



## wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 06:18 PM UTC

PDB ID : 8SUW / pdb\_00008suw  
EMDB ID : EMD-40778  
Title : E. coli SIR2-HerA complex (dodecamer SIR2 bound 4 protomers of HerA)  
Authors : Shen, Z.F.; Lin, Q.P.; Fu, T.M.  
Deposited on : 2023-05-13  
Resolution : 3.15 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:

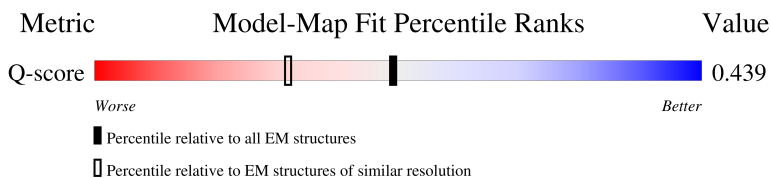
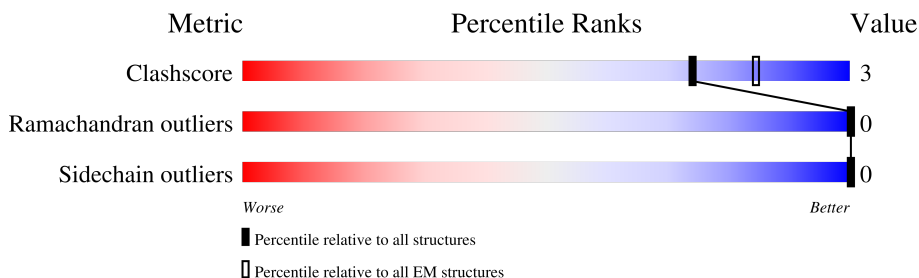
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

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

The reported resolution of this entry is 3.15 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.



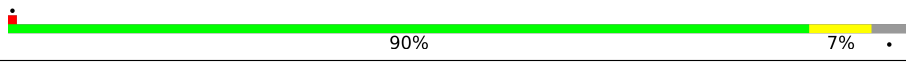




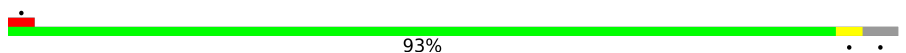

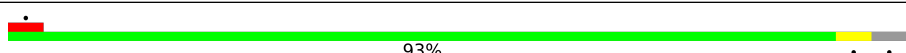
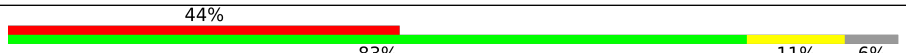
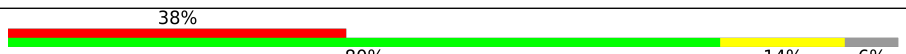
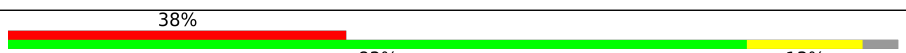

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14486 ( 2.65 - 3.65 )

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	93% <span style="float: right;">. .</span>
1	B	415	91% <span style="float: right;">5% .</span>
1	C	415	93% <span style="float: right;">. .</span>
1	D	415	92% <span style="float: right;">5% .</span>

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Mol	Chain	Length	Quality of chain
1	E	415	 90% 7%
1	F	415	 89% 7%
1	G	415	 9% 83% 11% 6%
1	H	415	 6% 90% 6%
1	I	415	 5% 82% 13% 5%
1	J	415	 93%
1	K	415	 91% 5%
1	L	415	 93%
2	M	610	 44% 83% 11% 6%
2	N	610	 38% 80% 14% 6%
2	O	610	 38% 83% 13%
2	P	610	 57% 74% 13% 13%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 56577 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	397	Total 3175	C 2044	N 528	O 597	S 6	0	0
1	C	398	Total 3185	C 2048	N 532	O 599	S 6	0	0
1	D	400	Total 3192	C 2053	N 532	O 601	S 6	0	0
1	E	400	Total 3194	C 2053	N 534	O 601	S 6	0	0
1	F	399	Total 3187	C 2050	N 531	O 600	S 6	0	0
1	G	390	Total 3119	C 2006	N 520	O 587	S 6	0	0
1	H	400	Total 3192	C 2053	N 532	O 601	S 6	0	0
1	I	394	Total 3145	C 2021	N 525	O 593	S 6	0	0
1	J	399	Total 3188	C 2051	N 531	O 600	S 6	0	0
1	K	398	Total 3182	C 2047	N 532	O 597	S 6	0	0
1	L	399	Total 3188	C 2051	N 531	O 600	S 6	0	0

- Molecule 2 is a protein called Nucleoside triphosphate hydrolase.

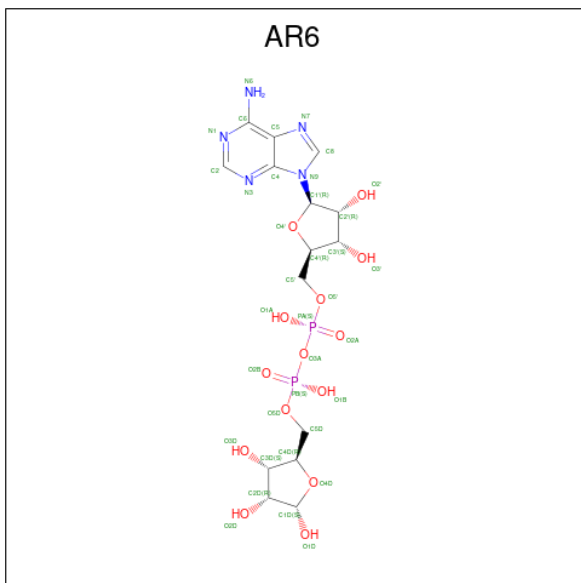
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	M	573	Total 4536	C 2887	N 798	O 838	S 13	0	0
2	N	574	Total 4548	C 2898	N 799	O 839	S 12	0	0
2	O	585	Total 4637	C 2951	N 812	O 862	S 12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	P	531	4208	2691	728	777	12	0	0

- 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-TRIHIDROXYOXOLAN-2-YL]METHOXY]PHOSPHORYL] HYDROGEN PHOSPHATE (CCD ID: 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).



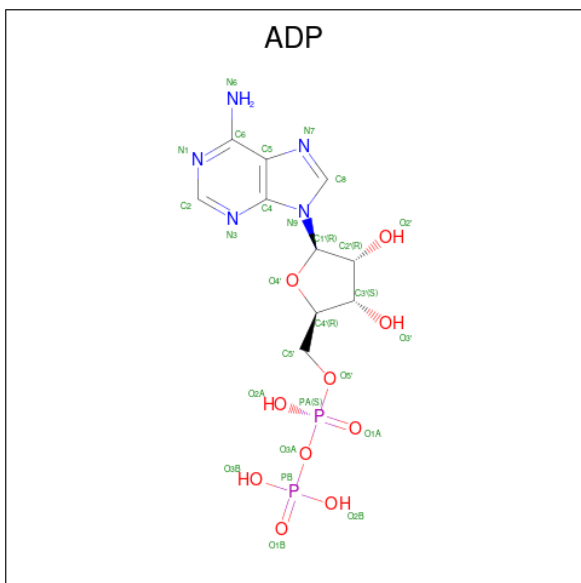
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	Total	C	N	O	P	0
			36	15	5	14	2	
3	B	1	Total	C	N	O	P	0
			36	15	5	14	2	
3	C	1	Total	C	N	O	P	0
			36	15	5	14	2	
3	D	1	Total	C	N	O	P	0
			36	15	5	14	2	
3	E	1	Total	C	N	O	P	0
			36	15	5	14	2	
3	F	1	Total	C	N	O	P	0
			36	15	5	14	2	
3	G	1	Total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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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	C	N	O	P	0
			27	10	5	10	2	
4	N	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	O	1	Total	C	N	O	P	0
			27	10	5	10	2	

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

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	M	1	Total	Mg	0
			1	1	
5	N	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	O	1	1	1	0

### 3 Residue-property plots [i](#)


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.

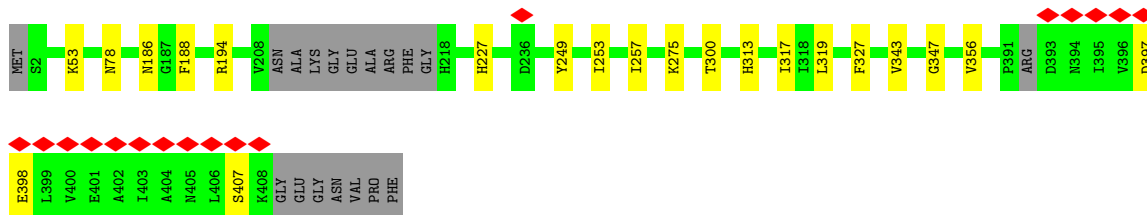
- Molecule 1: SIR2-like domain-containing protein

Chain A:  93%



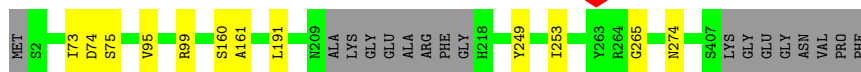
- Molecule 1: SIR2-like domain-containing protein

Chain B:  91% 5%



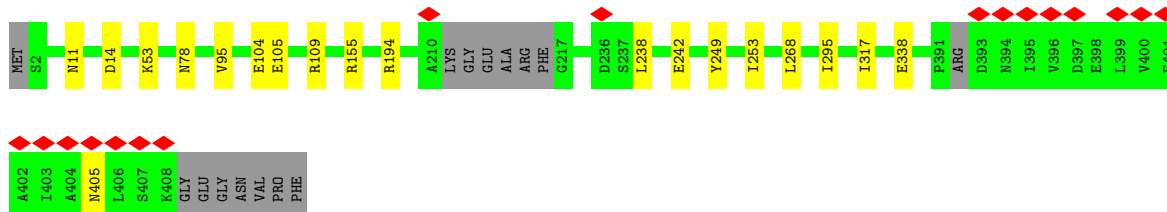
- Molecule 1: SIR2-like domain-containing protein

Chain C:  93%




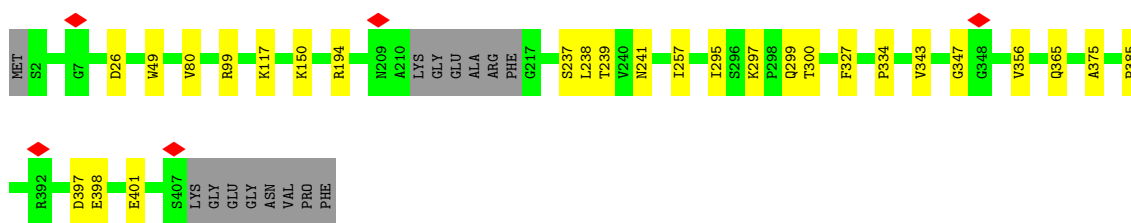
- Molecule 1: SIR2-like domain-containing protein

Chain D:  92% 5%




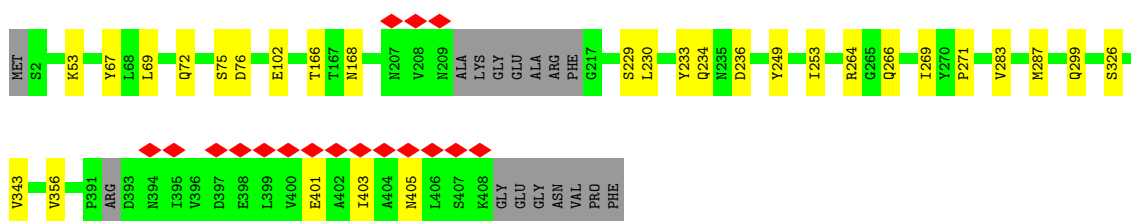
- Molecule 1: SIR2-like domain-containing protein

Chain E:  90% 7%




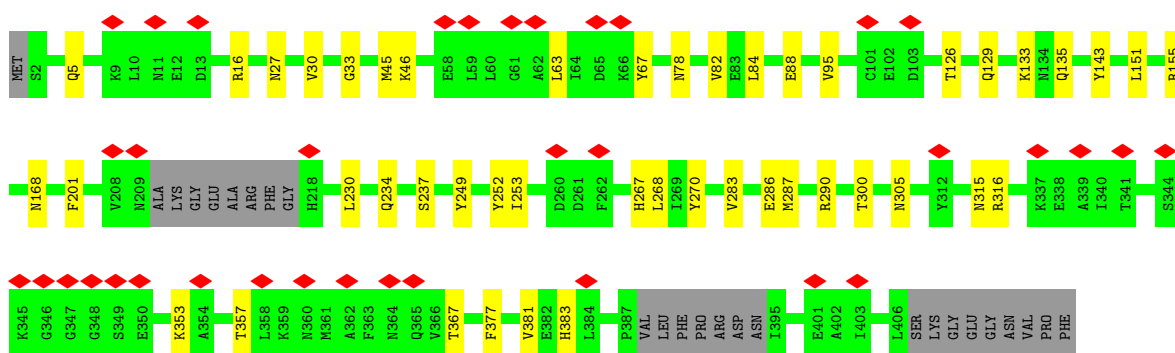
- Molecule 1: SIR2-like domain-containing protein

Chain F:  89% 7%

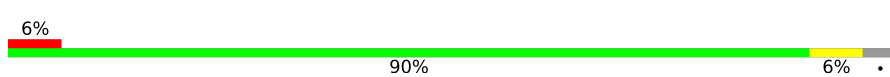


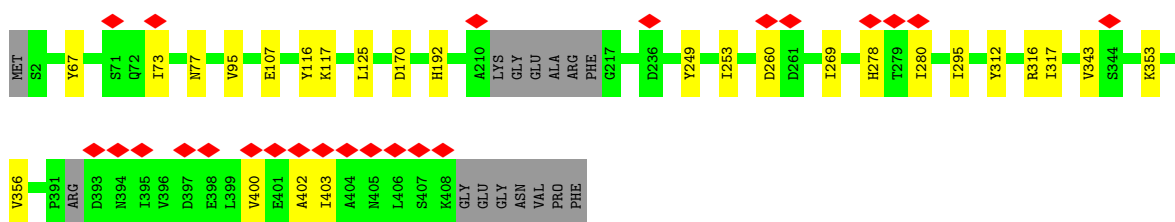
- Molecule 1: SIR2-like domain-containing protein

