



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 05:05 PM UTC

PDB ID : 8SU9 / pdb_00008su9
EMDB ID : EMD-40762
Title : E. coli SIR2-HerA complex (hexamer HerA bound with dodecamer Sir2)
Authors : Shen, Z.F.; Lin, Q.P.; Fu, T.M.
Deposited on : 2023-05-11
Resolution : 2.83 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

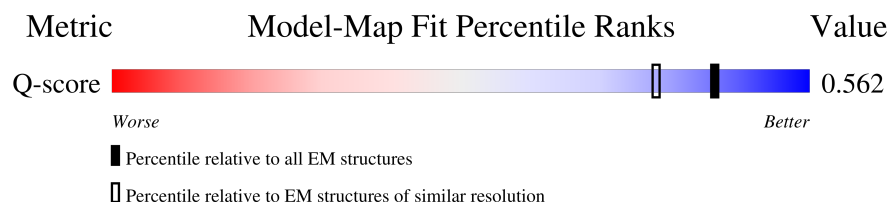
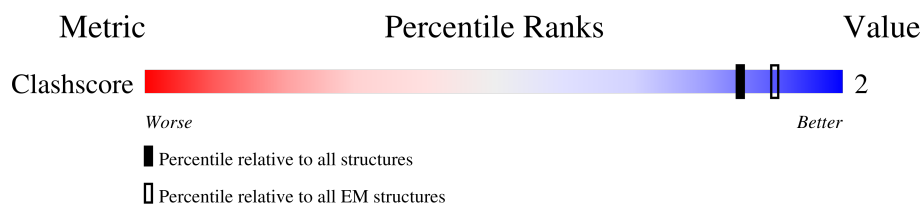
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

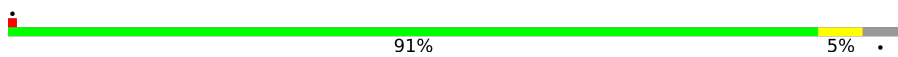
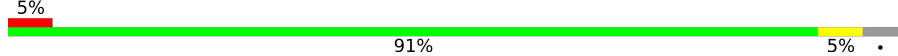
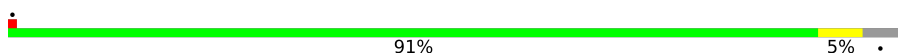
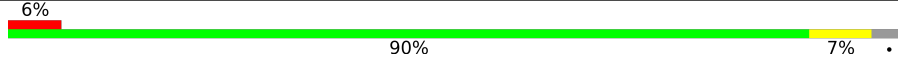
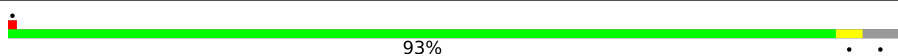
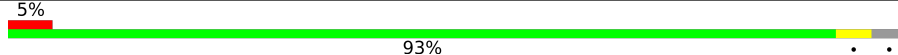
The reported resolution of this entry is 2.83 Å.

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.



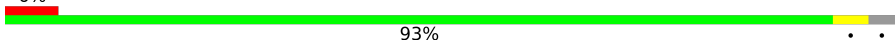
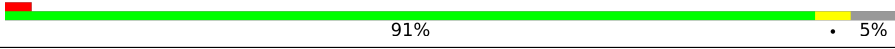
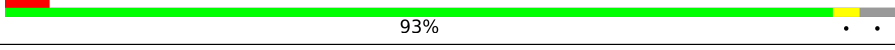
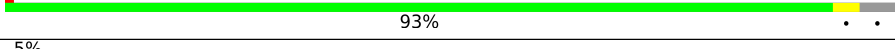
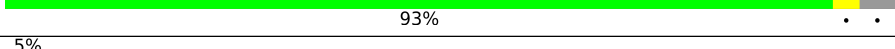
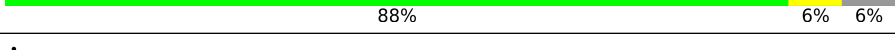
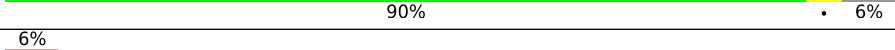
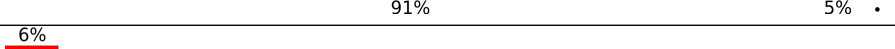
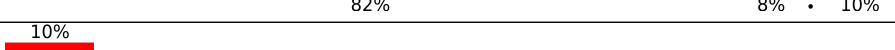
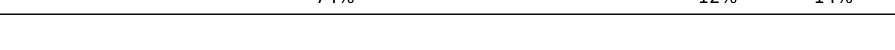
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Q-score	-	25397	11847 (2.33 - 3.33)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	415	 91% 5% .
1	B	415	 91% 5% .
1	C	415	 91% 5% .
1	D	415	 90% 7% .
1	E	415	 93% . .
1	F	415	 93% . .

