



# wwPDB EM Validation Summary Report

Mar 18, 2024 – 02:27 PM EDT

PDB ID : 8SUB  
EMDB ID : EMD-40763  
Title : E. coli SIR2-HerA complex (dodecamer SIR2 pentamer HerA)  
Authors : Shen, Z.F.; Lin, Q.P.; Fu, T.M.  
Deposited on : 2023-05-11  
Resolution : 2.89 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](mailto: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>.

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

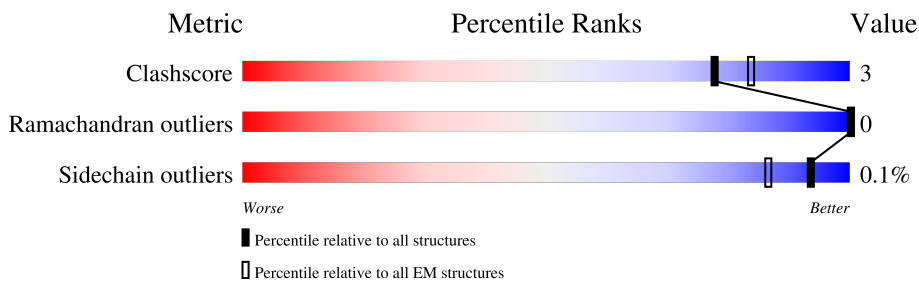
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 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 2.89 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.



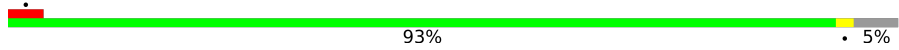

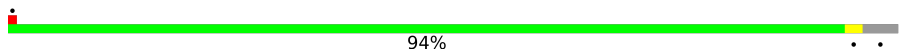
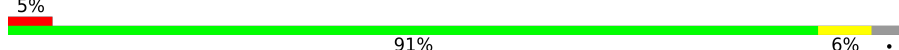

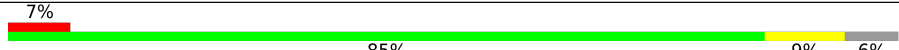
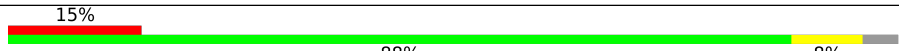


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	415	<p>93% 5%</p>
1	B	415	<p>92% 6%</p>
1	C	415	<p>89% 7%</p>
1	D	415	<p>91% 6%</p>
1	E	415	<p>91% 6%</p>
1	F	415	<p>90% 7%</p>
1	G	415	<p>86% 8% 6%</p>
1	H	415	<p>91% 5%</p>

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Mol	Chain	Length	Quality of chain
1	I	415	 93% 5%
1	J	415	 90% 6%
1	K	415	 94%
1	L	415	 91% 6%
2	M	610	 84% 10% 19% 6%
2	N	610	 85% 9% 7%
2	O	610	 88% 8% 15%
2	P	610	 77% 13% 27% 10%
2	Q	610	 73% 18% 53% 10%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 61226 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 SIR2-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	398	Total 3185	C 2048	N 532	O 599	S 6	0	0
1	B	398	Total 3186	C 2050	N 532	O 598	S 6	0	0
1	C	398	Total 3185	C 2048	N 532	O 599	S 6	0	0
1	D	401	Total 3203	C 2059	N 536	O 602	S 6	0	0
1	E	400	Total 3194	C 2053	N 534	O 601	S 6	0	0
1	F	400	Total 3198	C 2056	N 535	O 601	S 6	0	0
1	G	390	Total 3119	C 2006	N 520	O 587	S 6	0	0
1	H	401	Total 3203	C 2059	N 536	O 602	S 6	0	0
1	I	394	Total 3145	C 2021	N 525	O 593	S 6	0	0
1	J	400	Total 3199	C 2057	N 535	O 601	S 6	0	0
1	K	398	Total 3182	C 2047	N 532	O 597	S 6	0	0
1	L	400	Total 3199	C 2057	N 535	O 601	S 6	0	0

- Molecule 2 is a protein called Nucleoside triphosphate hydrolase.

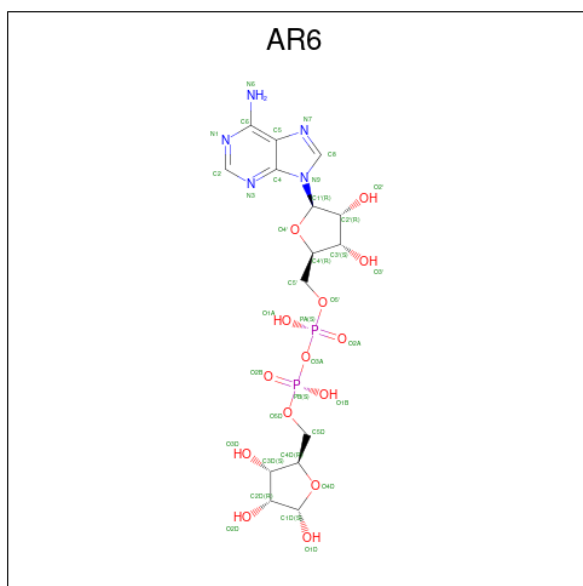
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	M	573	Total 4536	C 2887	N 798	O 838	S 13	0	0
2	N	574	Total 4548	C 2898	N 799	O 839	S 12	0	0
2	O	585	Total 4637	C 2951	N 812	O 862	S 12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	P	549	Total	C	N	O	S	0	0
			4346	2777	752	805	12		
2	Q	552	Total	C	N	O	S	0	0
			4389	2806	765	805	13		

- Molecule 3 is [(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHYL [HYDROXY-[[[(2R,3S,4R,5S)-3,4,5-TRIHYDROXYOXOLAN-2-YL]METHOXY]PHOSPHORYL] HYDROGEN PHOSPHATE (three-letter code: AR6) (formula: C<sub>15</sub>H<sub>23</sub>N<sub>5</sub>O<sub>14</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



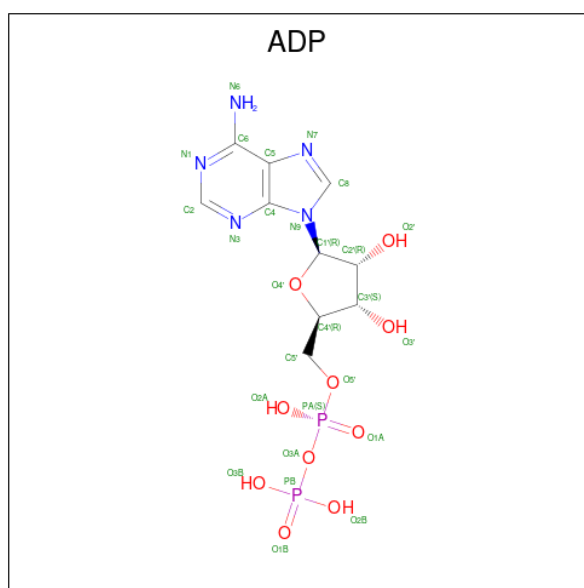
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	Total	C	N	O	P	0
			36	15	5	14	2	
3	B	1	Total	C	N	O	P	0
			36	15	5	14	2	
3	C	1	Total	C	N	O	P	0
			36	15	5	14	2	
3	D	1	Total	C	N	O	P	0
			36	15	5	14	2	
3	E	1	Total	C	N	O	P	0
			36	15	5	14	2	
3	F	1	Total	C	N	O	P	0
			36	15	5	14	2	
3	G	1	Total	C	N	O	P	0
			36	15	5	14	2	
3	H	1	Total	C	N	O	P	0
			36	15	5	14	2	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	I	1	Total 36	C 15	N 5	O 14	P 2	0
3	J	1	Total 36	C 15	N 5	O 14	P 2	0
3	K	1	Total 36	C 15	N 5	O 14	P 2	0
3	L	1	Total 36	C 15	N 5	O 14	P 2	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	M	1	Total 27	C 10	N 5	O 10	P 2	0
4	N	1	Total 27	C 10	N 5	O 10	P 2	0
4	O	1	Total 27	C 10	N 5	O 10	P 2	0
4	P	1	Total 27	C 10	N 5	O 10	P 2	0
4	Q	1	Total 27	C 10	N 5	O 10	P 2	0

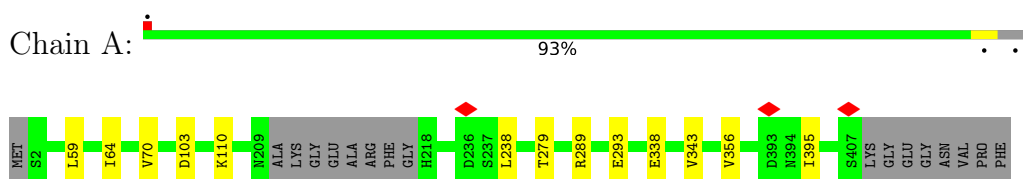
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
5	M	1	Total 1	Mg 1	0
5	N	1	Total 1	Mg 1	0
5	O	1	Total 1	Mg 1	0
5	P	1	Total 1	Mg 1	0
5	Q	1	Total 1	Mg 1	0

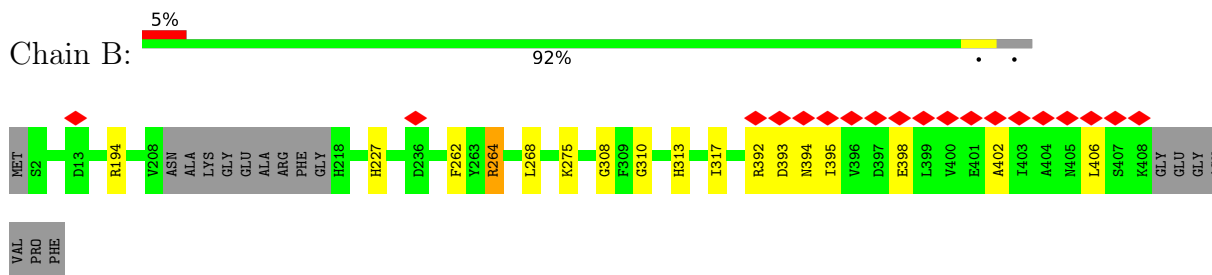
### 3 Residue-property plots

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.

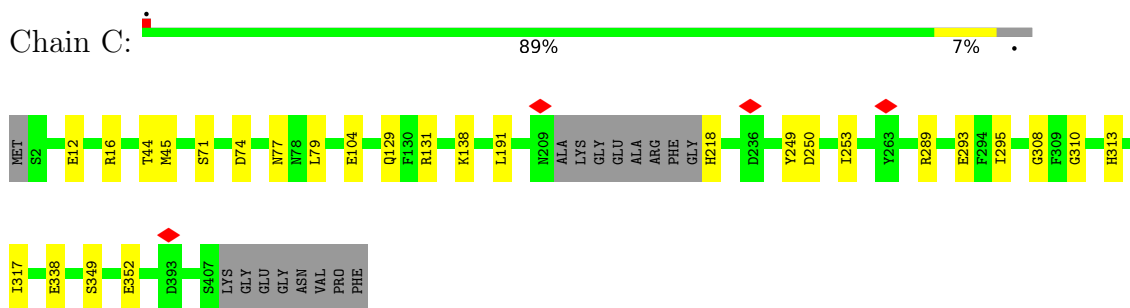
- Molecule 1: SIR2-like domain-containing protein



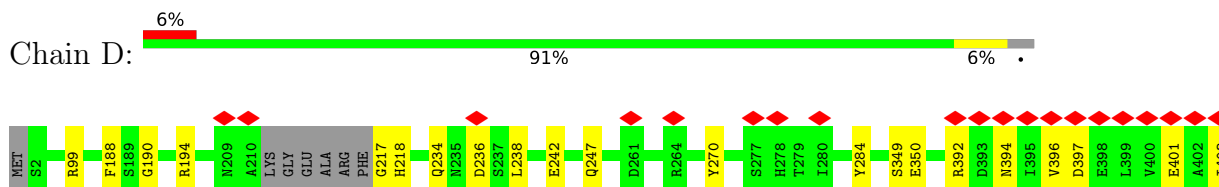
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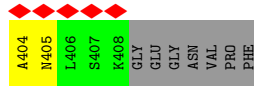
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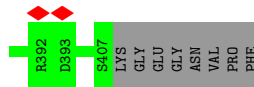
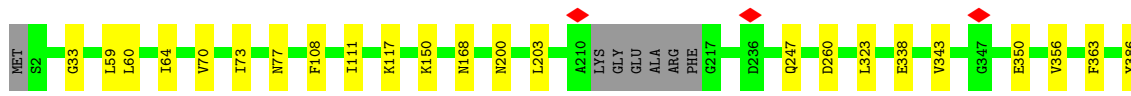
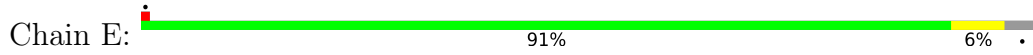
- Molecule 1: SIR2-like domain-containing protein



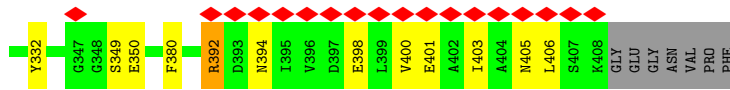
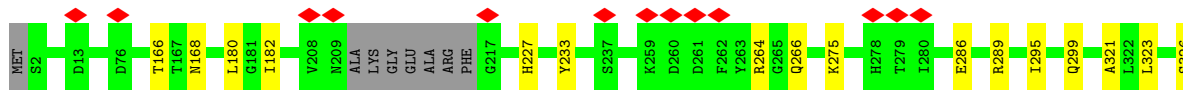
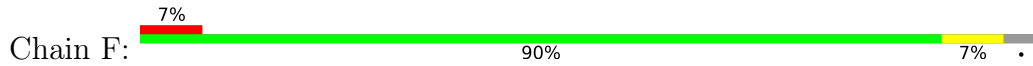




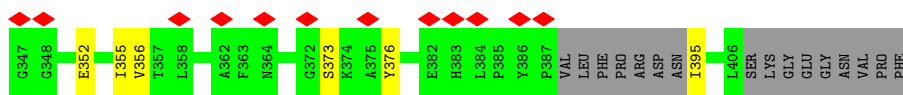
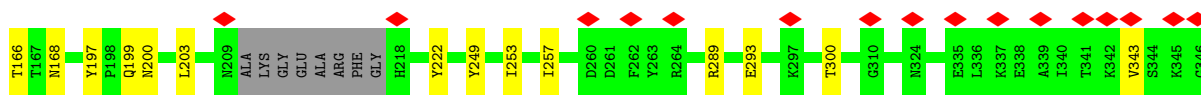
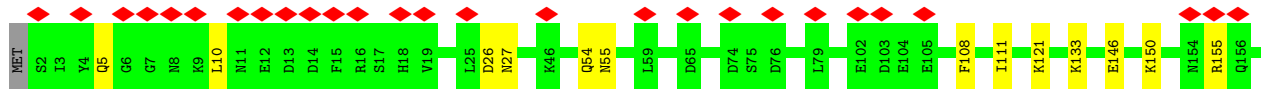
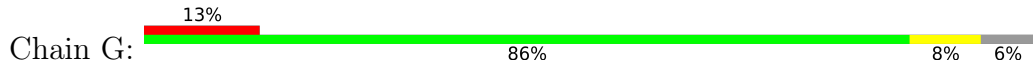
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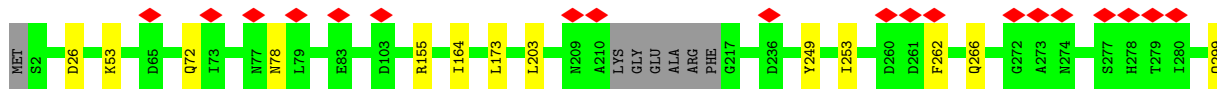
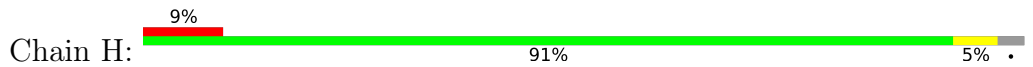
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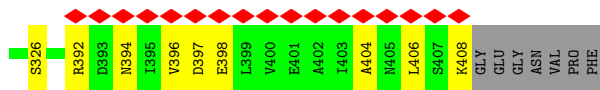


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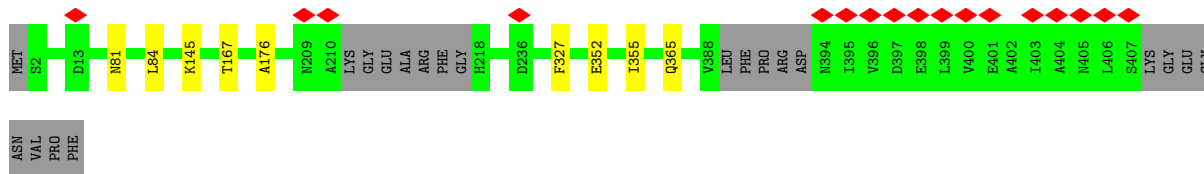
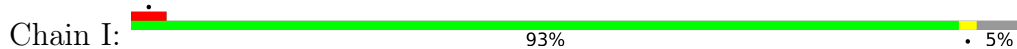