Chain G:  9% 83% 11% 6%




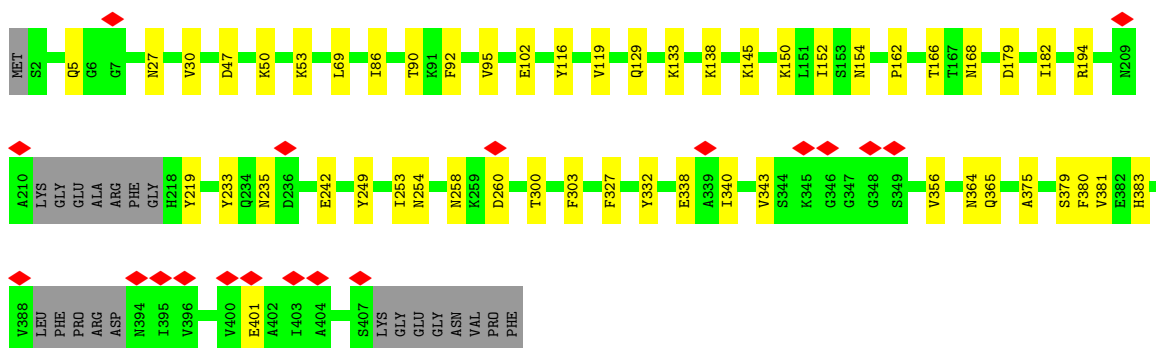
- Molecule 1: SIR2-like domain-containing protein

Chain H:  6% 90% 6%



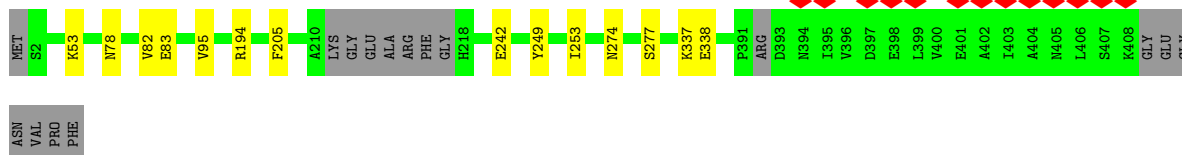
- Molecule 1: SIR2-like domain-containing protein

Chain I: 

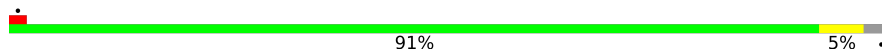


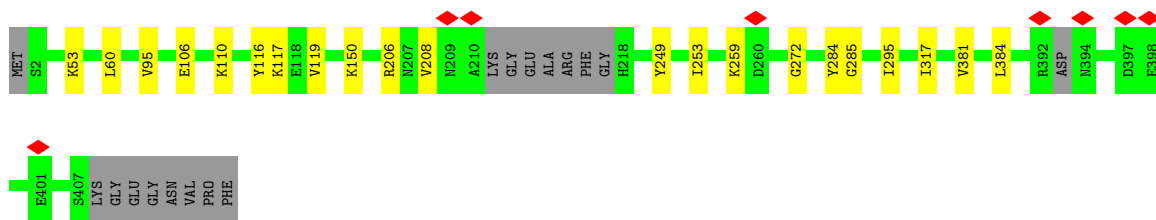
- Molecule 1: SIR2-like domain-containing protein

Chain J: 



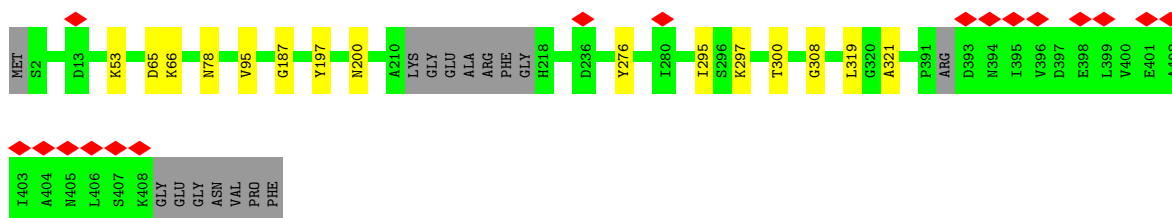
- Molecule 1: SIR2-like domain-containing protein

Chain K: 




- Molecule 1: SIR2-like domain-containing protein

Chain L: 



- Molecule 2: Nucleoside triphosphate hydrolase

Chain M: 





Q566	Q567	Q568	Q569	Q570	Q571	Q572	Q573	Q574	Q575	Q576	Q577	Q578	Q579	Q580	Q581	Q582	Q583	Q584	Q585	GLN	ALA	ARG	PRO	PRO	GLY	LYS	SER	ASP	ALA	VAL	PHE	SER	GLU	TRP	ALA	ASN	CYS	THR	GLU	LEU	ARG	CYS																		
Q422	K423	M429	D430	W431	W432	W433	V436	W437	M438	K439	M440	L441	A442	Q443	D444	H445	A446	P447	M448	L449	L450	S451	A452	L453	L454	E455	M456	F457	A458	E459	I460	L461	F462	R463	R464	G465	R466	S467	Y470	L475	E478	A479	H480	H481	Y482	L483	R484	ASP	PRO	TYR	ALA	GLU	ILE	ASP						
SER	GLN	ILE	K495	A496	Y497	E498	R499	L500	A501	K502	E503	G504	R505	K506	F507	R508	C509	S510	L511	I512	V513	Q516	R517	P518	S519	E520	L521	S522	P523	T524	V525	L526	A527	W532	F533	S534	L535	R536	L537	T538	N539	E540	R541	D542	L543	Q544	A545	L546	R547	Y548	A549	M550	E551	S552	G553	N554	E555			
E237	K238	K239	Q240	Q241	K242	G243	E244	L245	Y246	S247	E248	E249	Y250	Y251	C252	Y253	K254	K255	I256	A260	L261	G262	F263	A264	G265	L266	I267	K268	L269	L270	R271	P272	S273	D274	K275	T276	Q277	L278	P279	A280	L281	R282	N283	A284	L285	S286	A287	I288	N289	R290	T291	H292	F293	K294	S295	R296	N297	I298		
Y299	L300	E301	K302	D303	D304	G305	E306	T307	F308	L309	L310	Y311	D312	D313	C314	R315	D316	T317	N318	Q319	S320	K321	L322	A323	E324	W325	L326	D327	L328	LEU	ARG	ARG	ARG	ARG	LEU	LYS	R336	T337	N338	V339	W340	F341	P342	L281	F343	K344	S345	L346	A347	T348	L349	V350	A351	E352	F353	G354	C355	VAL	ALA	ALA
ASP	ARG	SER	ASN	GLY	SER	LYS	ARG	ASP	ALA	PHE	GLY	PHE	SER	ASN	V374	L375	P376	L377	V378	K379	I380	I381	Q382	Q383	L384	A385	E386	D387	I388	R389	F390	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	F421		

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62864	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	1.860	Depositor
Minimum map value	-1.060	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.192	Depositor
Map size ( $\text{\AA}$ )	355.2, 355.2, 355.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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	0.12	0/3259	0.28	0/4406
1	B	0.11	0/3248	0.29	0/4389
1	C	0.11	0/3259	0.26	0/4406
1	D	0.10	0/3265	0.28	0/4412
1	E	0.10	0/3268	0.28	0/4418
1	F	0.09	0/3260	0.28	0/4405
1	G	0.10	0/3190	0.27	0/4310
1	H	0.09	0/3265	0.27	0/4412
1	I	0.10	0/3216	0.26	0/4346
1	J	0.11	0/3261	0.27	0/4407
1	K	0.10	0/3255	0.30	1/4399 (0.0%)
1	L	0.10	0/3261	0.27	0/4407
2	M	0.10	0/4624	0.28	0/6243
2	N	0.11	0/4637	0.30	0/6260
2	O	0.10	0/4729	0.29	0/6388
2	P	0.10	0/4288	0.29	0/5790
All	All	0.10	0/57285	0.28	1/77398 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	208	VAL	N-CA-C	-5.73	107.54	113.10

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	3185	0	3109	8	0
1	B	3175	0	3102	14	0
1	C	3185	0	3109	8	0
1	D	3192	0	3116	13	0
1	E	3194	0	3117	16	0
1	F	3187	0	3111	17	0
1	G	3119	0	3044	29	0
1	H	3192	0	3116	15	0
1	I	3145	0	3069	31	0
1	J	3188	0	3113	10	0
1	K	3182	0	3109	12	0
1	L	3188	0	3113	10	0
2	M	4536	0	4576	44	0
2	N	4548	0	4592	52	0
2	O	4637	0	4664	54	0
2	P	4208	0	4256	46	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
3	G	36	0	21	0	0
3	H	36	0	21	0	0
3	I	36	0	21	0	0
3	J	36	0	21	1	0
3	K	36	0	21	0	0
3	L	36	0	21	1	0
4	M	27	0	12	3	0
4	N	27	0	12	1	0
4	O	27	0	12	2	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
5	O	1	0	0	0	0
All	All	56577	0	55604	359	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 359 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)
2:N:272:PRO:HG3	2:N:281:LEU:HD13	1.69	0.74
1:H:73:ILE:O	1:H:77:ASN:ND2	2.23	0.72
1:K:106:GLU:OE2	1:K:110:LYS:NZ	2.22	0.71
1:H:249:TYR:HA	1:H:253:ILE:HG22	1.73	0.70
1:H:400:VAL:HA	1:H:403:ILE:HD12	1.75	0.69

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%)	376 (95%)	18 (5%)	0	100	100
1	B	391/415 (94%)	379 (97%)	12 (3%)	0	100	100
1	C	394/415 (95%)	383 (97%)	11 (3%)	0	100	100
1	D	394/415 (95%)	380 (96%)	14 (4%)	0	100	100
1	E	396/415 (95%)	376 (95%)	20 (5%)	0	100	100
1	F	393/415 (95%)	378 (96%)	15 (4%)	0	100	100
1	G	384/415 (92%)	368 (96%)	16 (4%)	0	100	100
1	H	394/415 (95%)	381 (97%)	13 (3%)	0	100	100
1	I	388/415 (94%)	370 (95%)	18 (5%)	0	100	100
1	J	393/415 (95%)	381 (97%)	12 (3%)	0	100	100
1	K	392/415 (94%)	373 (95%)	19 (5%)	0	100	100
1	L	393/415 (95%)	376 (96%)	17 (4%)	0	100	100
2	M	567/610 (93%)	541 (95%)	26 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	568/610 (93%)	530 (93%)	38 (7%)	0	100	100
2	O	581/610 (95%)	559 (96%)	22 (4%)	0	100	100
2	P	521/610 (85%)	502 (96%)	19 (4%)	0	100	100
All	All	6943/7420 (94%)	6653 (96%)	290 (4%)	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	339/351 (97%)	339 (100%)	0	100	100
1	C	340/351 (97%)	340 (100%)	0	100	100
1	D	340/351 (97%)	340 (100%)	0	100	100
1	E	340/351 (97%)	340 (100%)	0	100	100
1	F	340/351 (97%)	340 (100%)	0	100	100
1	G	332/351 (95%)	332 (100%)	0	100	100
1	H	340/351 (97%)	340 (100%)	0	100	100
1	I	335/351 (95%)	335 (100%)	0	100	100
1	J	340/351 (97%)	340 (100%)	0	100	100
1	K	339/351 (97%)	339 (100%)	0	100	100
1	L	340/351 (97%)	340 (100%)	0	100	100
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%)	499 (100%)	0	100	100
2	P	455/519 (88%)	455 (100%)	0	100	100
All	All	5997/6288 (95%)	5997 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	274	ASN
2	O	241	GLN
1	K	241	ASN
2	O	214	GLN
2	N	432	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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 18 ligands modelled in this entry, 3 are monoatomic - leaving 15 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	K	501	-	39,39,39	1.27	2 (5%)	56,60,60	0.77	0
3	AR6	B	501	-	39,39,39	1.17	2 (5%)	56,60,60	0.73	0
3	AR6	A	501	-	39,39,39	1.29	2 (5%)	56,60,60	0.68	0
3	AR6	G	501	-	39,39,39	1.26	2 (5%)	56,60,60	0.80	1 (1%)
3	AR6	F	501	-	39,39,39	1.25	2 (5%)	56,60,60	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ADP	N	701	5	28,29,29	1.42	4 (14%)	43,45,45	1.82	9 (20%)
3	AR6	J	501	-	39,39,39	1.23	2 (5%)	56,60,60	0.72	0
4	ADP	O	701	-	28,29,29	1.41	4 (14%)	43,45,45	1.83	9 (20%)
3	AR6	H	501	-	39,39,39	1.25	2 (5%)	56,60,60	0.69	0
3	AR6	L	501	-	39,39,39	1.24	2 (5%)	56,60,60	0.70	0
3	AR6	E	501	-	39,39,39	1.27	2 (5%)	56,60,60	0.74	1 (1%)
3	AR6	D	501	-	39,39,39	1.29	2 (5%)	56,60,60	0.66	0
4	ADP	M	701	5	28,29,29	1.41	4 (14%)	43,45,45	1.83	9 (20%)
3	AR6	C	501	-	39,39,39	1.26	2 (5%)	56,60,60	0.73	0
3	AR6	I	501	-	39,39,39	1.24	2 (5%)	56,60,60	0.70	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AR6	K	501	-	-	9/22/54/54	0/4/4/4
3	AR6	B	501	-	-	12/22/54/54	0/4/4/4
3	AR6	A	501	-	-	11/22/54/54	0/4/4/4
3	AR6	G	501	-	-	8/22/54/54	0/4/4/4
3	AR6	F	501	-	-	12/22/54/54	0/4/4/4
4	ADP	N	701	5	-	3/16/32/32	0/3/3/3
3	AR6	J	501	-	-	12/22/54/54	0/4/4/4
4	ADP	O	701	-	-	1/16/32/32	0/3/3/3
3	AR6	H	501	-	-	9/22/54/54	0/4/4/4
3	AR6	L	501	-	-	13/22/54/54	0/4/4/4
3	AR6	E	501	-	-	8/22/54/54	0/4/4/4
3	AR6	D	501	-	-	9/22/54/54	0/4/4/4
4	ADP	M	701	5	-	1/16/32/32	0/3/3/3
3	AR6	C	501	-	-	14/22/54/54	0/4/4/4
3	AR6	I	501	-	-	9/22/54/54	0/4/4/4

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	AR6	PB-O3A	4.91	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	AR6	PB-O3A	4.89	1.64	1.59
3	E	501	AR6	PB-O3A	4.79	1.64	1.59
3	G	501	AR6	PB-O3A	4.75	1.64	1.59
4	M	701	ADP	C5-C4	4.73	1.47	1.39

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	701	ADP	C5-C4-N3	-5.86	118.65	126.72
4	M	701	ADP	C5-C4-N3	-5.81	118.71	126.72
4	N	701	ADP	C5-C4-N3	-5.76	118.78	126.72
4	O	701	ADP	N3-C4-N9	4.66	135.09	127.17
4	M	701	ADP	N3-C4-N9	4.62	135.02	127.17

There are no chirality outliers.