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Mol	Chain	Length	Quality of chain
1	G	415	
1	H	415	
1	I	415	
1	J	415	
1	K	415	
1	L	415	
2	M	610	
2	N	610	
2	O	610	
2	P	610	
2	Q	610	
2	R	610	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 65385 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
1	A	398	Total	C	N	O	S	0	0
			3185	2048	532	599	6		
1	B	398	Total	C	N	O	S	0	0
			3186	2050	532	598	6		
1	C	398	Total	C	N	O	S	0	0
			3185	2048	532	599	6		
1	D	400	Total	C	N	O	S	0	0
			3192	2053	532	601	6		
1	E	400	Total	C	N	O	S	0	0
			3194	2053	534	601	6		
1	F	400	Total	C	N	O	S	0	0
			3198	2056	535	601	6		
1	G	390	Total	C	N	O	S	0	0
			3119	2006	520	587	6		
1	H	401	Total	C	N	O	S	0	0
			3203	2059	536	602	6		
1	I	394	Total	C	N	O	S	0	0
			3145	2021	525	593	6		
1	J	400	Total	C	N	O	S	0	0
			3199	2057	535	601	6		
1	K	398	Total	C	N	O	S	0	0
			3182	2047	532	597	6		
1	L	400	Total	C	N	O	S	0	0
			3199	2057	535	601	6		

- Molecule 2 is a protein called Nucleoside triphosphate hydrolase.

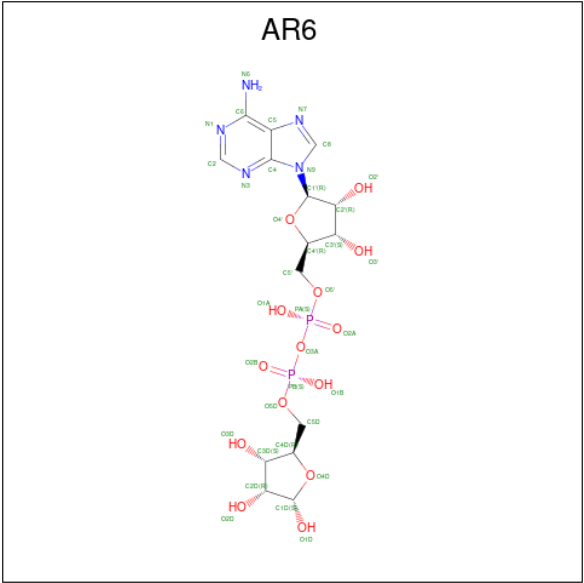
Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	573	Total	C	N	O	S	0	0
			4536	2887	798	838	13		
2	N	574	Total	C	N	O	S	0	0
			4548	2898	799	839	12		
2	O	585	Total	C	N	O	S	0	0
			4637	2951	812	862	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
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		
2	R	524	Total	C	N	O	S	0	0
			4170	2660	728	771	11		

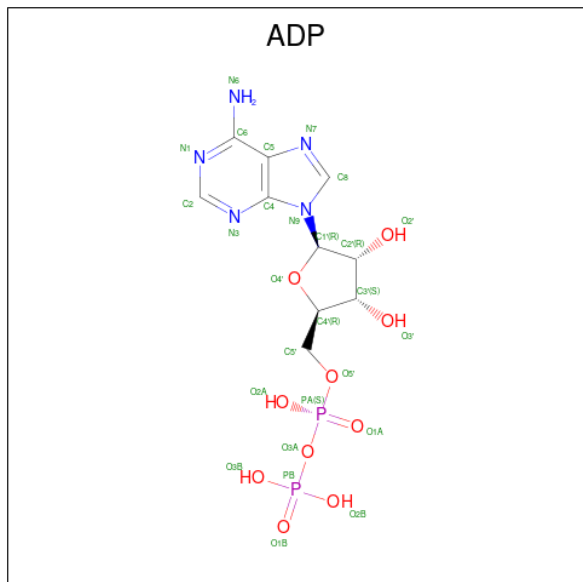
- Molecule 3 is [(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHYL [HYDROXY-[(2R,3S,4R,5S)-3,4,5-TRIHIDROXYOXOLAN-2-YL]METHOXY]PHOSPHORYL] HYDROGEN PHOSPHATE (CCD ID: AR6) (formula: C₁₅H₂₃N₅O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					AltConf
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	
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: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

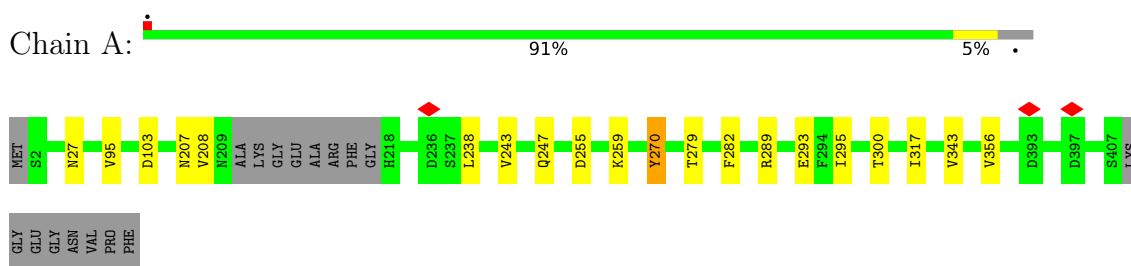
Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
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