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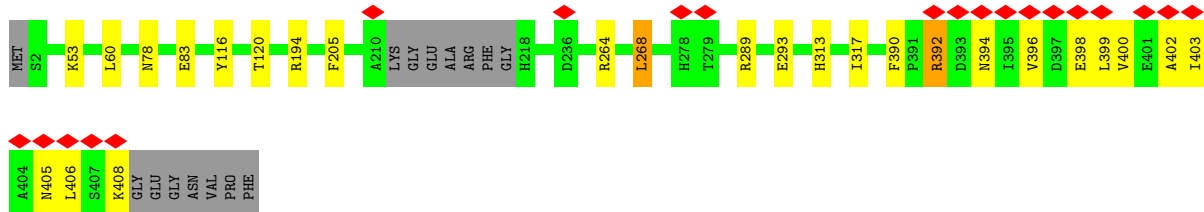
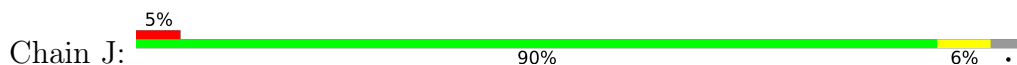




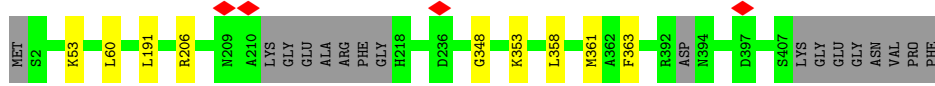
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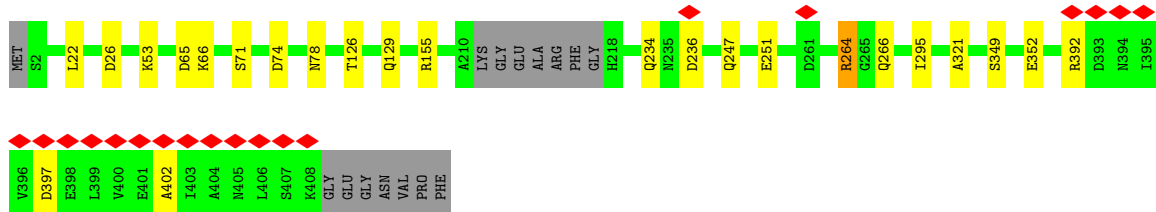
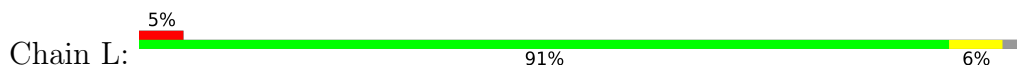
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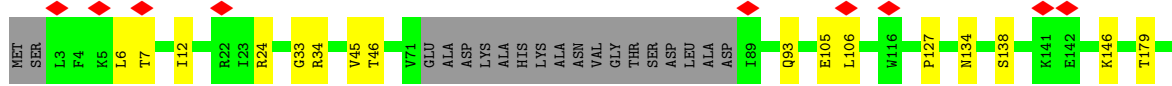
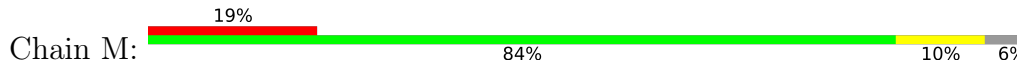
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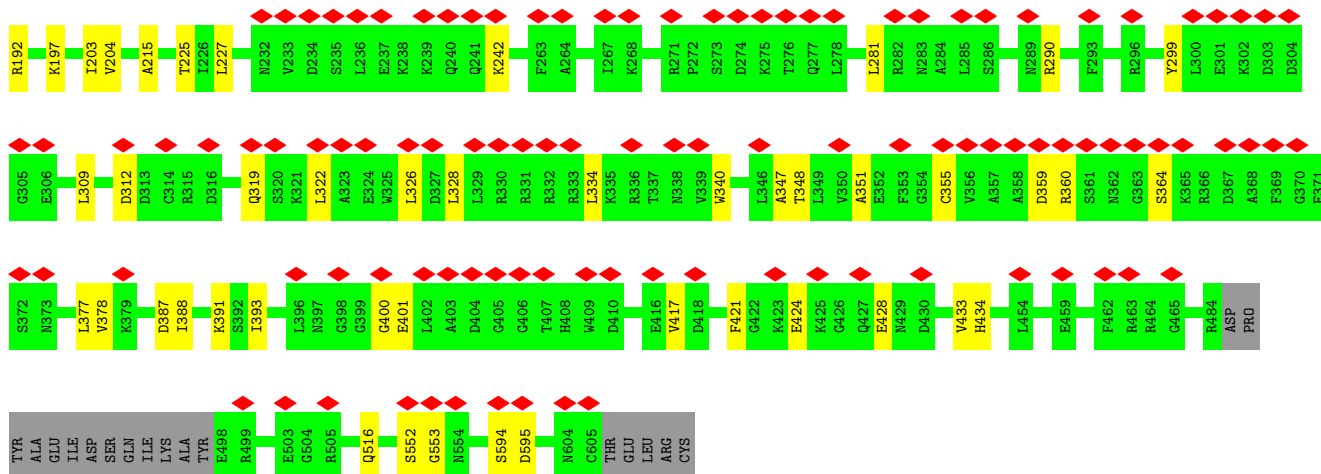


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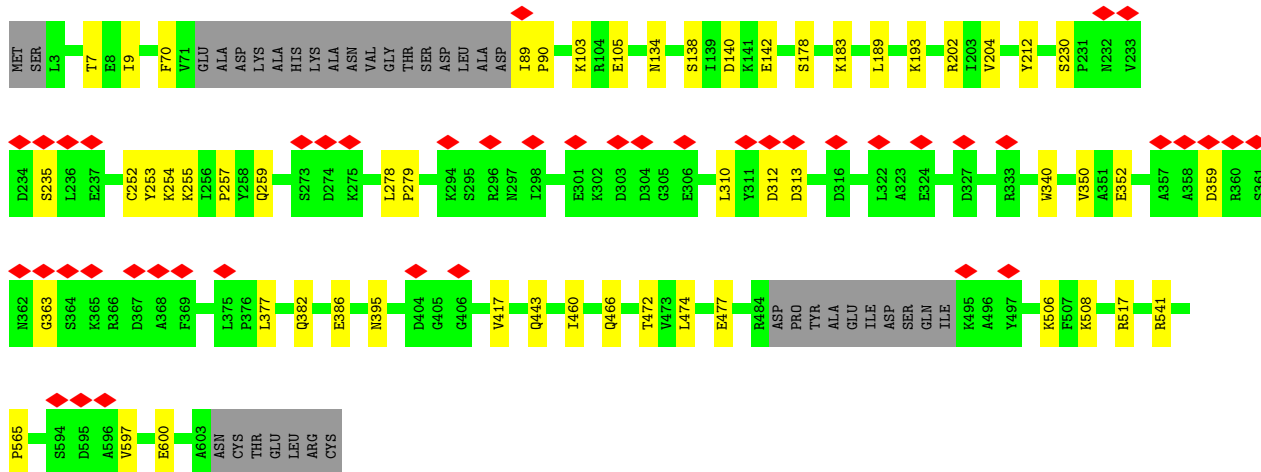
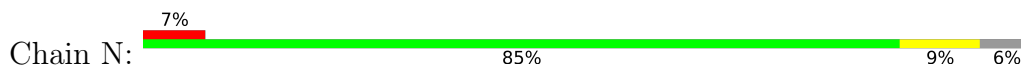


• Molecule 2: Nucleoside triphosphate hydrolase

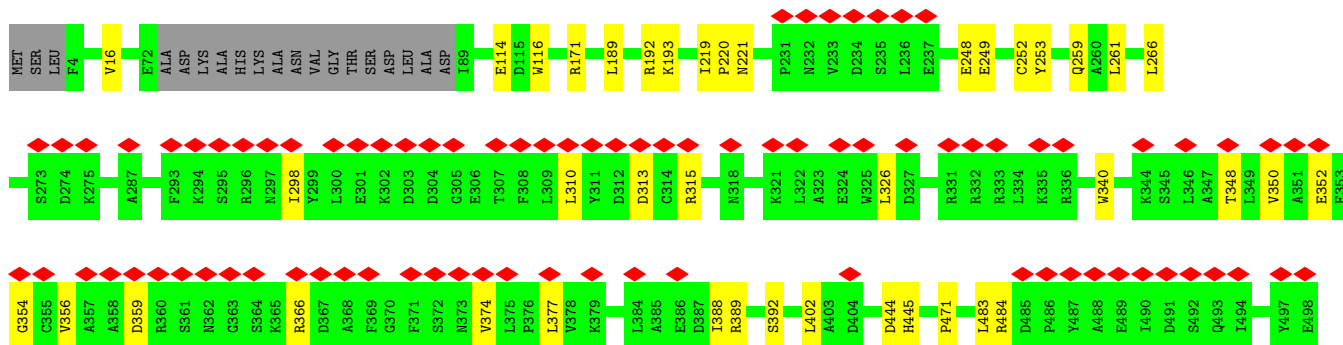
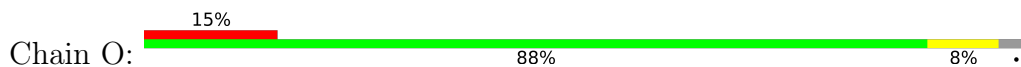


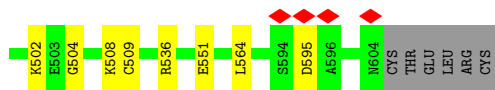


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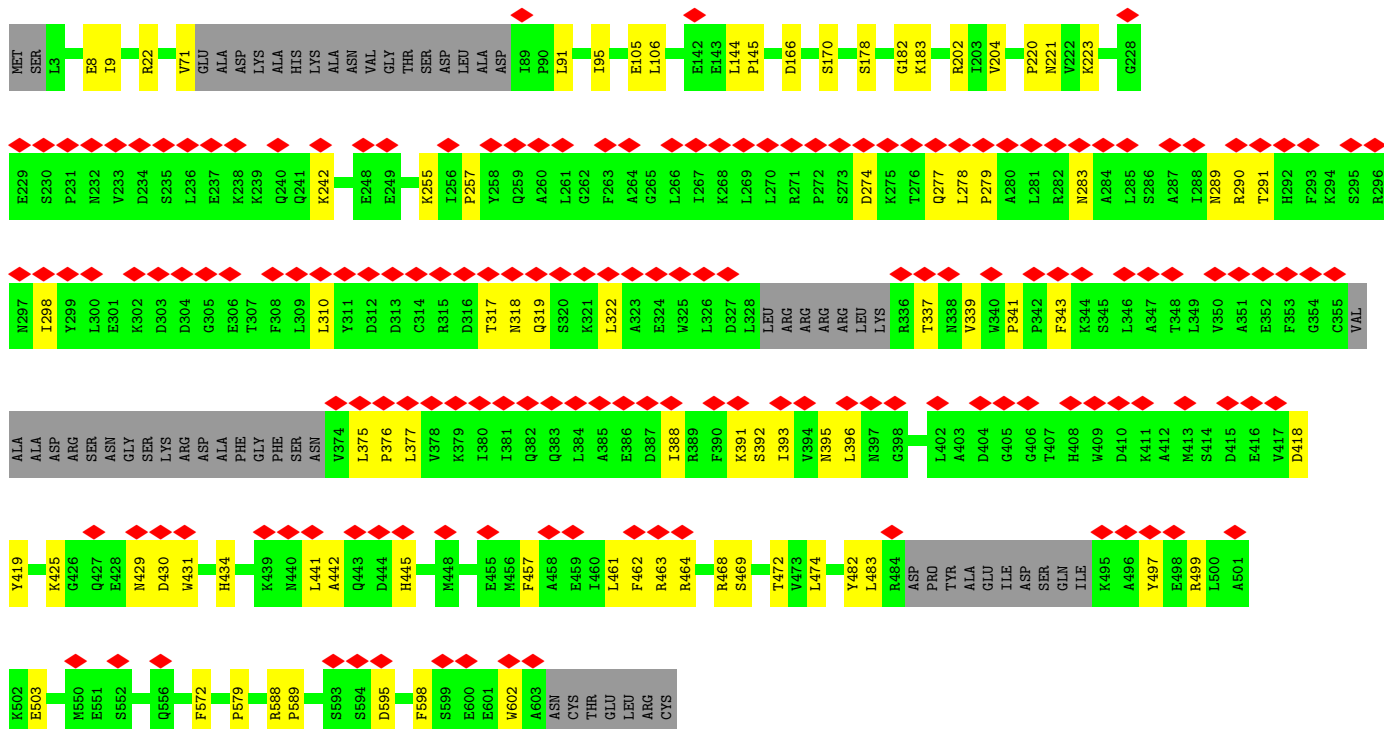
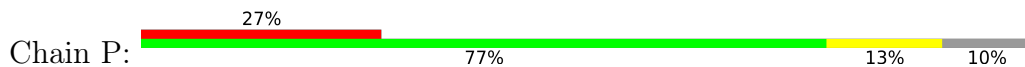


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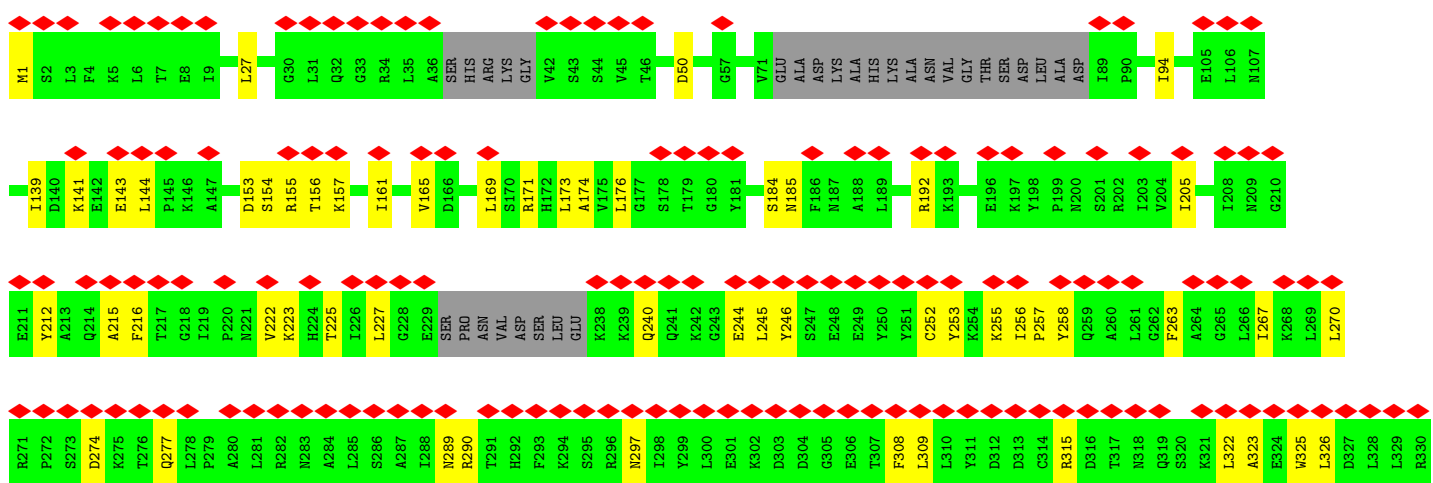




• Molecule 2: Nucleoside triphosphate hydrolase



• Molecule 2: Nucleoside triphosphate hydrolase



ARG	CYS	P518	SS19	E520	L521	SS22	P523	L526	WS32	R536	L537	TS38	N539	E540	R541	DS42	L543	MS50	E555	QS56	K559	QS60	I561	SS62	GS63	L564	P565	R566	I582	N585	QS86	A587	R588	P589	GS90	P591	K592	SS93	SS94	DS95	A596	V597	F598	SS99	E600	E601	W602	ALA	ASN	CYS	THR	GLU	LEU	P518	SS19	E520	L521	SS22	P523	L526	WS32	R536	L537	TS38	N539	E540	R541	DS42	L543	MS50	E555	QS56	K559	QS60	I561	SS62	GS63	L564	P565	R566	I582	N585	QS86	A587	R588	P589	GS90	P591	K592	SS93	SS94	DS95	A596	V597	F598	SS99	E600	E601	W602	ALA	ASN	CYS	THR	GLU	LEU	A452	L453	L454	E455	M456	F457	A458	E459	I460	L461	F462	R463	R464	G465	Q466	E467	R468	S469	Y470	P471	T472	V473	L474	L475	L476	E477	E478	A479	H480	H481	Y482	L483	R484	ASP	PRO	TYR	ALA	GLU	ILE	ASP	SER	GLN	ILE	LYS	ALA	Y497	E498	R499	L500	A501	KS02	ES03	G504	R505	C509	T515	QS16	R517	K391	S392	I393	V394	N395	L396	N397	G398	G399	G400	E401	L402	A403	D404	G405	G406	T407	H408	W409	D410	K411	A412	M413	S414	D415	E416	V417	F420	F421	G422	K423	E424	K425	G426	Q427	E428	M429	D430	W431	M432	V433	H434	I435	V436	M437	M438	K439	M440	L441	A442	Q443	D444	H445	A446	P447	M448	L449	L450	S451	R331	R332	R333	L334	K335	R336	T337	N338	V339	W340	P341	P342	F343	K344	S345	L346	A347	T348	L349	V350	A351	E352	F353	G354	C355	VAL	ALA	ALA	ASP	ARG	SER	ASN	GLY	S364	K365	R366	D367	A368	F369	G370	F371	S372	N373	V374	L375	P376	L377	V378	K379	I380	I381	Q382	Q383	L384	A385	E386	D387	I388	R389	F390
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	200494	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.655	Depositor
Minimum map value	-1.978	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.090	Depositor
Recommended contour level	0.264	Depositor
Map size (Å)	355.2, 355.2, 355.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	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: AR6, MG, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.34	0/3259	0.53	0/4406
1	B	0.31	0/3260	0.51	1/4406 (0.0%)
1	C	0.32	0/3259	0.51	0/4406
1	D	0.30	0/3276	0.52	0/4426
1	E	0.31	0/3268	0.50	1/4418 (0.0%)
1	F	0.28	0/3272	0.48	0/4422
1	G	0.27	0/3190	0.45	0/4310
1	H	0.28	0/3277	0.48	0/4429
1	I	0.30	0/3216	0.49	0/4346
1	J	0.32	0/3272	0.50	1/4421 (0.0%)
1	K	0.33	0/3255	0.52	0/4399
1	L	0.32	0/3273	0.53	1/4424 (0.0%)
2	M	0.26	0/4624	0.53	0/6243
2	N	0.28	0/4637	0.53	0/6260
2	O	0.28	0/4729	0.54	0/6388
2	P	0.27	0/4431	0.53	0/5985
2	Q	0.26	0/4473	0.52	0/6033
All	All	0.29	0/61971	0.51	4/83722 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	22	LEU	CA-CB-CG	5.67	128.33	115.30
1	J	268	LEU	CA-CB-CG	5.54	128.05	115.30
1	B	268	LEU	CA-CB-CG	5.42	127.77	115.30
1	E	323	LEU	CA-CB-CG	5.21	127.28	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	218	HIS	Peptide

## 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	3185	0	3109	8	0
1	B	3186	0	3116	10	0
1	C	3185	0	3109	18	0
1	D	3203	0	3129	17	0
1	E	3194	0	3117	16	0
1	F	3198	0	3125	21	0
1	G	3119	0	3044	21	0
1	H	3203	0	3130	13	0
1	I	3145	0	3069	5	0
1	J	3199	0	3126	17	0
1	K	3182	0	3109	6	0
1	L	3199	0	3127	12	0
2	M	4536	0	4576	37	0
2	N	4548	0	4592	32	0
2	O	4637	0	4664	30	0
2	P	4346	0	4380	50	0
2	Q	4389	0	4439	67	0
3	A	36	0	21	0	0
3	B	36	0	21	0	0
3	C	36	0	21	0	0
3	D	36	0	21	0	0
3	E	36	0	21	0	0
3	F	36	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	36	0	21	0	0
3	H	36	0	21	0	0
3	I	36	0	21	1	0
3	J	36	0	21	1	0
3	K	36	0	21	0	0
3	L	36	0	21	0	0
4	M	27	0	12	0	0
4	N	27	0	12	0	0
4	O	27	0	12	0	0
4	P	27	0	12	1	0
4	Q	27	0	12	3	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
5	O	1	0	0	0	0
5	P	1	0	0	0	0
5	Q	1	0	0	0	0
All	All	61226	0	60273	352	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 3.