5 of 131 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	C5'-O5'-PA-O3A
3	B	501	AR6	C2'-C1'-N9-C4
3	B	501	AR6	C2'-C1'-N9-C8

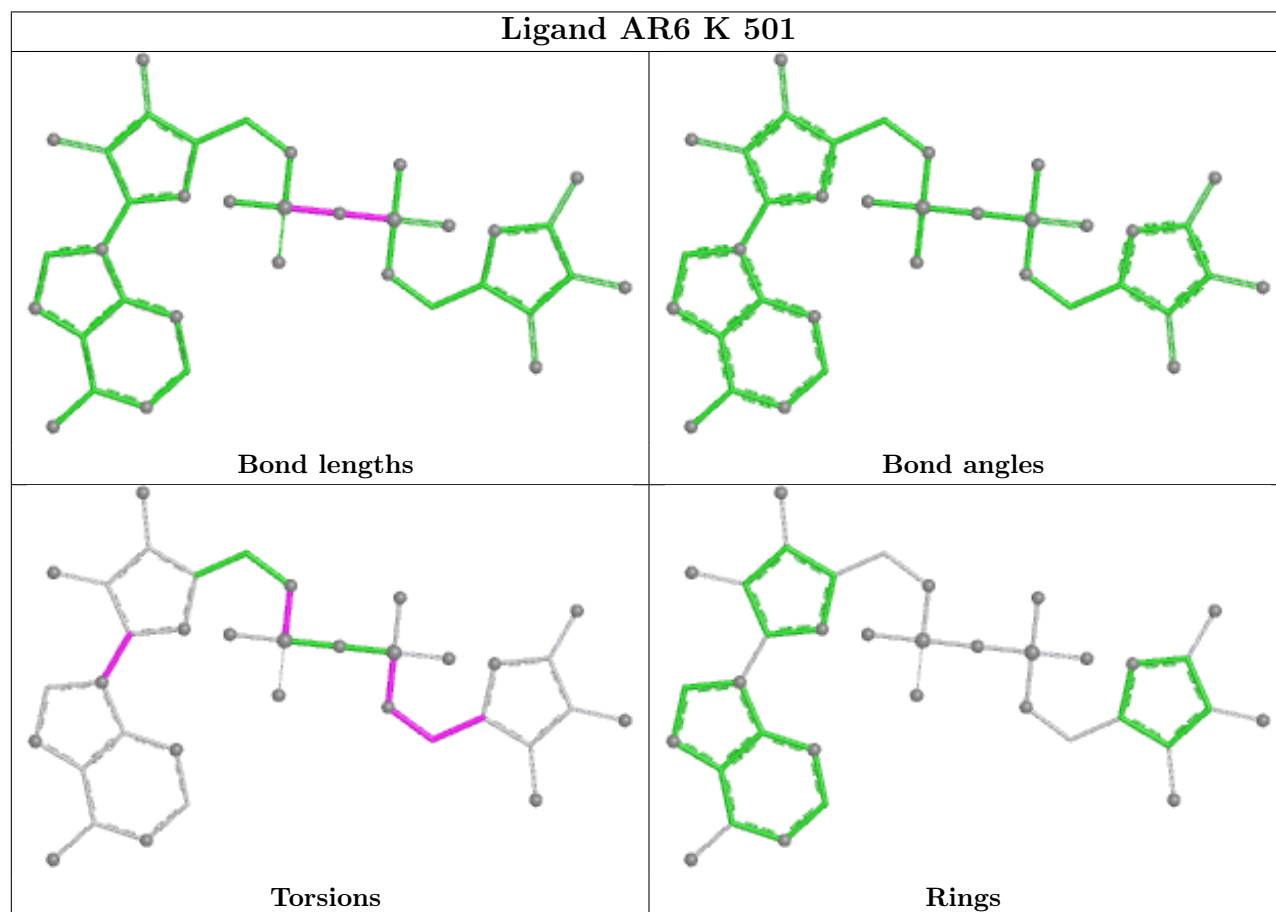
There are no ring outliers.

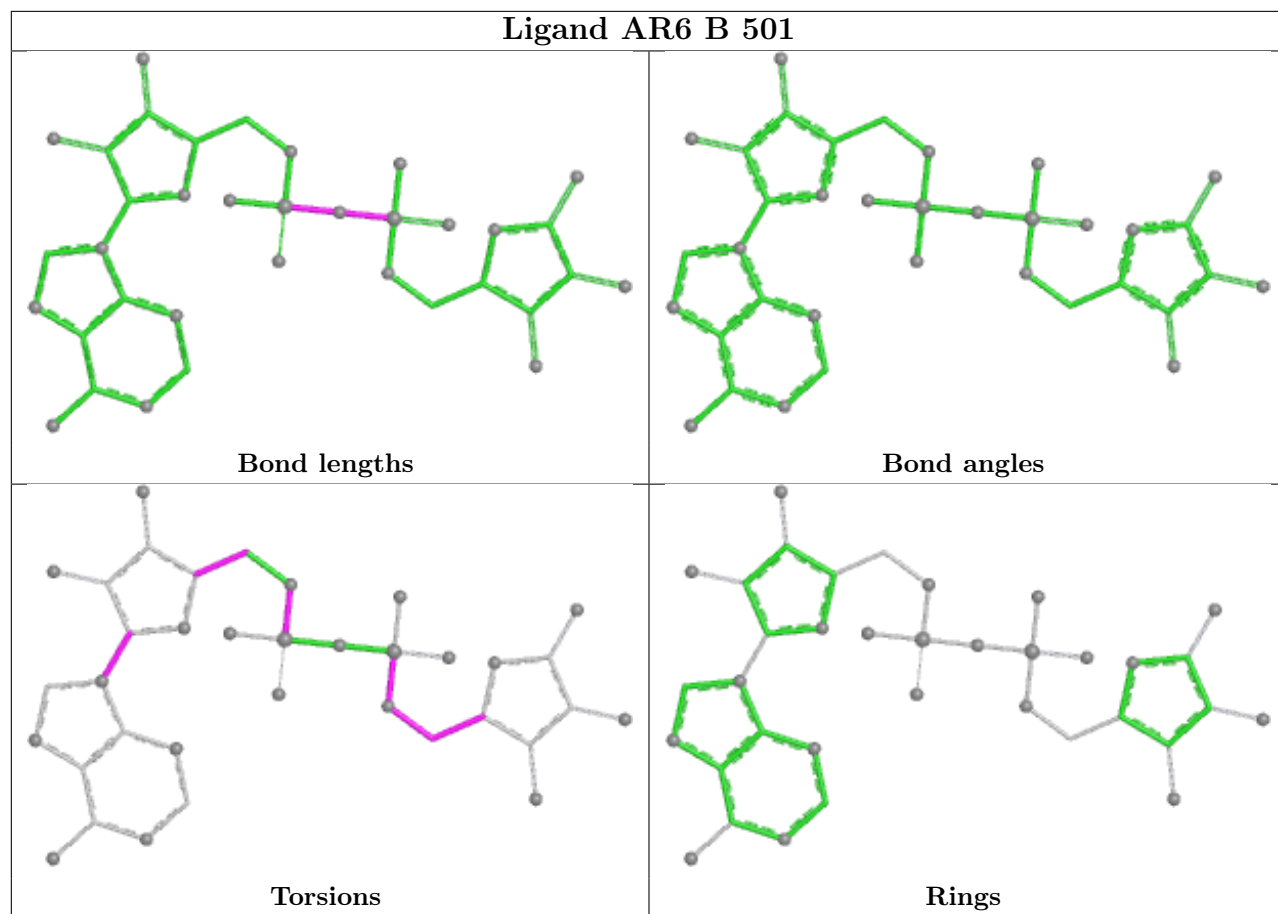
5 monomers are involved in 8 short contacts:

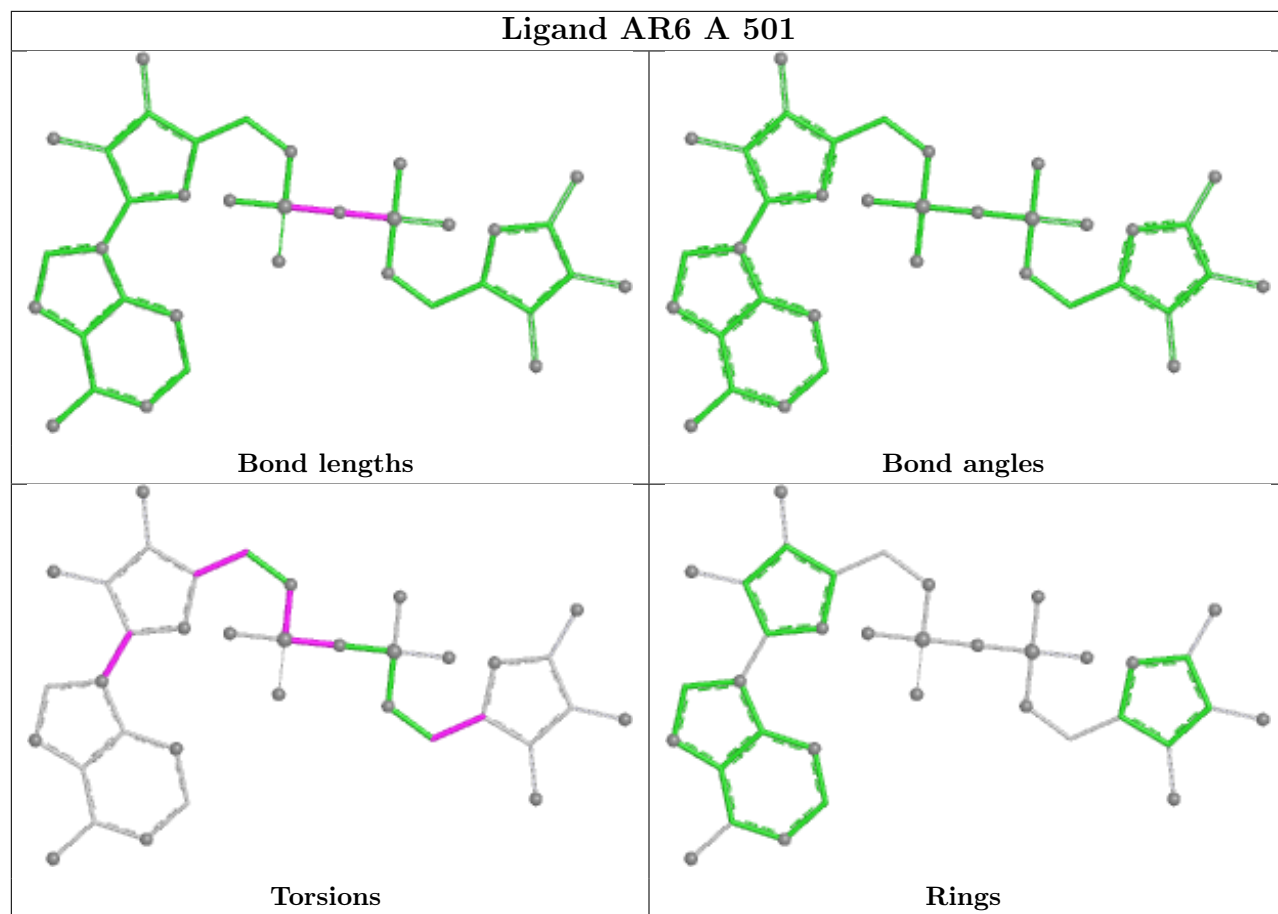
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	701	ADP	1	0
3	J	501	AR6	1	0
4	O	701	ADP	2	0
3	L	501	AR6	1	0
4	M	701	ADP	3	0

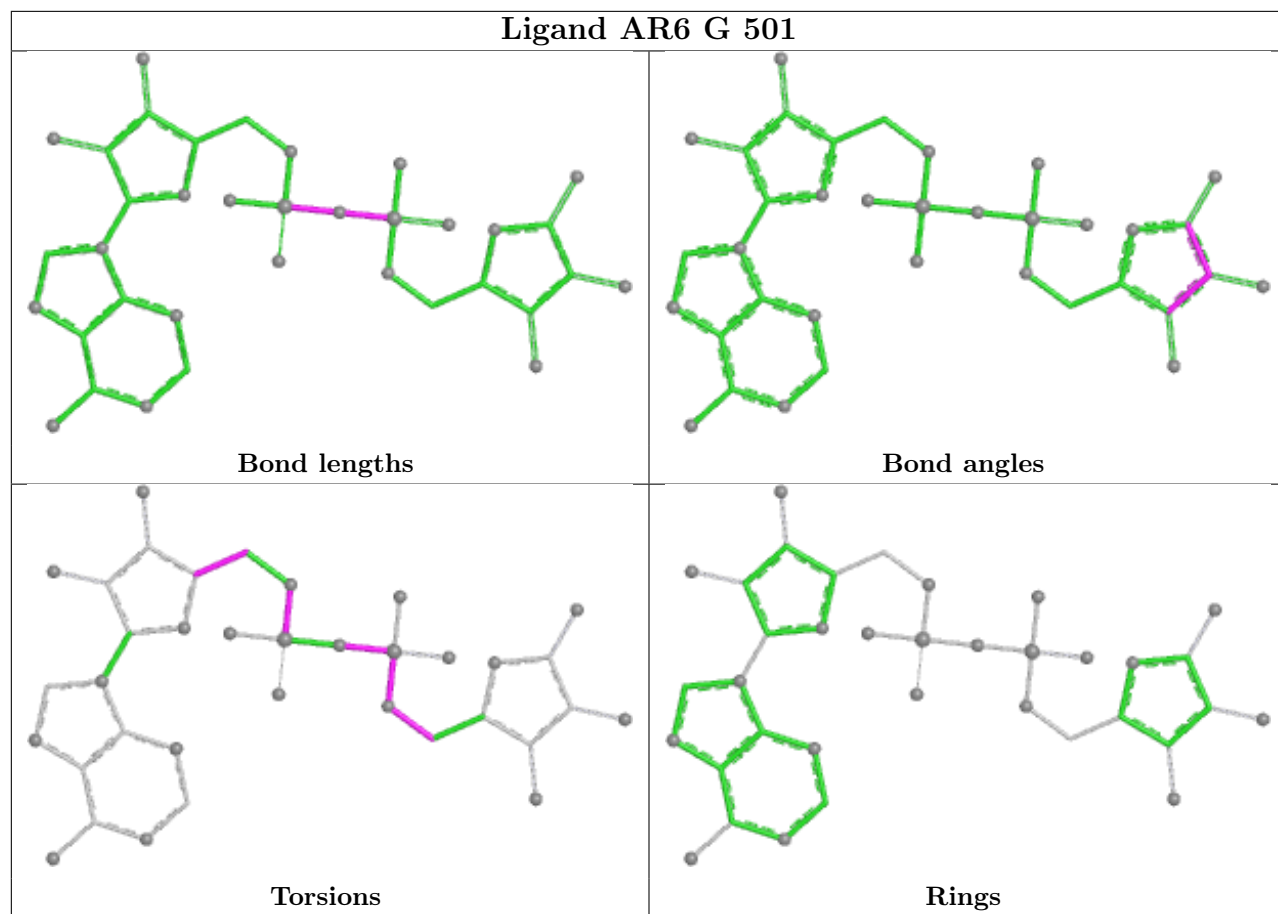
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

