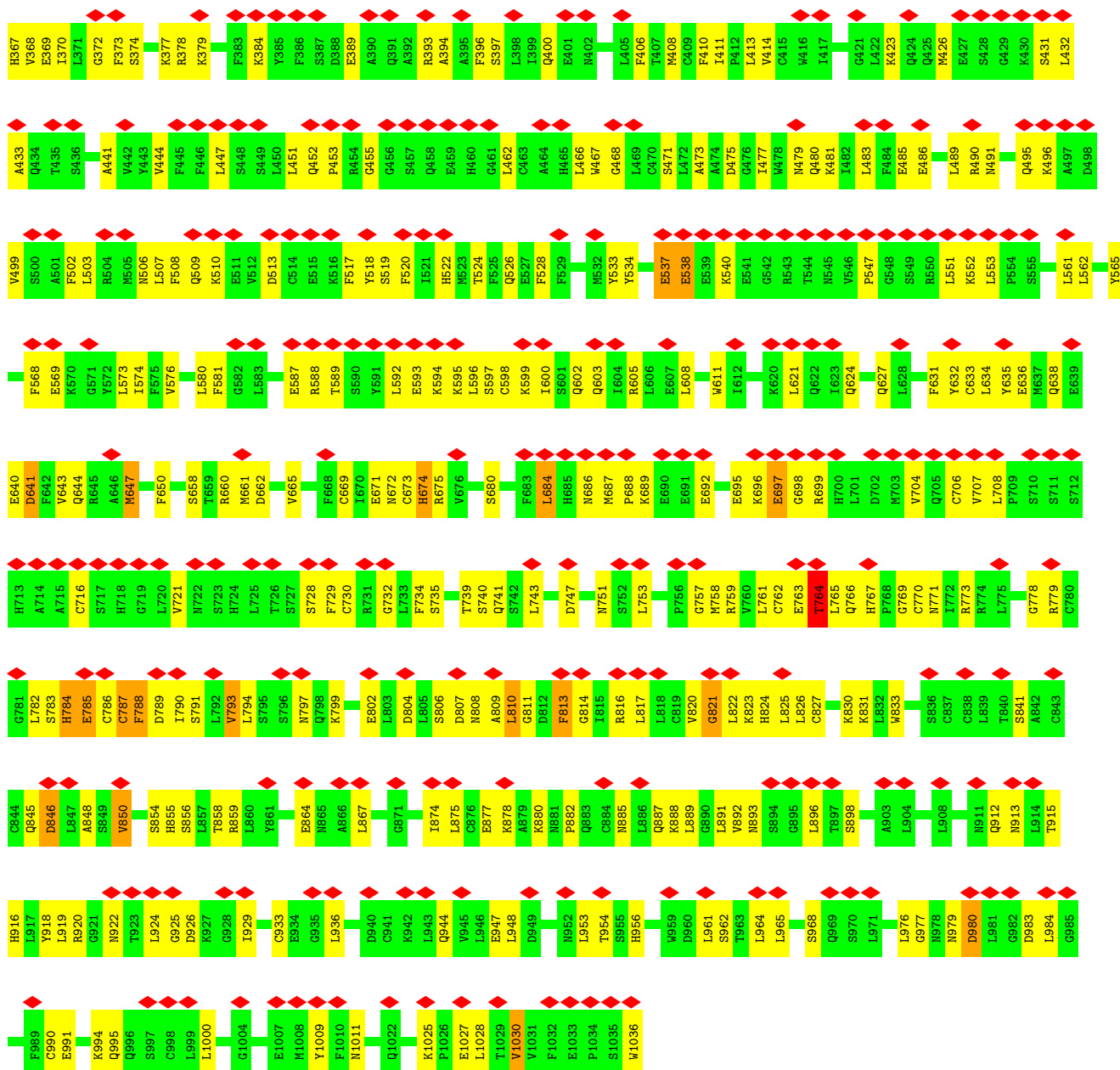
- Molecule 1: NACHT, LRR and PYD domains-containing protein 3



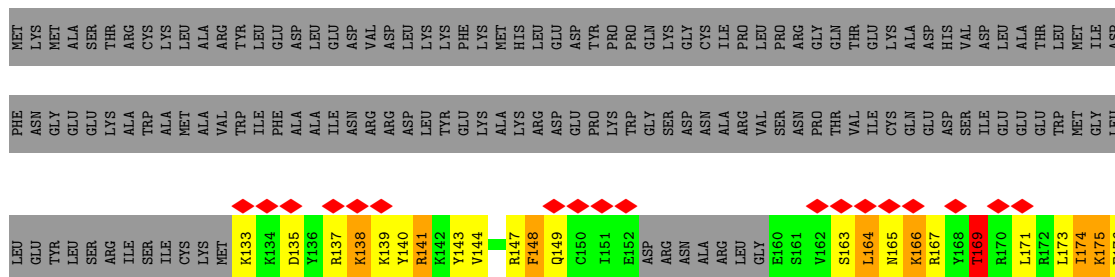


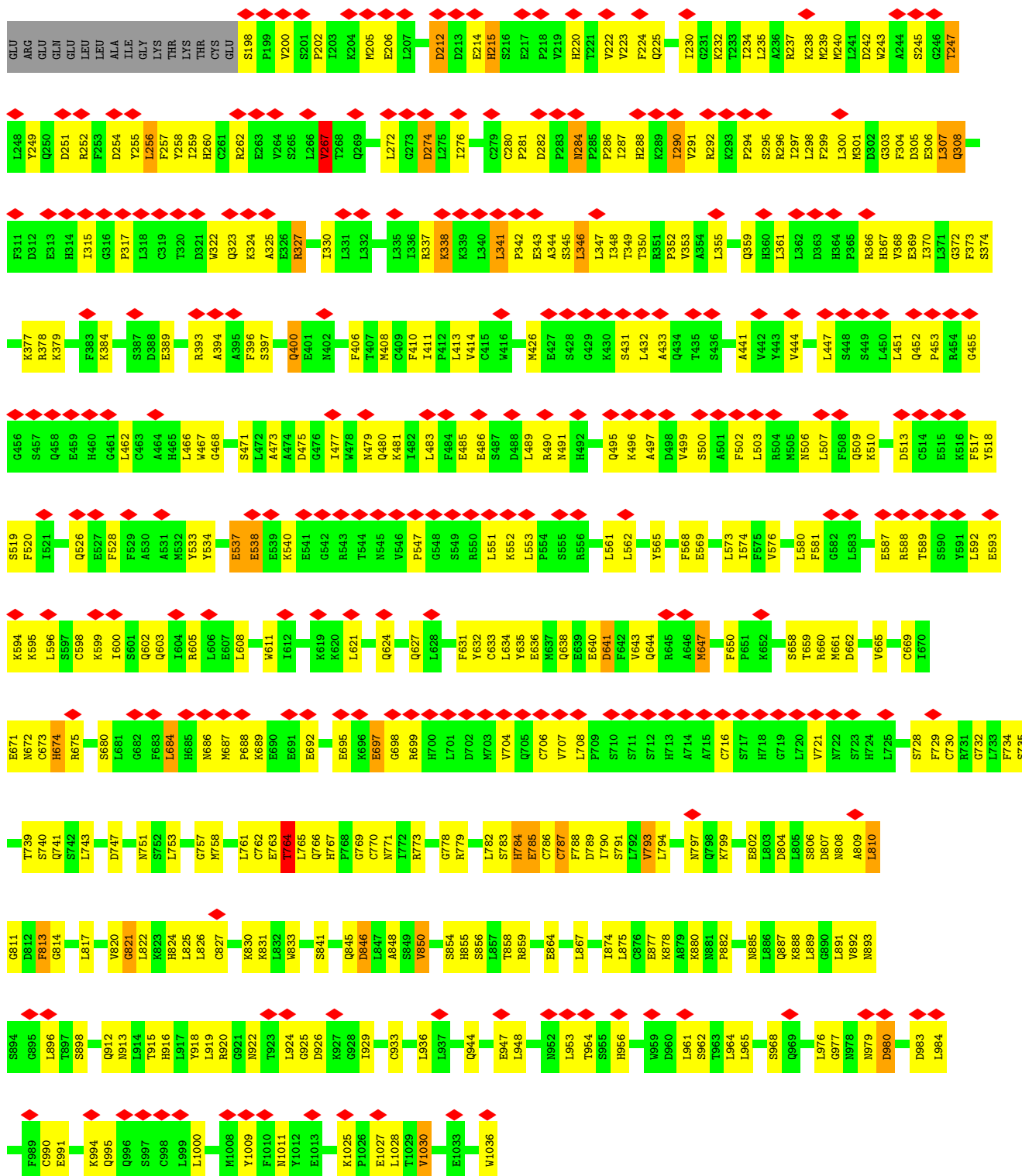
• Molecule 1: NACHT, LRR and PYD domains-containing protein 3





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

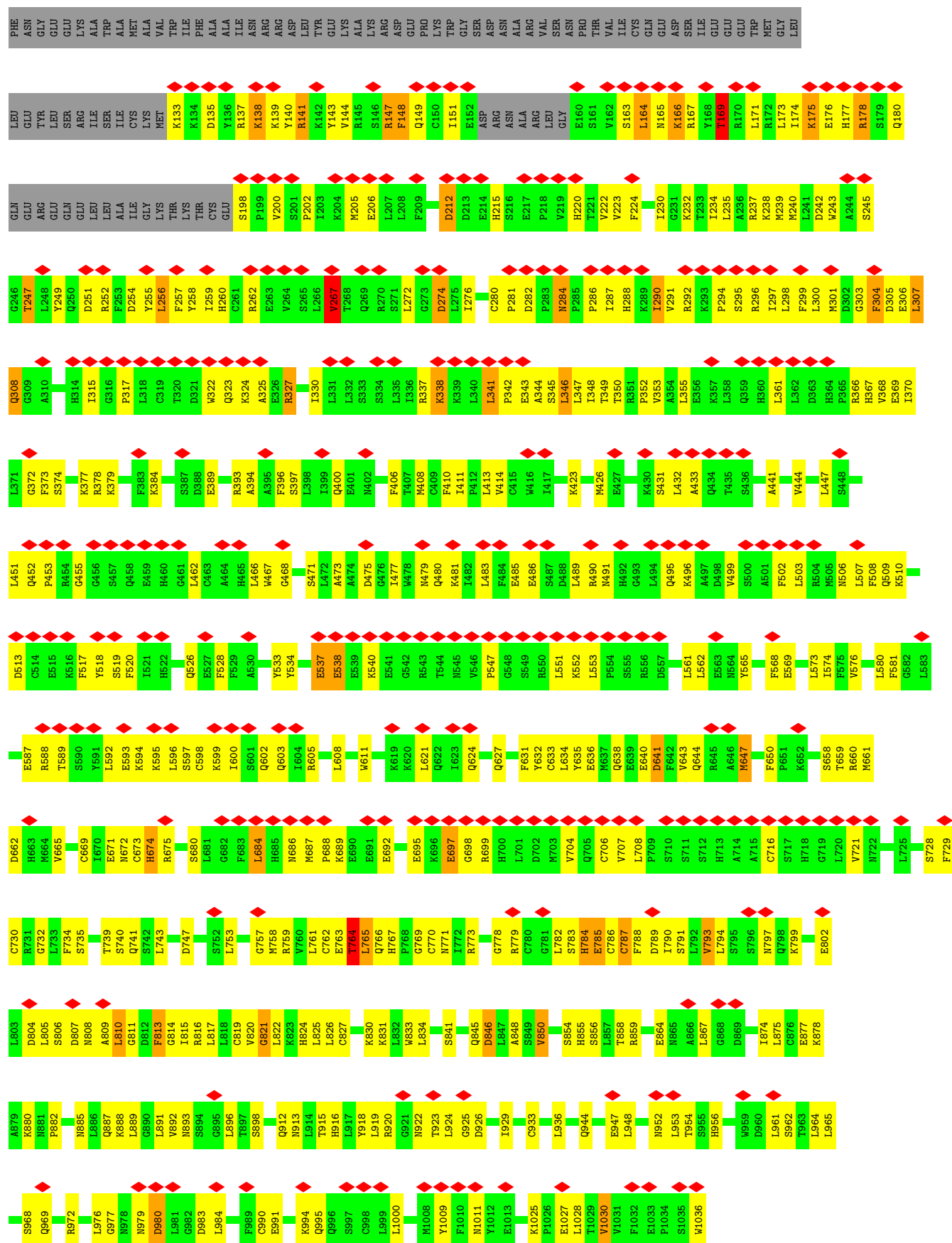




- Molecule 1: NACHT, LRR and PYD domains-containing protein 3



MET	LYS	MET	ALA	THR	THR	ARG	CYS	LYS	LEU	LEU	ALA	ILE	GLY	LYS	THR	LYS	THR	CYS	GLU	ASP	LYS	LYS	PHE	LYS	MET	HIS	LEU	GLU	ASP	THR	PRO	PRO	GLN	GLY	GLY	CYS	ILE	PRO	PRO	ARG	GLY	GLN	GLU	LYS	ALA	ASP	HIS	VAL	ASP	LEU	ALA	THR	LEU	MET	ILE	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D5	Depositor
Number of particles used	161351	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.046	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00515	Depositor
Map size (Å)	309.59998, 309.59998, 309.59998	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2899998, 1.2899998, 1.2899998	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, 8GI

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	0.52	3/8223 (0.0%)	0.82	18/11088 (0.2%)
1	B	0.42	3/7144 (0.0%)	0.74	18/9632 (0.2%)
1	C	0.42	3/7144 (0.0%)	0.74	18/9632 (0.2%)
1	D	0.42	3/7144 (0.0%)	0.74	18/9632 (0.2%)
1	E	0.42	3/7144 (0.0%)	0.74	18/9632 (0.2%)
1	F	0.42	3/7144 (0.0%)	0.74	18/9632 (0.2%)
1	G	0.42	3/7144 (0.0%)	0.74	18/9632 (0.2%)
1	H	0.62	12/8223 (0.1%)	0.82	28/11088 (0.3%)
1	I	0.42	3/7144 (0.0%)	0.74	18/9632 (0.2%)
1	J	0.42	3/7144 (0.0%)	0.74	18/9632 (0.2%)
All	All	0.46	39/73598 (0.1%)	0.76	190/99232 (0.2%)

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	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
All	All	0	10

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	29	LEU	C-O	-8.41	1.14	1.24
1	H	51	HIS	C-O	-6.61	1.16	1.24
1	H	28	HIS	C-O	-6.55	1.16	1.24
1	H	26	LYS	C-O	-6.36	1.16	1.24
1	H	27	MET	C-O	-6.21	1.16	1.24

The worst 5 of 190 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	640	GLU	N-CA-C	9.82	121.67	110.97
1	G	640	GLU	N-CA-C	9.80	121.66	110.97
1	F	640	GLU	N-CA-C	9.80	121.65	110.97
1	A	640	GLU	N-CA-C	9.79	121.64	110.97
1	J	640	GLU	N-CA-C	9.79	121.64	110.97

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	809	ALA	Mainchain
1	B	809	ALA	Mainchain
1	C	809	ALA	Mainchain
1	D	809	ALA	Mainchain
1	E	809	ALA	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8065	0	8081	333	0
1	B	7009	0	7038	300	0
1	C	7009	0	7038	303	0
1	D	7009	0	7038	328	0
1	E	7009	0	7038	302	0
1	F	7009	0	7038	306	0
1	G	7009	0	7038	302	0
1	H	8065	0	8081	363	0
1	I	7009	0	7038	288	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	7009	0	7038	297	0
2	A	27	0	12	2	0
2	B	27	0	12	2	0
2	C	27	0	12	2	0
2	D	27	0	12	2	0
2	E	27	0	12	2	0
2	F	27	0	12	2	0
2	G	27	0	12	2	0
2	H	27	0	12	2	0
2	I	27	0	12	2	0
2	J	27	0	12	2	0
3	A	28	0	0	1	0
3	B	28	0	0	1	0
3	C	28	0	0	1	0
3	D	28	0	0	1	0
3	E	28	0	0	1	0
3	F	28	0	0	1	0
3	G	28	0	0	1	0
3	H	28	0	0	1	0
3	I	28	0	0	1	0
3	J	28	0	0	1	0
All	All	72752	0	72586	2950	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 20.