The worst 5 of 352 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:188:PHE:HB3	1:D:194:ARG:HD2	1.61	0.82
2:P:8:GLU:HG3	2:P:9:ILE:HD12	1.60	0.81
2:P:429:ASN:ND2	2:P:431:TRP:O	2.15	0.79
2:M:134:ASN:O	2:M:138:SER:OG	2.03	0.77
2:P:242:LYS:NZ	2:P:430:ASP:O	2.18	0.77

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	394/415 (95%)	372 (94%)	22 (6%)	0	100	100
1	B	394/415 (95%)	371 (94%)	23 (6%)	0	100	100
1	C	394/415 (95%)	380 (96%)	14 (4%)	0	100	100
1	D	395/415 (95%)	375 (95%)	20 (5%)	0	100	100
1	E	396/415 (95%)	371 (94%)	25 (6%)	0	100	100
1	F	396/415 (95%)	373 (94%)	23 (6%)	0	100	100
1	G	384/415 (92%)	361 (94%)	23 (6%)	0	100	100
1	H	397/415 (96%)	376 (95%)	21 (5%)	0	100	100
1	I	388/415 (94%)	366 (94%)	22 (6%)	0	100	100
1	J	394/415 (95%)	377 (96%)	17 (4%)	0	100	100
1	K	392/415 (94%)	366 (93%)	26 (7%)	0	100	100
1	L	396/415 (95%)	378 (96%)	18 (4%)	0	100	100
2	M	567/610 (93%)	521 (92%)	46 (8%)	0	100	100
2	N	568/610 (93%)	528 (93%)	40 (7%)	0	100	100
2	O	581/610 (95%)	548 (94%)	33 (6%)	0	100	100
2	P	539/610 (88%)	504 (94%)	35 (6%)	0	100	100
2	Q	540/610 (88%)	515 (95%)	25 (5%)	0	100	100
All	All	7515/8030 (94%)	7082 (94%)	433 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	340/351 (97%)	340 (100%)	0	100	100
1	B	340/351 (97%)	339 (100%)	1 (0%)	92	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	340/351 (97%)	340 (100%)	0	100	100
1	D	341/351 (97%)	341 (100%)	0	100	100
1	E	340/351 (97%)	340 (100%)	0	100	100
1	F	341/351 (97%)	340 (100%)	1 (0%)	92	98
1	G	332/351 (95%)	332 (100%)	0	100	100
1	H	341/351 (97%)	341 (100%)	0	100	100
1	I	335/351 (95%)	335 (100%)	0	100	100
1	J	341/351 (97%)	339 (99%)	2 (1%)	86	96
1	K	339/351 (97%)	339 (100%)	0	100	100
1	L	341/351 (97%)	340 (100%)	1 (0%)	92	98
2	M	489/519 (94%)	489 (100%)	0	100	100
2	N	489/519 (94%)	489 (100%)	0	100	100
2	O	499/519 (96%)	497 (100%)	2 (0%)	91	97
2	P	469/519 (90%)	469 (100%)	0	100	100
2	Q	473/519 (91%)	473 (100%)	0	100	100
All	All	6490/6807 (95%)	6483 (100%)	7 (0%)	93	98

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	392	ARG
1	L	264	ARG
2	O	484	ARG
2	O	171	ARG
1	J	264	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	54	GLN
1	J	313	HIS
2	Q	480	HIS
2	Q	481	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 5 are monoatomic - leaving 17 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
3	AR6	H	501	-	34,39,39	1.00	1 (2%)	40,60,60	1.12	2 (5%)
3	AR6	G	501	-	34,39,39	0.91	1 (2%)	40,60,60	1.04	2 (5%)
3	AR6	L	501	-	34,39,39	1.00	1 (2%)	40,60,60	0.99	2 (5%)
4	ADP	Q	701	5	24,29,29	0.95	1 (4%)	29,45,45	1.57	4 (13%)
3	AR6	C	501	-	34,39,39	1.03	1 (2%)	40,60,60	1.01	2 (5%)
3	AR6	E	501	-	34,39,39	1.00	1 (2%)	40,60,60	0.86	1 (2%)
4	ADP	M	701	5	24,29,29	0.96	1 (4%)	29,45,45	1.45	4 (13%)
4	ADP	N	701	5	24,29,29	0.97	1 (4%)	29,45,45	1.43	4 (13%)
4	ADP	O	701	5	24,29,29	0.95	1 (4%)	29,45,45	1.41	4 (13%)
3	AR6	K	501	-	34,39,39	1.05	1 (2%)	40,60,60	0.92	2 (5%)
3	AR6	B	501	-	34,39,39	1.03	1 (2%)	40,60,60	0.95	2 (5%)
3	AR6	I	501	-	34,39,39	1.01	1 (2%)	40,60,60	0.87	0
3	AR6	J	501	-	34,39,39	1.01	1 (2%)	40,60,60	0.91	2 (5%)
4	ADP	P	701	5	24,29,29	0.97	1 (4%)	29,45,45	1.48	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	AR6	D	501	-	34,39,39	0.99	1 (2%)	40,60,60	0.93	2 (5%)
3	AR6	F	501	-	34,39,39	0.97	1 (2%)	40,60,60	0.89	1 (2%)
3	AR6	A	501	-	34,39,39	1.05	1 (2%)	40,60,60	0.92	1 (2%)

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	AR6	H	501	-	-	9/18/54/54	0/4/4/4
3	AR6	G	501	-	-	7/18/54/54	0/4/4/4
3	AR6	L	501	-	-	7/18/54/54	0/4/4/4
4	ADP	Q	701	5	-	4/12/32/32	0/3/3/3
3	AR6	C	501	-	-	9/18/54/54	0/4/4/4
3	AR6	E	501	-	-	8/18/54/54	0/4/4/4
4	ADP	M	701	5	-	7/12/32/32	0/3/3/3
4	ADP	N	701	5	-	6/12/32/32	0/3/3/3
4	ADP	O	701	5	-	3/12/32/32	0/3/3/3
3	AR6	K	501	-	-	10/18/54/54	0/4/4/4
3	AR6	B	501	-	-	9/18/54/54	0/4/4/4
3	AR6	I	501	-	-	8/18/54/54	0/4/4/4
3	AR6	J	501	-	-	9/18/54/54	0/4/4/4
4	ADP	P	701	5	-	3/12/32/32	0/3/3/3
3	AR6	D	501	-	-	7/18/54/54	0/4/4/4
3	AR6	F	501	-	-	7/18/54/54	0/4/4/4
3	AR6	A	501	-	-	11/18/54/54	0/4/4/4

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	AR6	C8-N7	-2.64	1.30	1.34
3	K	501	AR6	C8-N7	-2.60	1.30	1.34
3	C	501	AR6	C8-N7	-2.59	1.30	1.34
3	B	501	AR6	C8-N7	-2.52	1.30	1.34
3	L	501	AR6	C8-N7	-2.46	1.30	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	701	ADP	PA-O3A-PB	-4.32	118.01	132.83
3	G	501	AR6	C1D-C2D-C3D	-3.86	97.46	102.30
4	P	701	ADP	PA-O3A-PB	-3.77	119.89	132.83
3	H	501	AR6	PB-O3A-PA	-3.43	121.07	132.83
4	Q	701	ADP	C3'-C2'-C1'	3.41	106.11	100.98

There are no chirality outliers.

5 of 124 torsion outliers are listed below:

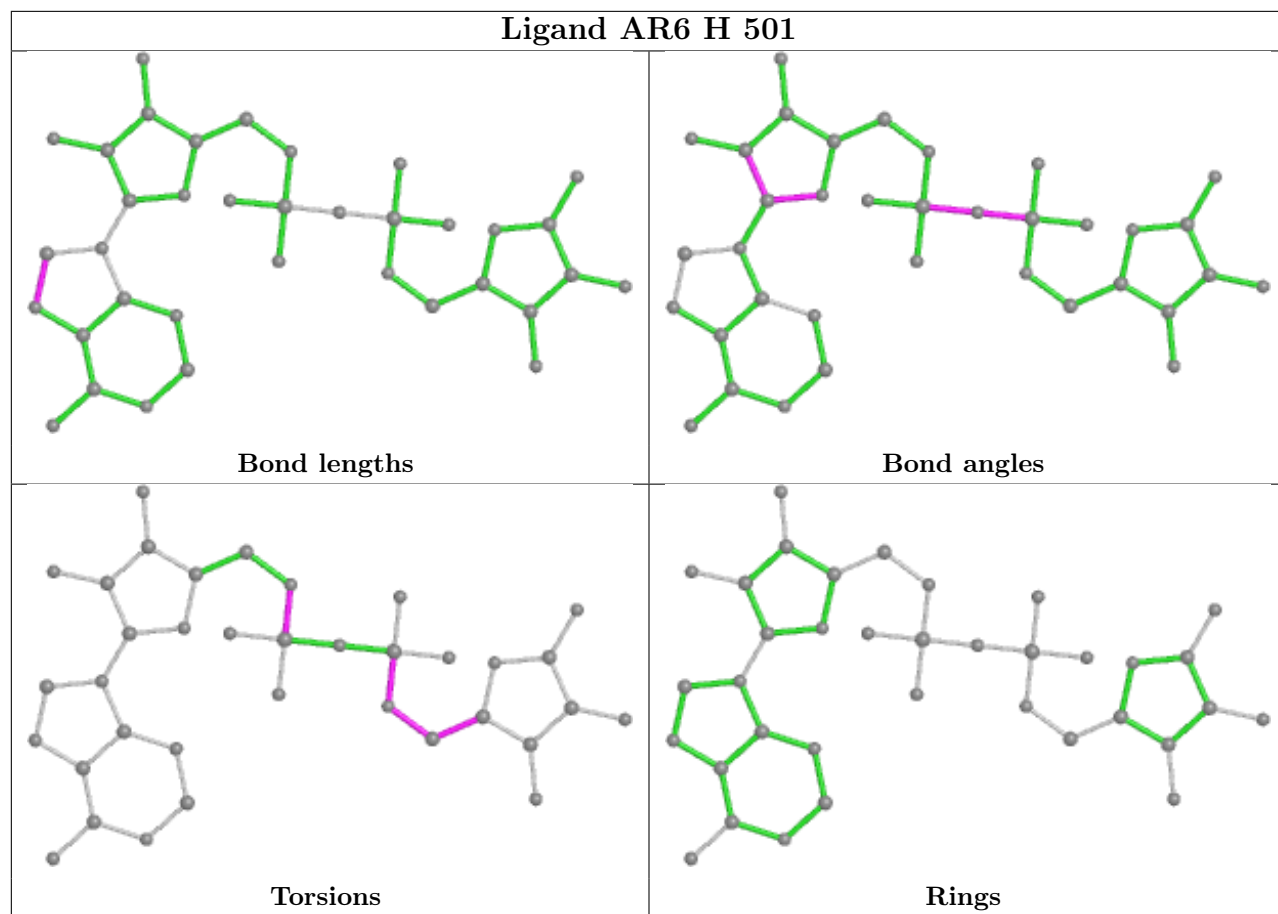
Mol	Chain	Res	Type	Atoms
3	A	501	AR6	C5'-O5'-PA-O1A
3	A	501	AR6	C5'-O5'-PA-O2A
3	A	501	AR6	C5D-O5D-PB-O1B
3	A	501	AR6	O4D-C4D-C5D-O5D
3	A	501	AR6	C4D-C5D-O5D-PB

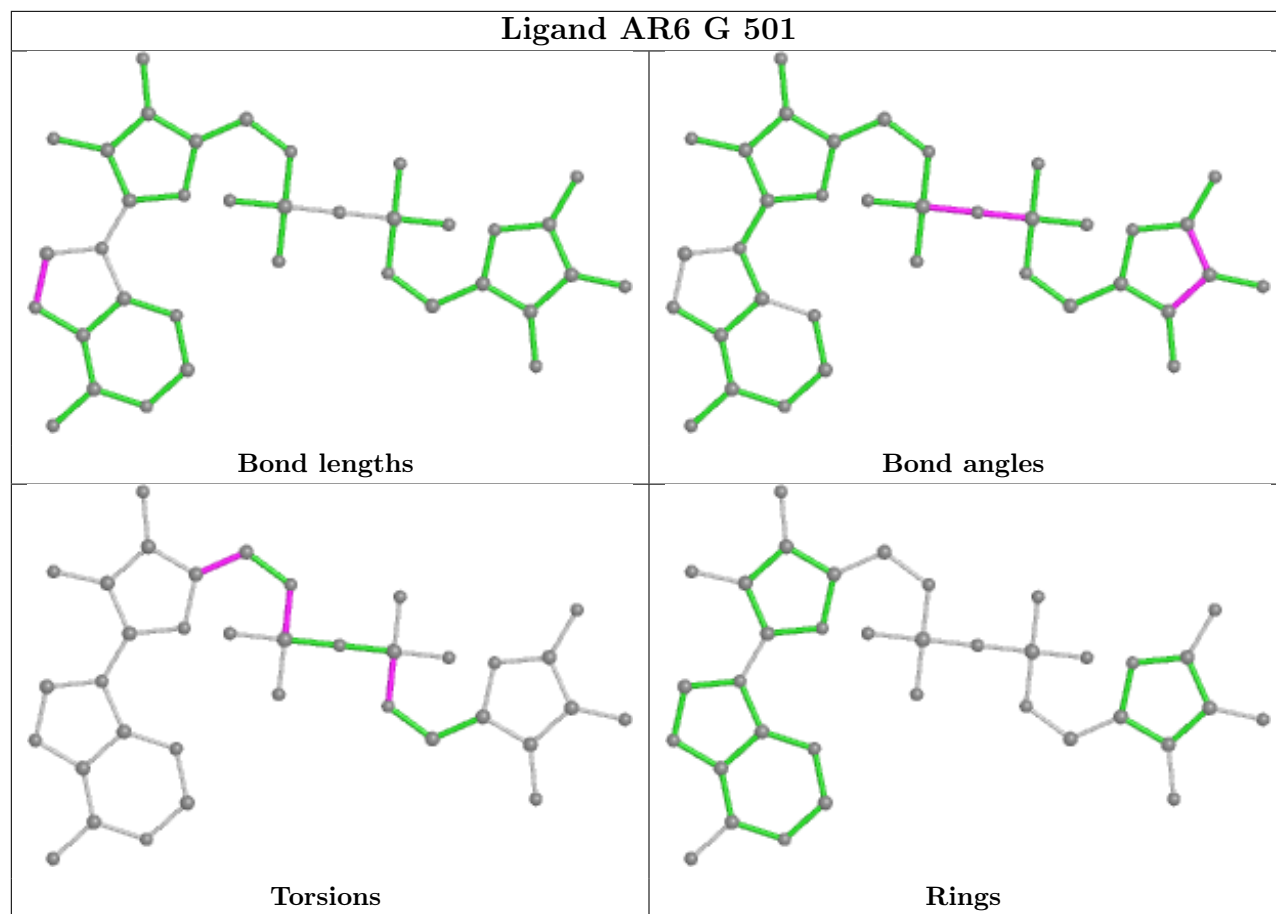
There are no ring outliers.