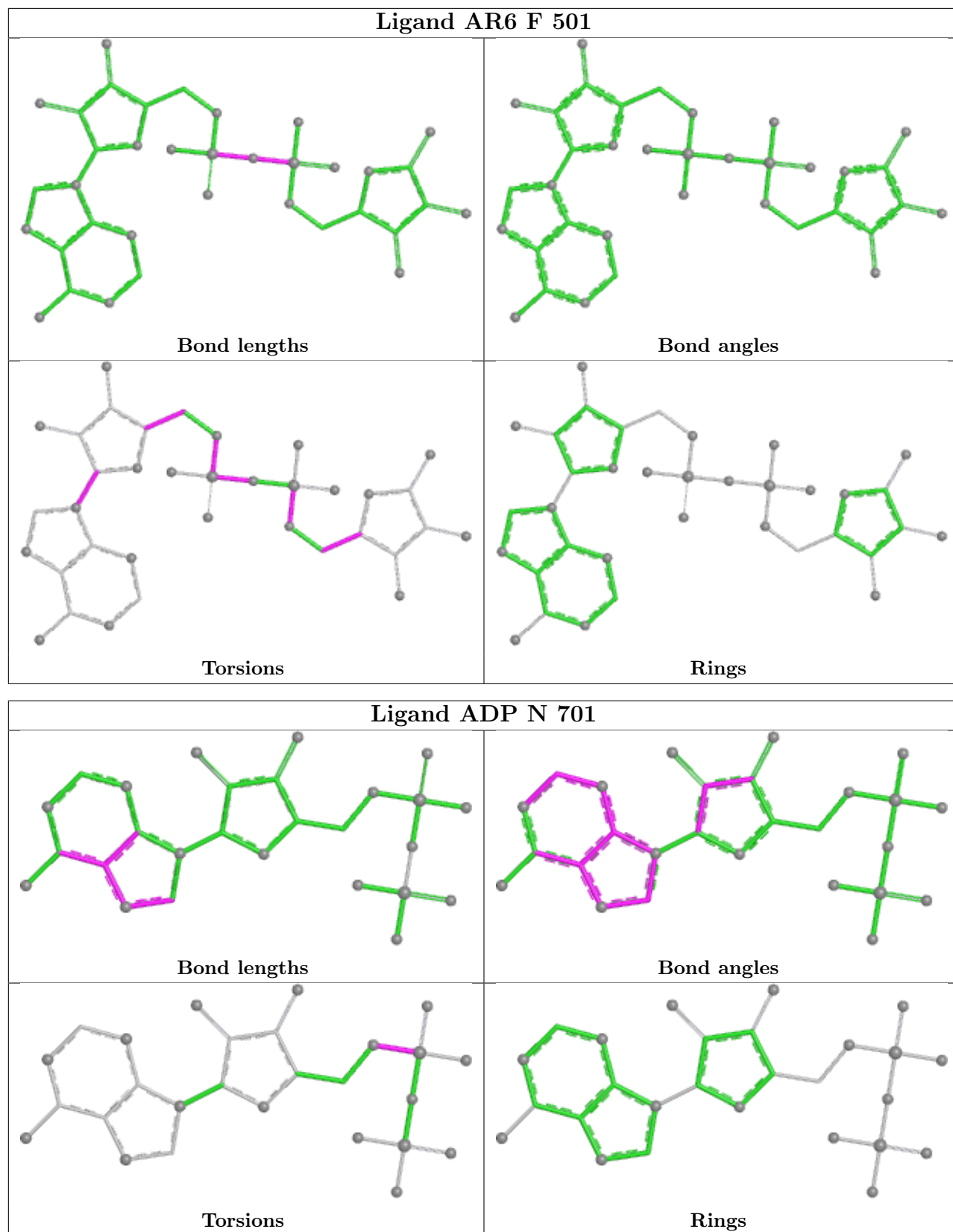
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