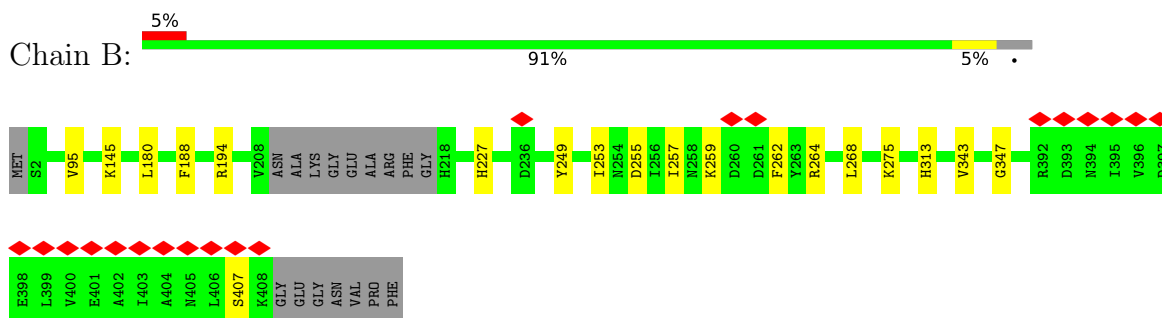
3 Residue-property plots

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.

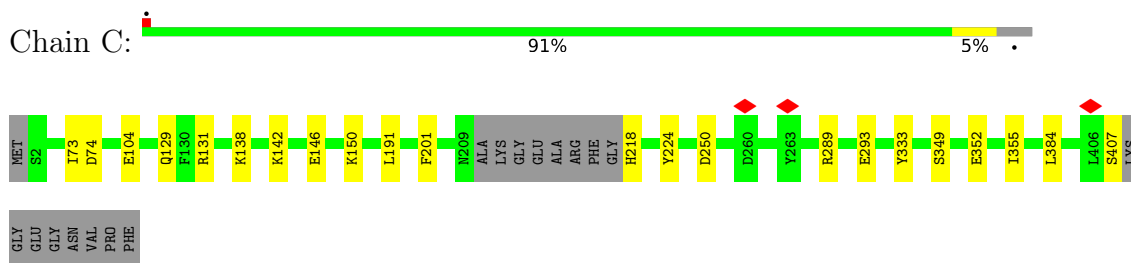
- Molecule 1: SIR2-like domain-containing protein



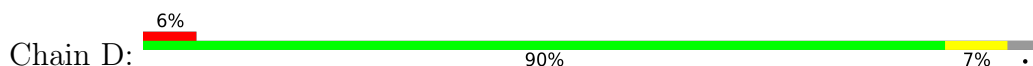
- Molecule 1: SIR2-like domain-containing protein

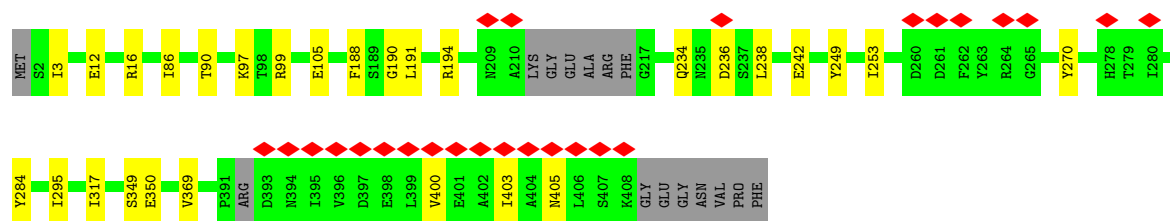


- Molecule 1: SIR2-like domain-containing protein



- Molecule 1: SIR2-like domain-containing protein





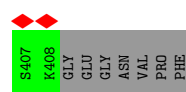
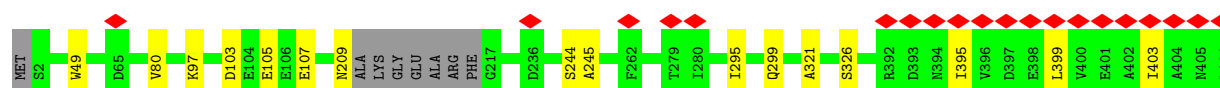
- Molecule 1: SIR2-like domain-containing protein

Chain E: 93%



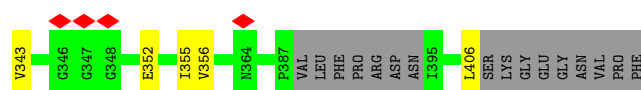
- Molecule 1: SIR2-like domain-containing protein