4 monomers are involved in 6 short contacts:

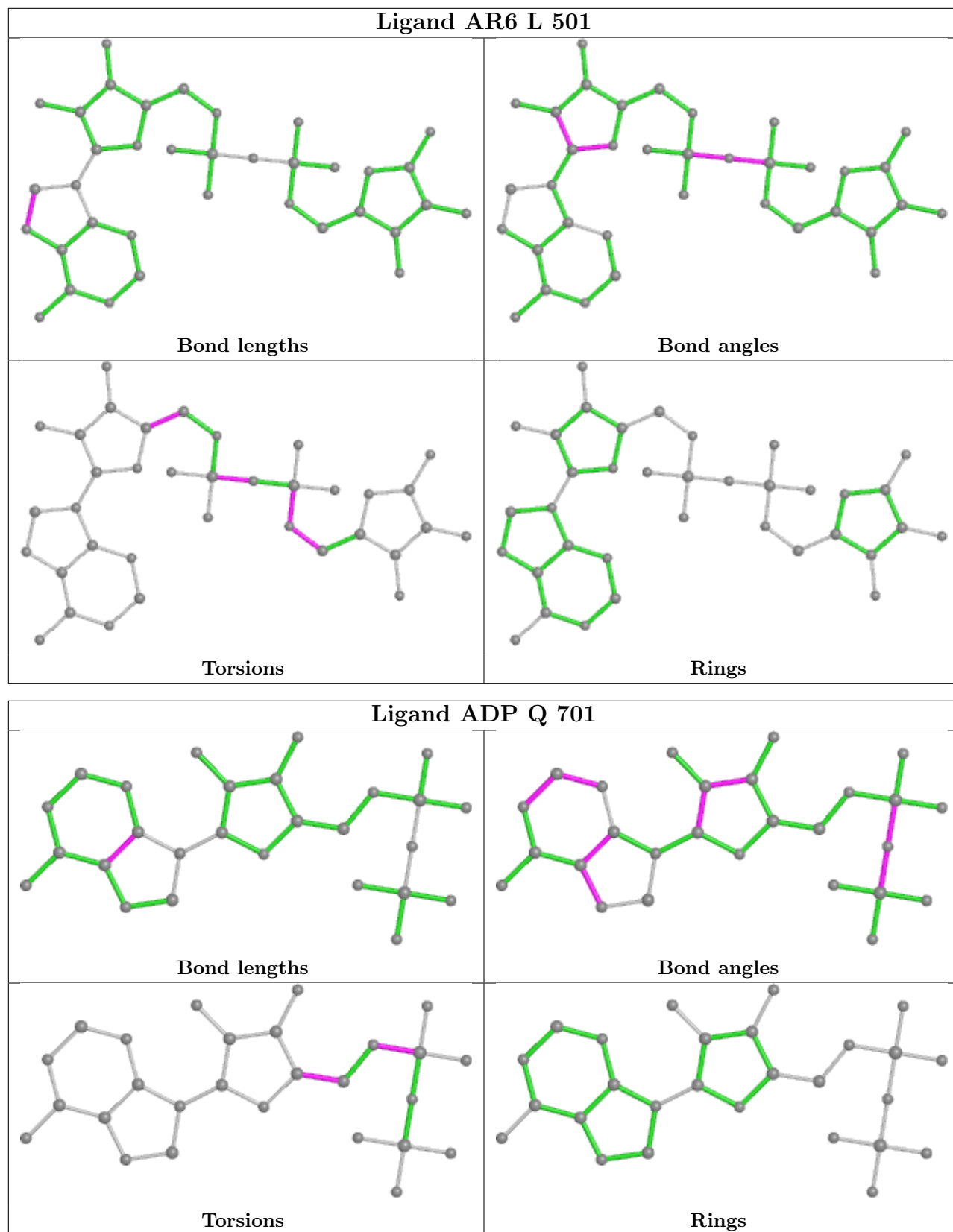
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Q	701	ADP	3	0
3	I	501	AR6	1	0
3	J	501	AR6	1	0
4	P	701	ADP	1	0

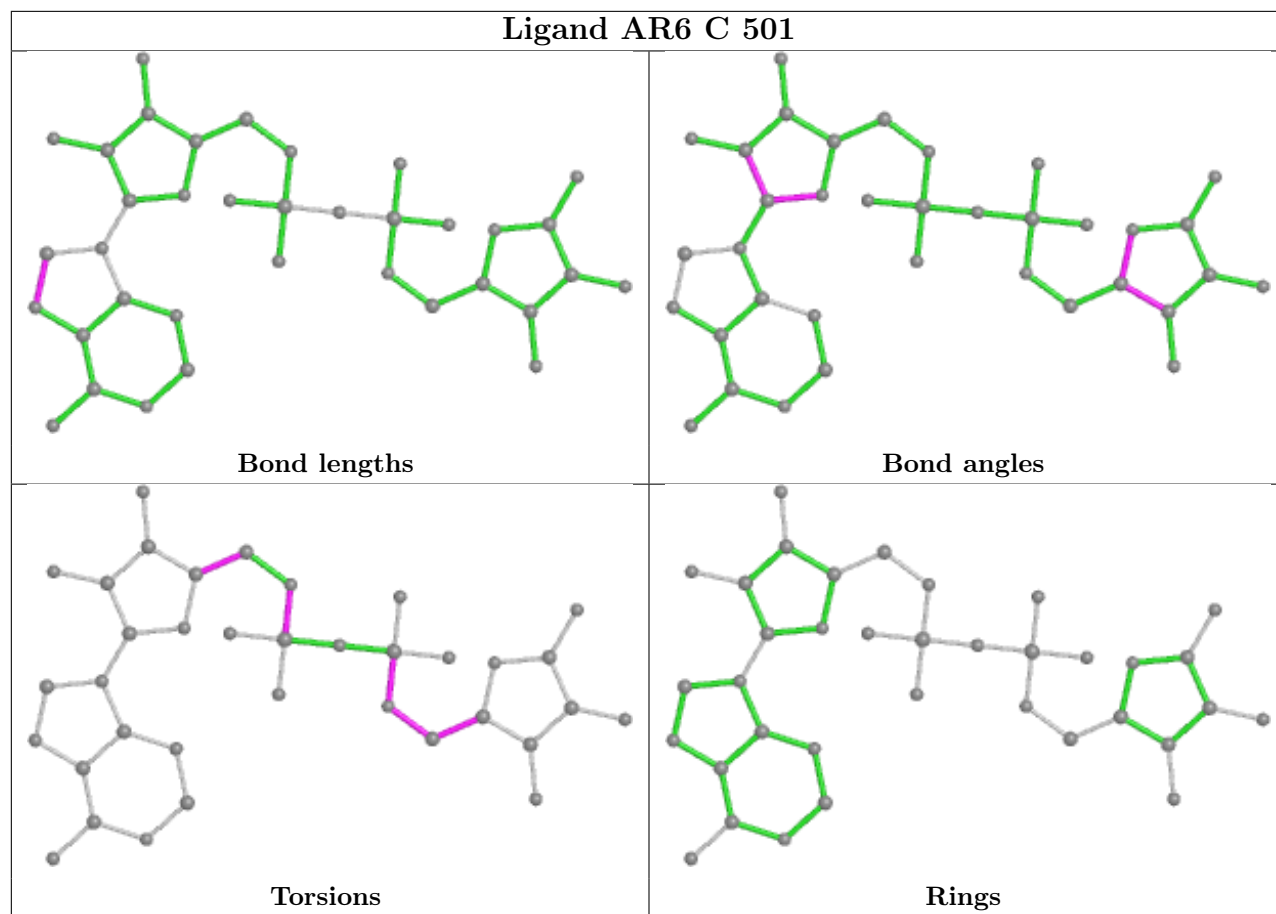
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

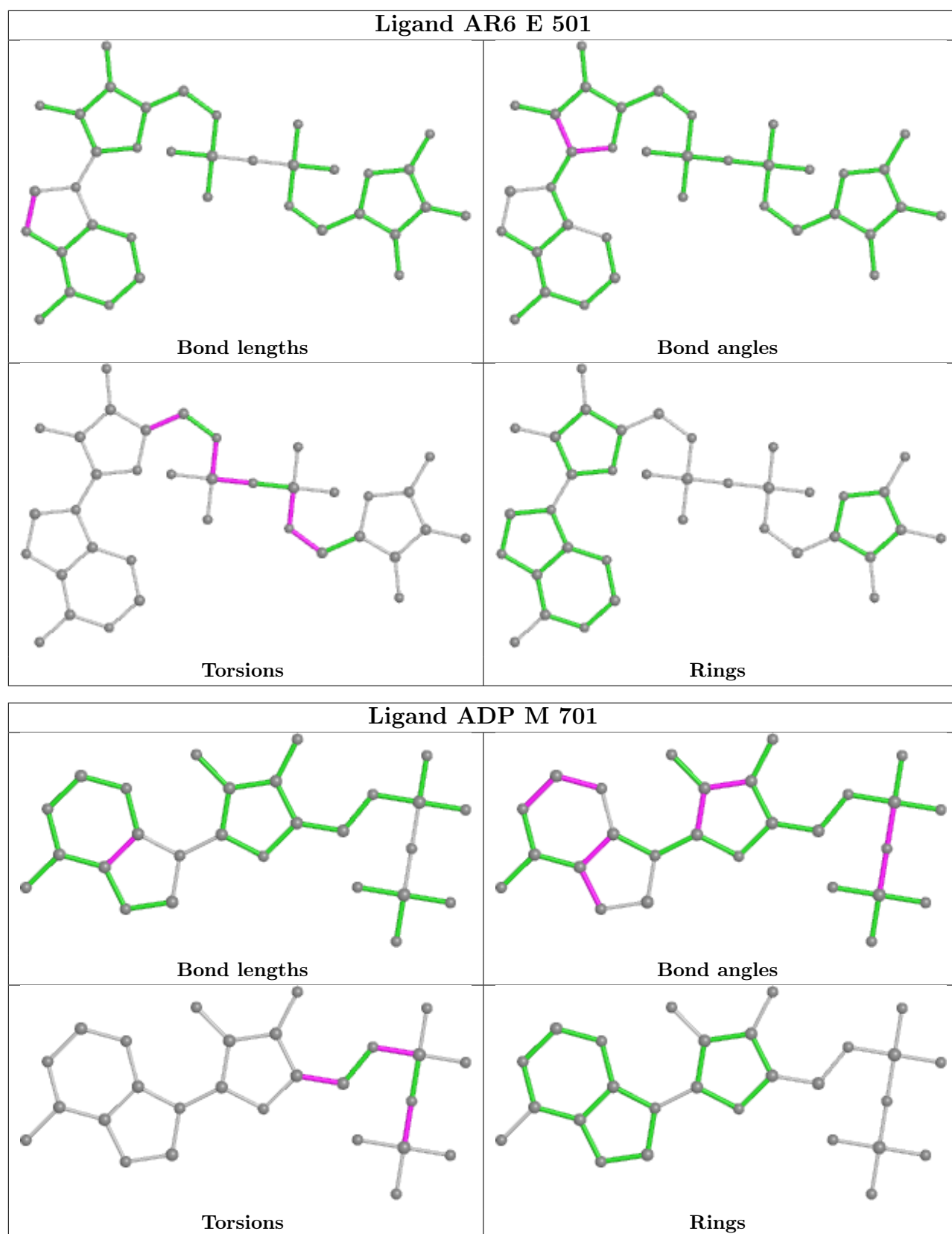


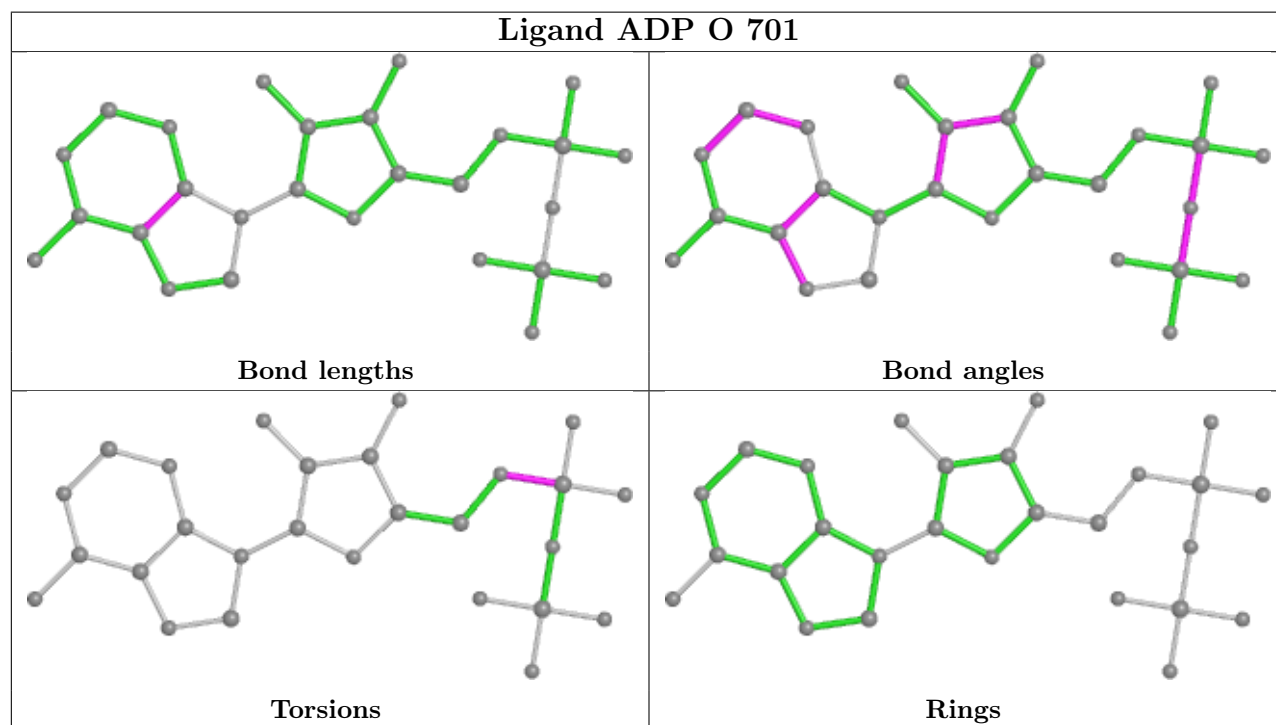
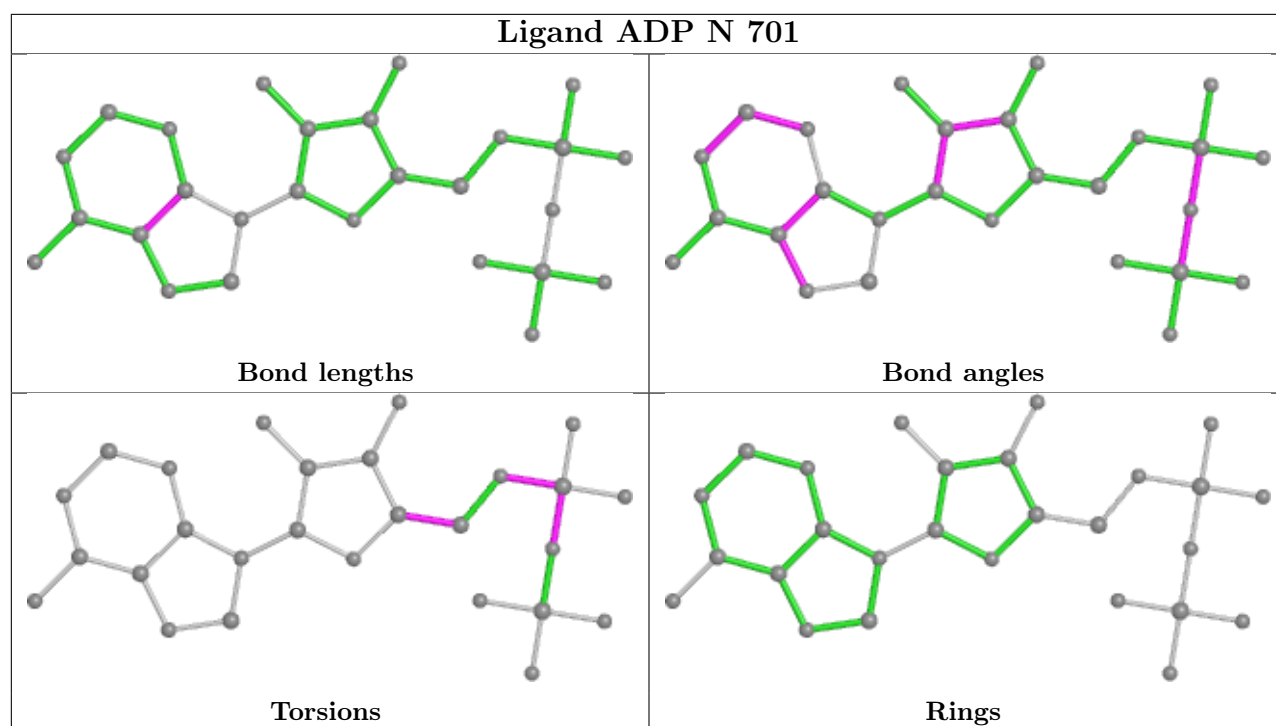