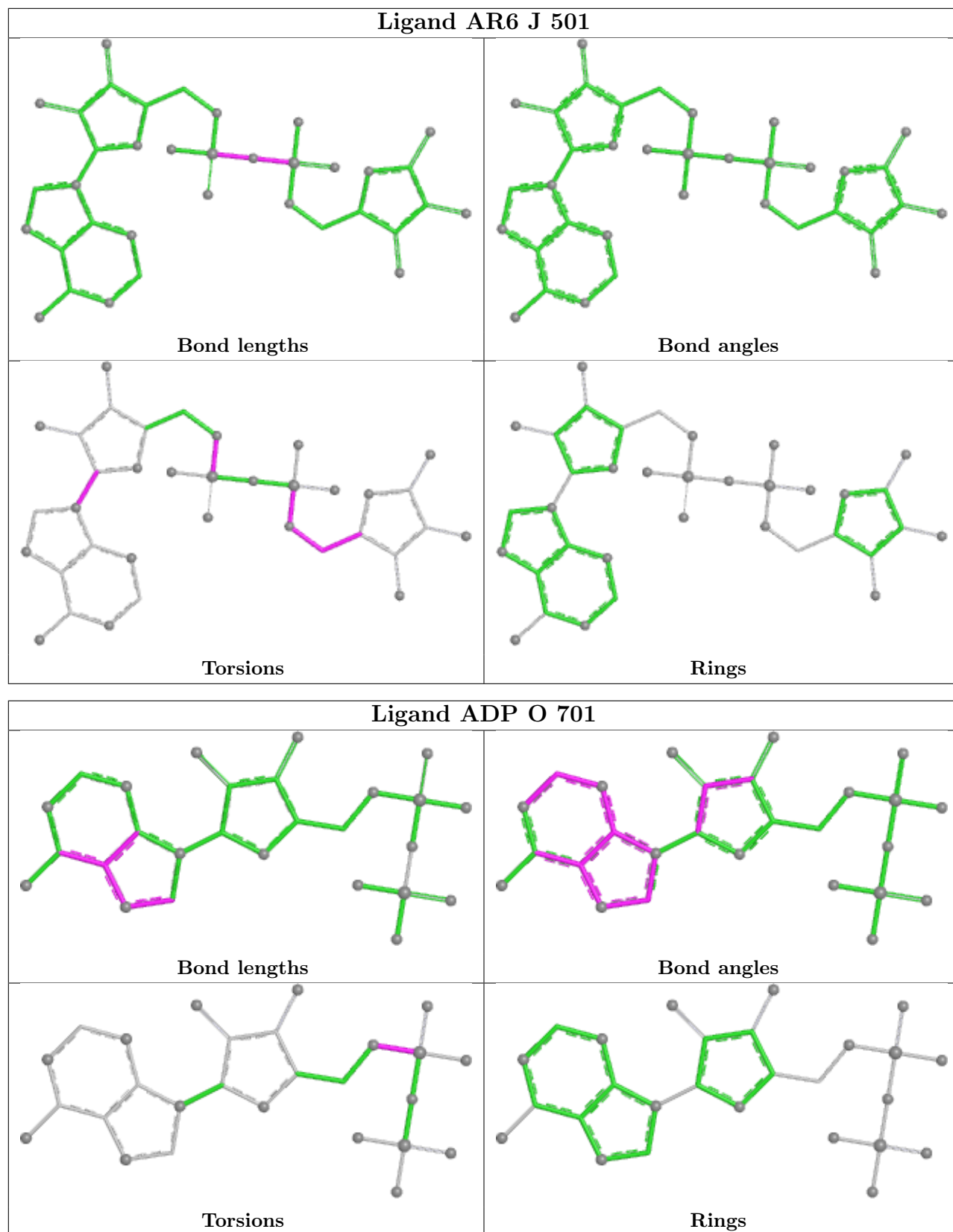


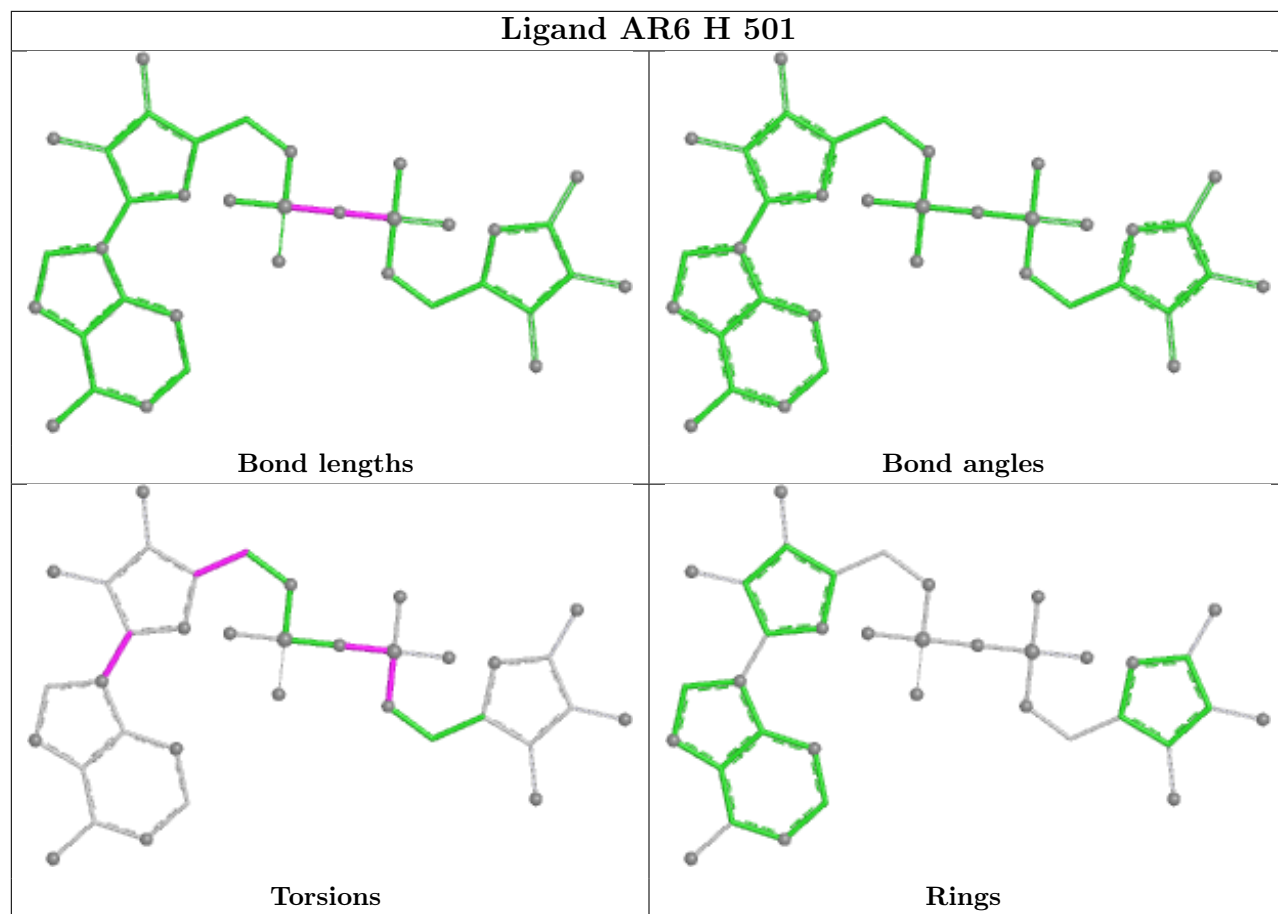


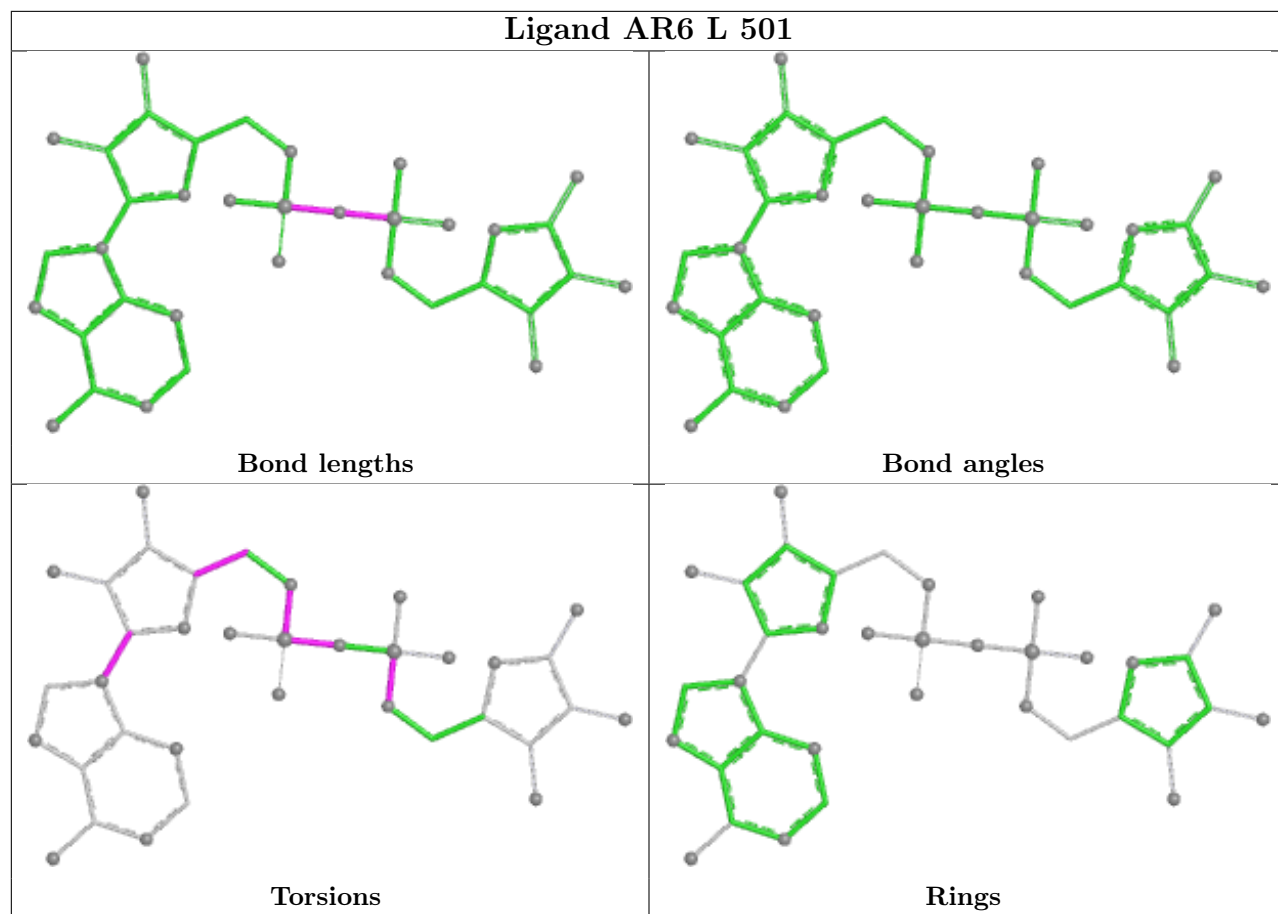


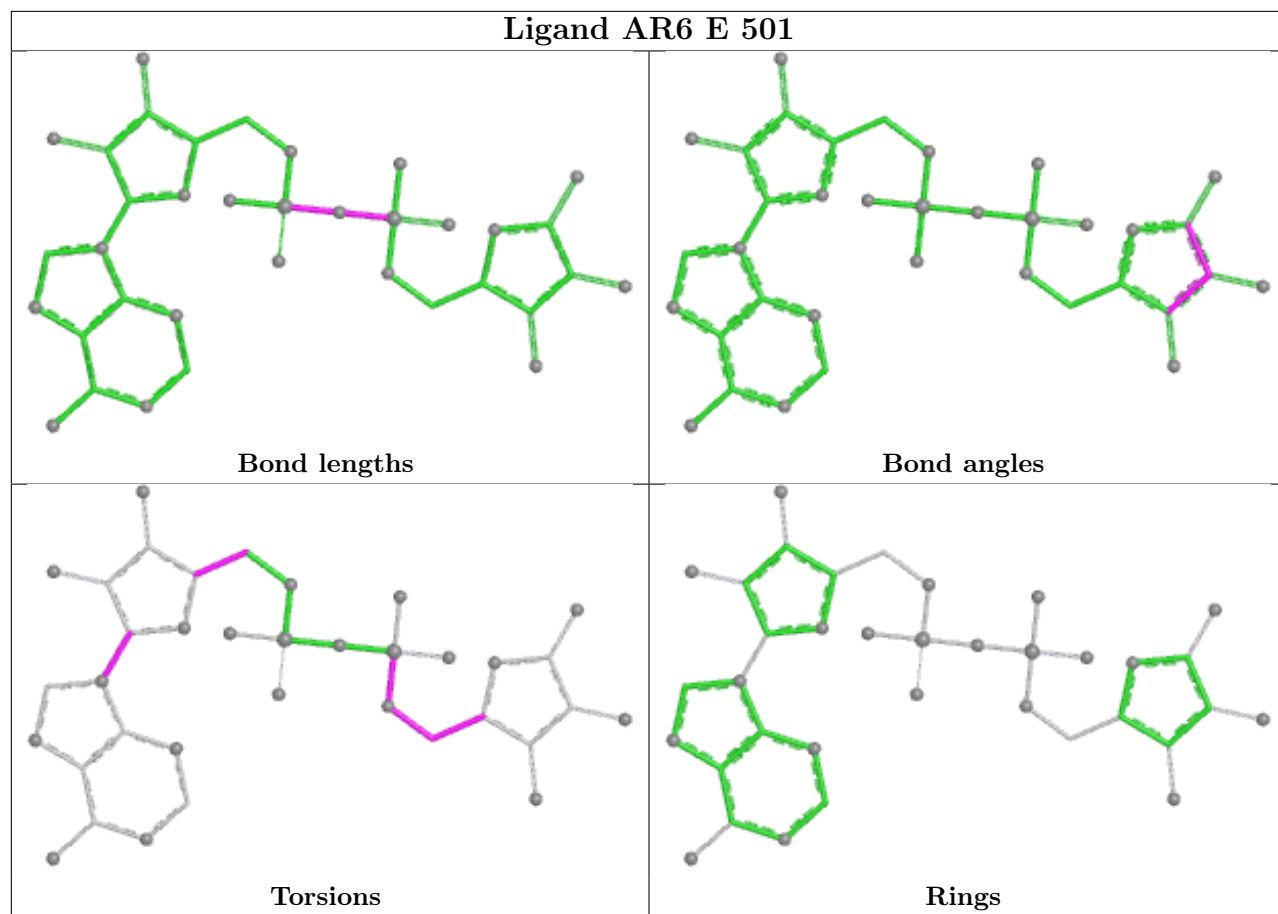


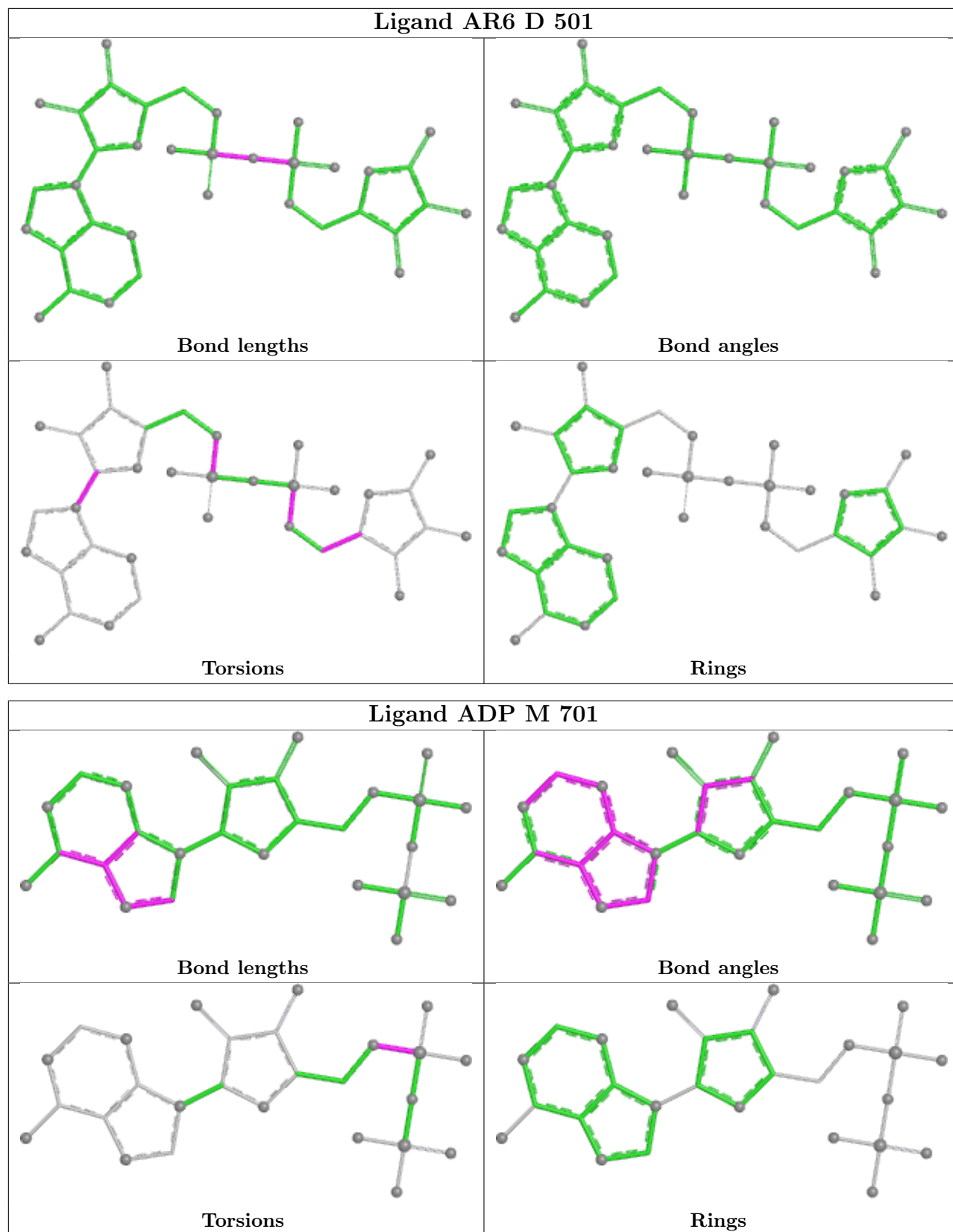


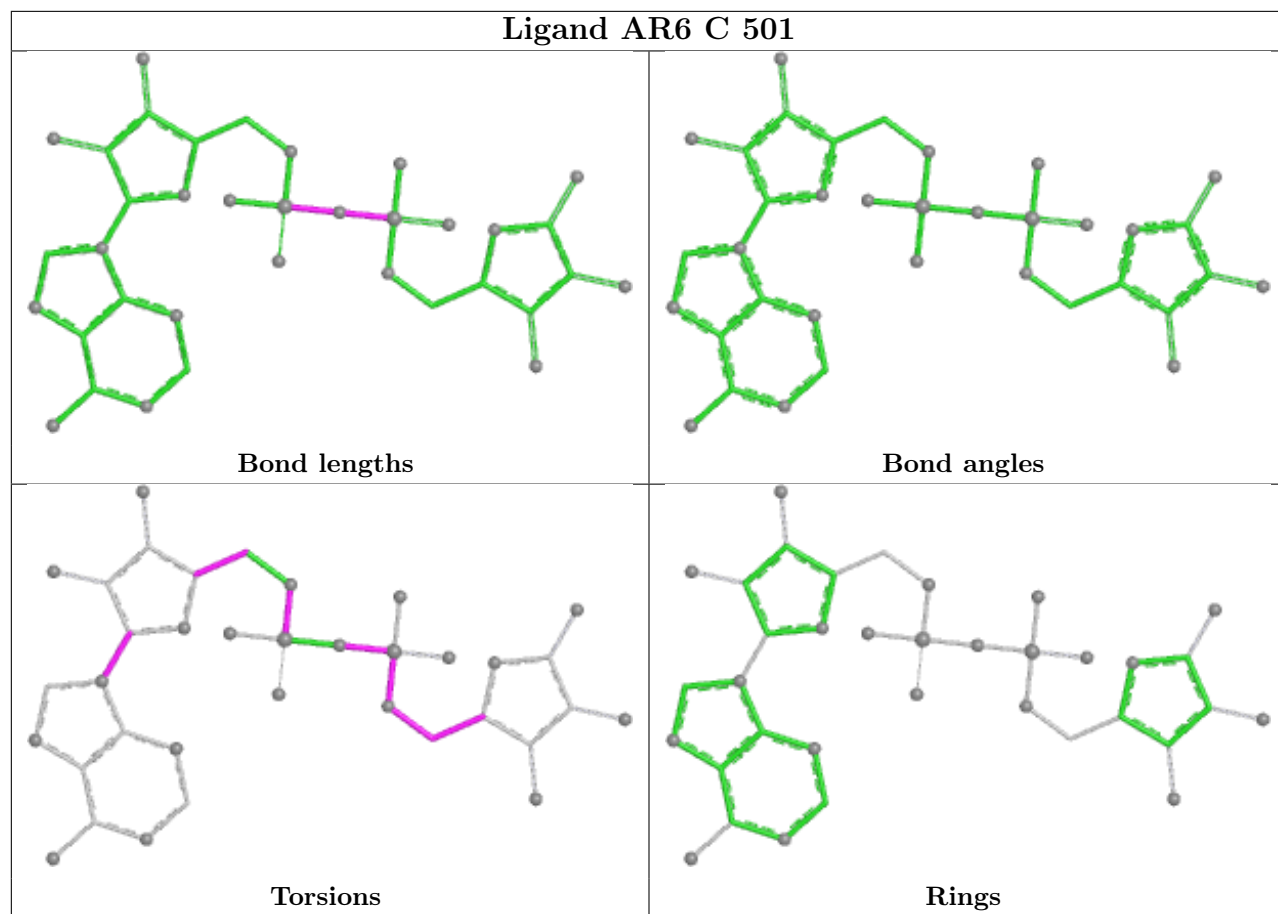


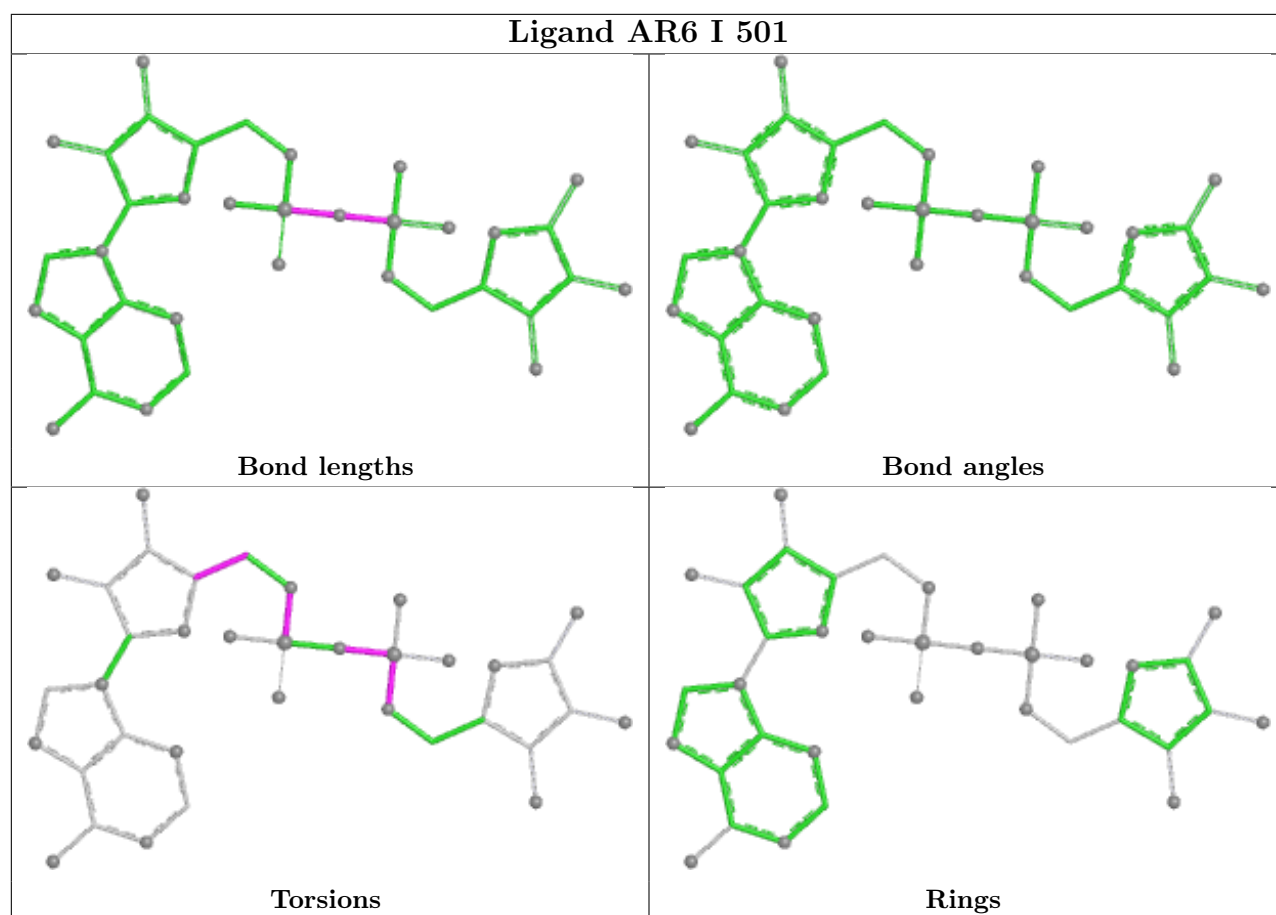












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

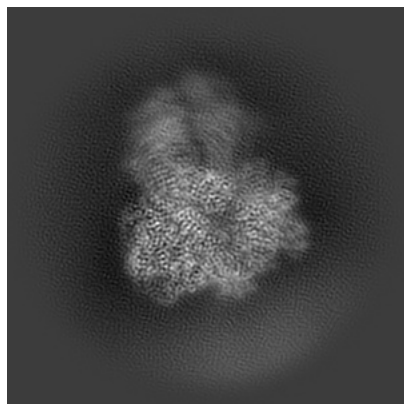
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40778. These allow visual inspection of the internal detail of the map and identification of artifacts.