The worst 5 of 2950 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:D:133:LYS:HZ1	1:H:3:MET:CG	1.10	1.62
1:D:133:LYS:CE	1:H:3:MET:HG3	1.42	1.49
1:D:133:LYS:NZ	1:H:3:MET:HG3	1.15	1.47
1:D:133:LYS:NZ	1:H:3:MET:CG	1.82	1.13
1:D:133:LYS:NZ	1:H:3:MET:CB	2.11	1.12

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1004/1036 (97%)	878 (88%)	120 (12%)	6 (1%)	21	55
1	B	874/1036 (84%)	757 (87%)	113 (13%)	4 (0%)	24	59
1	C	874/1036 (84%)	757 (87%)	113 (13%)	4 (0%)	24	59
1	D	874/1036 (84%)	757 (87%)	113 (13%)	4 (0%)	24	59
1	E	874/1036 (84%)	757 (87%)	113 (13%)	4 (0%)	24	59
1	F	874/1036 (84%)	757 (87%)	113 (13%)	4 (0%)	24	59
1	G	874/1036 (84%)	757 (87%)	113 (13%)	4 (0%)	24	59
1	H	1004/1036 (97%)	872 (87%)	125 (12%)	7 (1%)	18	53
1	I	874/1036 (84%)	757 (87%)	113 (13%)	4 (0%)	24	59
1	J	874/1036 (84%)	757 (87%)	113 (13%)	4 (0%)	24	59
All	All	9000/10360 (87%)	7806 (87%)	1149 (13%)	45 (0%)	26	59

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	SER
1	H	127	ILE
1	H	131	LYS
1	A	303	GLY
1	A	721	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	
1	A	911/933 (98%)	828 (91%)	83 (9%)	9	31
1	B	797/933 (85%)	730 (92%)	67 (8%)	10	33
1	C	797/933 (85%)	730 (92%)	67 (8%)	10	33
1	D	797/933 (85%)	729 (92%)	68 (8%)	10	33
1	E	797/933 (85%)	729 (92%)	68 (8%)	10	33
1	F	797/933 (85%)	730 (92%)	67 (8%)	10	33
1	G	797/933 (85%)	729 (92%)	68 (8%)	10	33
1	H	911/933 (98%)	833 (91%)	78 (9%)	10	33
1	I	797/933 (85%)	729 (92%)	68 (8%)	10	33
1	J	797/933 (85%)	730 (92%)	67 (8%)	10	33
All	All	8198/9330 (88%)	7497 (91%)	701 (9%)	12	33

5 of 701 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	671	GLU
1	I	175	LYS
1	G	787	CYS
1	G	659	THR
1	H	338	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	545	ASN
1	H	797	ASN
1	G	705	GLN
1	G	1022	GLN
1	H	1022	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

20 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
3	8GI	F	1102	-	28,31,31	1.72	6 (21%)	35,48,48	2.54	14 (40%)
2	ADP	C	1101	-	28,29,29	1.39	4 (14%)	43,45,45	1.82	9 (20%)
3	8GI	J	1102	-	28,31,31	1.73	6 (21%)	35,48,48	2.53	14 (40%)
2	ADP	I	1101	-	28,29,29	1.39	4 (14%)	43,45,45	1.82	9 (20%)
2	ADP	F	1101	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	9 (20%)
3	8GI	I	1102	-	28,31,31	1.73	6 (21%)	35,48,48	2.54	13 (37%)
2	ADP	A	1101	-	28,29,29	1.39	4 (14%)	43,45,45	1.83	9 (20%)
3	8GI	C	1102	-	28,31,31	1.73	6 (21%)	35,48,48	2.53	14 (40%)
2	ADP	E	1101	-	28,29,29	1.39	4 (14%)	43,45,45	1.83	9 (20%)
2	ADP	J	1101	-	28,29,29	1.39	4 (14%)	43,45,45	1.82	9 (20%)
3	8GI	A	1102	-	28,31,31	1.74	6 (21%)	35,48,48	2.54	13 (37%)
3	8GI	E	1102	-	28,31,31	1.74	6 (21%)	35,48,48	2.53	14 (40%)
2	ADP	D	1101	-	28,29,29	1.39	4 (14%)	43,45,45	1.82	9 (20%)
3	8GI	B	1102	-	28,31,31	1.72	6 (21%)	35,48,48	2.52	13 (37%)
3	8GI	G	1102	-	28,31,31	1.73	6 (21%)	35,48,48	2.53	13 (37%)
2	ADP	G	1101	-	28,29,29	1.39	4 (14%)	43,45,45	1.83	9 (20%)
2	ADP	H	1101	-	28,29,29	1.39	5 (17%)	43,45,45	1.83	9 (20%)
3	8GI	D	1102	-	28,31,31	1.72	6 (21%)	35,48,48	2.54	14 (40%)
2	ADP	B	1101	-	28,29,29	1.39	4 (14%)	43,45,45	1.82	9 (20%)
3	8GI	H	1102	-	28,31,31	1.72	6 (21%)	35,48,48	2.53	14 (40%)

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
3	8GI	F	1102	-	-	2/19/33/33	0/4/4/4
2	ADP	C	1101	-	-	2/16/32/32	0/3/3/3
3	8GI	J	1102	-	-	2/19/33/33	0/4/4/4
2	ADP	I	1101	-	-	2/16/32/32	0/3/3/3
2	ADP	F	1101	-	-	3/16/32/32	0/3/3/3
3	8GI	I	1102	-	-	2/19/33/33	0/4/4/4
2	ADP	A	1101	-	-	2/16/32/32	0/3/3/3
3	8GI	C	1102	-	-	2/19/33/33	0/4/4/4
2	ADP	E	1101	-	-	2/16/32/32	0/3/3/3
2	ADP	J	1101	-	-	3/16/32/32	0/3/3/3
3	8GI	A	1102	-	-	2/19/33/33	0/4/4/4
3	8GI	E	1102	-	-	2/19/33/33	0/4/4/4
2	ADP	D	1101	-	-	3/16/32/32	0/3/3/3
3	8GI	B	1102	-	-	2/19/33/33	0/4/4/4
3	8GI	G	1102	-	-	2/19/33/33	0/4/4/4
2	ADP	G	1101	-	-	2/16/32/32	0/3/3/3
2	ADP	H	1101	-	-	3/16/32/32	0/3/3/3
3	8GI	D	1102	-	-	2/19/33/33	0/4/4/4
2	ADP	B	1101	-	-	3/16/32/32	0/3/3/3
3	8GI	H	1102	-	-	2/19/33/33	0/4/4/4

The worst 5 of 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1101	ADP	C5-C4	4.65	1.47	1.39
2	E	1101	ADP	C5-C4	4.64	1.47	1.39
2	A	1101	ADP	C5-C4	4.63	1.47	1.39
2	I	1101	ADP	C5-C4	4.62	1.47	1.39
2	H	1101	ADP	C5-C4	4.61	1.47	1.39

The worst 5 of 226 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1102	8GI	O28-S02-O01	-9.69	102.06	119.82
3	G	1102	8GI	O28-S02-O01	-9.66	102.10	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1102	8GI	O28-S02-O01	-9.66	102.10	119.82
3	D	1102	8GI	O28-S02-O01	-9.66	102.11	119.82
3	F	1102	8GI	O28-S02-O01	-9.66	102.12	119.82

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	ADP	C3'-C4'-C5'-O5'
2	B	1101	ADP	C3'-C4'-C5'-O5'
2	C	1101	ADP	C3'-C4'-C5'-O5'
2	D	1101	ADP	C3'-C4'-C5'-O5'
2	E	1101	ADP	C3'-C4'-C5'-O5'

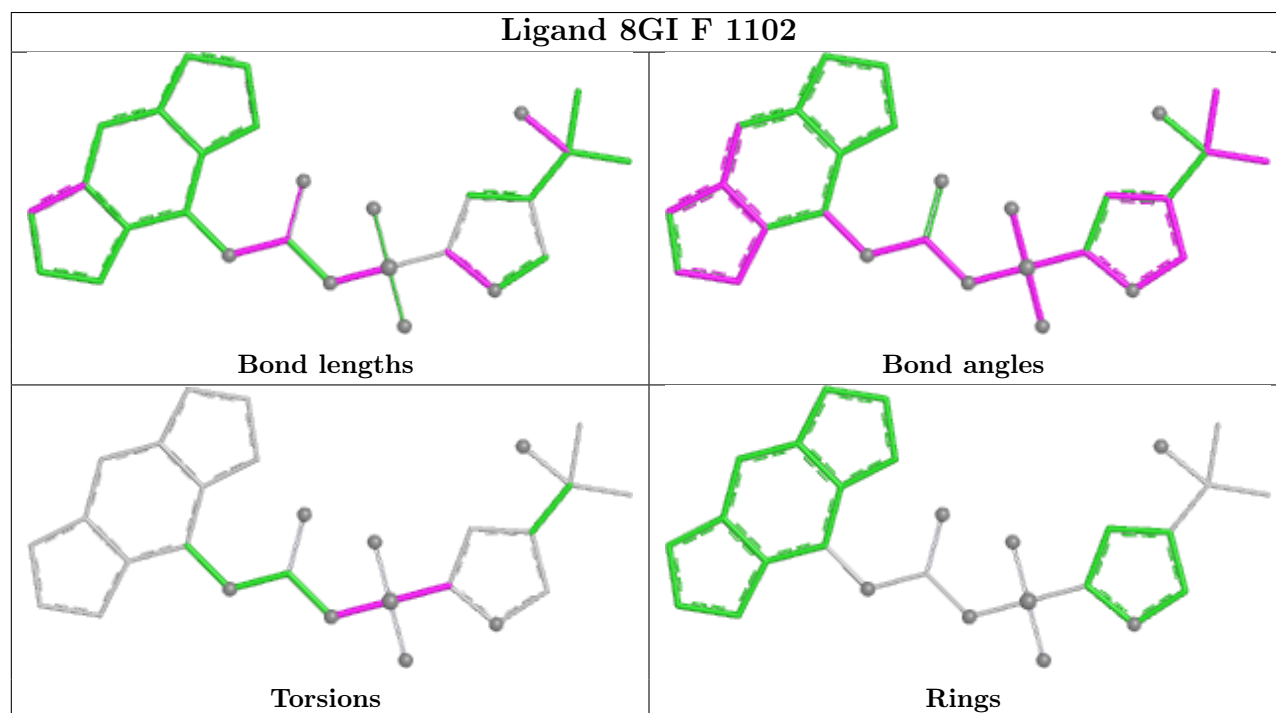
There are no ring outliers.