Chain F: 5% 93%



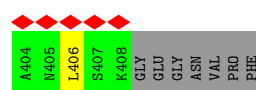
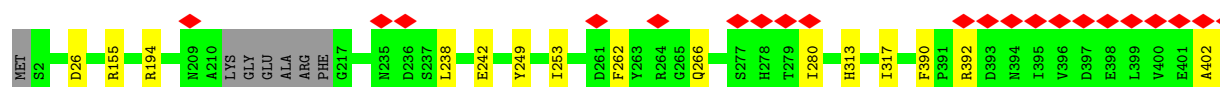
- Molecule 1: SIR2-like domain-containing protein

Chain G: 87% 7% 6%

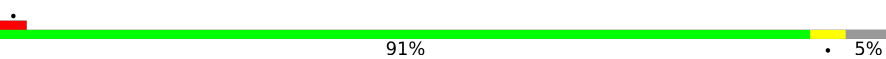


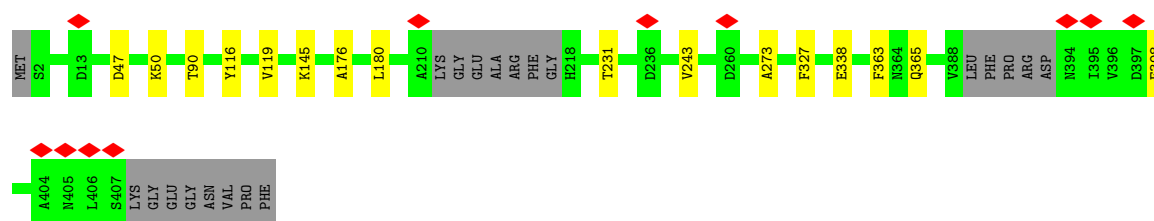
- Molecule 1: SIR2-like domain-containing protein

Chain H: 6% 93%

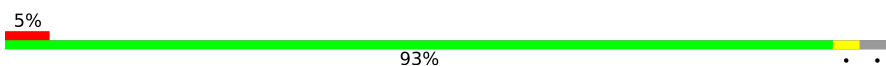


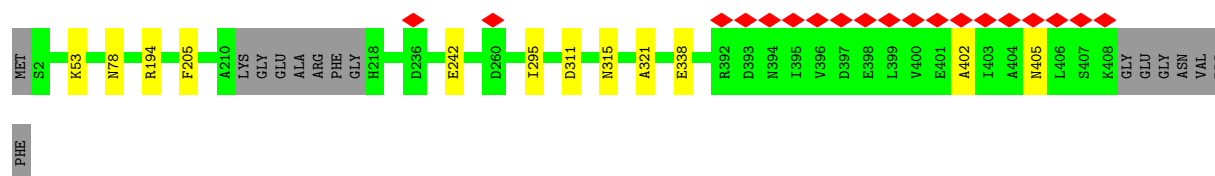
- Molecule 1: SIR2-like domain-containing protein

Chain I:  91% 5%

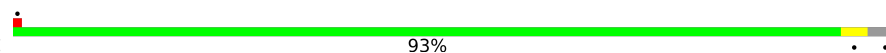


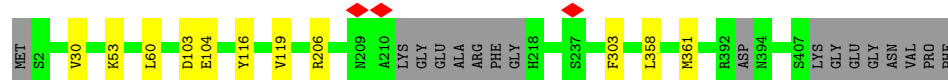
- Molecule 1: SIR2-like domain-containing protein

Chain J:  93% 5%

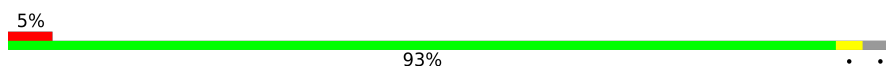


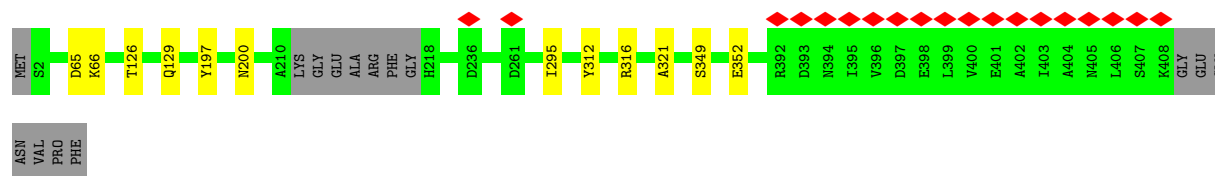
- Molecule 1: SIR2-like domain-containing protein