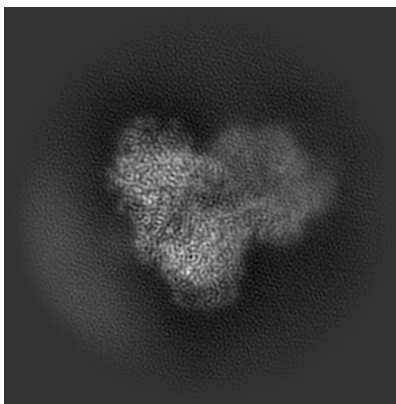
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

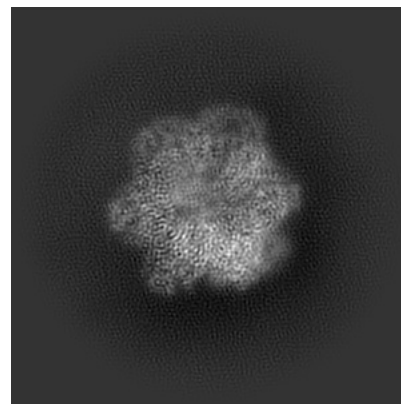
#### 6.1.1 Primary map



X

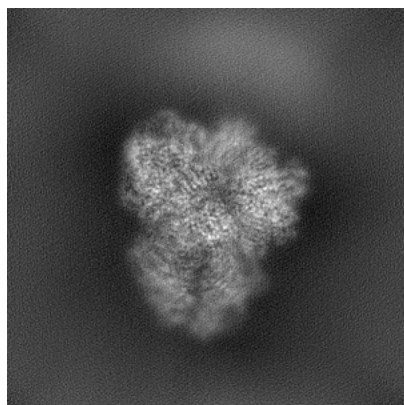


Y

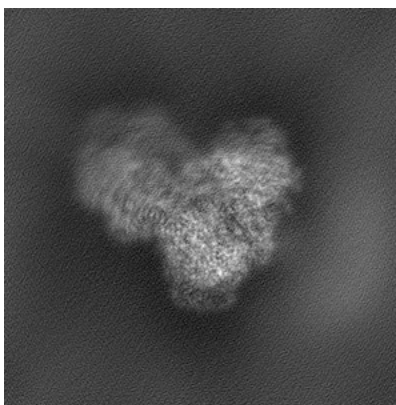


Z

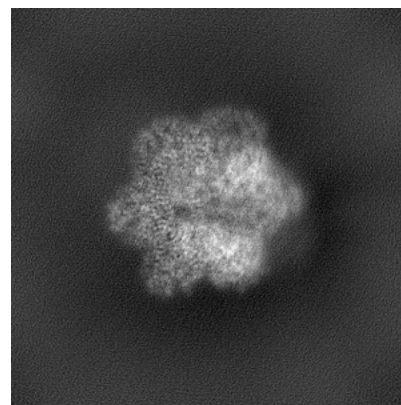
#### 6.1.2 Raw map



X



Y

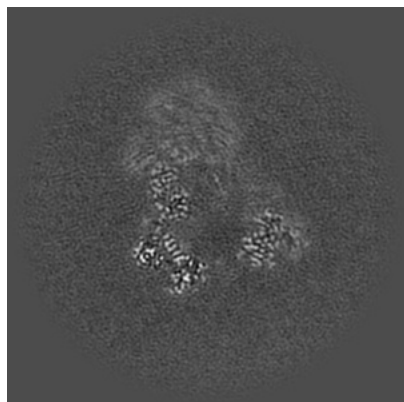


Z

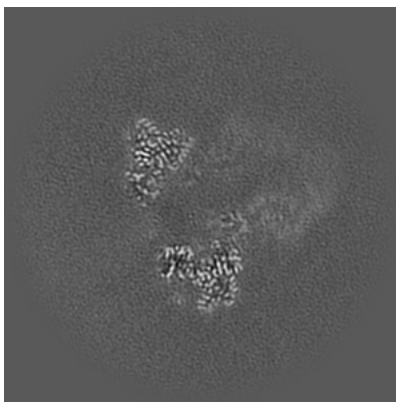
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

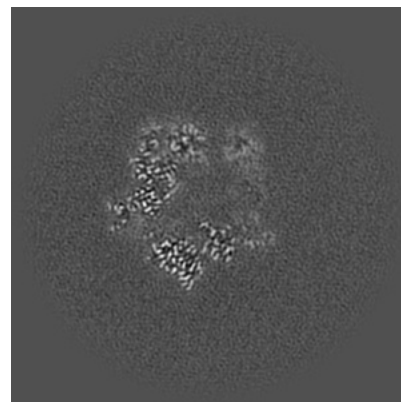
### 6.2.1 Primary map



X Index: 160

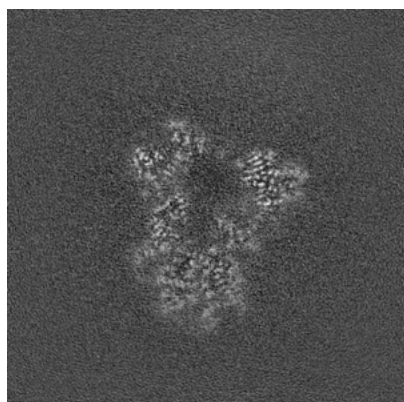


Y Index: 160

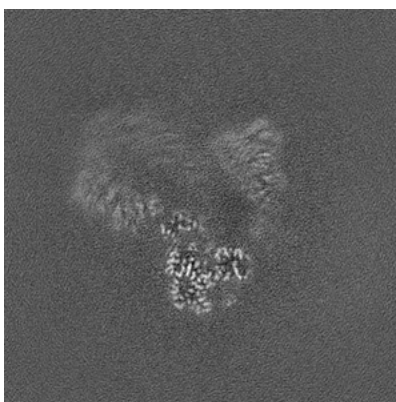


Z Index: 160

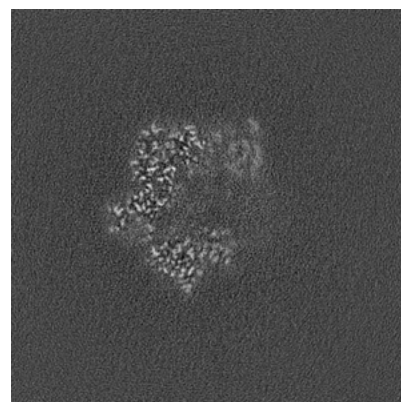
### 6.2.2 Raw map



X Index: 160



Y Index: 160

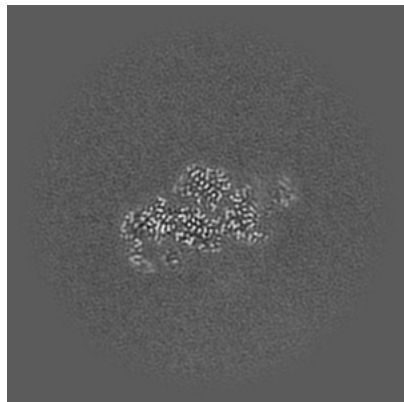


Z Index: 160

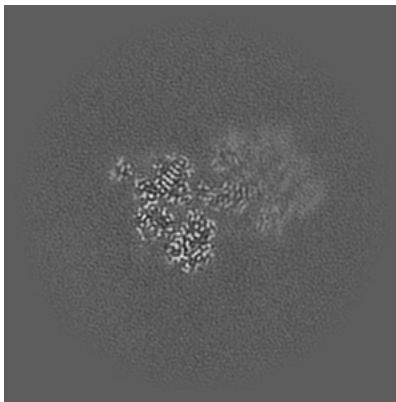
The images above show central slices of the map in three orthogonal directions.

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

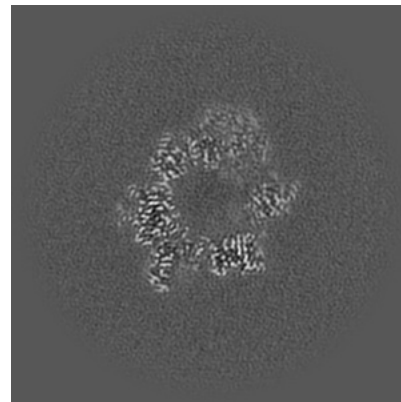
### 6.3.1 Primary map



X Index: 118

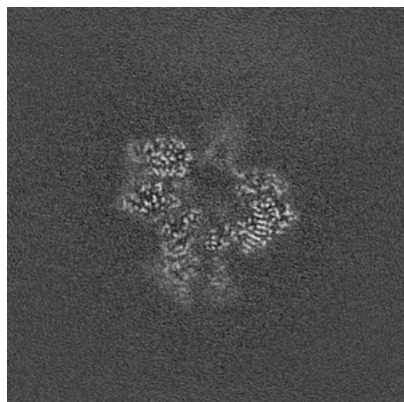


Y Index: 120

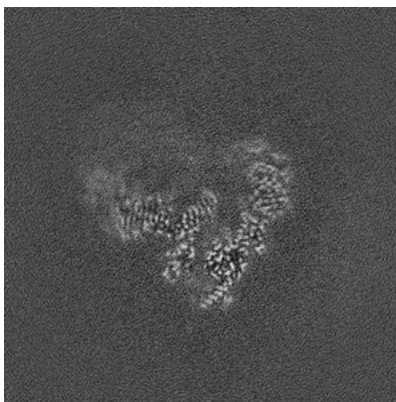


Z Index: 135

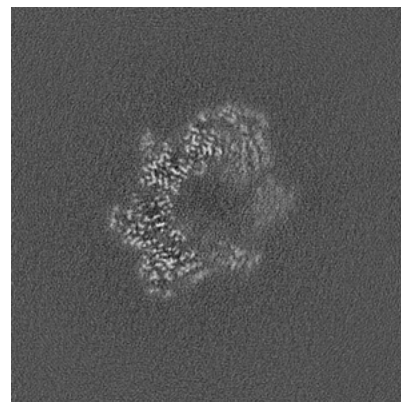
### 6.3.2 Raw map



X Index: 140



Y Index: 142

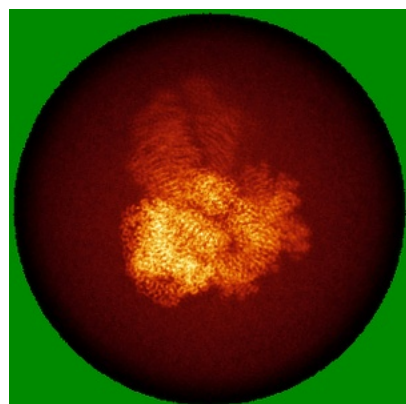


Z Index: 175

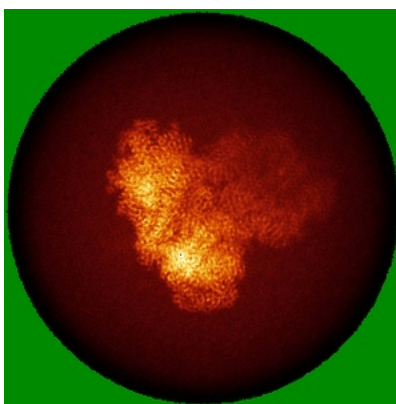
The images above show the largest variance slices of the map in three orthogonal directions.