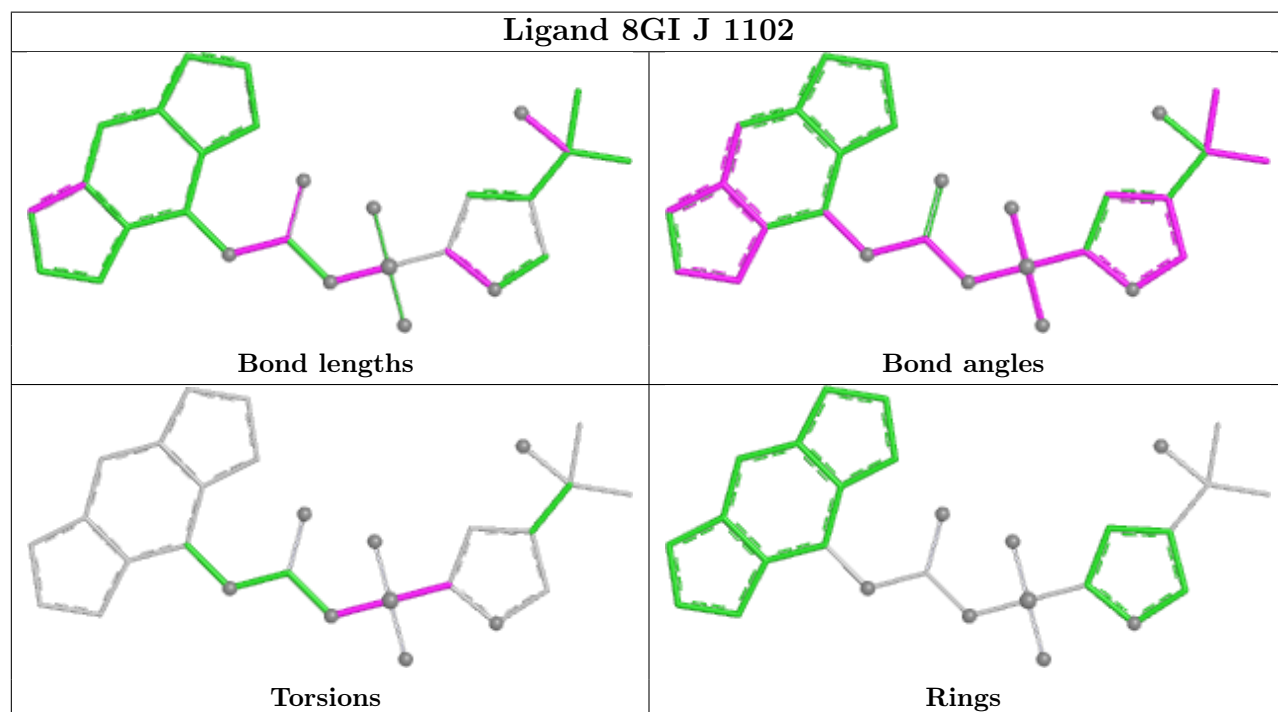
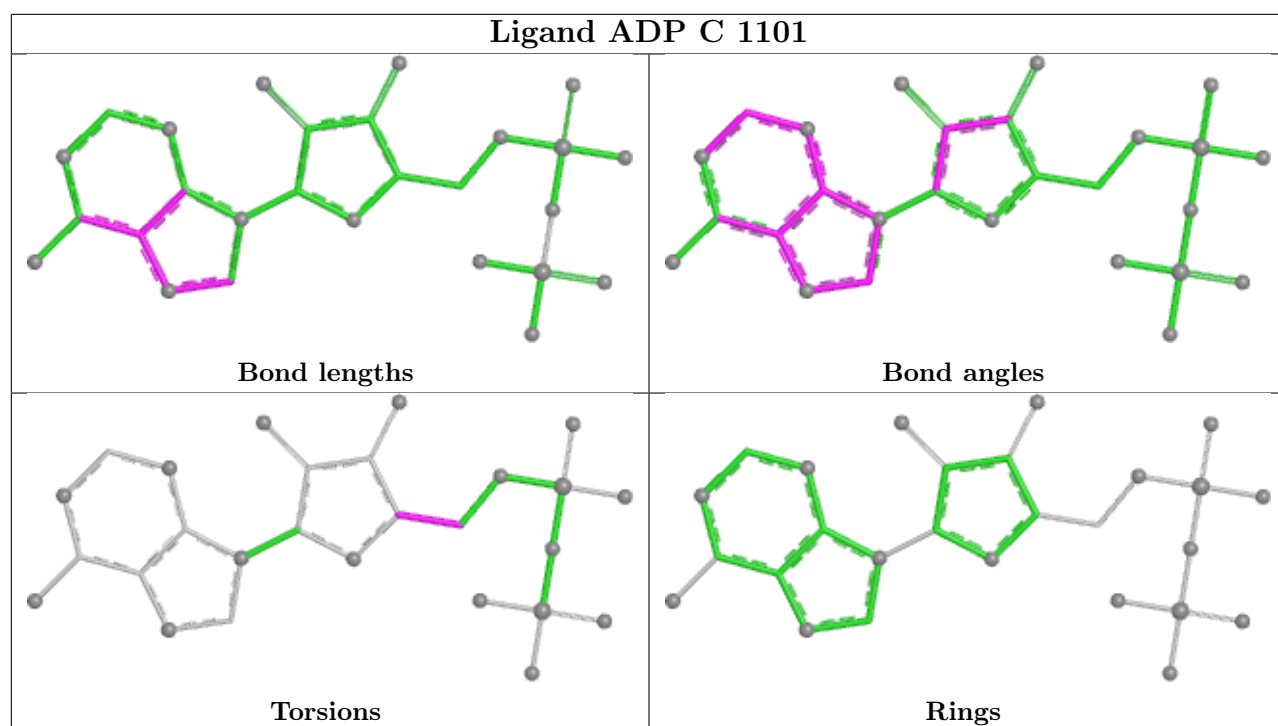
20 monomers are involved in 30 short contacts:

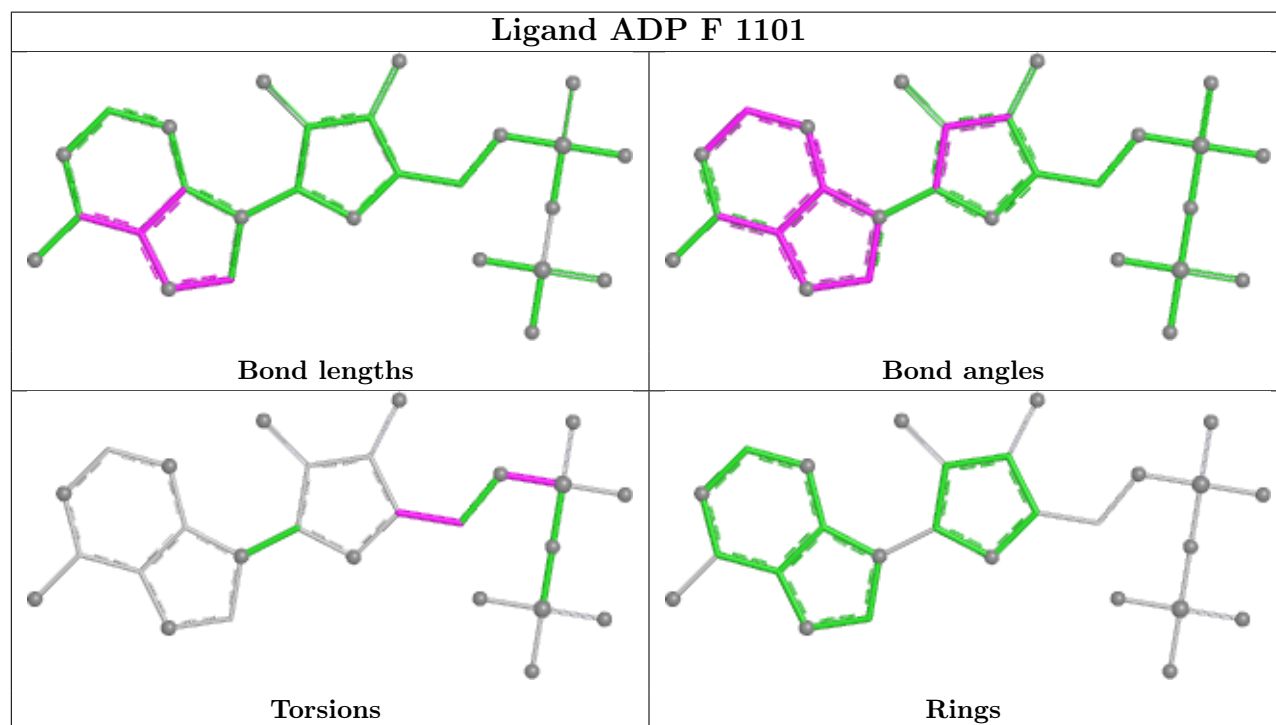
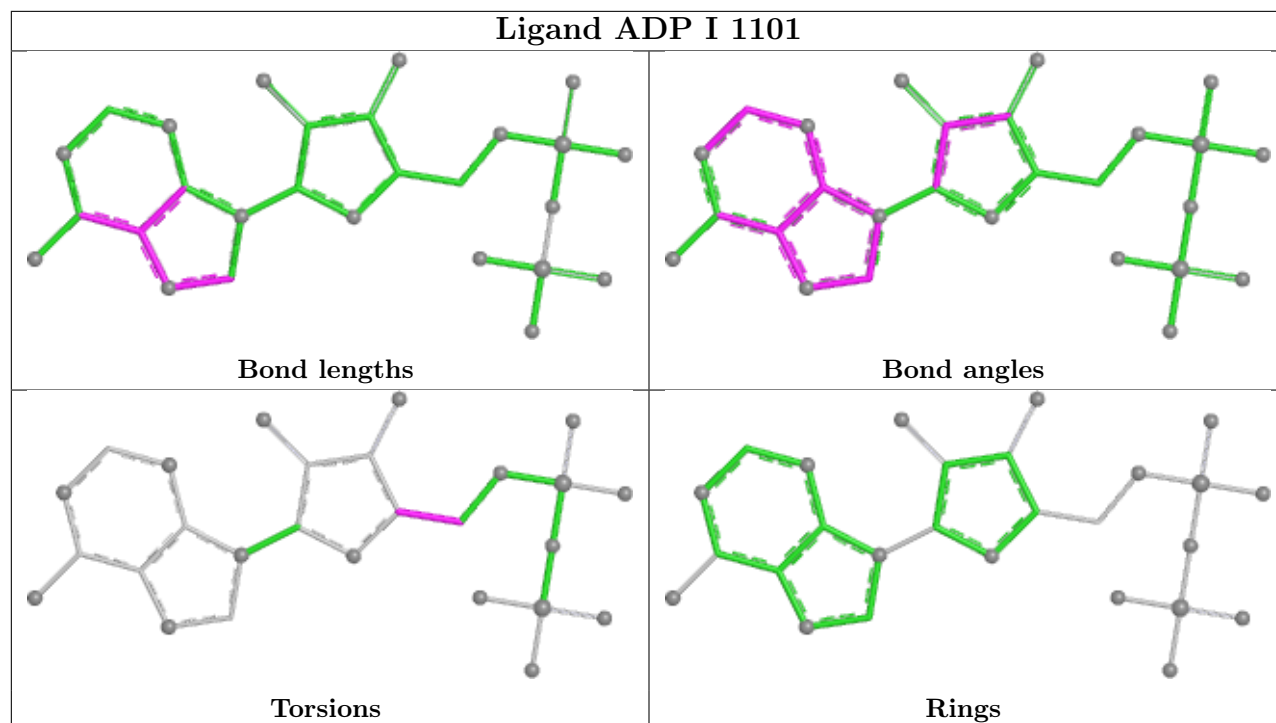
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1102	8GI	1	0
2	C	1101	ADP	2	0
3	J	1102	8GI	1	0
2	I	1101	ADP	2	0
2	F	1101	ADP	2	0
3	I	1102	8GI	1	0
2	A	1101	ADP	2	0
3	C	1102	8GI	1	0
2	E	1101	ADP	2	0
2	J	1101	ADP	2	0
3	A	1102	8GI	1	0
3	E	1102	8GI	1	0
2	D	1101	ADP	2	0
3	B	1102	8GI	1	0
3	G	1102	8GI	1	0
2	G	1101	ADP	2	0
2	H	1101	ADP	2	0
3	D	1102	8GI	1	0
2	B	1101	ADP	2	0
3	H	1102	8GI	1	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

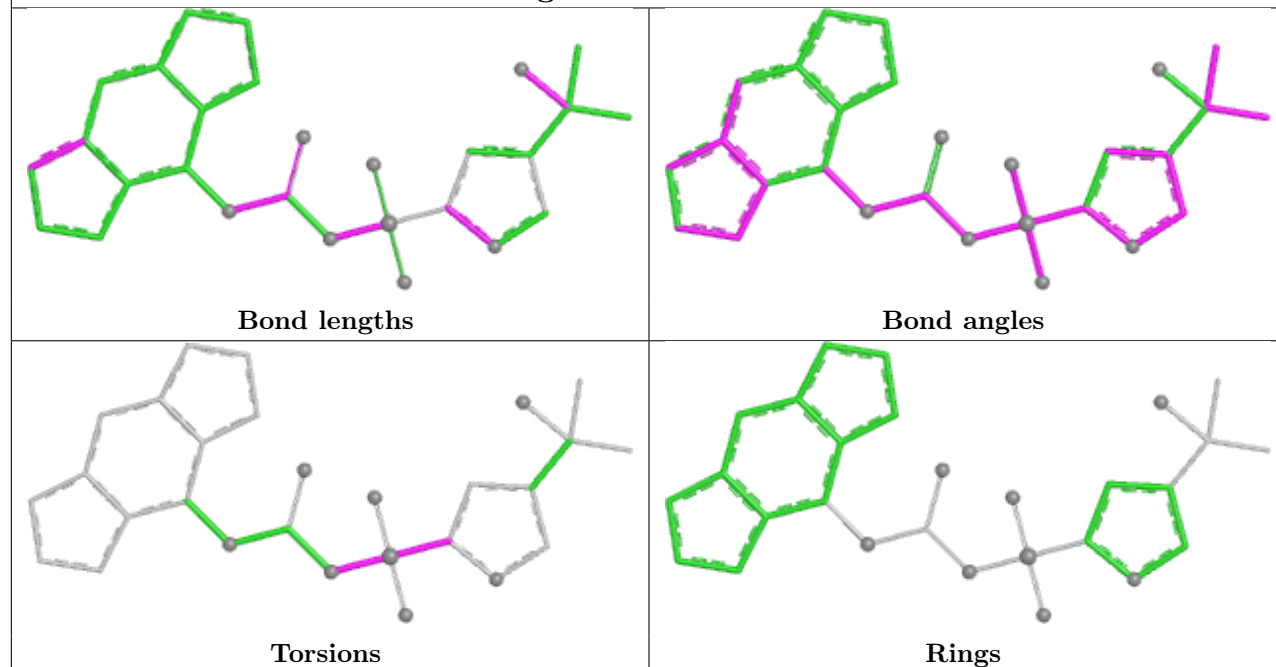
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