Chain K:  93% 5%

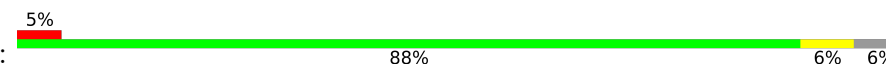


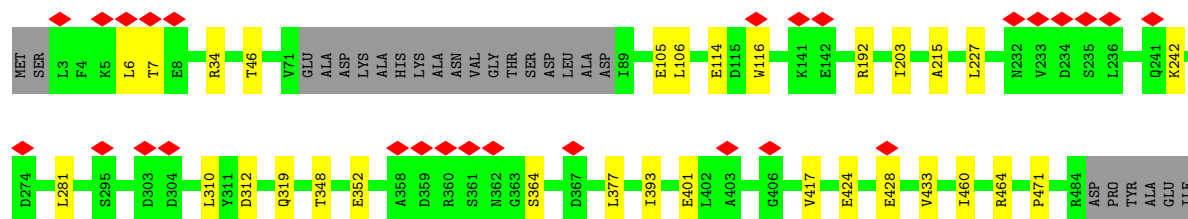
- Molecule 1: SIR2-like domain-containing protein

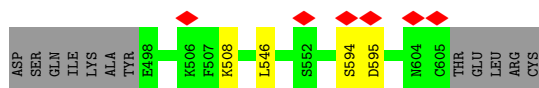
Chain L:  93% 5%



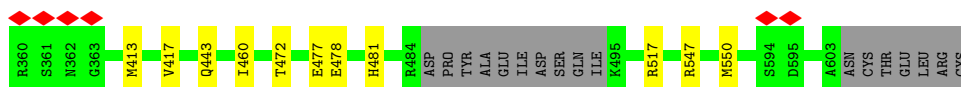
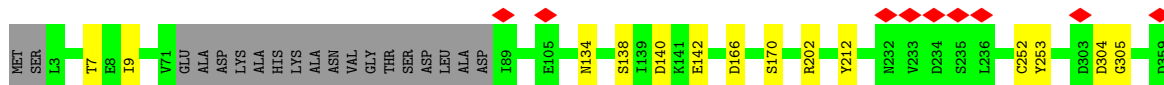
- Molecule 2: Nucleoside triphosphate hydrolase

Chain M:  88% 6% 6%

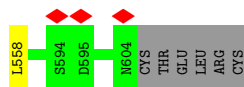
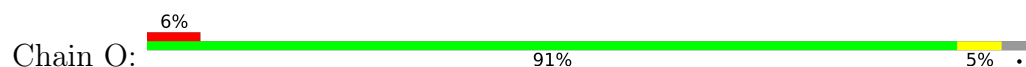




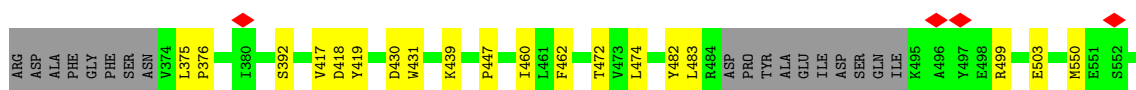
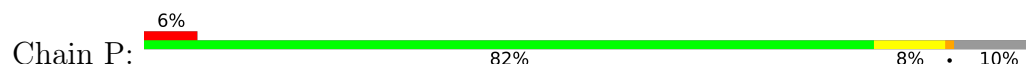
• Molecule 2: Nucleoside triphosphate hydrolase



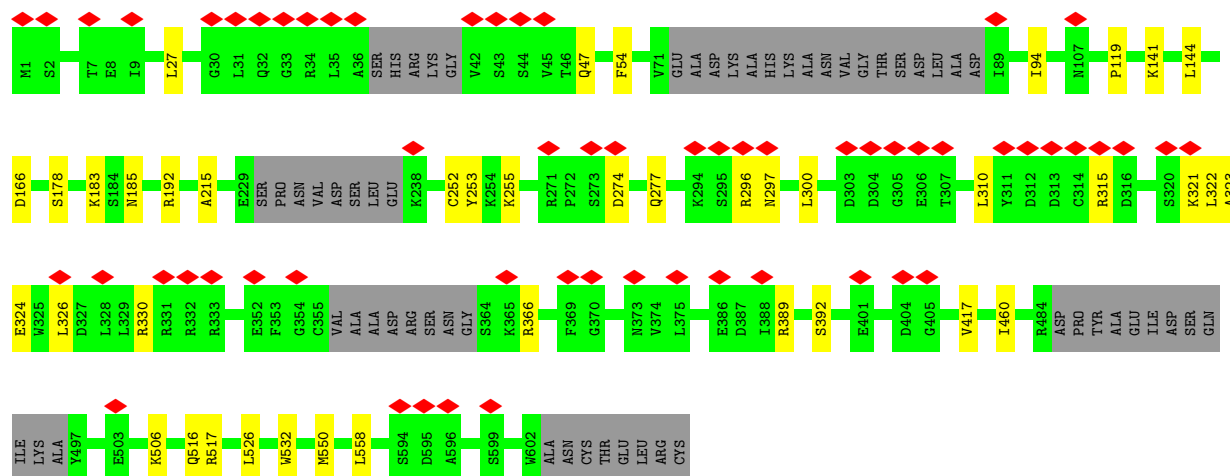
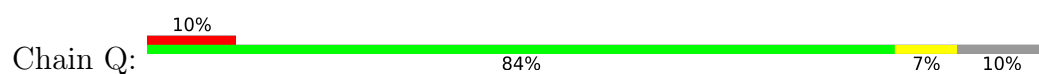
• Molecule 2: Nucleoside triphosphate hydrolase