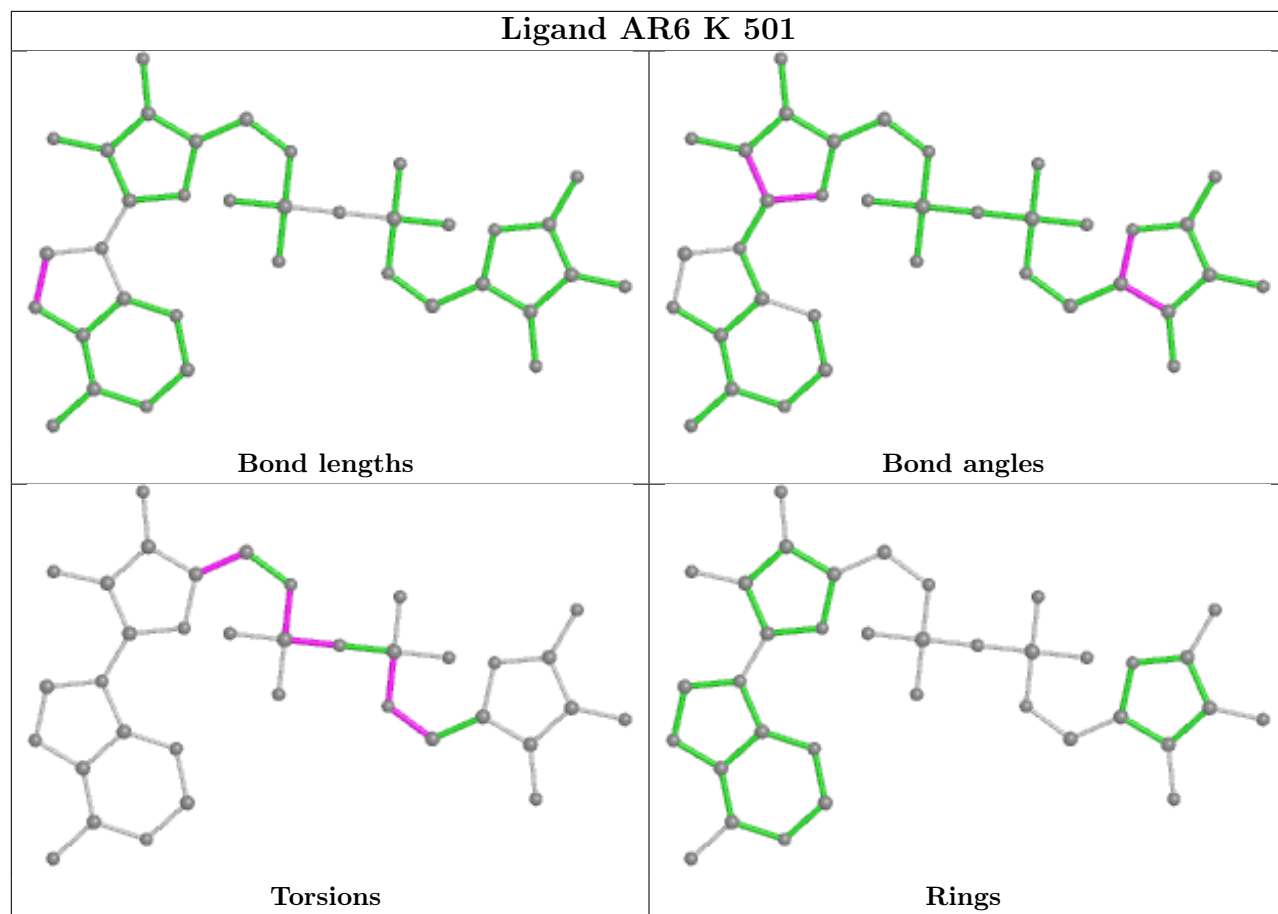


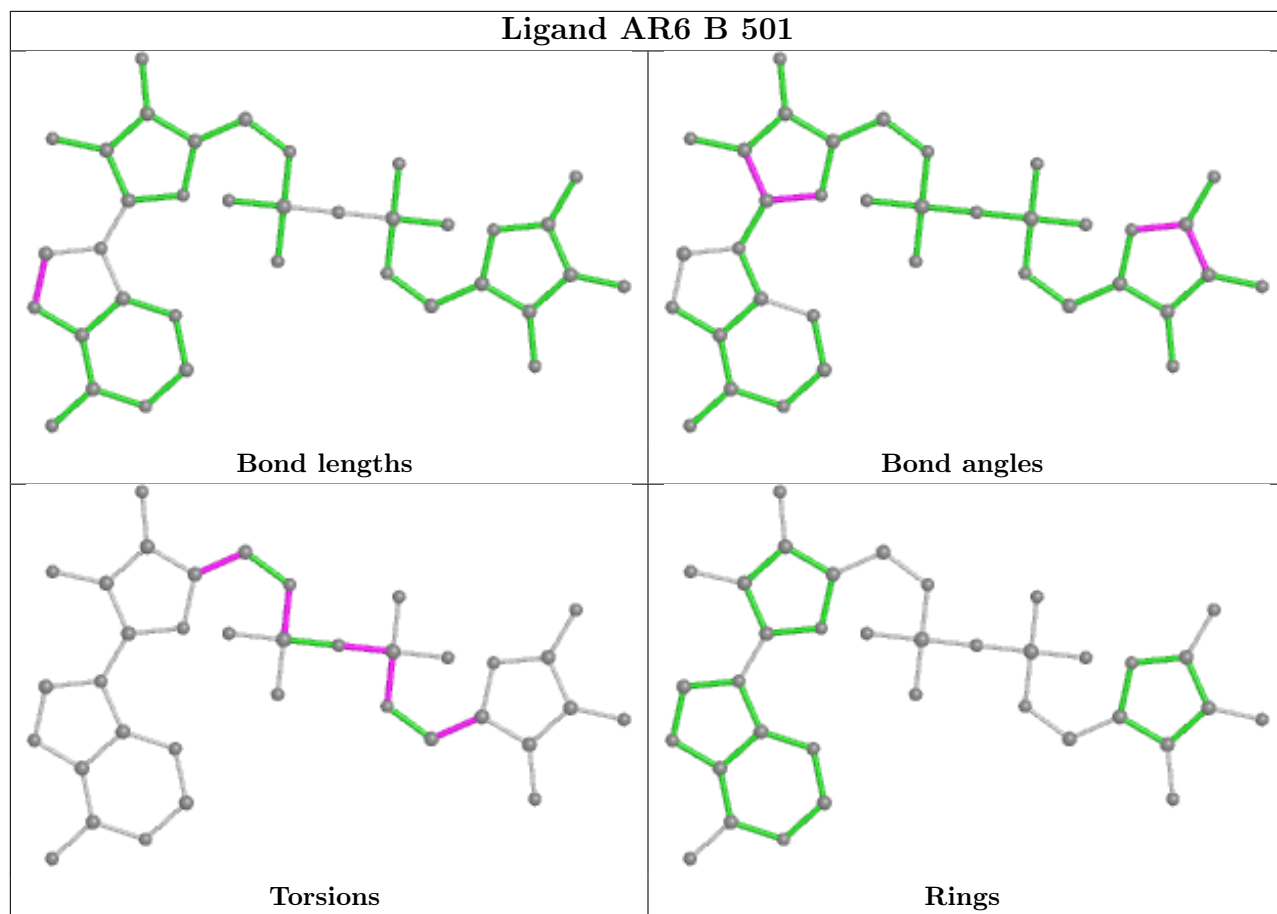


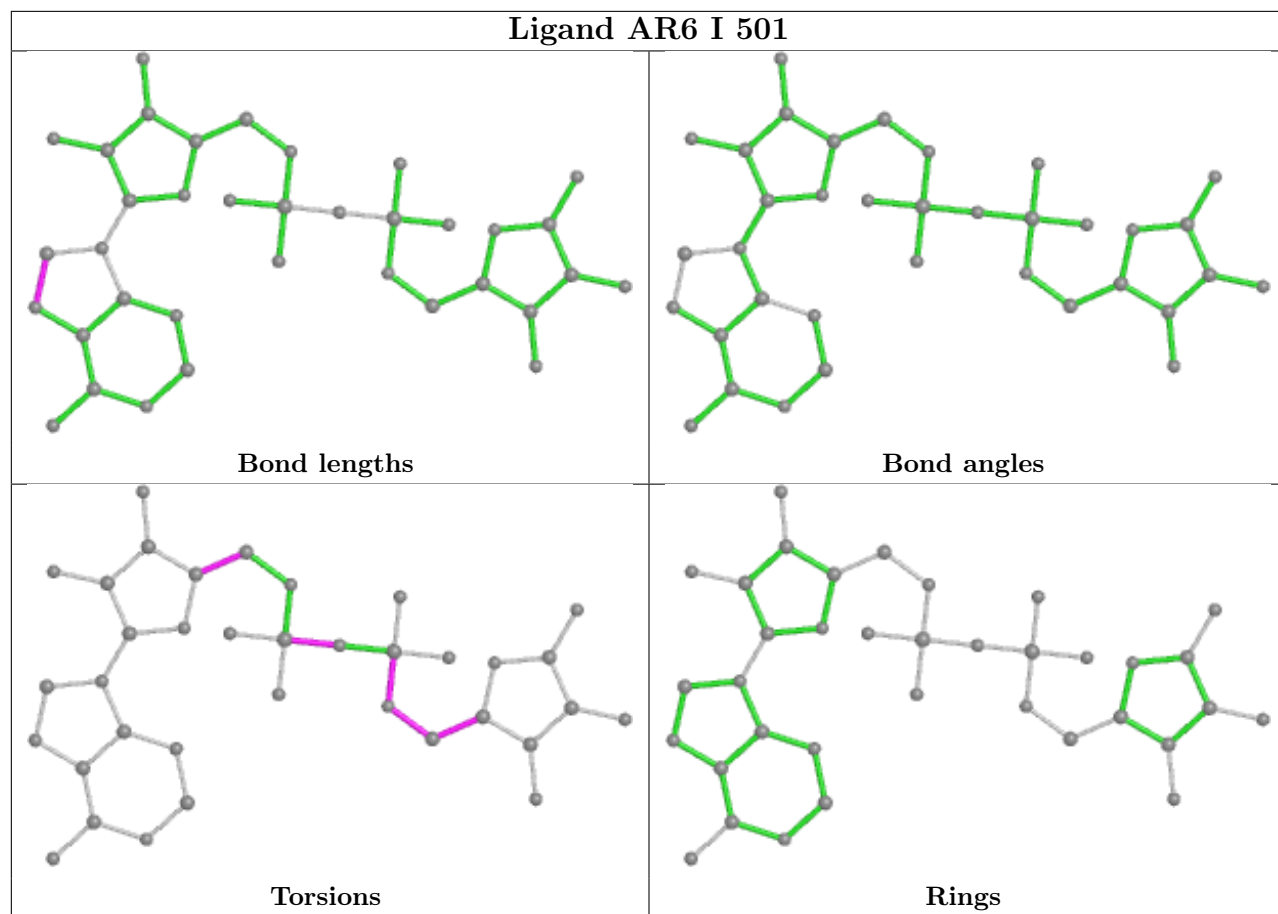


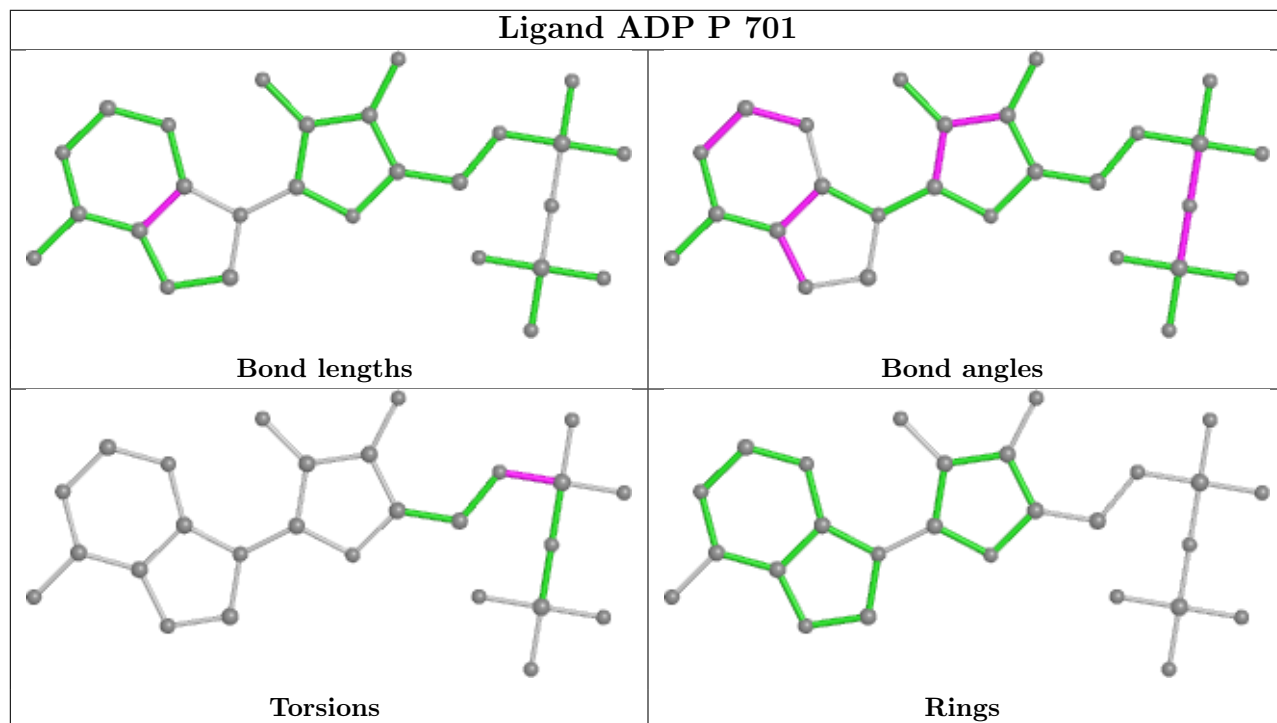
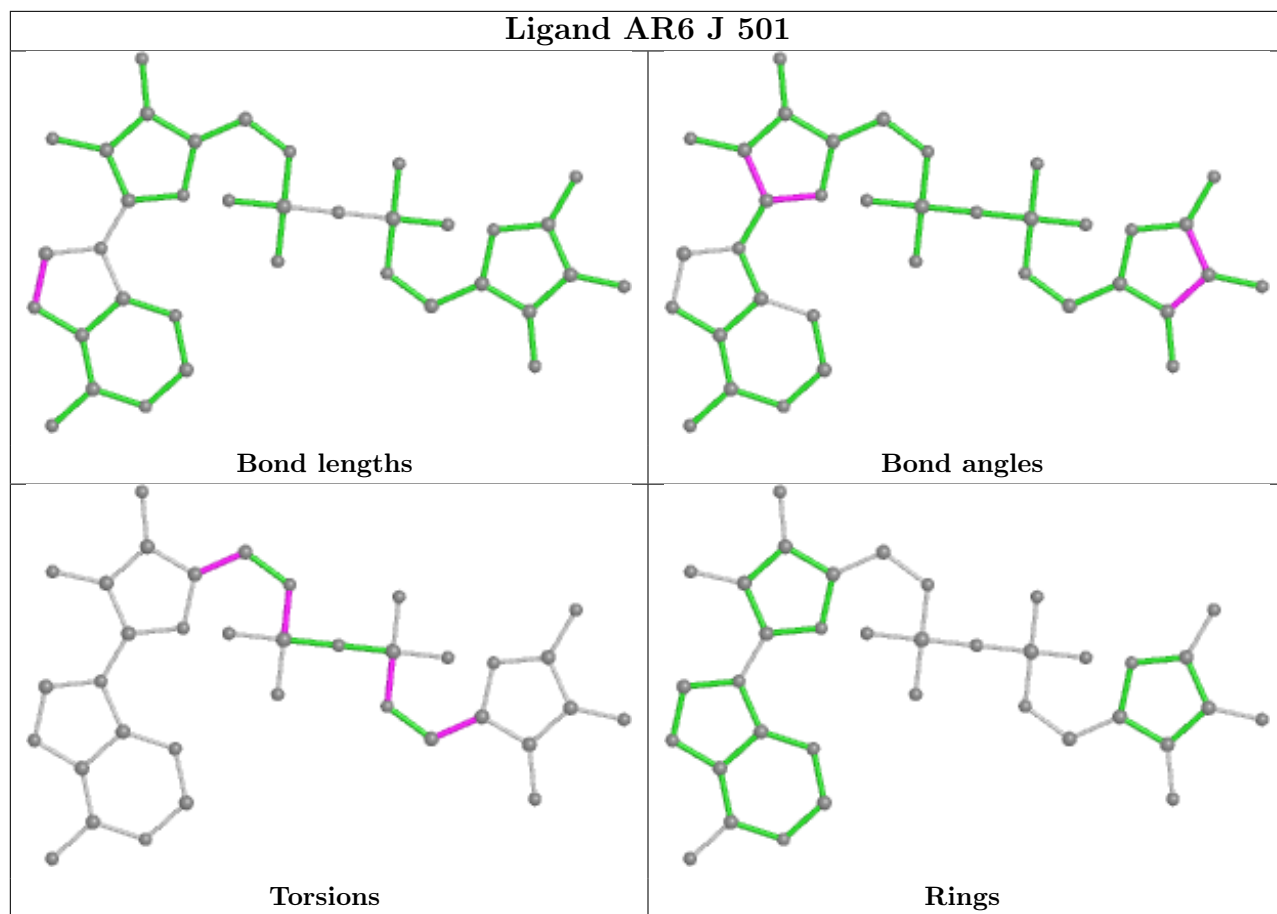