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

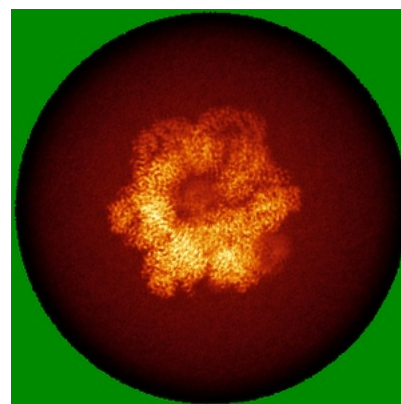
### 6.4.1 Primary map



X

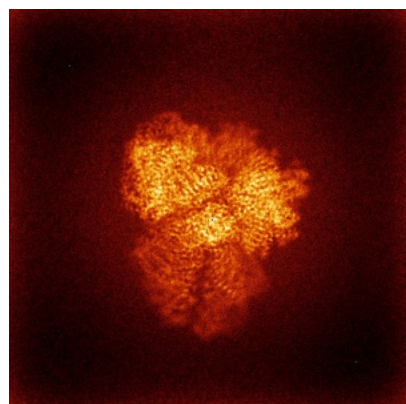


Y

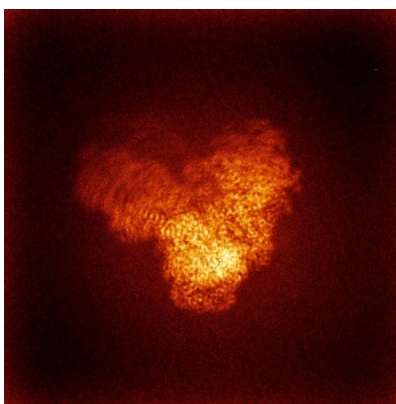


Z

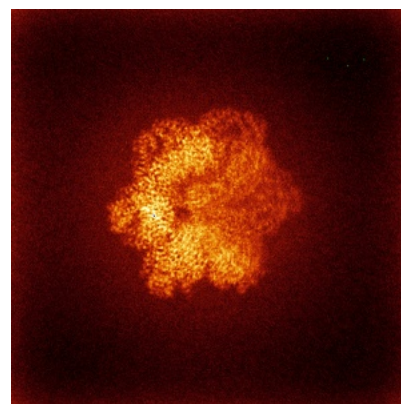
### 6.4.2 Raw map



X



Y

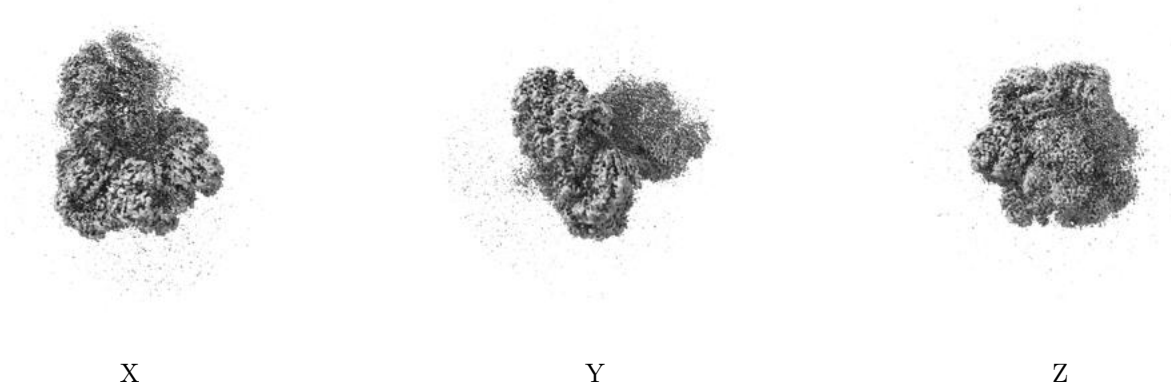


Z

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.

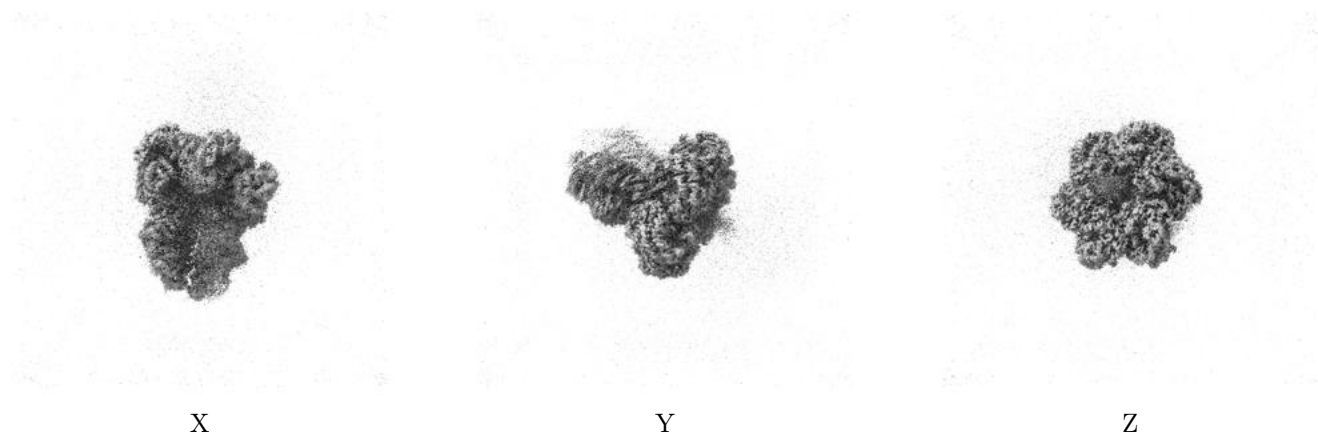
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.192. 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.

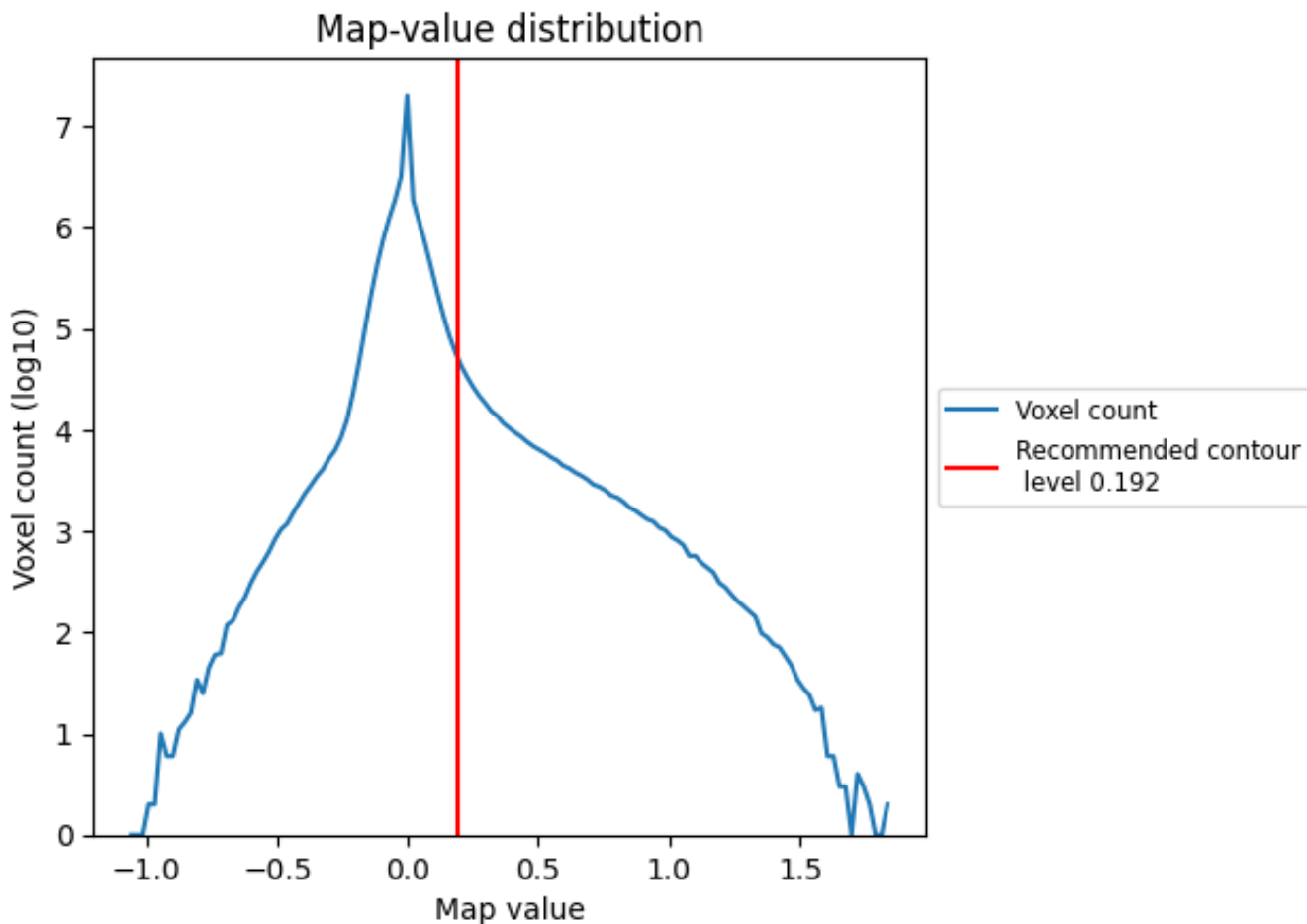
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

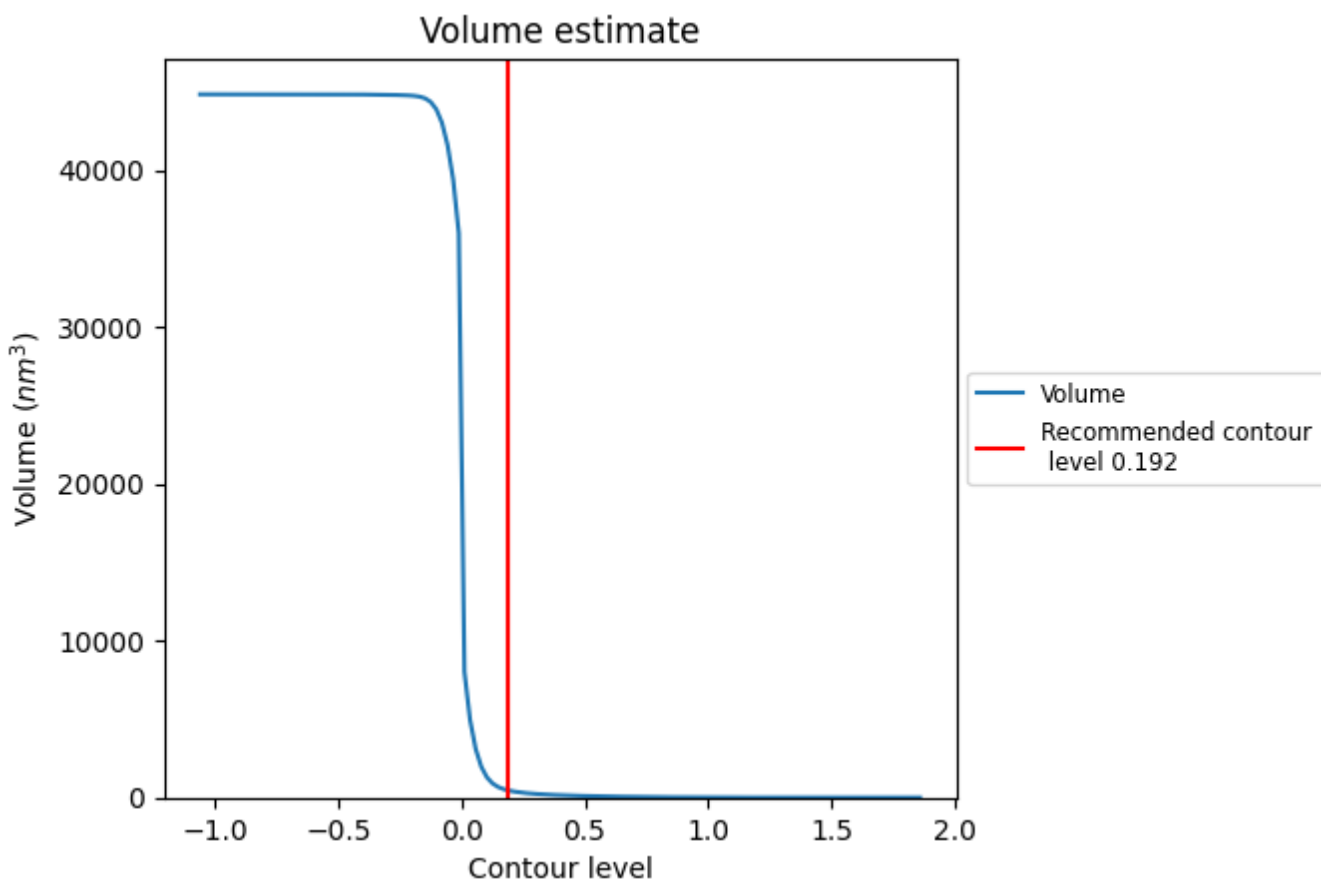
This section contains the results of statistical analysis of the map.

### 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.

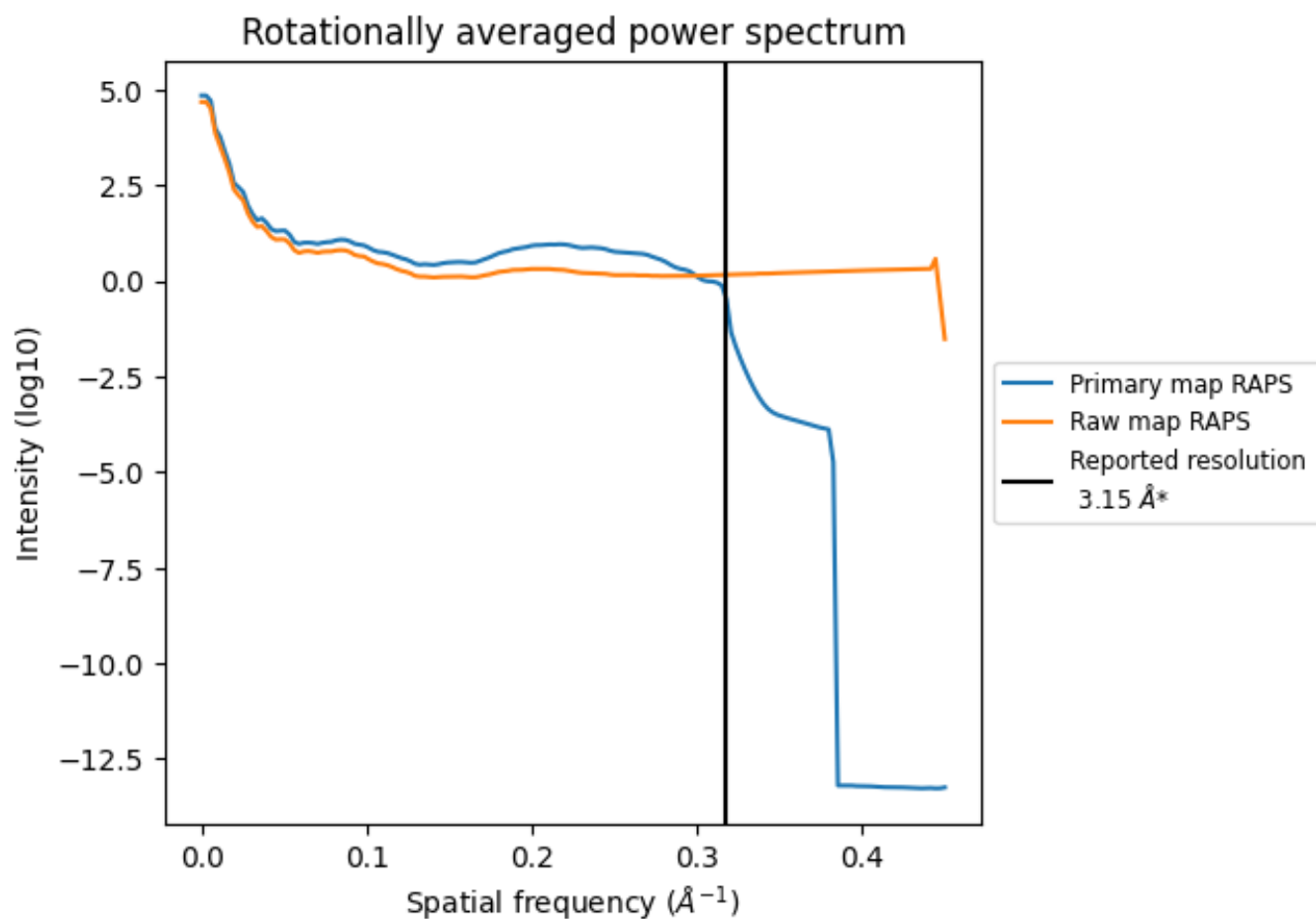
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 450 nm<sup>3</sup>; this corresponds to an approximate mass of 407 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](#)