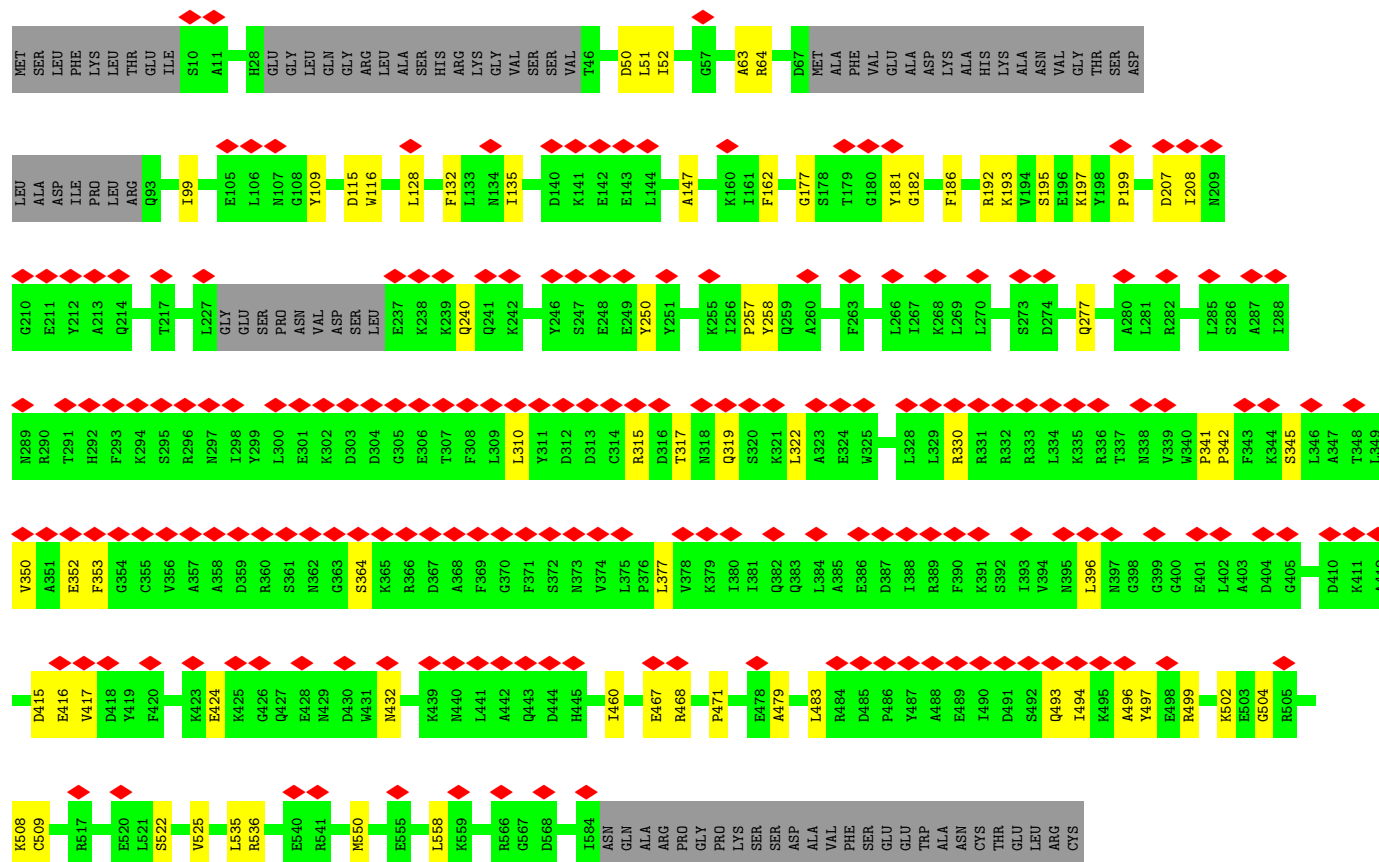
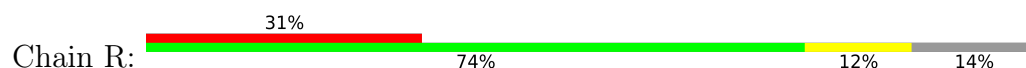
• Molecule 2: Nucleoside triphosphate hydrolase