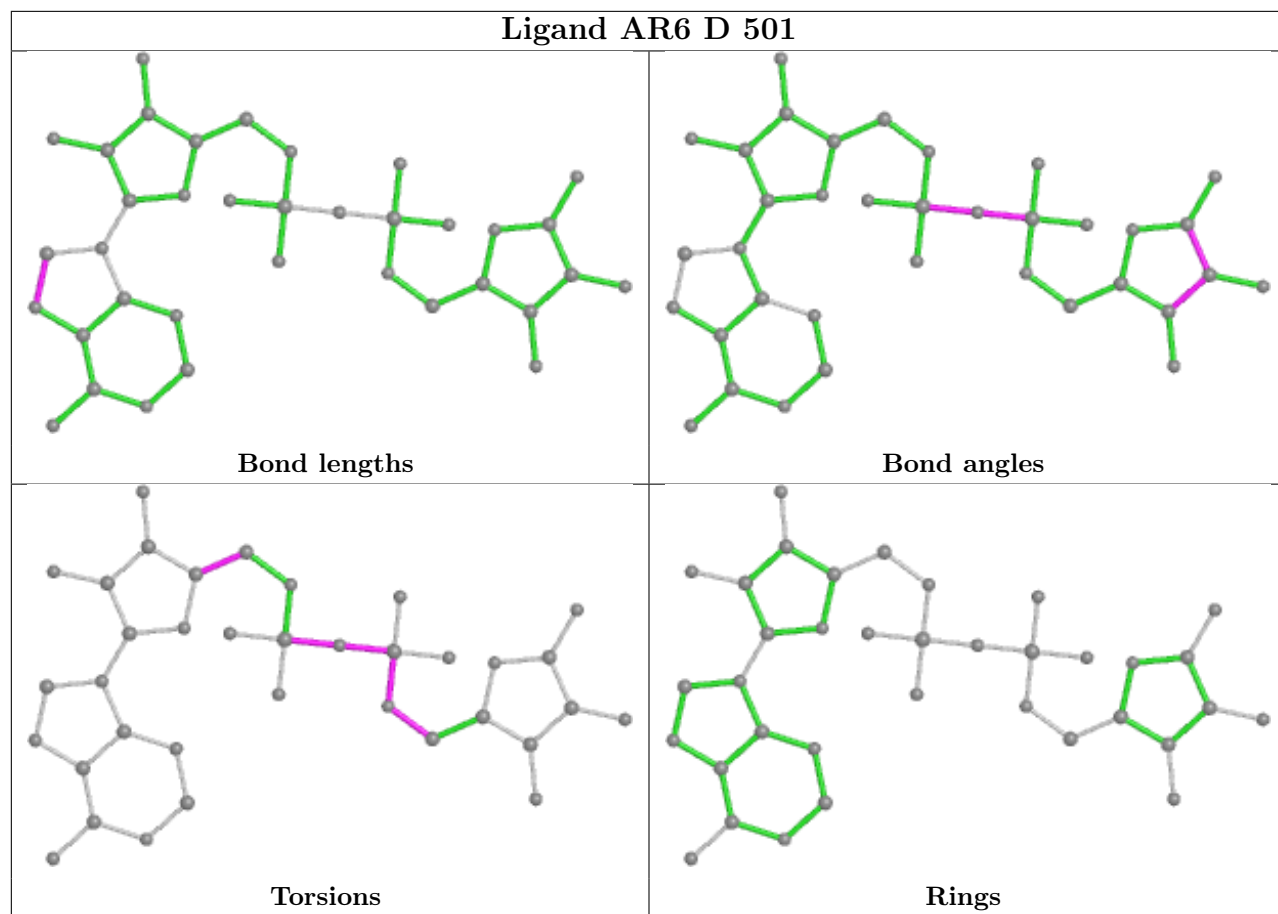


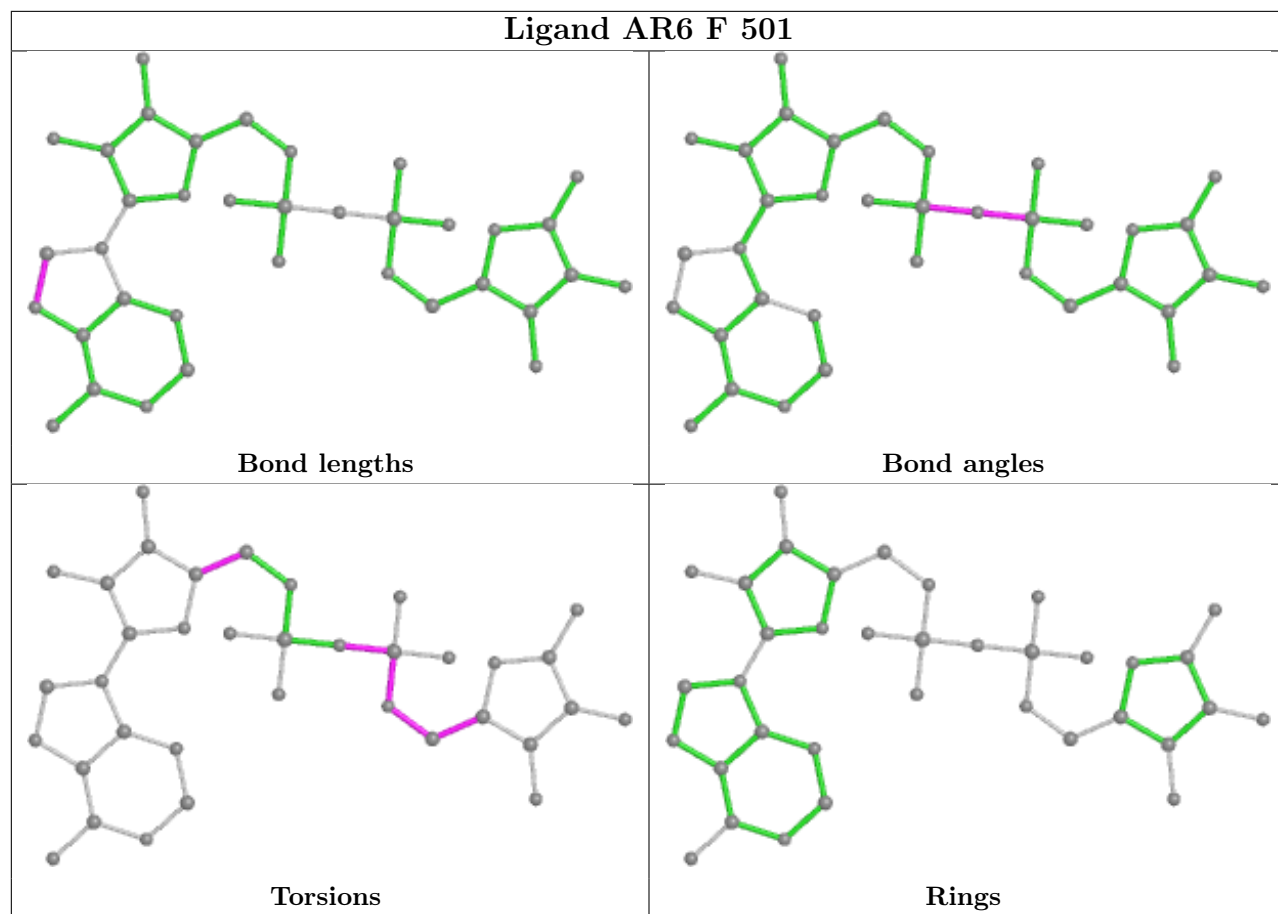


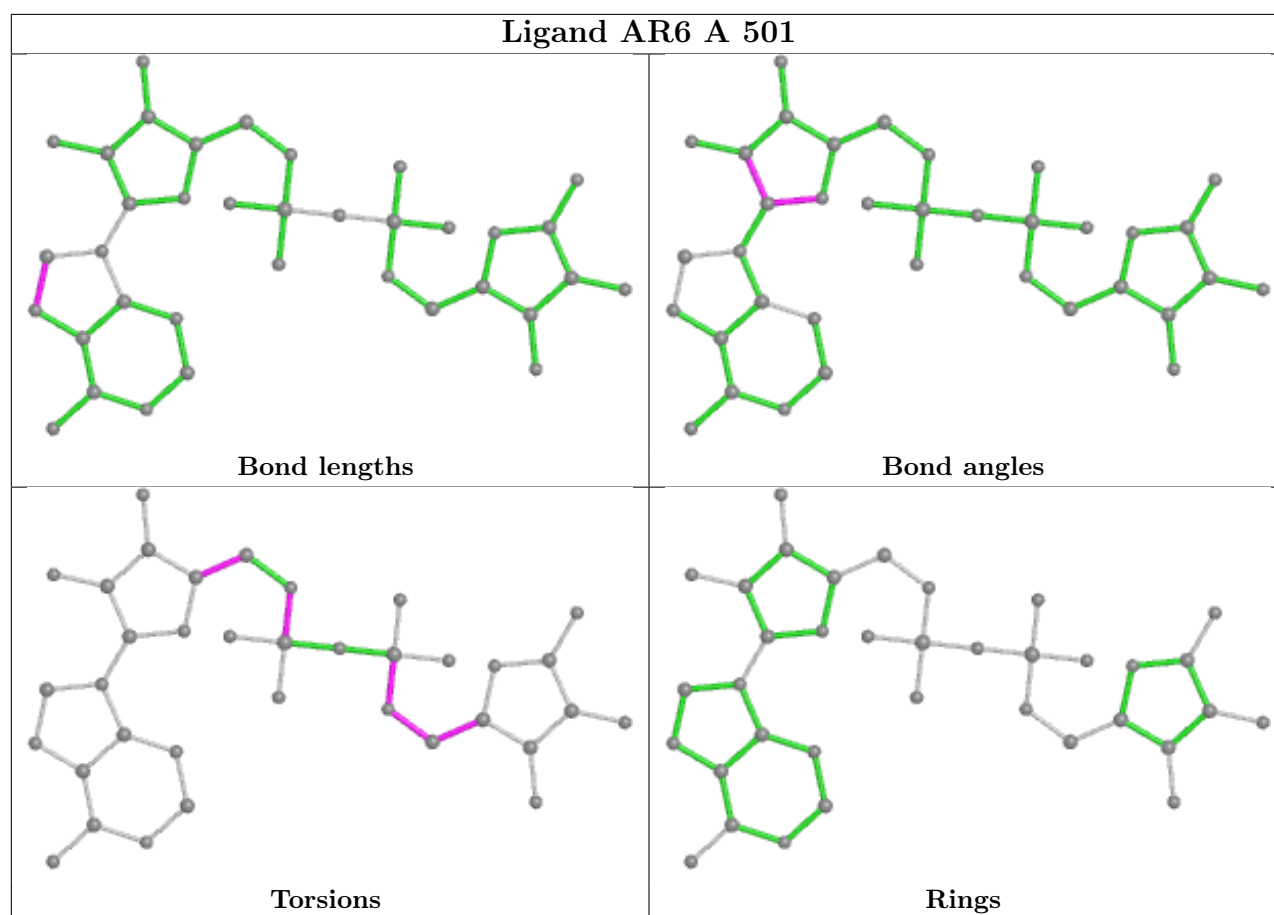












## 5.7 Other polymers [i](#)

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	J	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	391:PRO	C	392:ARG	N	3.68
1	D	391:PRO	C	392:ARG	N	3.15

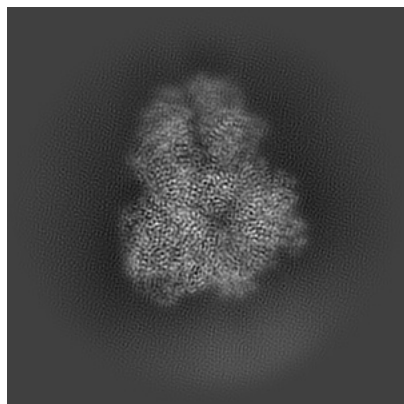
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40763. These allow visual inspection of the internal detail of the map and identification of artifacts.

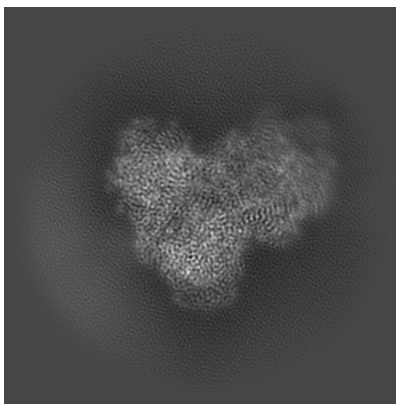
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

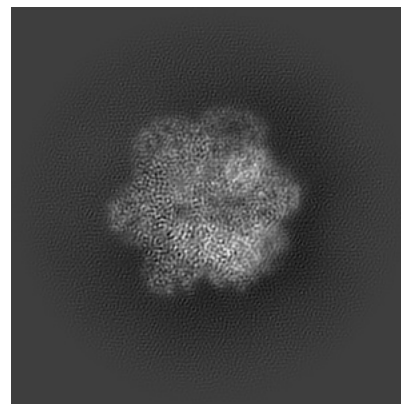
#### 6.1.1 Primary map



X

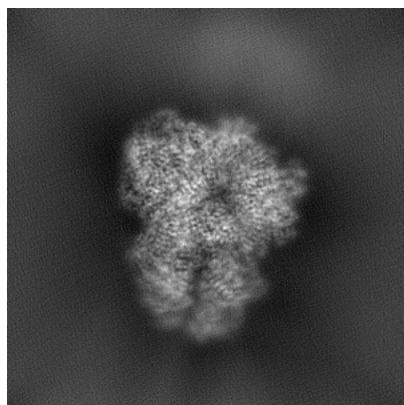


Y

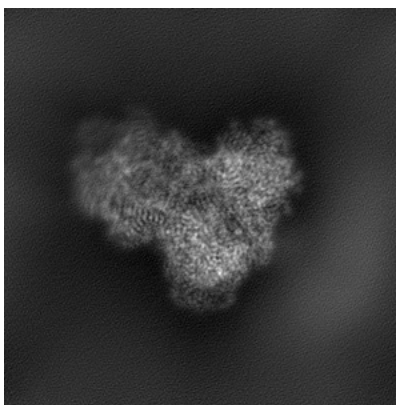


Z

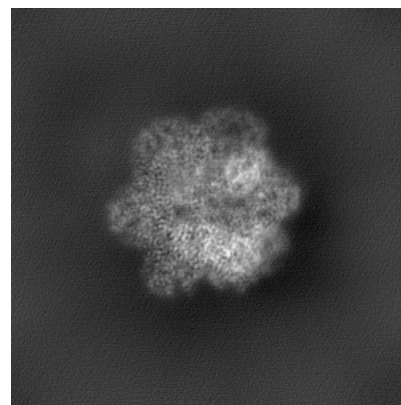
#### 6.1.2 Raw map



X



Y

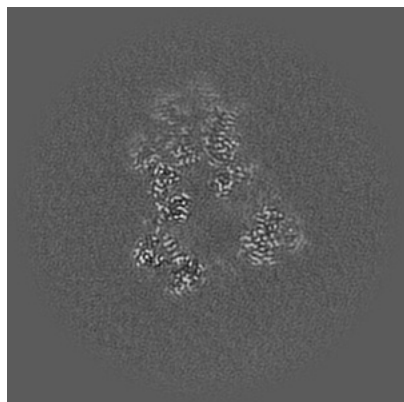


Z

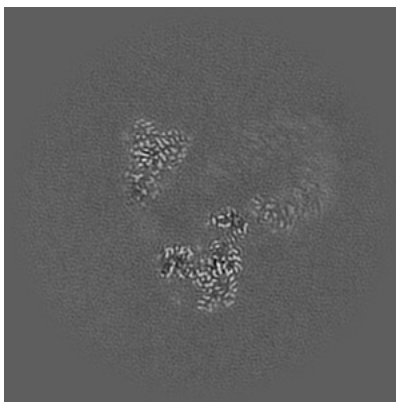
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

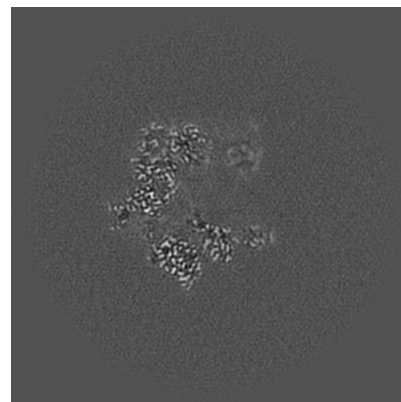
### 6.2.1 Primary map



X Index: 160

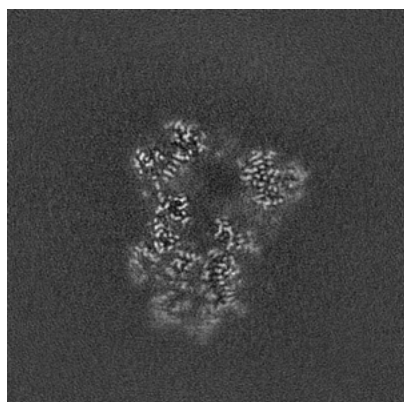


Y Index: 160

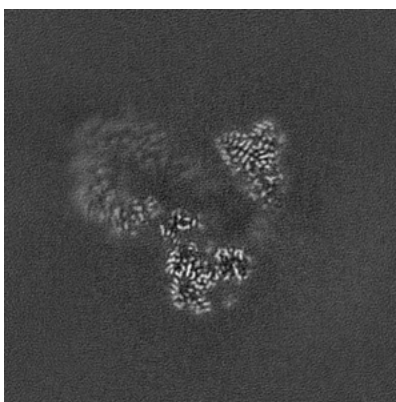


Z Index: 160

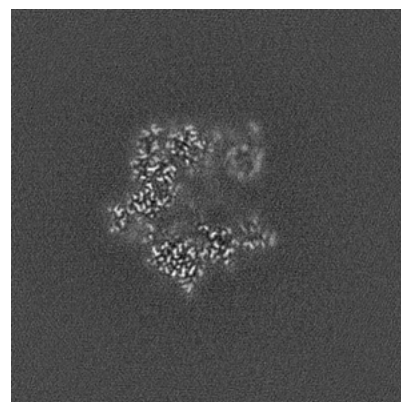
### 6.2.2 Raw map



X Index: 160



Y Index: 160

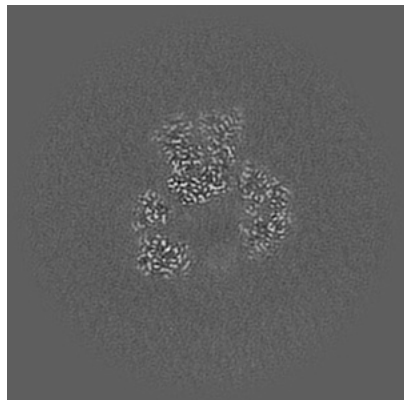


Z Index: 160

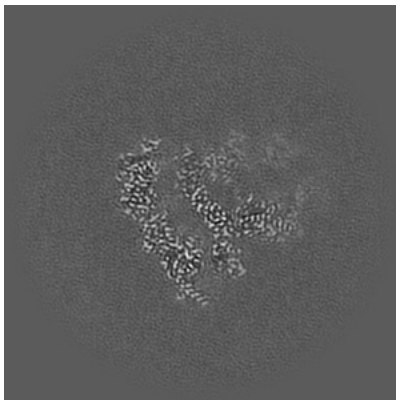
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