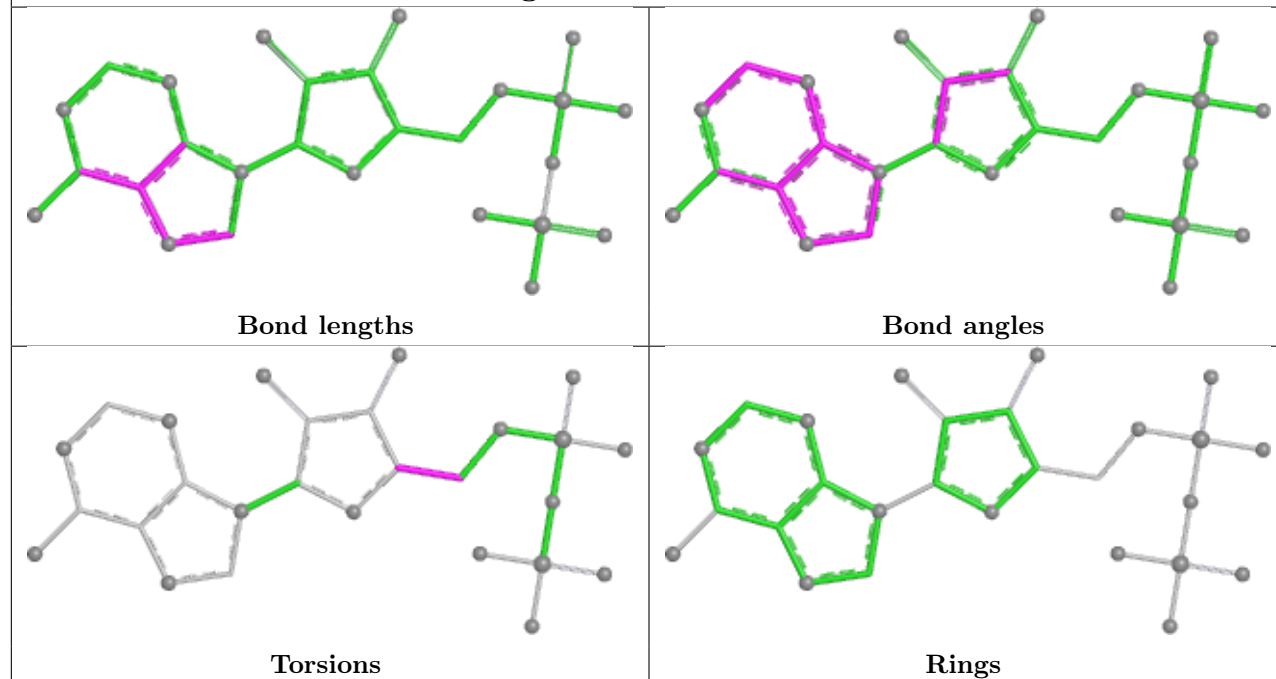


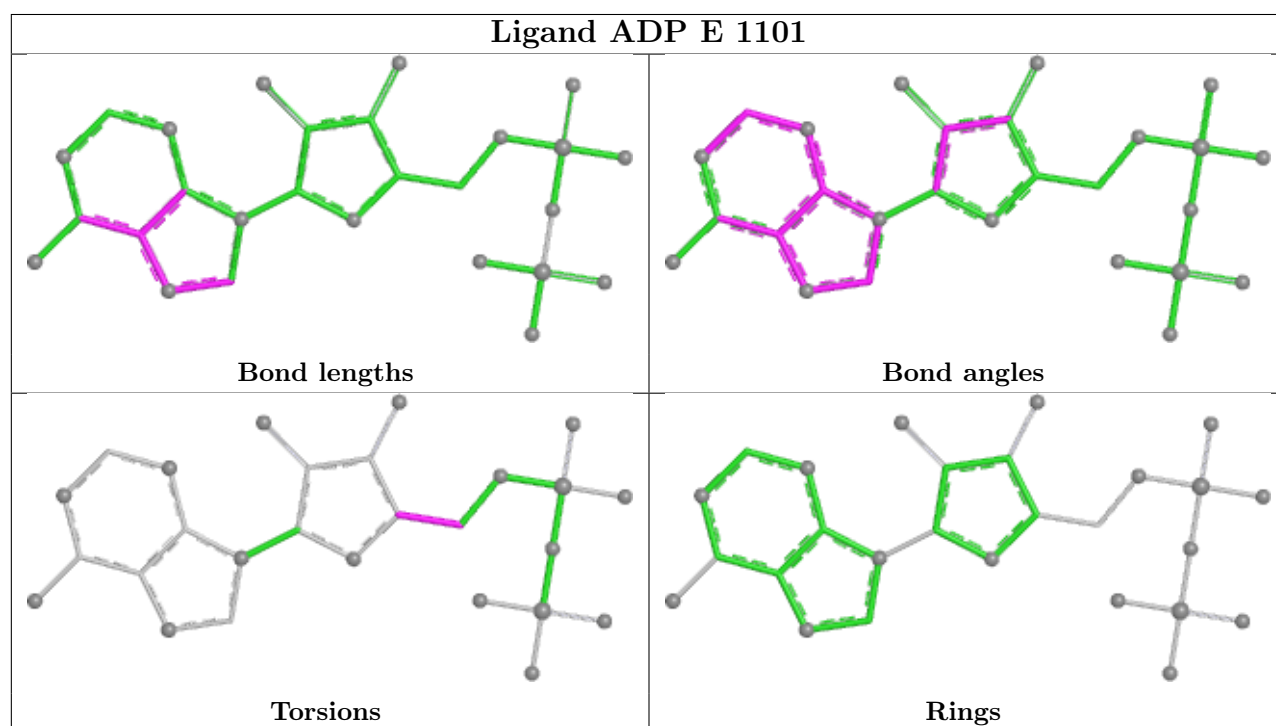
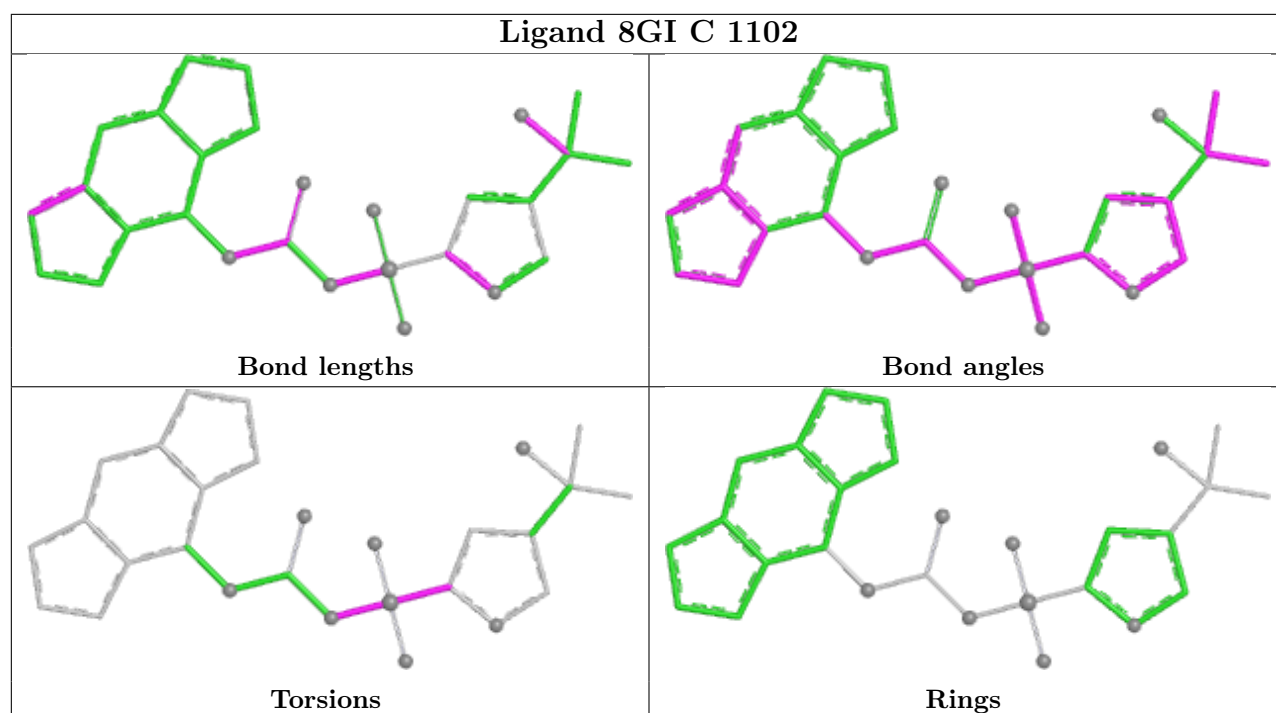


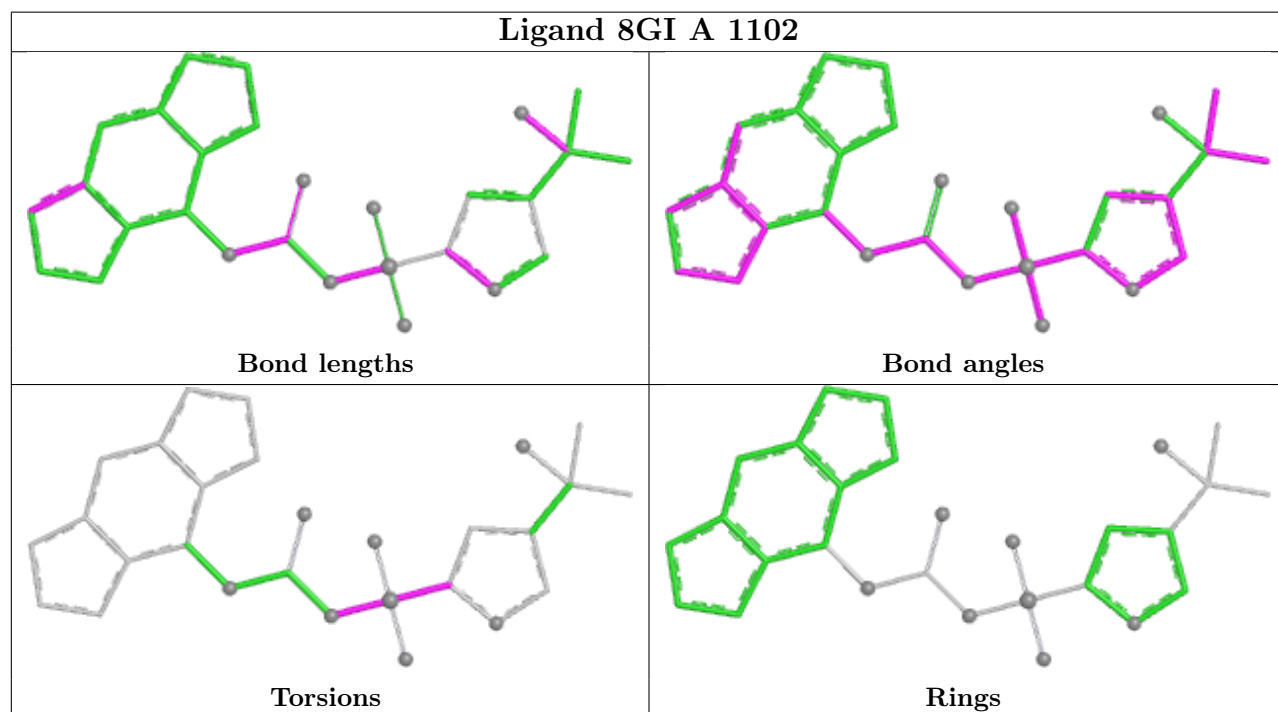
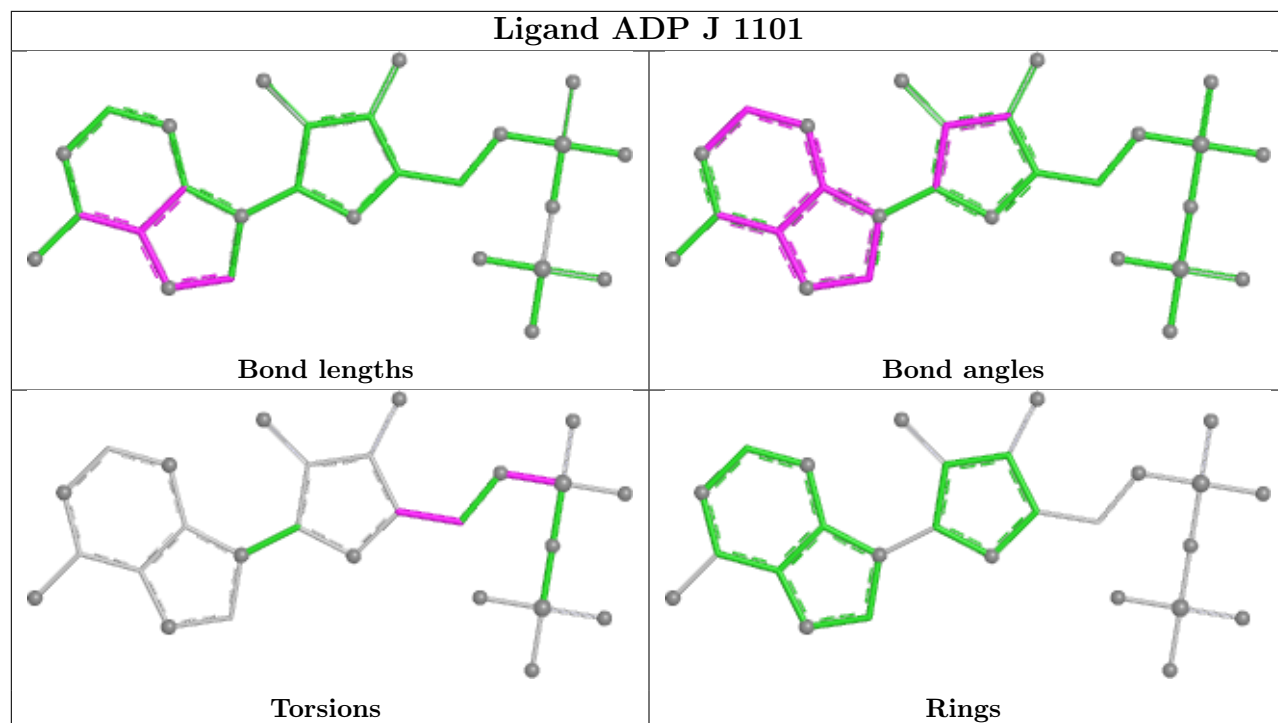
Ligand 8GI I 1102