• Molecule 2: Nucleoside triphosphate hydrolase



• Molecule 2: Nucleoside triphosphate hydrolase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	215970	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	2.913	Depositor
Minimum map value	-1.969	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.099	Depositor
Recommended contour level	0.286	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AR6, 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	0.19	0/3259	0.38	2/4406 (0.0%)
1	B	0.12	0/3260	0.32	0/4406
1	C	0.12	0/3259	0.29	0/4406
1	D	0.13	0/3265	0.32	0/4412
1	E	0.13	0/3268	0.29	0/4418
1	F	0.12	0/3272	0.30	0/4422
1	G	0.12	0/3190	0.27	0/4310
1	H	0.12	0/3277	0.32	0/4429
1	I	0.12	0/3216	0.29	0/4346
1	J	0.12	0/3273	0.30	0/4424
1	K	0.13	0/3255	0.29	0/4399
1	L	0.12	0/3273	0.29	0/4424
2	M	0.12	0/4624	0.30	0/6243
2	N	0.13	0/4637	0.32	0/6260
2	O	0.13	0/4729	0.32	0/6388
2	P	0.18	0/4431	0.44	4/5985 (0.1%)
2	Q	0.12	0/4473	0.30	0/6033
2	R	0.11	0/4250	0.30	0/5737
All	All	0.13	0/66211	0.32	6/89448 (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	A	0	1
2	P	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	320	SER	N-CA-C	-8.79	101.54	112.88
2	P	323	ALA	N-CA-C	-8.38	99.72	110.53
2	P	322	LEU	N-CA-C	-7.53	104.23	113.41
1	A	270	TYR	N-CA-C	-6.52	102.27	108.07
1	A	270	TYR	CA-C-O	-6.49	114.66	120.56
2	P	324	GLU	N-CA-C	-6.41	105.88	113.38

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	270	TYR	Peptide
2	P	290	ARG	Sidechain

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	11	0
1	B	3186	0	3116	14	0
1	C	3185	0	3109	14	0
1	D	3192	0	3116	17	0
1	E	3194	0	3117	9	0
1	F	3198	0	3125	9	0
1	G	3119	0	3044	15	0
1	H	3203	0	3130	13	0
1	I	3145	0	3069	10	0
1	J	3199	0	3127	9	0
1	K	3182	0	3109	6	0
1	L	3199	0	3127	6	0
2	M	4536	0	4576	22	0
2	N	4548	0	4591	14	0
2	O	4637	0	4664	20	0
2	P	4346	0	4381	47	0
2	Q	4389	0	4439	25	0
2	R	4170	0	4203	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	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	1	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	65385	0	64464	283	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 2.