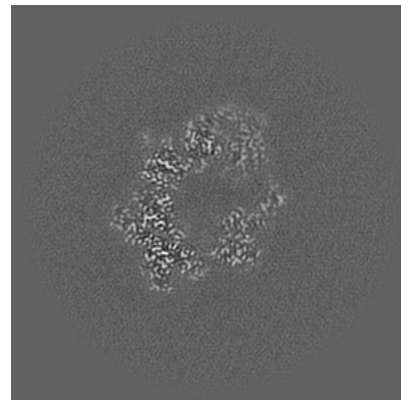
### 6.3.1 Primary map



X Index: 148

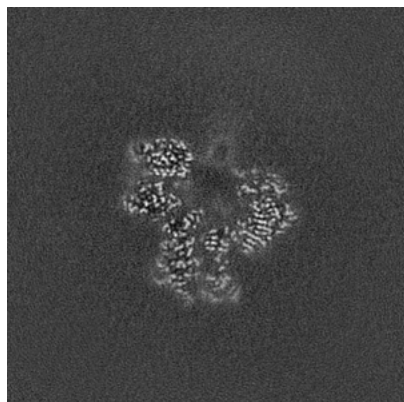


Y Index: 142

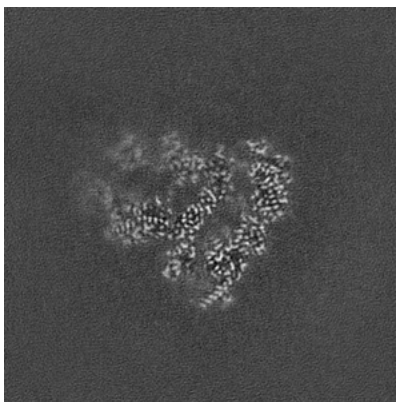


Z Index: 143

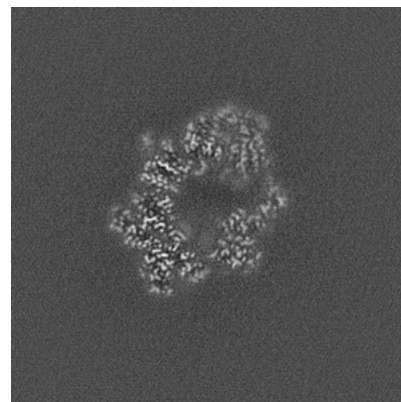
### 6.3.2 Raw map



X Index: 140



Y Index: 142

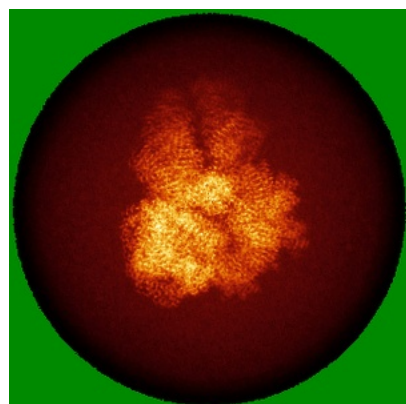


Z Index: 176

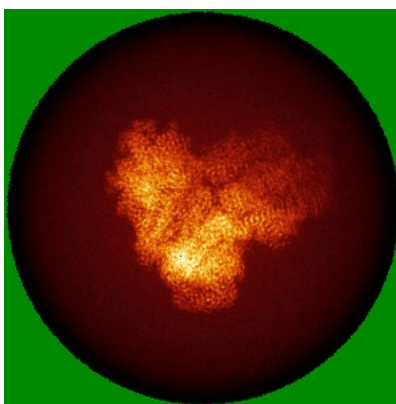
The images above show the largest variance slices of the map in three orthogonal directions.

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

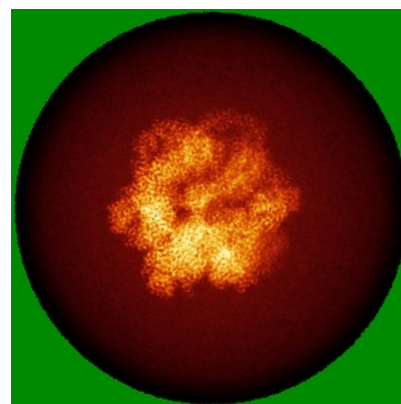
### 6.4.1 Primary map



X

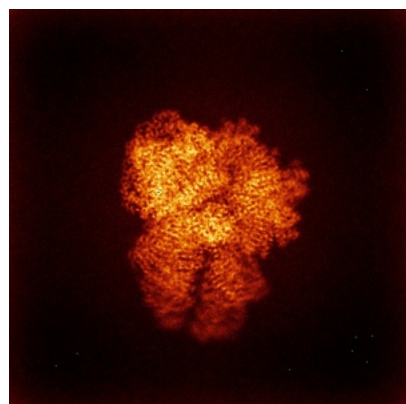


Y

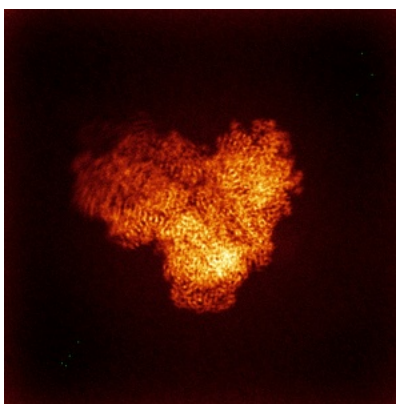


Z

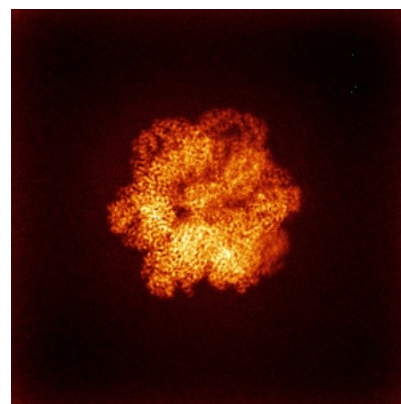
### 6.4.2 Raw map



X



Y

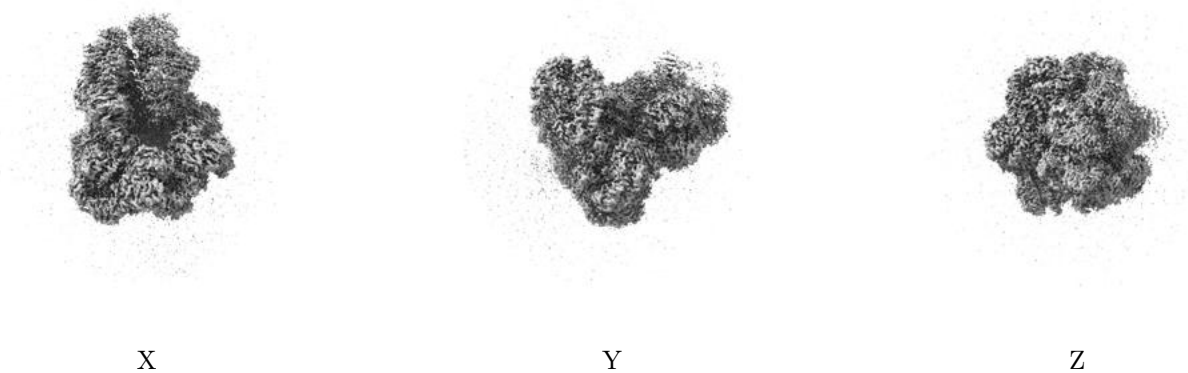


Z

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.

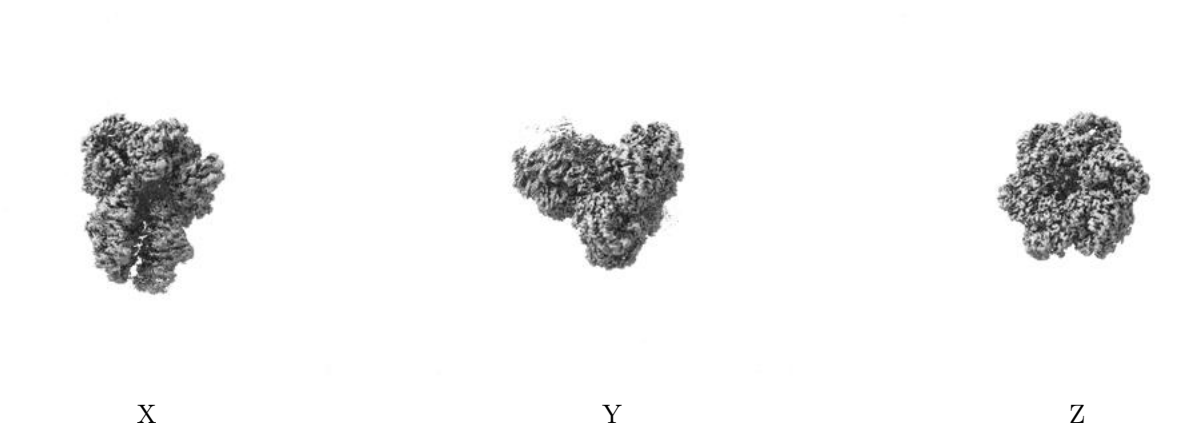
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.264. 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](#)

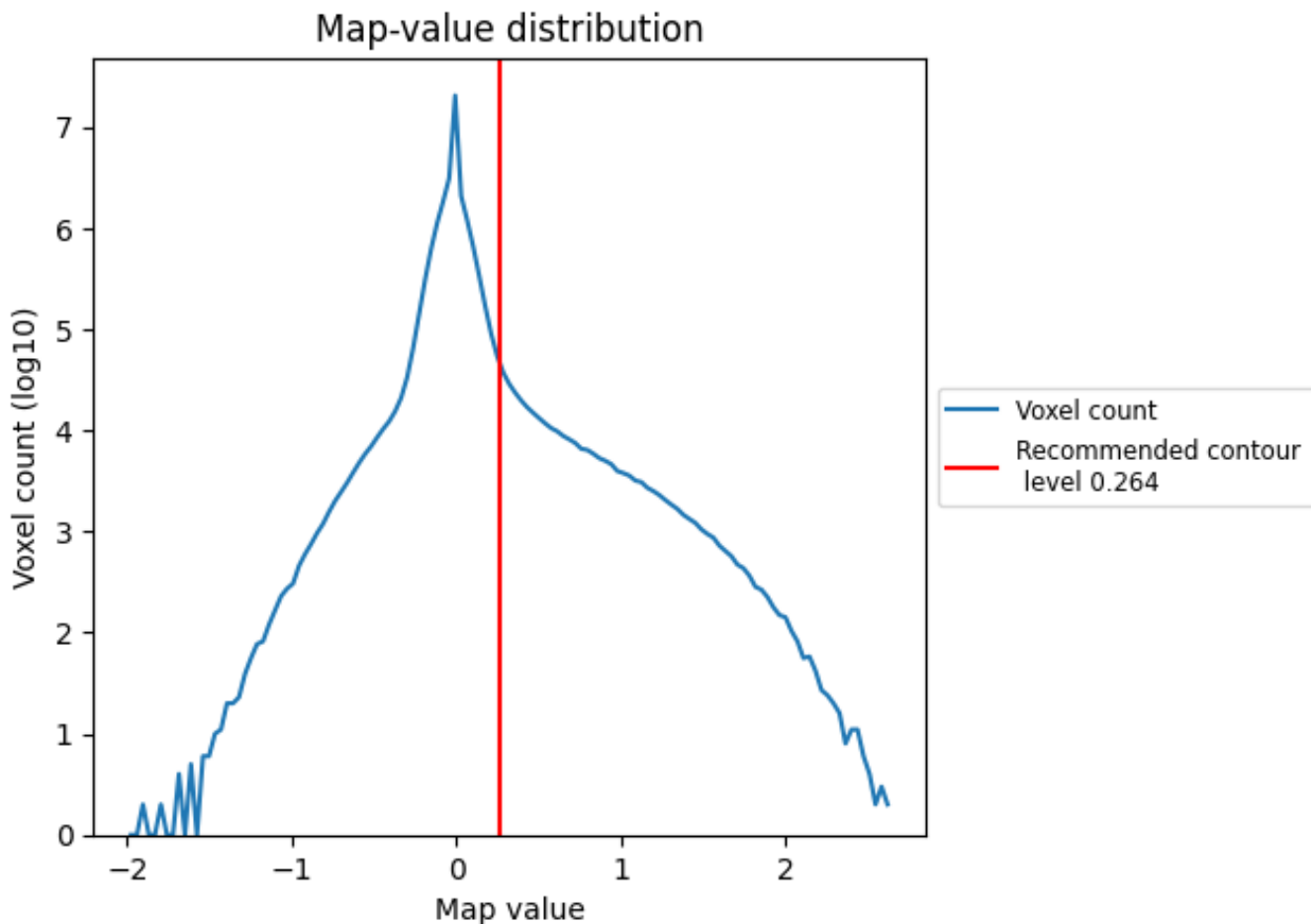
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

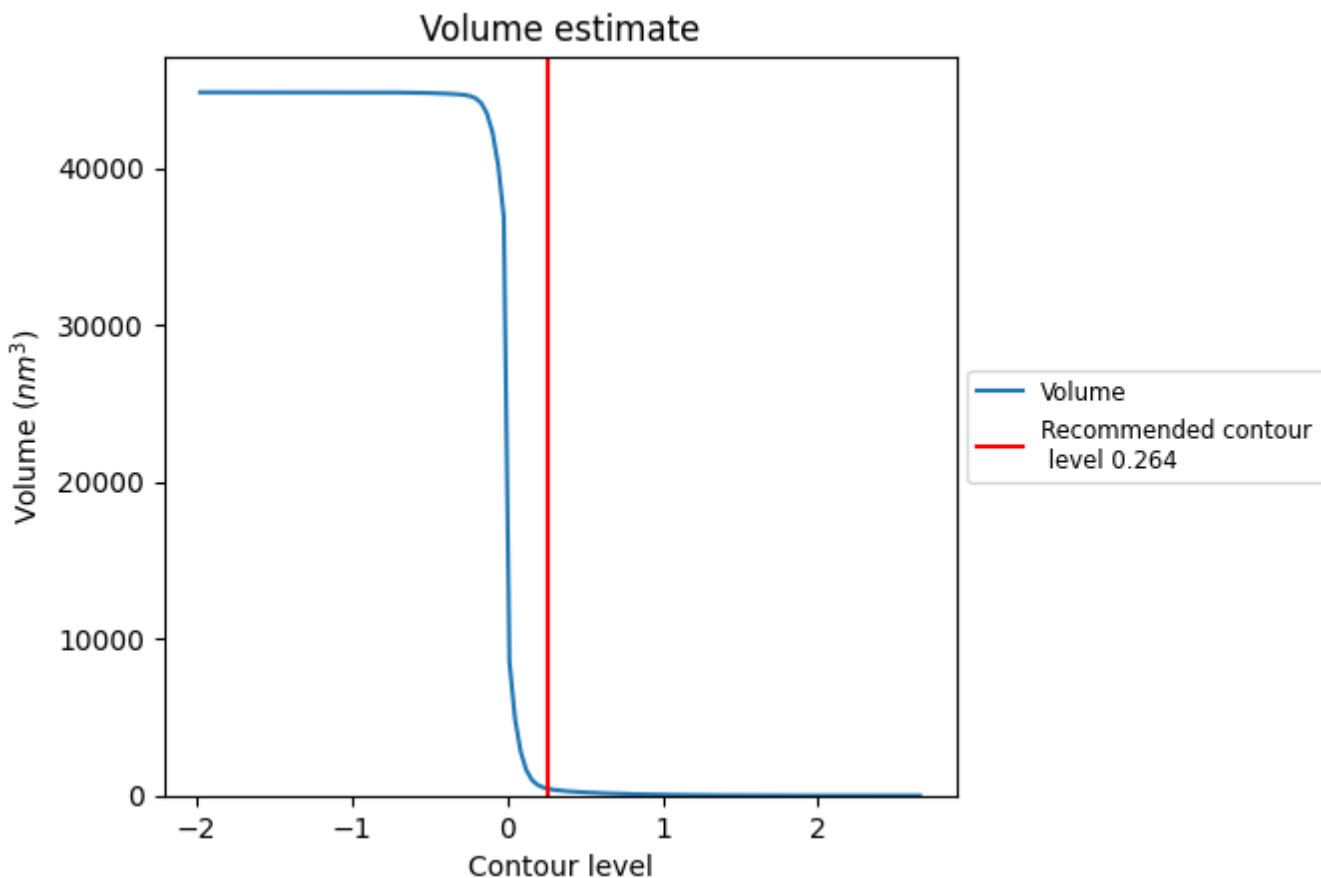
This section contains the results of statistical analysis of the map.