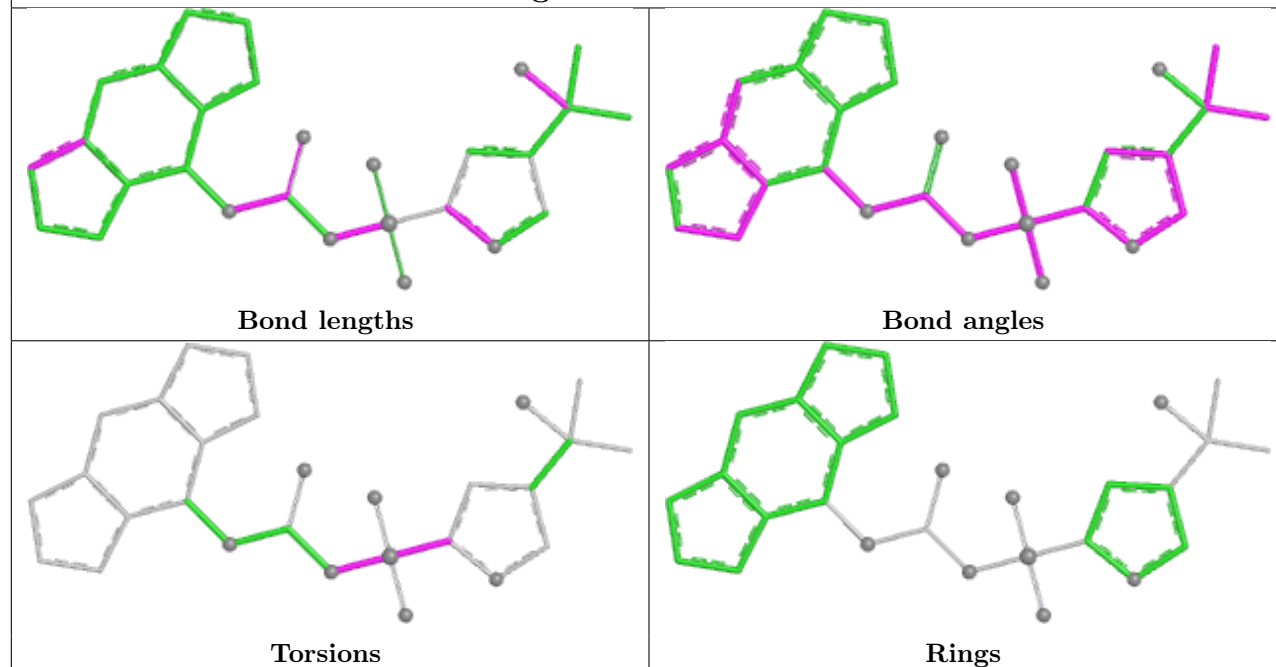
Ligand ADP A 1101



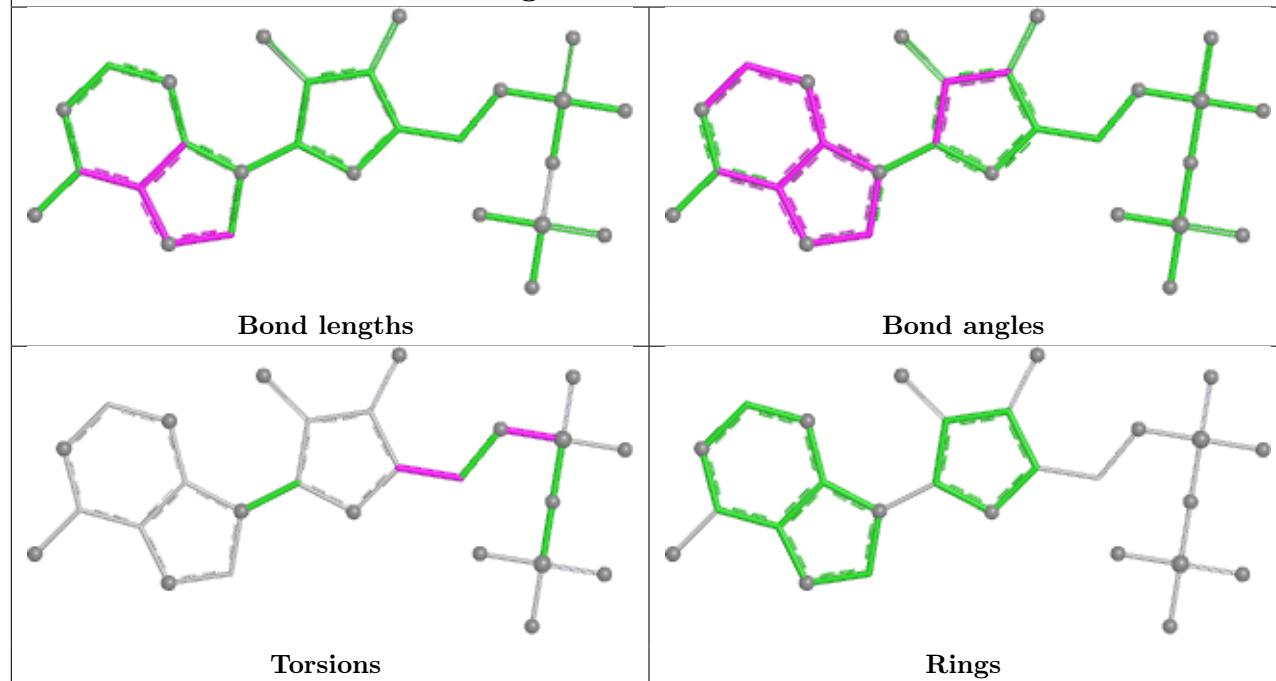


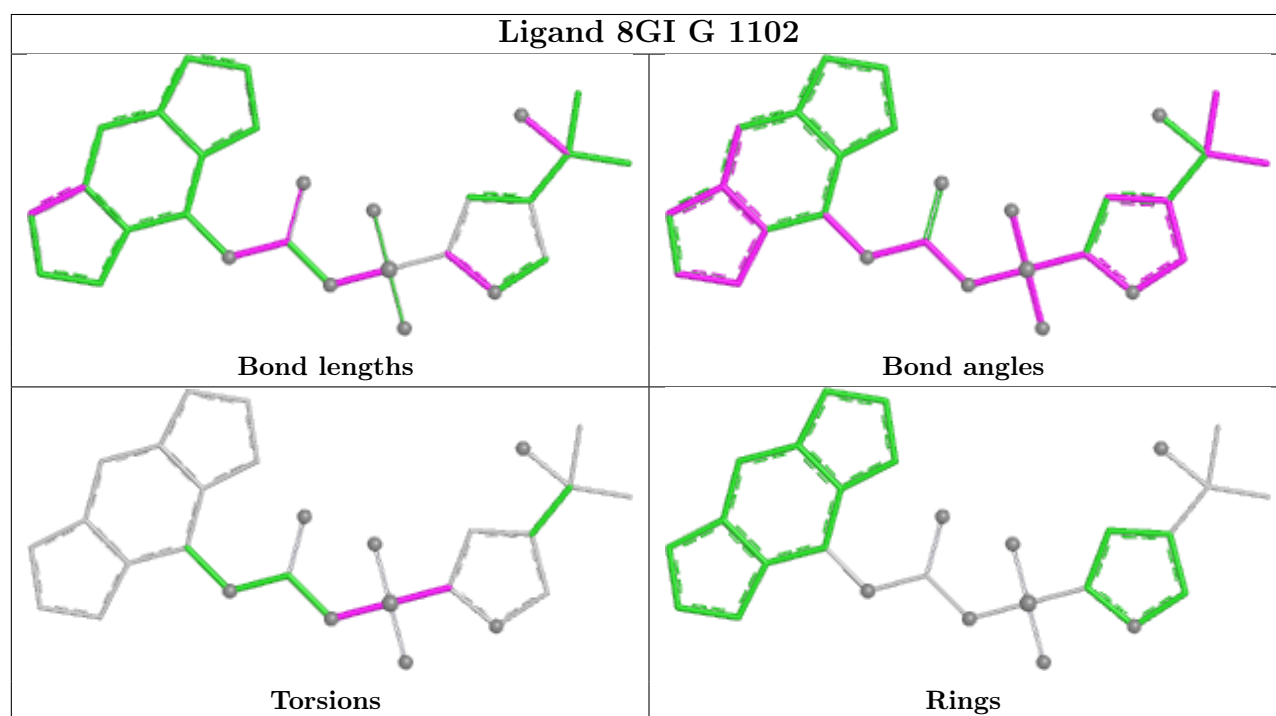
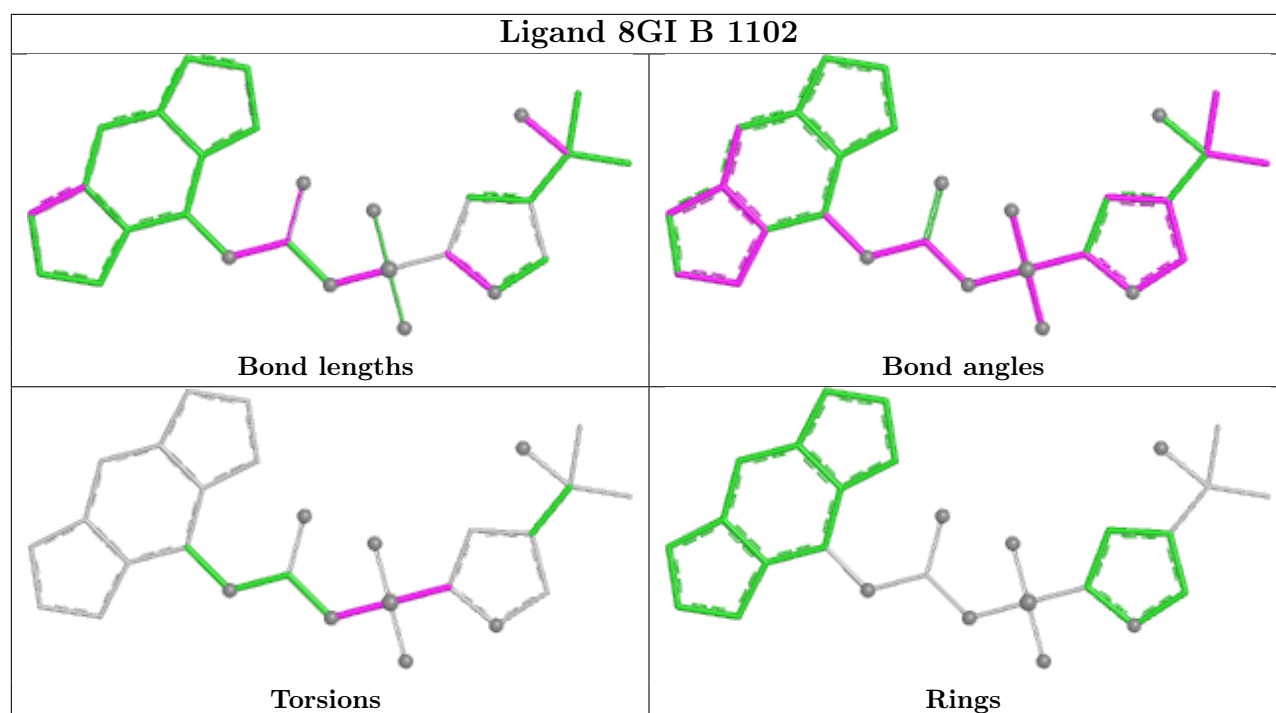


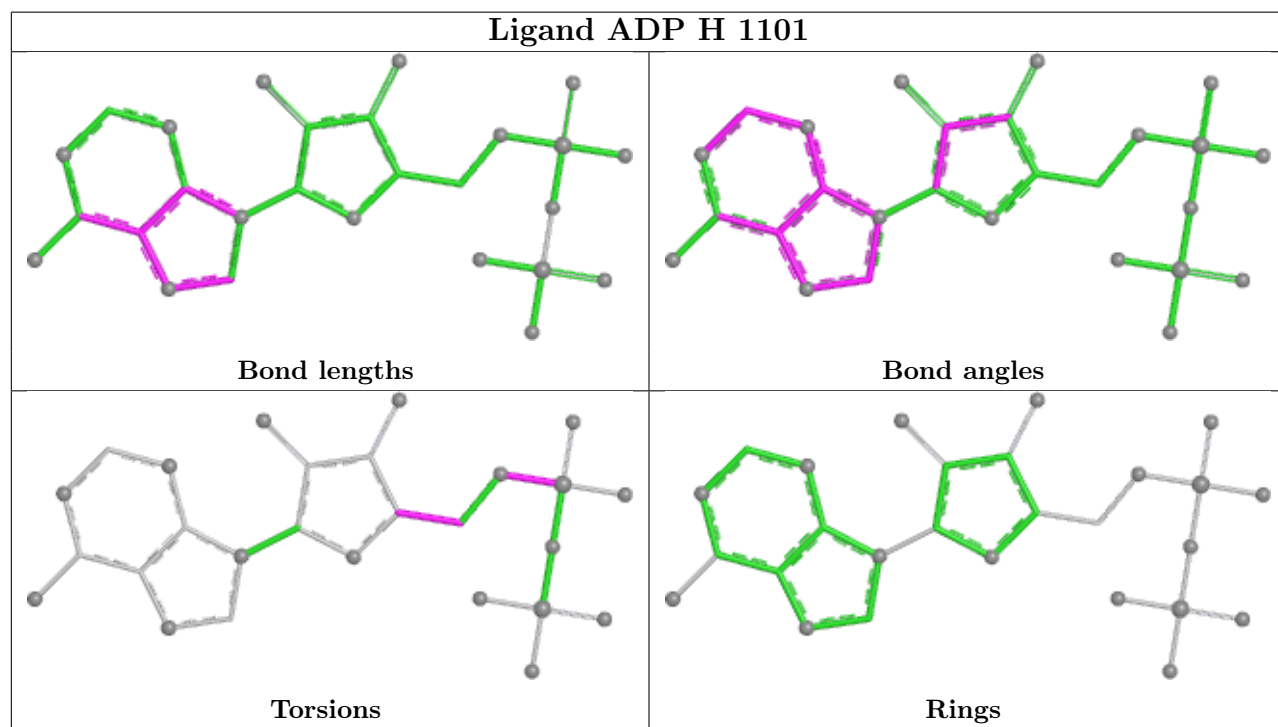
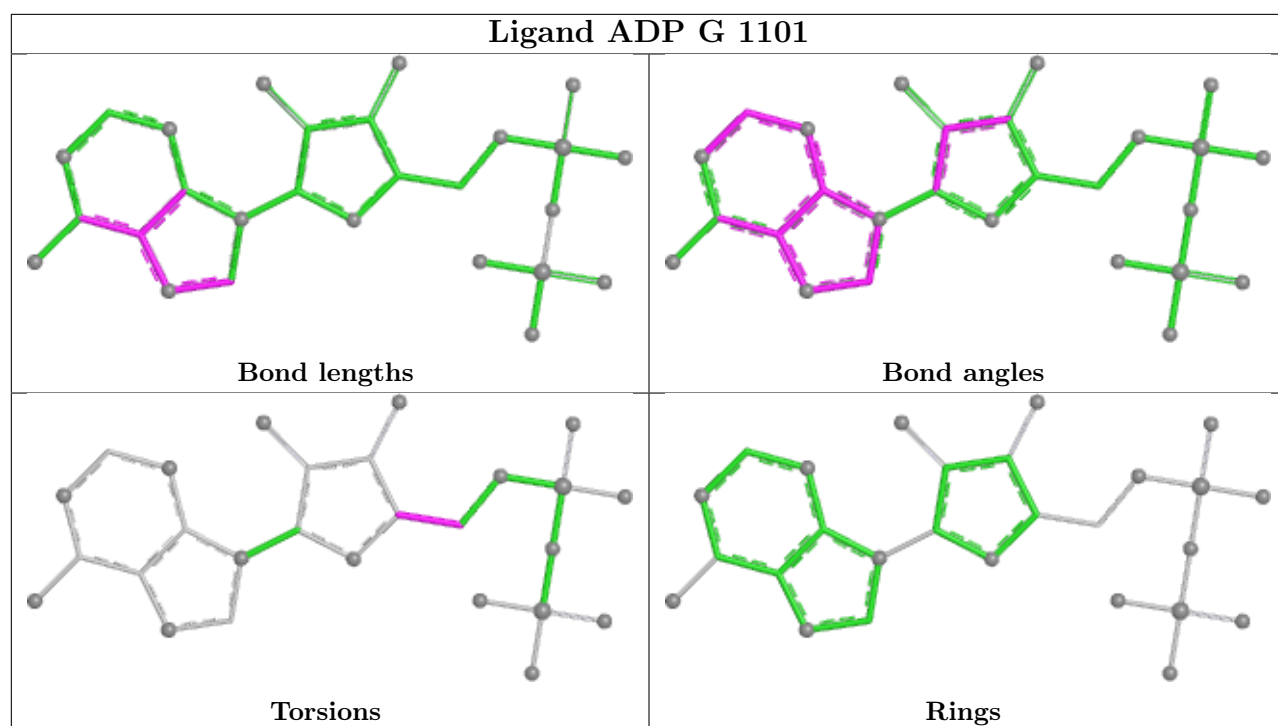
Ligand 8GI E 1102