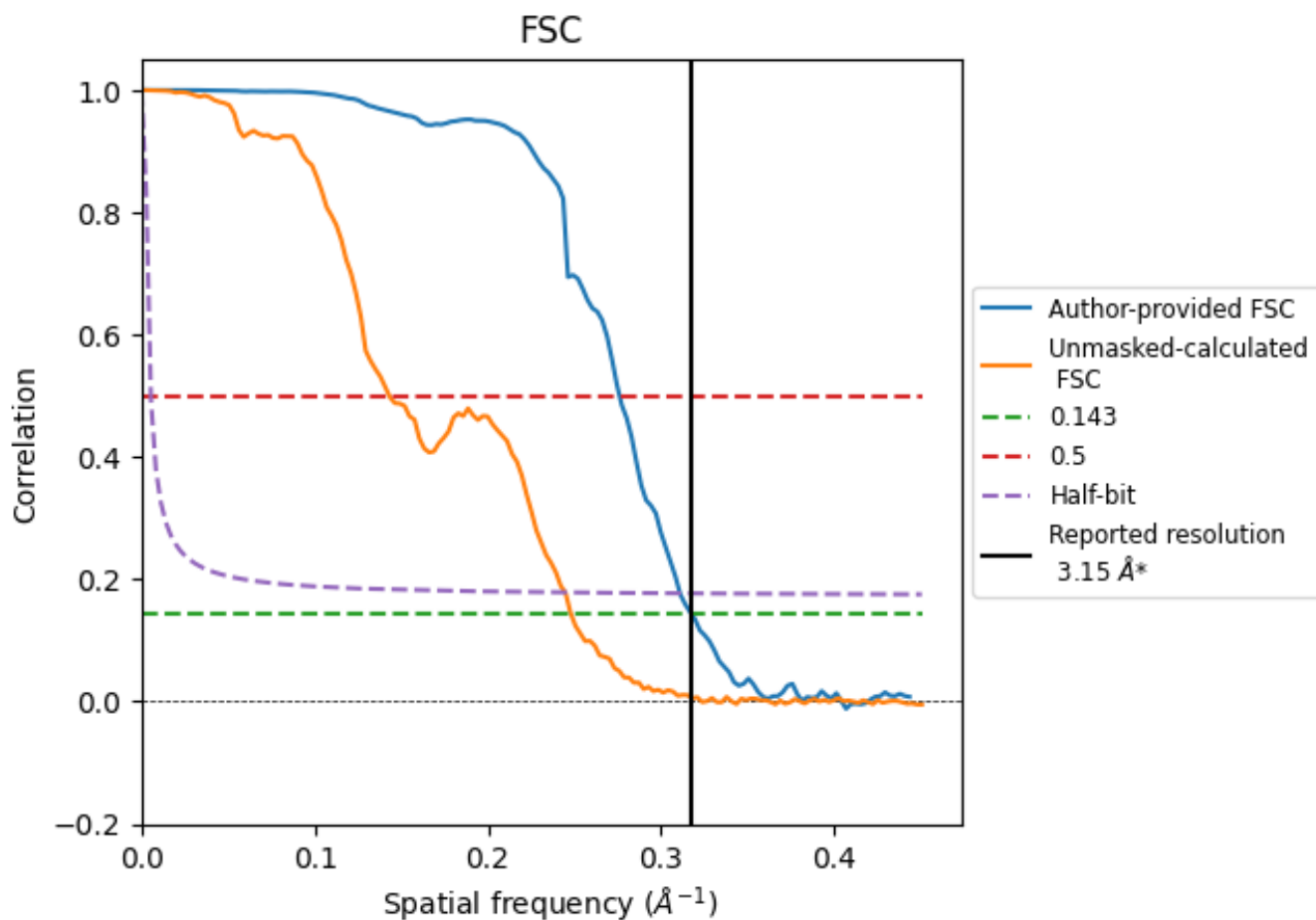


\*Reported resolution corresponds to spatial frequency of 0.317 Å<sup>-1</sup>

## 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 0.317 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

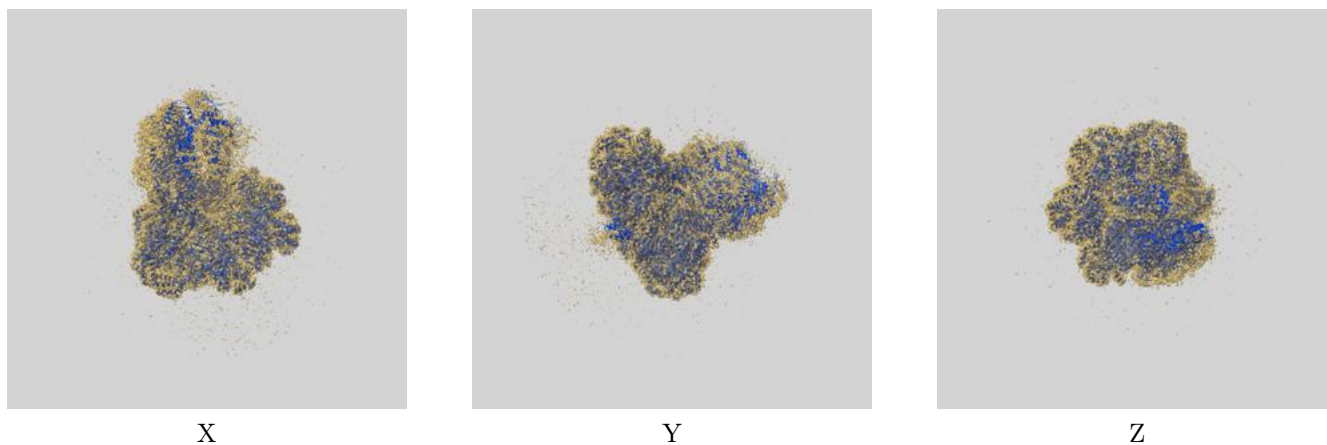
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.15	-	-
Author-provided FSC curve	3.15	3.62	3.22
Unmasked-calculated*	4.03	6.99	4.09

\*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 4.03 differs from the reported value 3.15 by more than 10 %

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

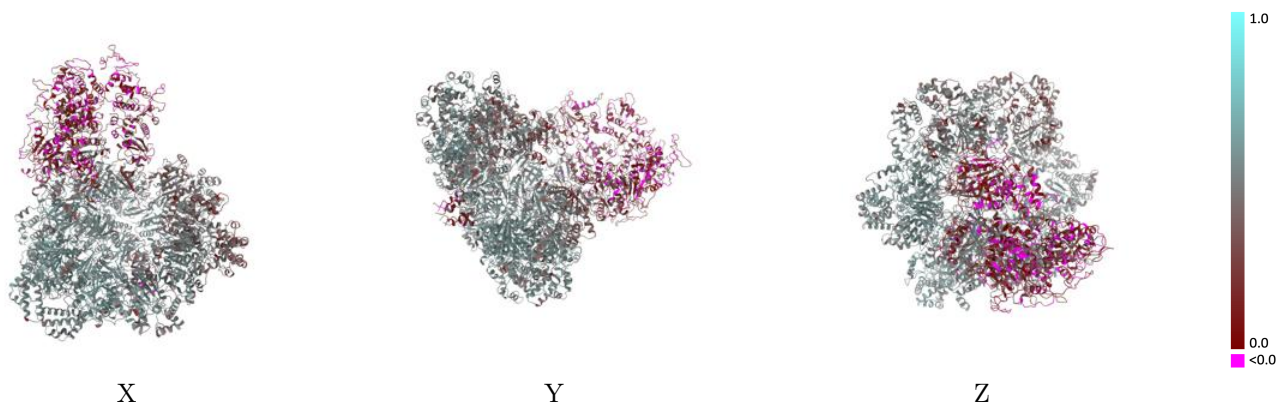
This section contains information regarding the fit between EMDB map EMD-40778 and PDB model 8SUW. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



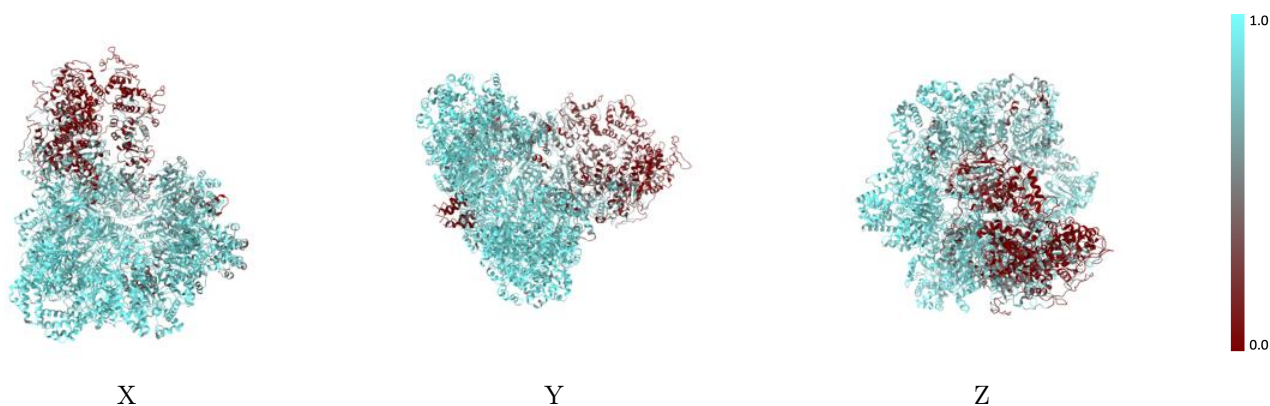
The images above show the 3D surface view of the map at the recommended contour level 0.192 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



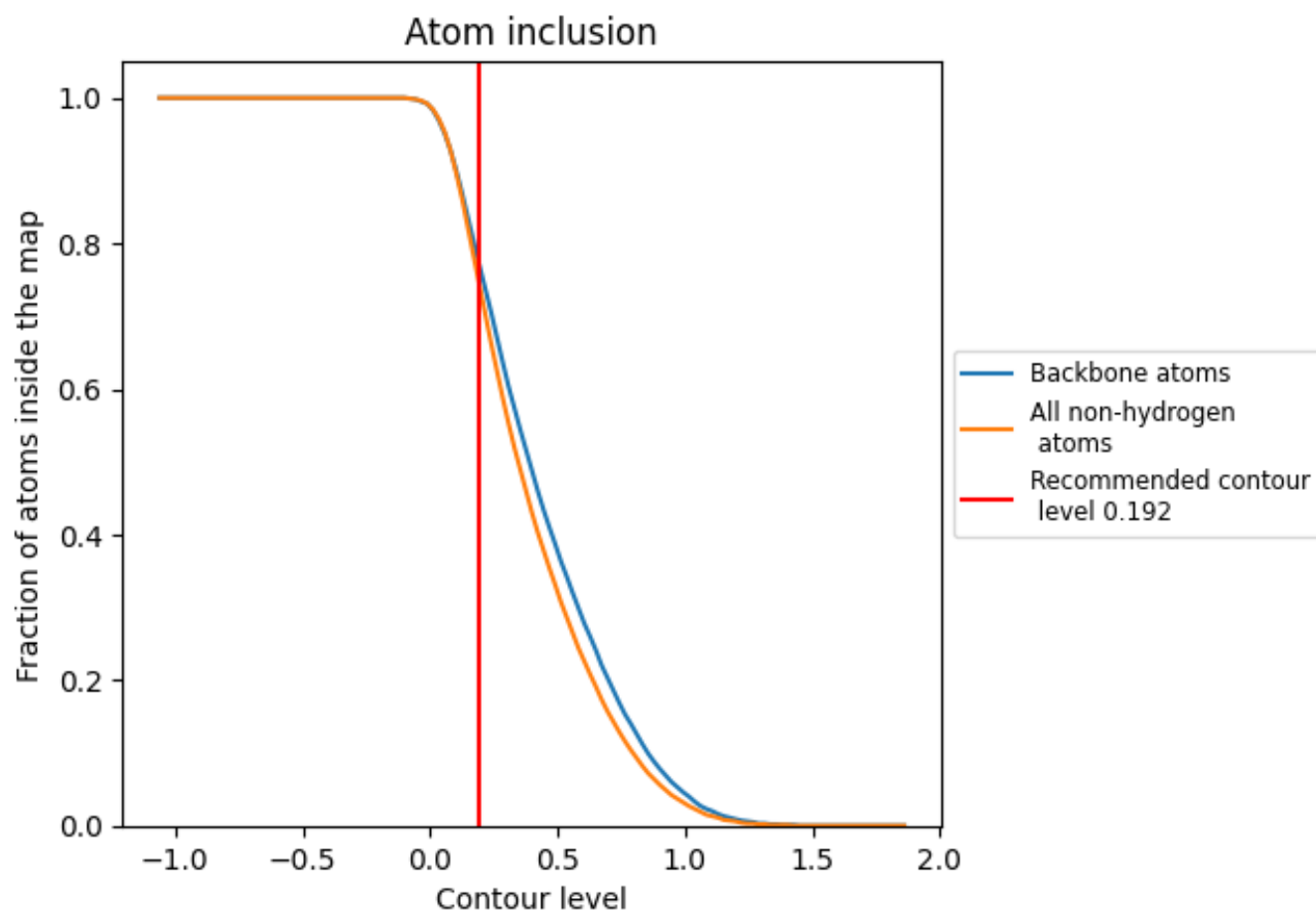
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.192).



































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 74% 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 (0.192) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7450	 0.4390
A	 0.9410	 0.5640
B	 0.9140	 0.5500
C	 0.9390	 0.5580
D	 0.8950	 0.5360
E	 0.9040	 0.5230
F	 0.8590	 0.5080
G	 0.7470	 0.4060
H	 0.8350	 0.4860
I	 0.8080	 0.4500
J	 0.9010	 0.5230
K	 0.9170	 0.5440
L	 0.9150	 0.5500
M	 0.4600	 0.2910
N	 0.5100	 0.2950
O	 0.5110	 0.2940
P	 0.3050	 0.2020