### 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.

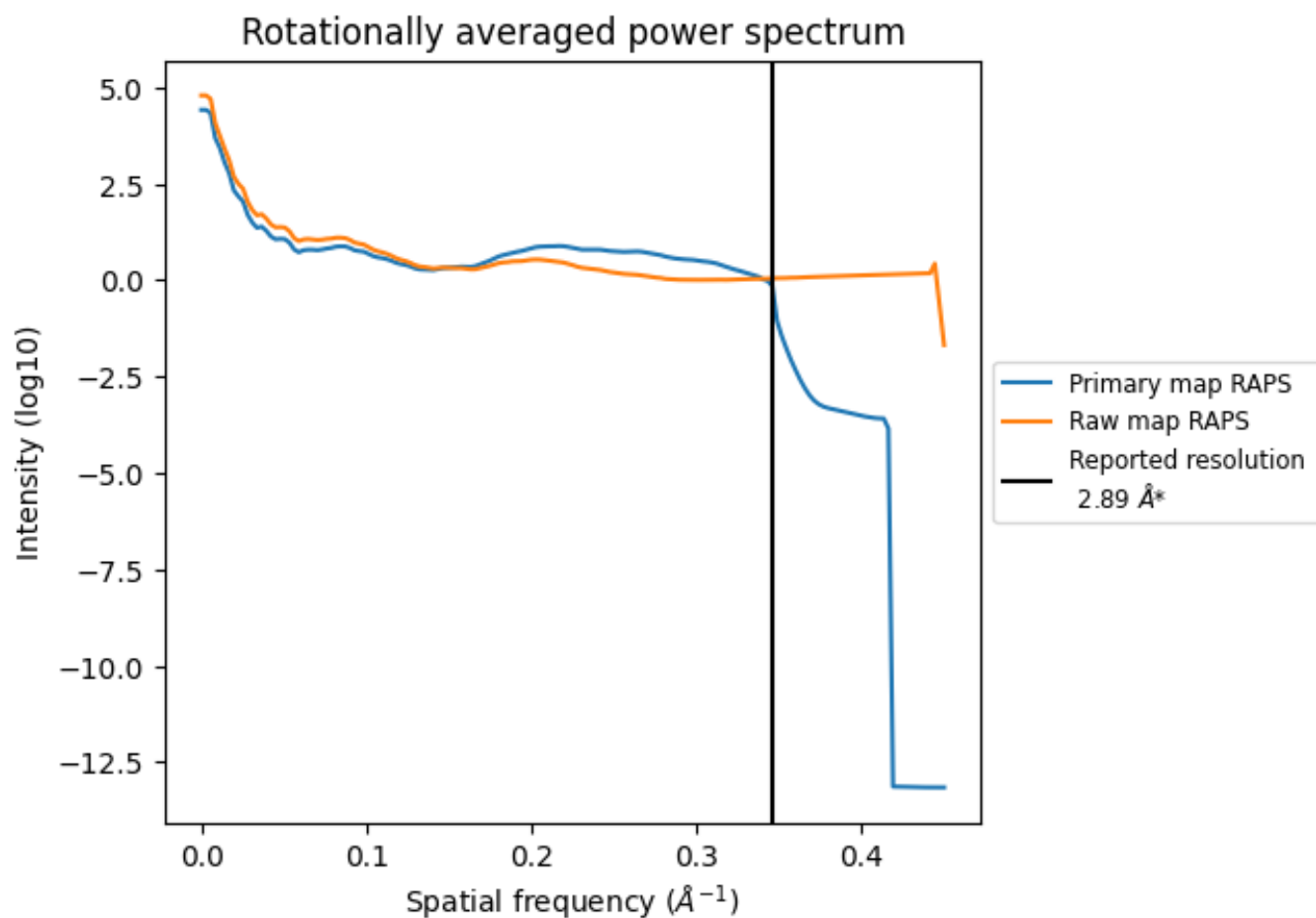
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 431  $\text{nm}^3$ ; this corresponds to an approximate mass of 389 kDa.

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

### 7.3 Rotationally averaged power spectrum i

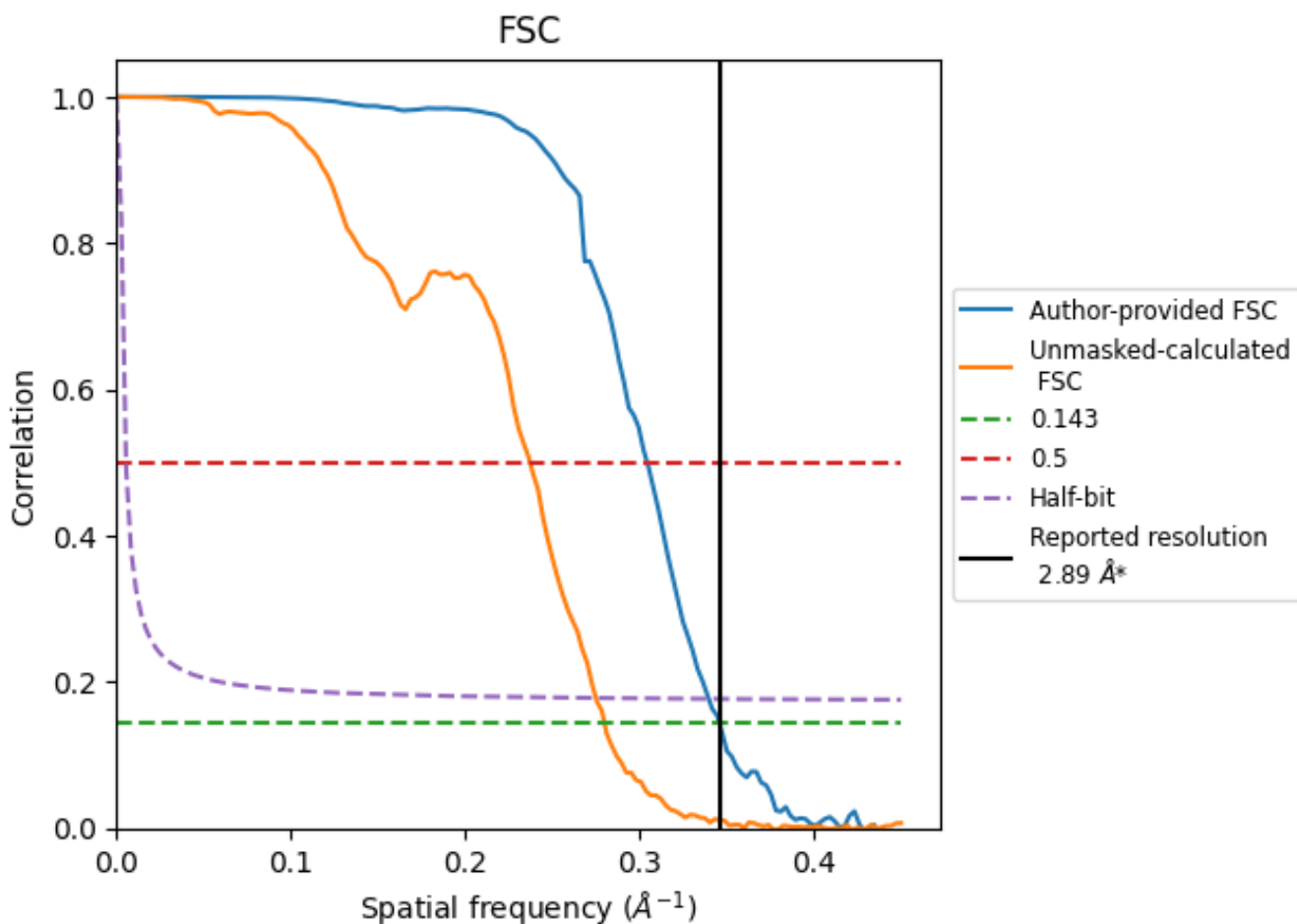


\*Reported resolution corresponds to spatial frequency of  $0.346 \text{ \AA}^{-1}$

## 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 0.346  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

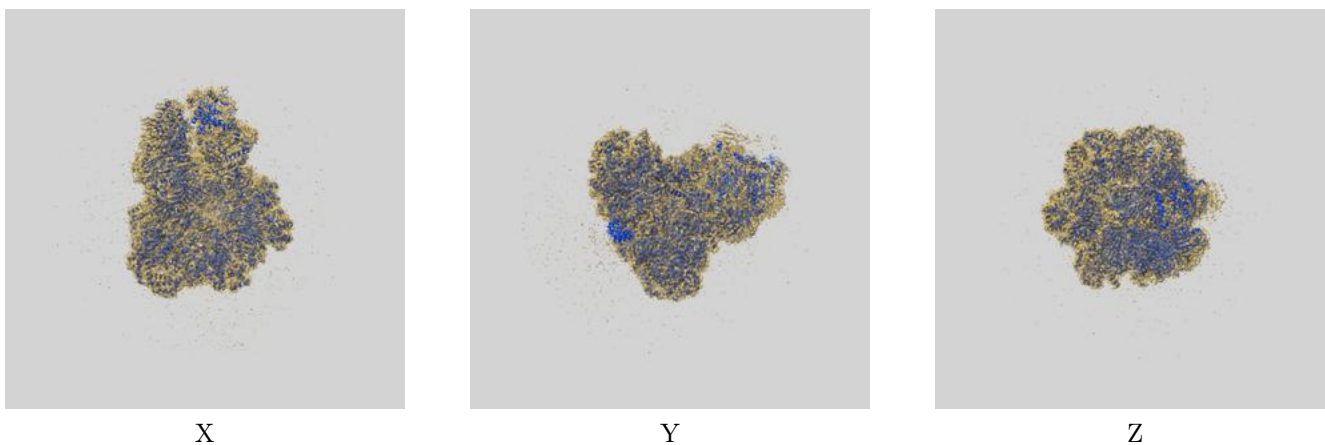
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.89	-	-
Author-provided FSC curve	2.89	3.28	2.94
Unmasked-calculated*	3.57	4.21	3.63

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.57 differs from the reported value 2.89 by more than 10 %

## 9 Map-model fit [i](#)

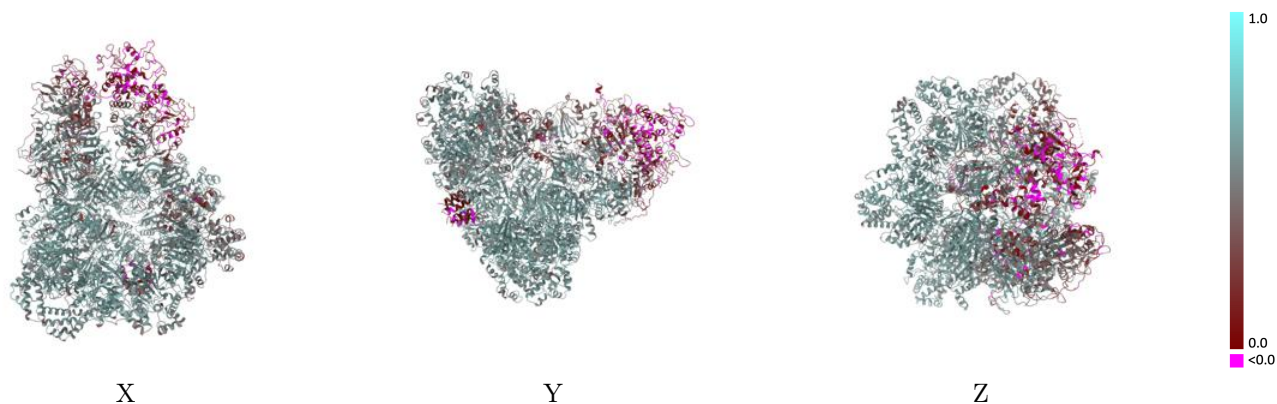
This section contains information regarding the fit between EMDB map EMD-40763 and PDB model 8SUB. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlay [i](#)



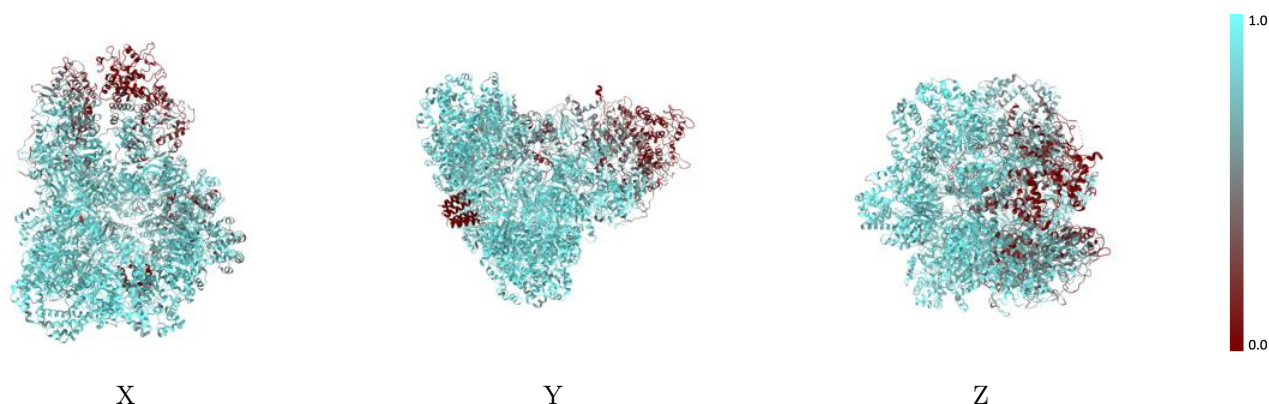
The images above show the 3D surface view of the map at the recommended contour level 0.264 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



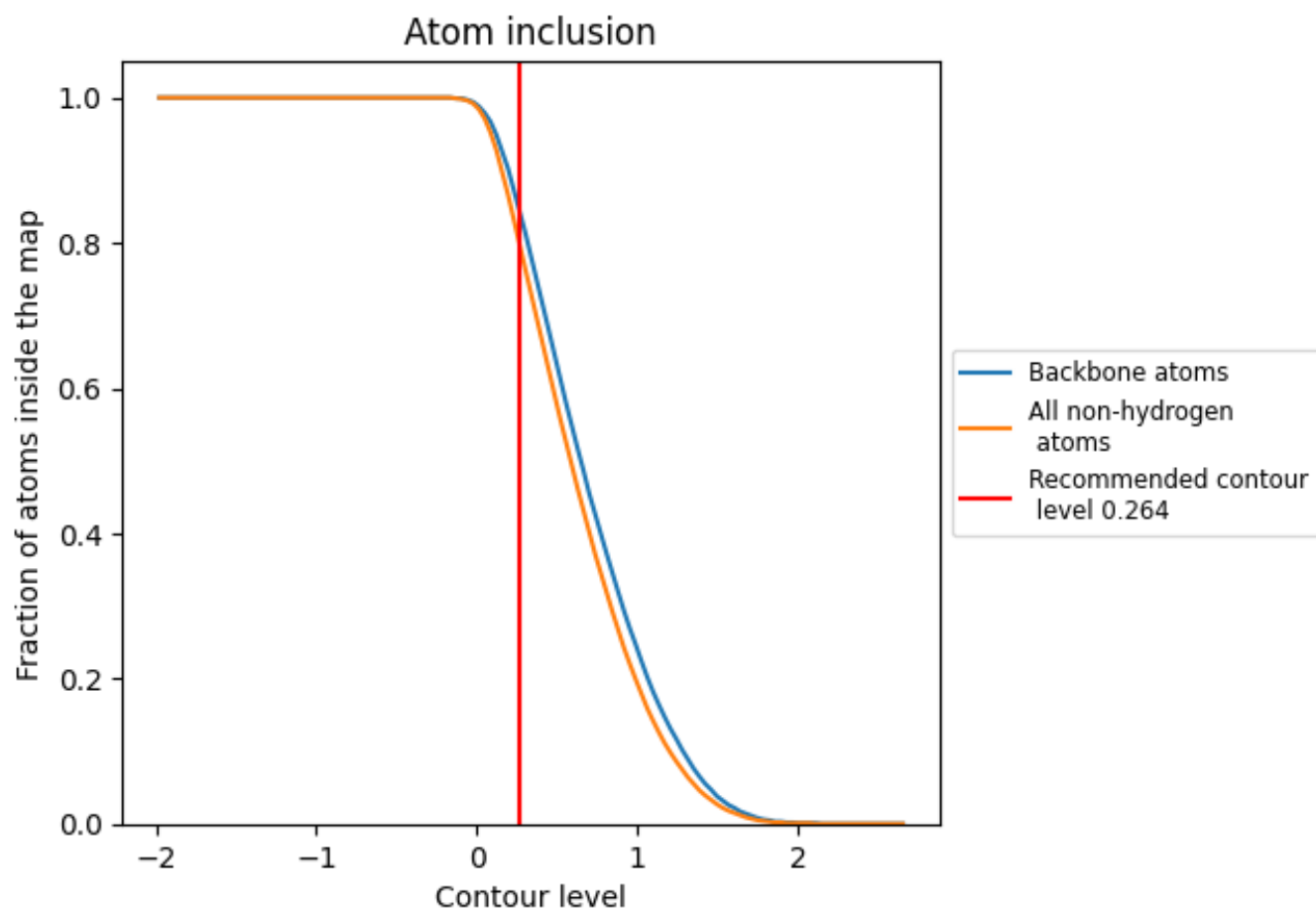
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.264).

## 9.4 Atom inclusion [i](#)







































At the recommended contour level, 85% of all backbone atoms, 80% 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 (0.264) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8000	 0.5150
A	 0.9430	 0.6120
B	 0.9020	 0.5870
C	 0.9280	 0.5910
D	 0.8780	 0.5650
E	 0.9060	 0.5770
F	 0.8460	 0.5470
G	 0.7090	 0.4520
H	 0.8220	 0.5370
I	 0.8960	 0.5770
J	 0.8900	 0.5740
K	 0.9380	 0.6100
L	 0.9060	 0.5850
M	 0.6820	 0.4460
N	 0.8250	 0.5390
O	 0.7710	 0.5040
P	 0.6350	 0.3960
Q	 0.3810	 0.2260