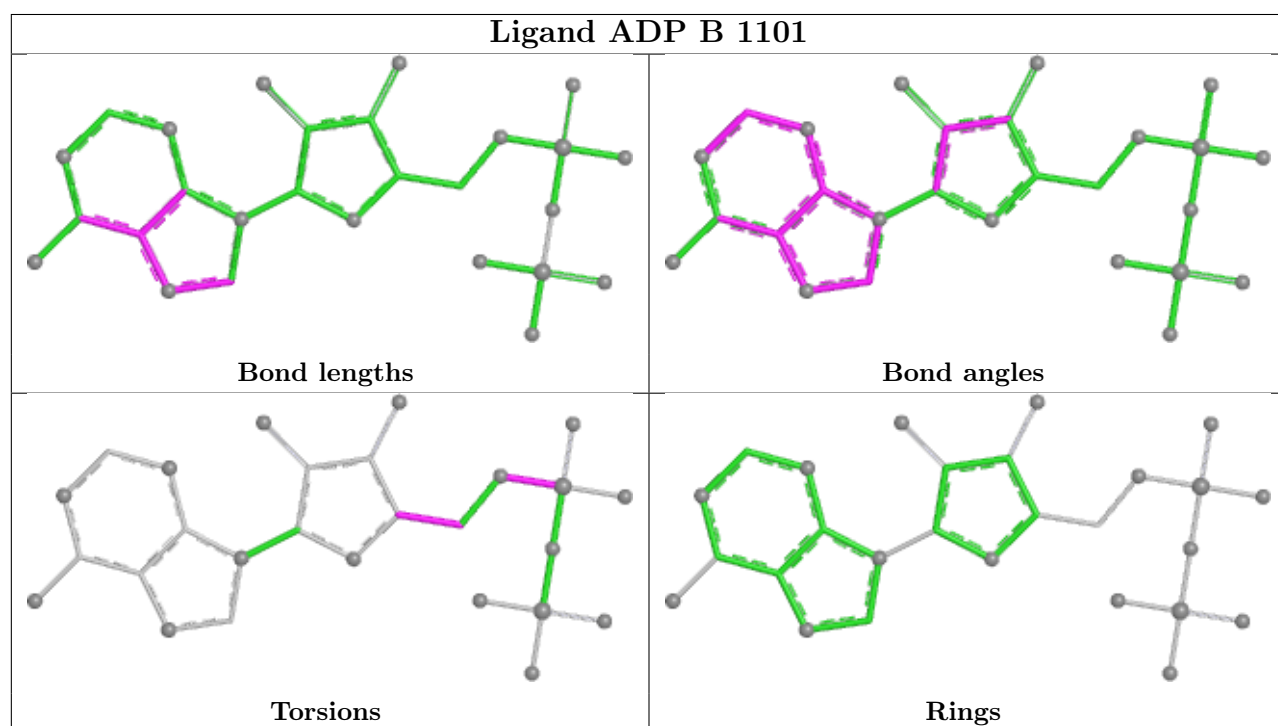
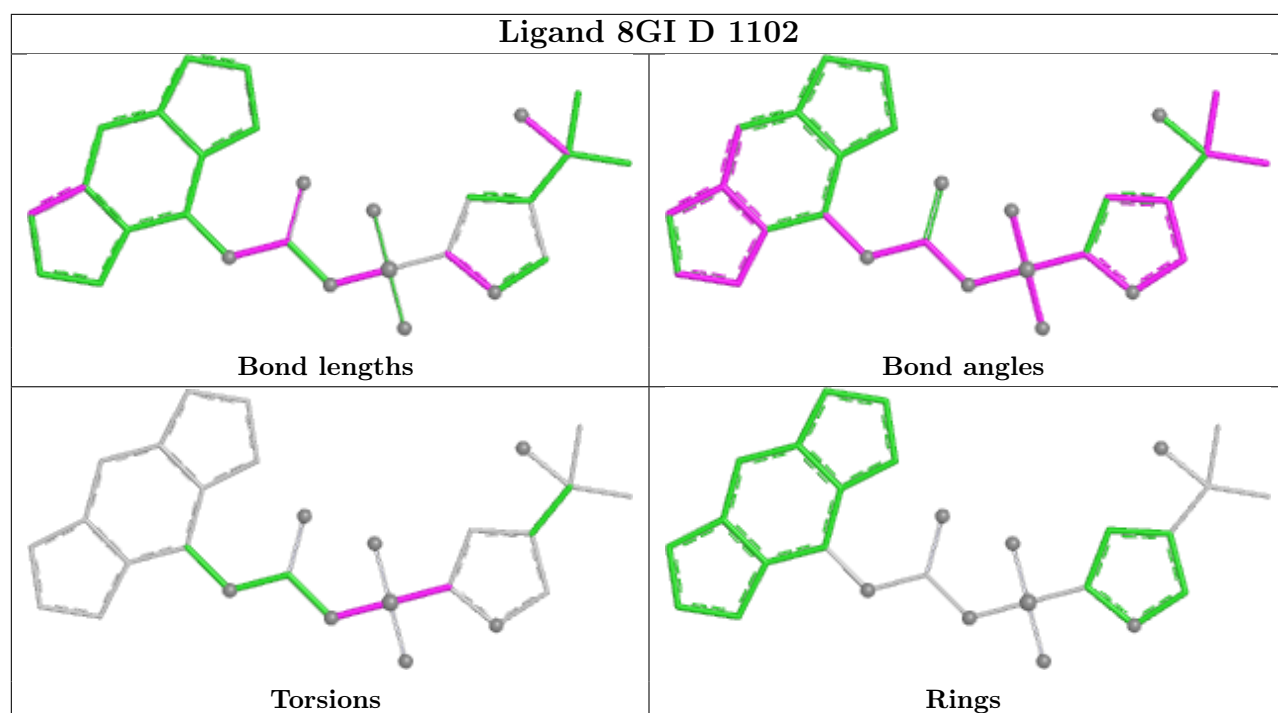


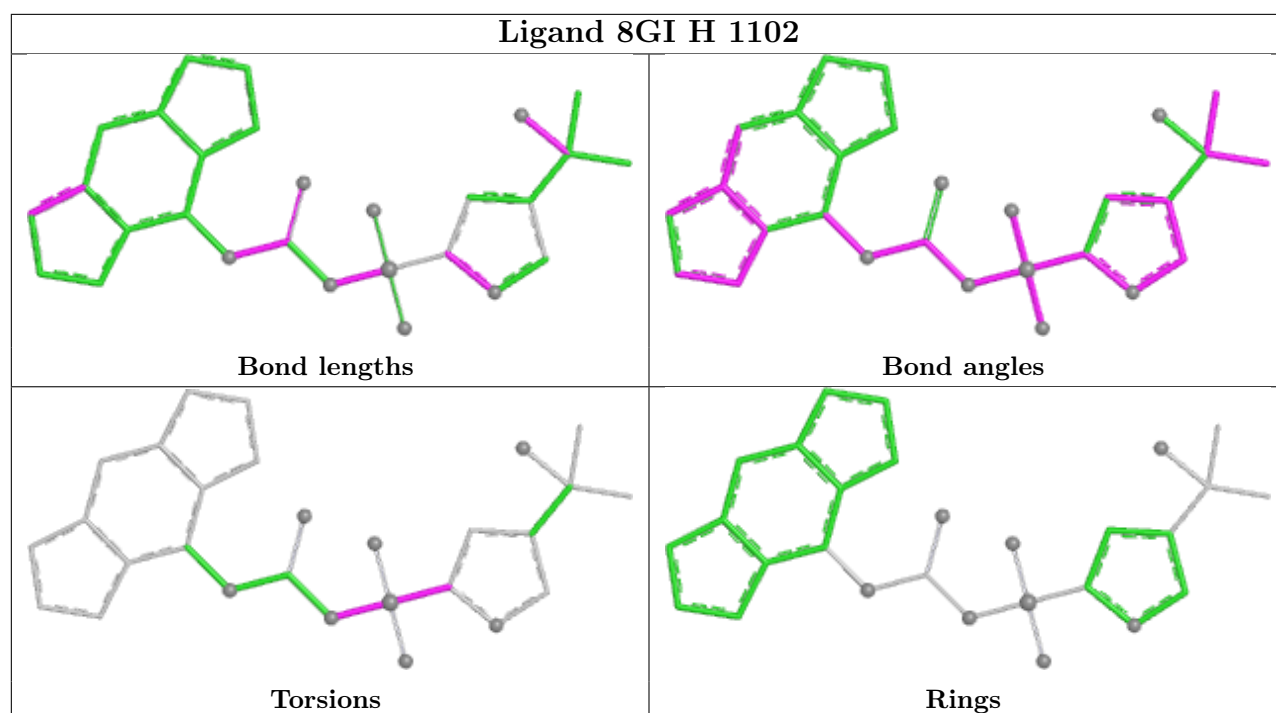
Ligand ADP D 1101











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.

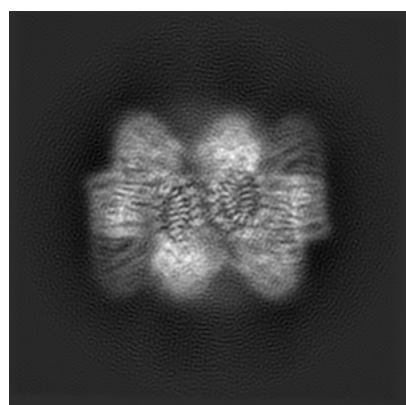
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13686. These allow visual inspection of the internal detail of the map and identification of artifacts.

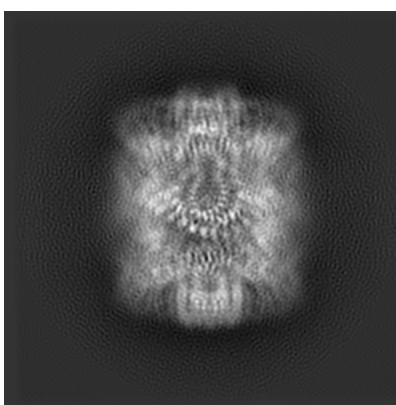
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

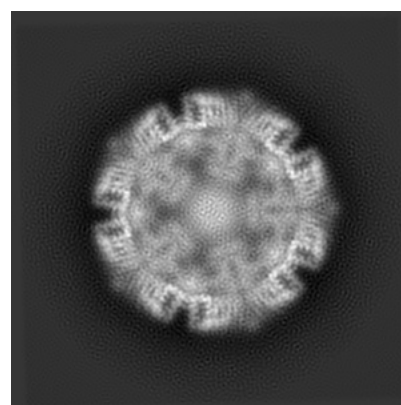
6.1.1 Primary map



X



Y

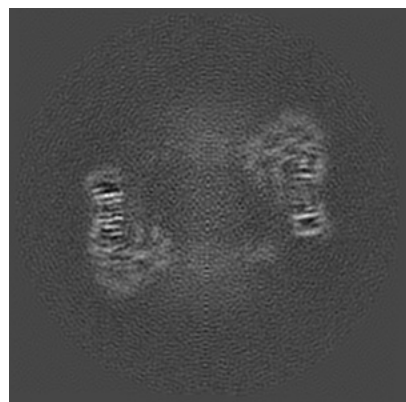


Z

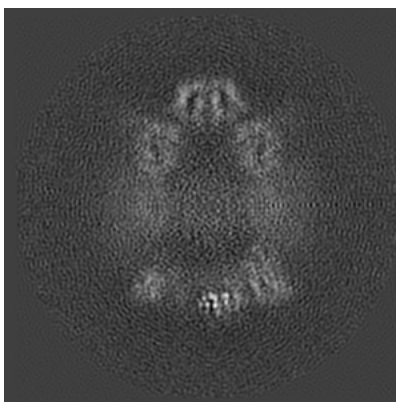
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

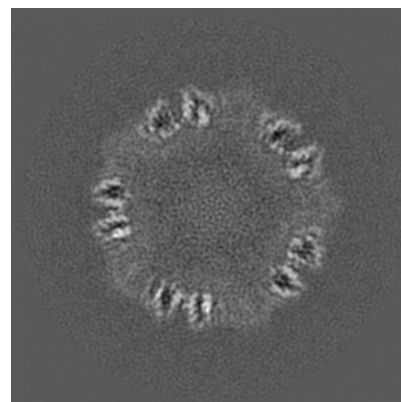
6.2.1 Primary map



X Index: 120



Y Index: 120

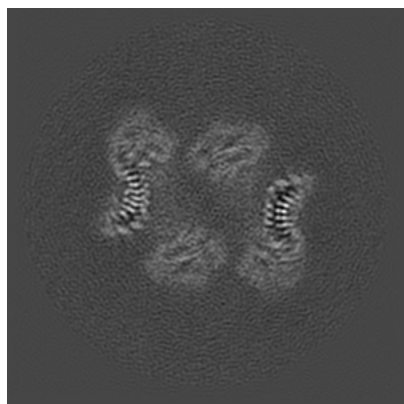


Z Index: 120

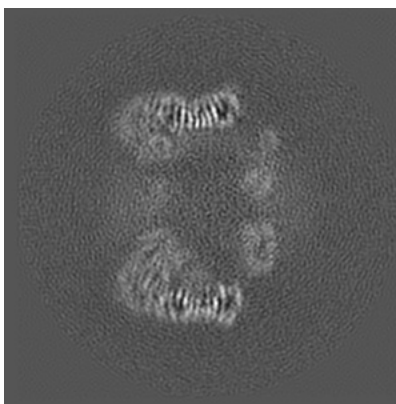
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

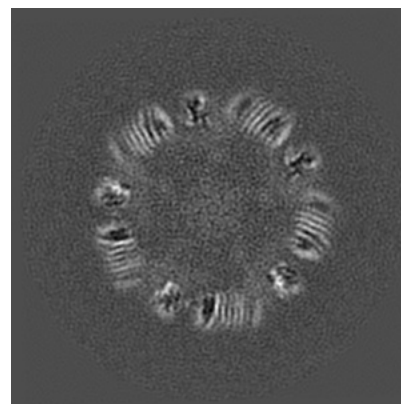
6.3.1 Primary map



X Index: 158



Y Index: 100

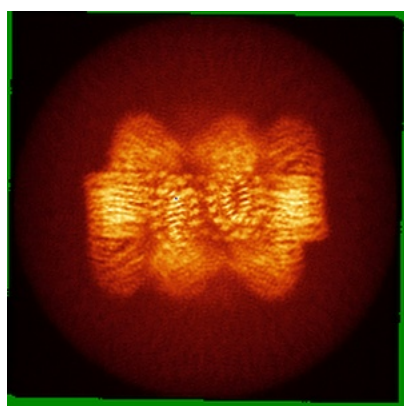


Z Index: 130

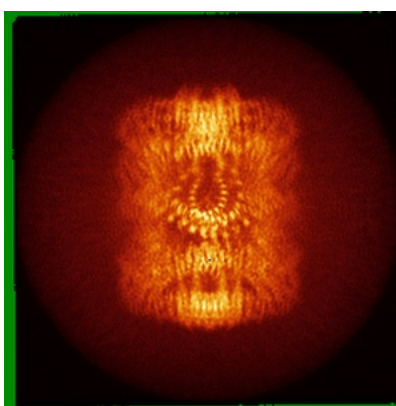
The images above show the largest variance slices of the map in three orthogonal directions.

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

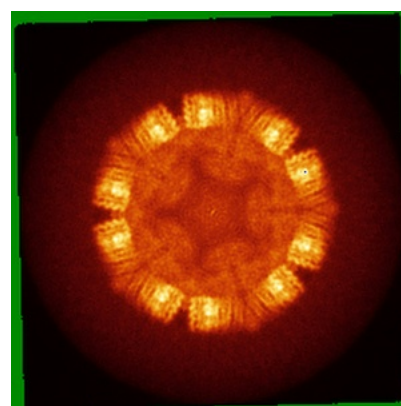
6.4.1 Primary map



X



Y

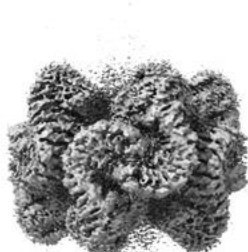


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00515. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

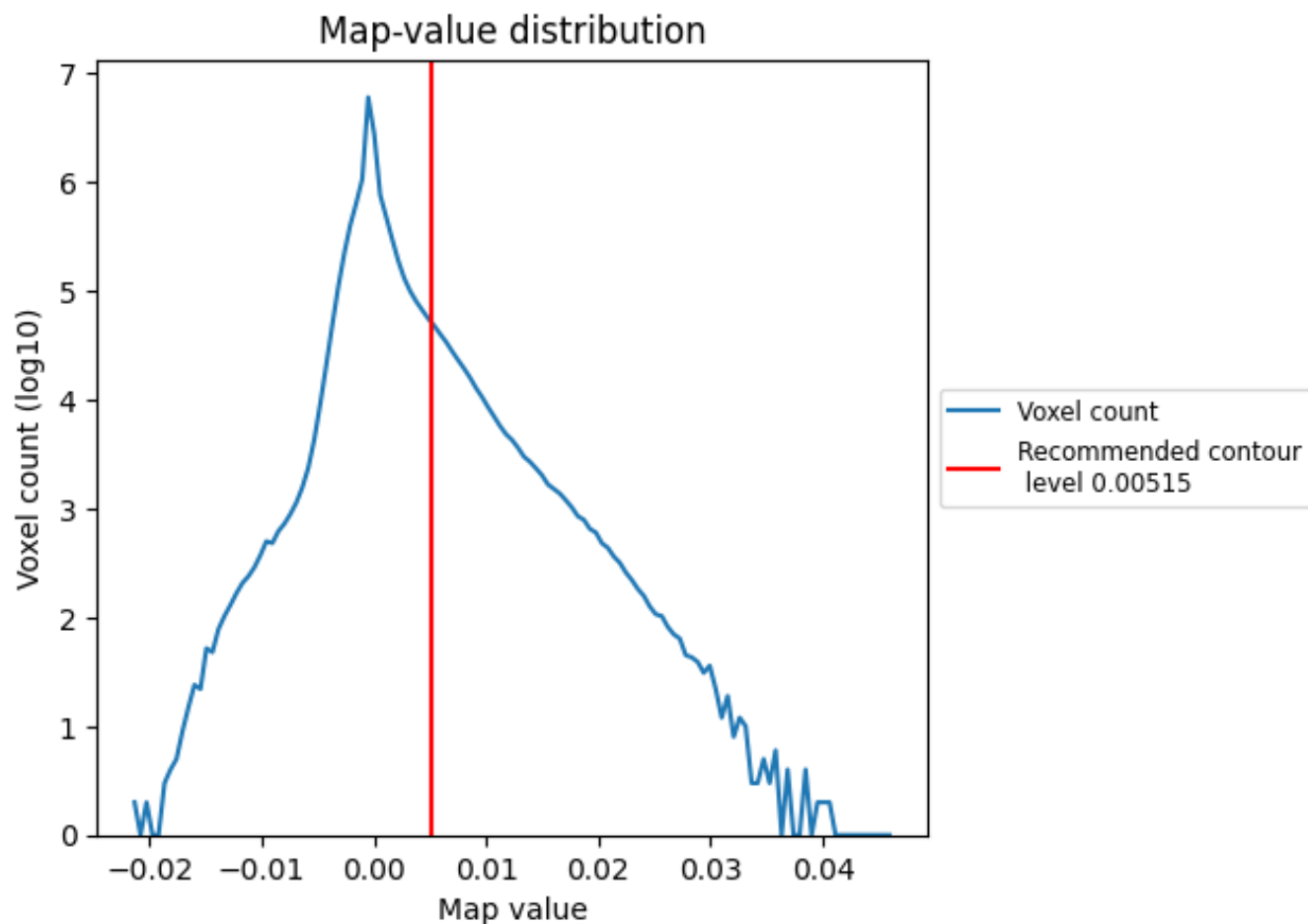
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

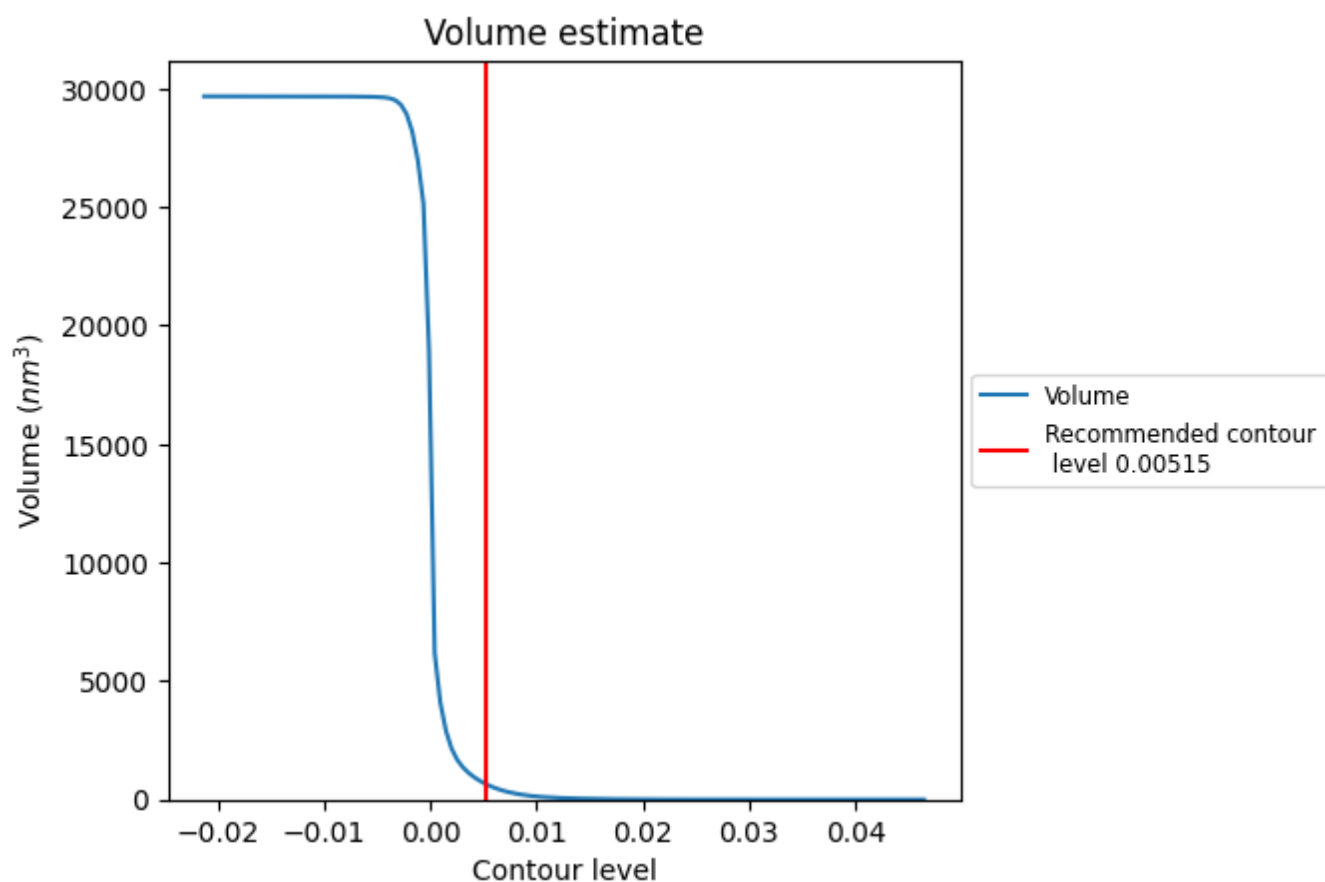
This section contains the results of statistical analysis of the map.

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.

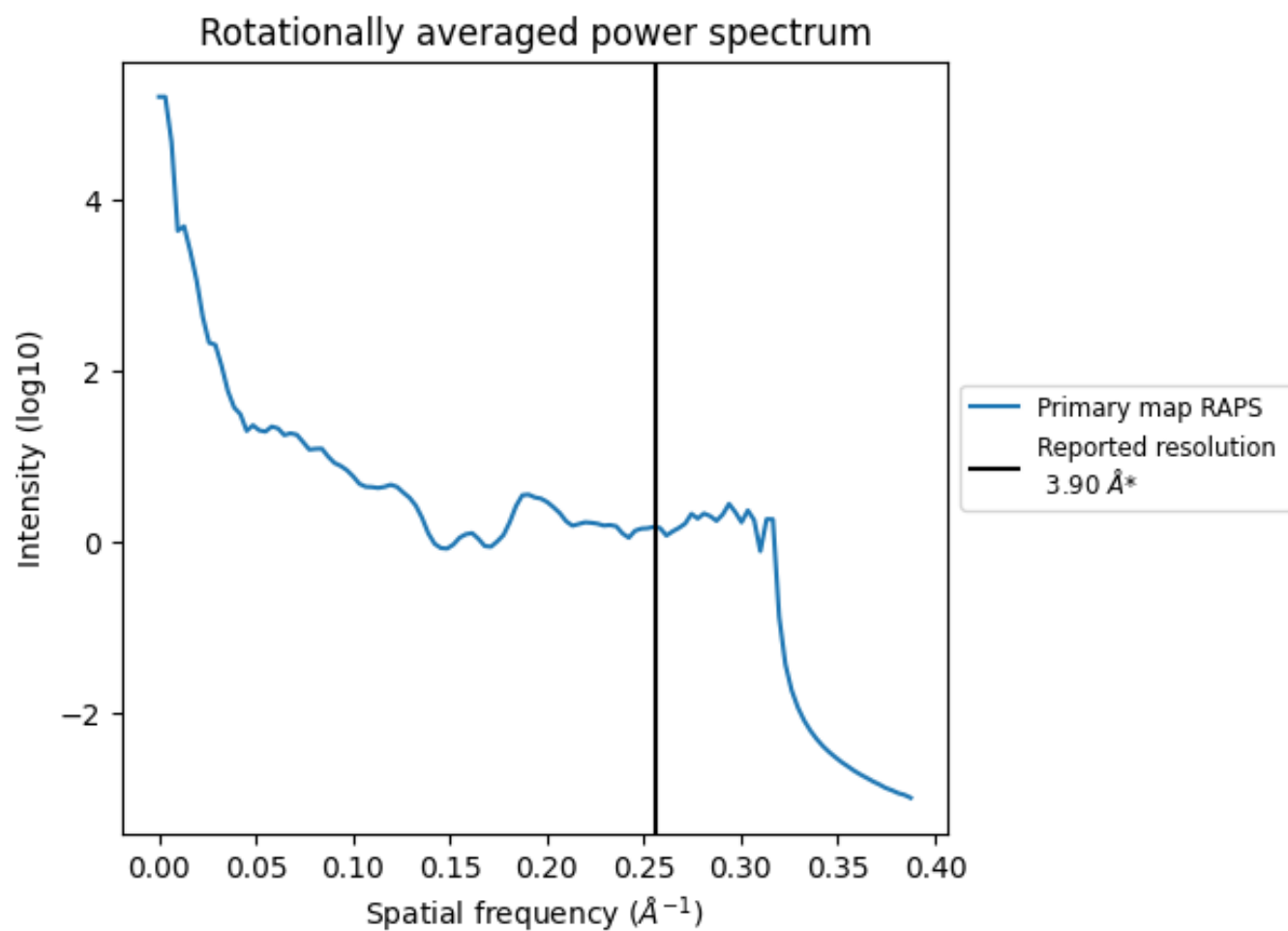
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 670 nm³; this corresponds to an approximate mass of 605 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 ⓘ

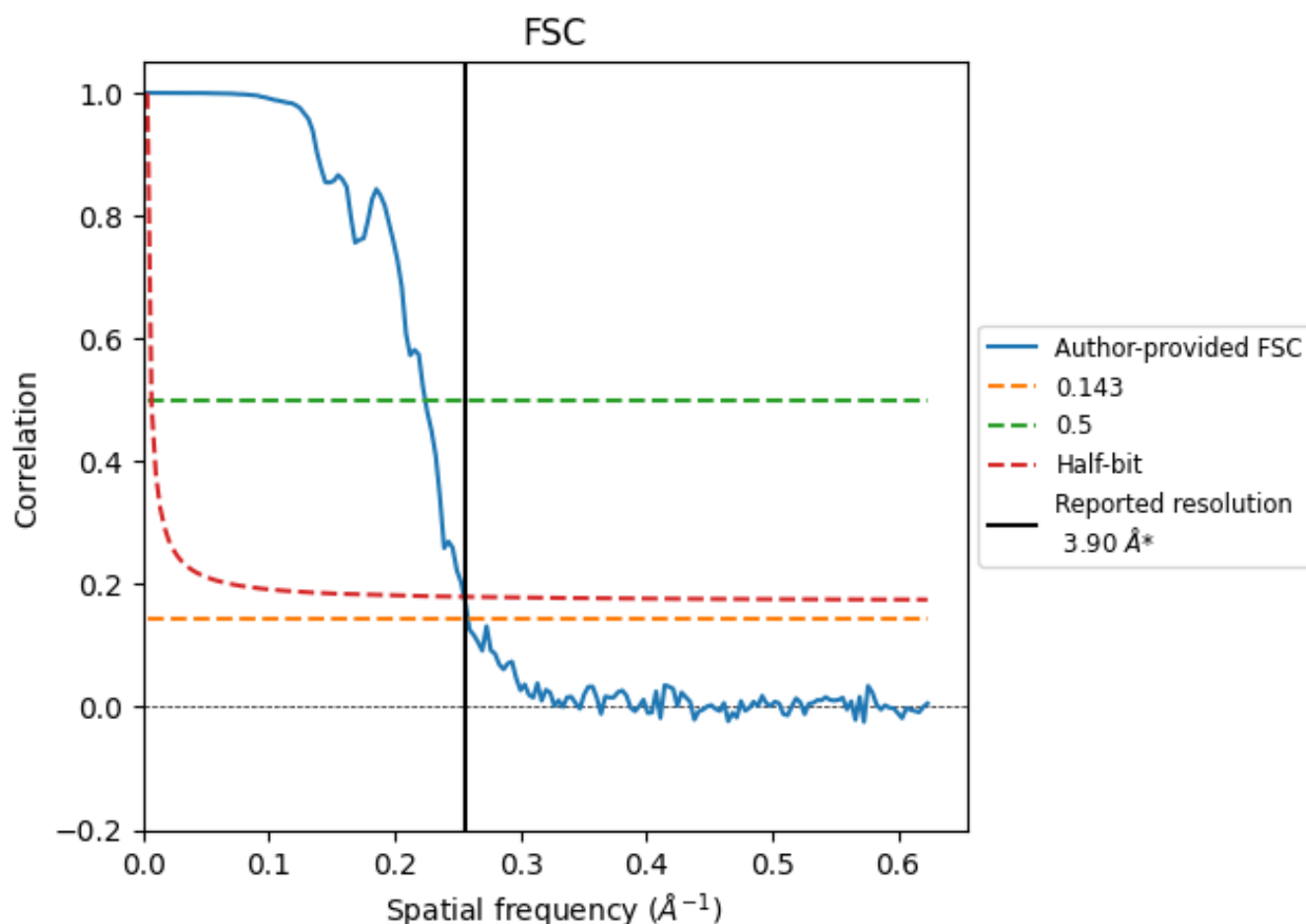


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

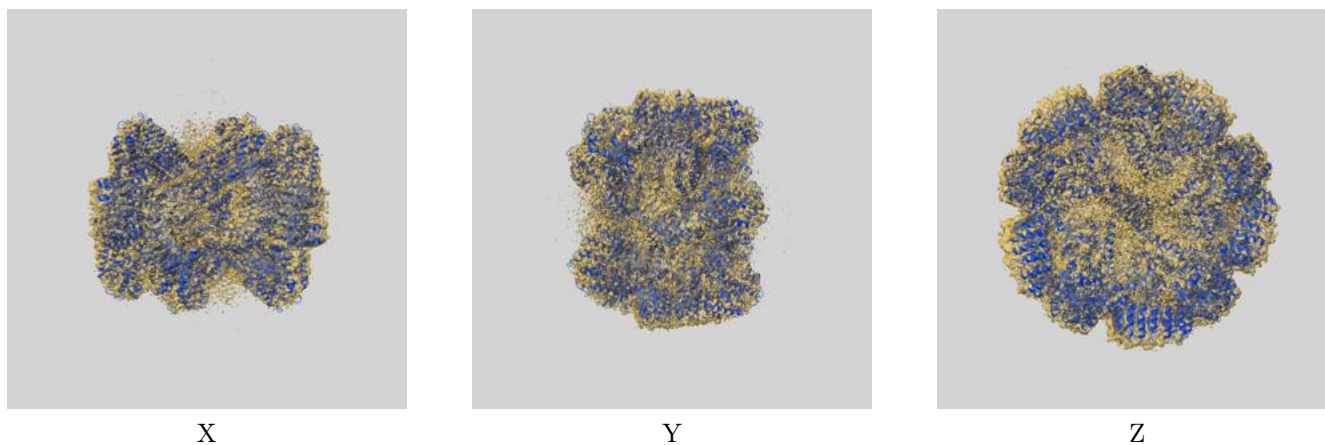
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.87	4.46	3.92
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

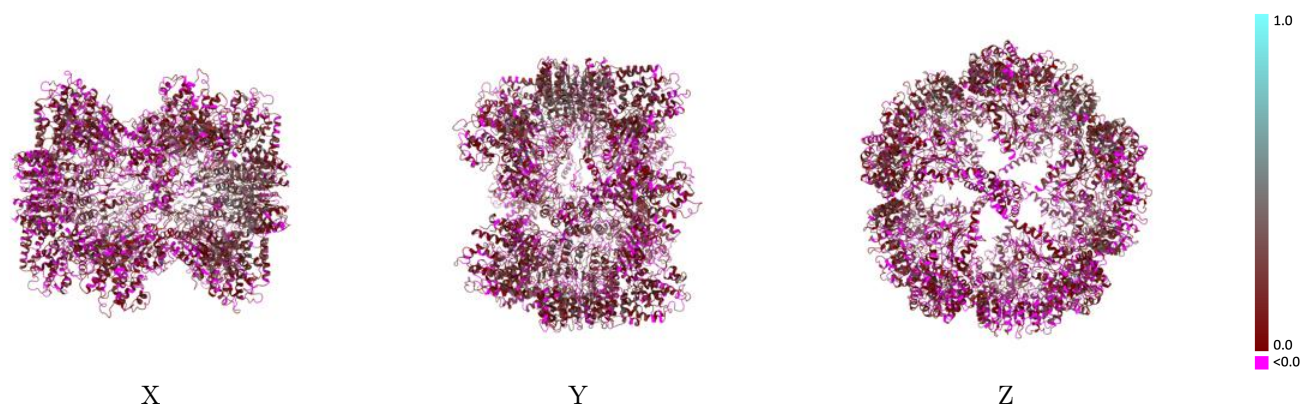
This section contains information regarding the fit between EMDB map EMD-13686 and PDB model 7PZC. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



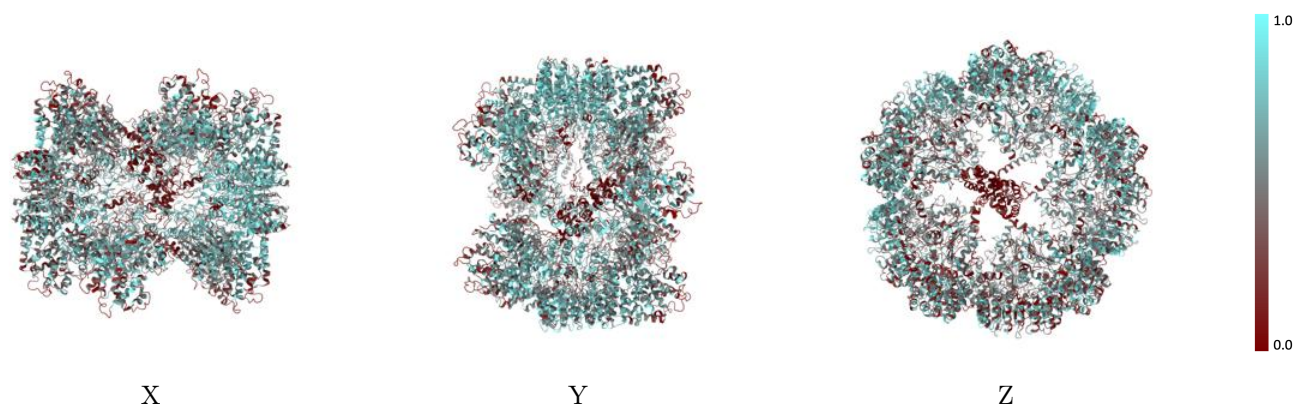
The images above show the 3D surface view of the map at the recommended contour level 0.00515 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



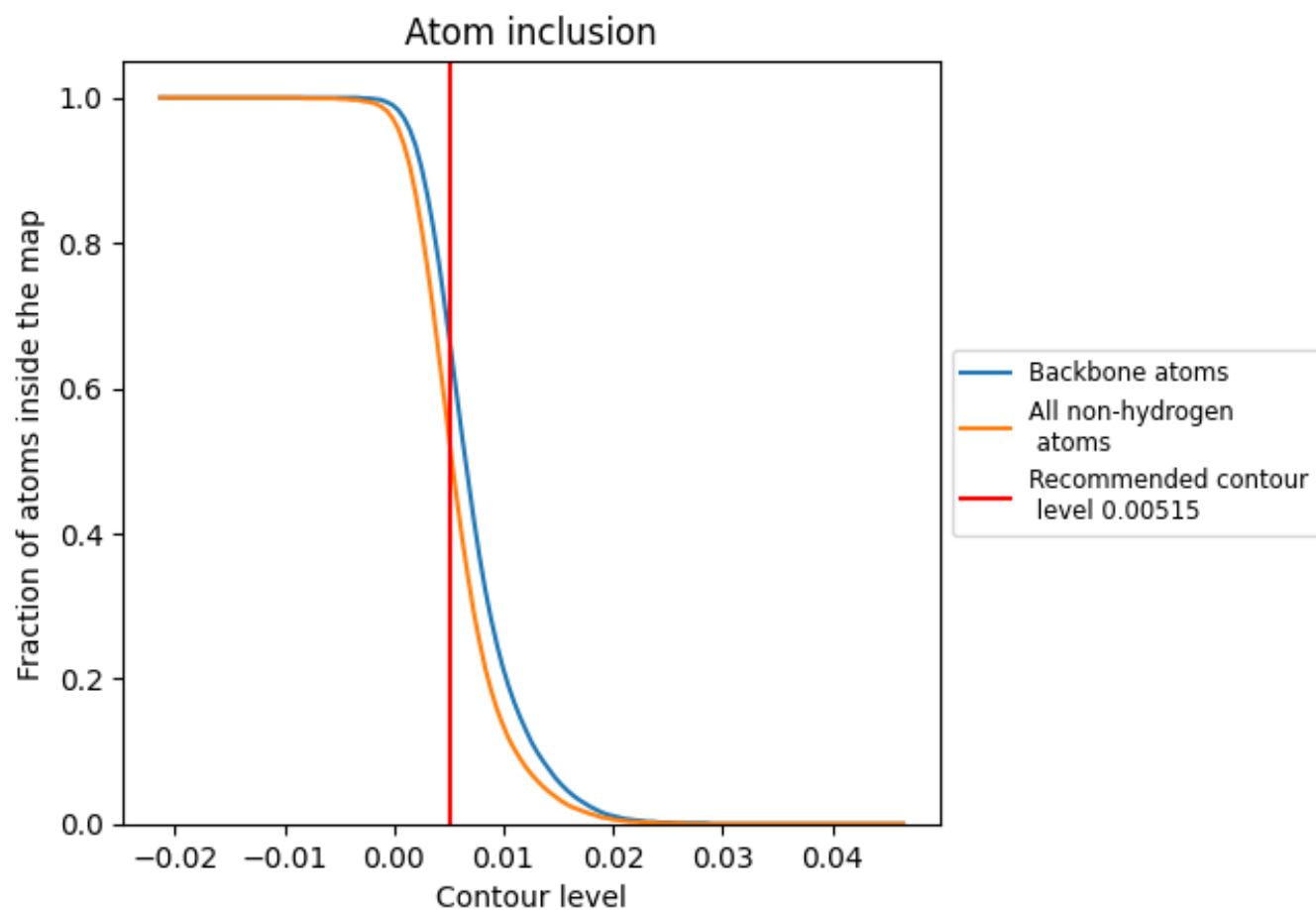
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00515).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 52% 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 (0.00515) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5160	0.1140
A	0.5090	0.1460
B	0.5570	0.1380
C	0.5320	0.1080
D	0.5740	0.1570
E	0.4780	0.0670
F	0.5130	0.0950
G	0.5170	0.1060
H	0.4250	0.0620
I	0.5500	0.1460
J	0.5230	0.1190

1.0

0.0

<0.0