All (283) 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:P:290:ARG:NH1	2:P:336:ARG:HD2	1.61	1.14
2:P:322:LEU:HD22	2:P:325:TRP:HZ3	1.15	1.11
2:P:290:ARG:NH1	2:P:336:ARG:CD	2.19	1.06
2:P:322:LEU:HD22	2:P:325:TRP:CZ3	1.90	1.05
2:P:322:LEU:CD2	2:P:325:TRP:CZ3	2.42	1.01
2:P:322:LEU:CD2	2:P:325:TRP:HZ3	1.75	0.99
2:P:290:ARG:HH11	2:P:336:ARG:CD	1.82	0.92
2:P:290:ARG:HH11	2:P:336:ARG:CG	1.86	0.89
2:P:290:ARG:HG2	2:P:336:ARG:HG2	1.60	0.83
2:P:322:LEU:HD23	2:P:325:TRP:CE3	2.18	0.78
2:P:322:LEU:HA	2:P:325:TRP:HE3	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:443:GLN:HG2	2:O:502:LYS:HD2	1.68	0.75
2:R:417:VAL:HG11	2:R:460:ILE:HG13	1.69	0.74
2:P:322:LEU:CD2	2:P:325:TRP:CE3	2.71	0.73
2:Q:296:ARG:O	2:Q:297:ASN:OD1	2.09	0.71
1:D:188:PHE:HB3	1:D:194:ARG:HD2	1.72	0.71
2:P:290:ARG:CZ	2:P:336:ARG:HD2	2.19	0.70
2:P:322:LEU:HD23	2:P:325:TRP:CZ3	2.26	0.70
2:P:290:ARG:HH11	2:P:336:ARG:HG3	1.56	0.70
2:O:315:ARG:O	2:O:366:ARG:NH1	2.26	0.68
1:I:327:PHE:O	1:I:365:GLN:NE2	2.23	0.68
2:R:240:GLN:HE22	2:R:250:TYR:HB3	1.60	0.67
1:I:363:PHE:CE2	1:I:365:GLN:HB2	2.31	0.66
2:Q:252:CYS:SG	2:Q:253:TYR:N	2.69	0.66
1:L:349:SER:OG	1:L:352:GLU:OE1	2.12	0.65
2:R:199:PRO:O	2:R:432:ASN:ND2	2.30	0.65
2:M:281:LEU:HD12	2:M:377:LEU:HD21	1.79	0.65
2:Q:141:LYS:HA	2:Q:144:LEU:HD23	1.78	0.65
2:R:193:LYS:O	2:R:197:LYS:NZ	2.30	0.65
1:F:295:ILE:HD12	1:F:321:ALA:HB2	1.79	0.64
1:E:194:ARG:HG2	1:E:242:GLU:HB3	1.79	0.64
1:F:299:GLN:H	1:F:326:SER:HB2	1.62	0.64
2:R:319:GLN:O	2:R:364:SER:OG	2.16	0.64
1:A:289:ARG:NH1	1:A:293:GLU:OE2	2.31	0.63
2:N:417:VAL:HG21	2:N:460:ILE:HD13	1.79	0.63
1:H:406:LEU:HB2	1:J:405:ASN:HD22	1.63	0.63
2:M:203:ILE:HB	2:M:433:VAL:HG12	1.81	0.62
2:M:310:LEU:HD12	2:M:352:GLU:HG3	1.81	0.62
2:O:354:GLY:HA3	2:O:374:VAL:HG21	1.81	0.61
2:Q:315:ARG:O	2:Q:366:ARG:NH1	2.33	0.61
2:M:227:LEU:HD21	2:M:393:ILE:HG23	1.82	0.61
1:A:95:VAL:HG21	1:B:95:VAL:HG11	1.83	0.61
2:R:181:TYR:OH	2:R:536:ARG:NH1	2.34	0.61
2:P:279:PRO:O	2:P:283:ASN:ND2	2.34	0.60
2:R:315:ARG:NH1	2:R:317:THR:OG1	2.33	0.60
2:Q:178:SER:O	2:Q:183:LYS:NZ	2.35	0.60
2:R:415:ASP:OD1	2:R:416:GLU:N	2.35	0.60
2:R:483:LEU:O	2:R:493:GLN:NE2	2.34	0.59
2:R:522:SER:HB3	2:R:525:VAL:HG23	1.85	0.59
2:P:202:ARG:HD2	2:P:472:THR:HG22	1.83	0.59
2:Q:322:LEU:HD23	2:Q:326:LEU:HD23	1.85	0.59
2:R:128:LEU:HD11	2:R:132:PHE:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:289:ARG:NH2	1:G:293:GLU:OE2	2.37	0.58
1:F:403:ILE:HD11	1:H:402:ALA:HA	1.85	0.57
2:Q:192:ARG:NH1	2:Q:215:ALA:O	2.37	0.57
2:P:313:ASP:OD1	2:Q:330:ARG:NH1	2.38	0.57
1:C:349:SER:OG	1:C:352:GLU:OE1	2.19	0.57
2:P:289:ASN:OD1	2:P:290:ARG:HG3	2.05	0.56
2:Q:550:MET:HE1	2:Q:558:LEU:HD21	1.87	0.56
2:R:479:ALA:HB1	2:R:483:LEU:HD12	1.87	0.56
1:G:145:LYS:HG3	1:G:176:ALA:HB1	1.88	0.56
1:K:30:VAL:HG12	1:K:303:PHE:HB2	1.87	0.56
2:M:105:GLU:N	2:M:105:GLU:OE1	2.37	0.56
2:M:312:ASP:HB3	2:M:348:THR:HG22	1.88	0.56
2:O:252:CYS:SG	2:O:253:TYR:N	2.78	0.56
1:D:270:TYR:HE2	1:D:284:TYR:HB2	1.70	0.56
2:R:258:TYR:OH	2:R:341:PRO:O	2.24	0.56
1:G:260:ASP:OD1	1:G:261:ASP:N	2.38	0.55
2:Q:255:LYS:NZ	2:Q:392:SER:O	2.39	0.55
1:E:64:ILE:HG12	1:E:70:VAL:HG13	1.88	0.55
1:G:26:ASP:O	1:G:155:ARG:NH2	2.39	0.55
2:M:242:LYS:NZ	2:M:428:GLU:OE2	2.37	0.55
1:B:194:ARG:NH1	1:C:191:LEU:HD13	2.22	0.55
1:D:191:LEU:HD22	1:E:194:ARG:HH12	1.72	0.55
2:P:308:PHE:CD1	2:P:321:LYS:HG3	2.42	0.55
2:R:494:ILE:HA	2:R:497:TYR:CE2	2.41	0.55
1:H:390:PHE:HB3	1:H:392:ARG:HH12	1.70	0.55
2:P:247:SER:OG	2:P:249:GLU:OE1	2.22	0.55
1:G:343:VAL:HG21	1:G:356:VAL:HG21	1.89	0.55
2:R:207:ASP:OD1	2:R:208:ILE:N	2.40	0.54
1:J:53:LYS:NZ	1:J:78:ASN:OD1	2.40	0.54
1:B:262:PHE:O	1:B:264:ARG:NH1	2.40	0.54
1:J:205:PHE:O	1:K:206:ARG:NH1	2.39	0.54
1:H:403:ILE:HA	1:J:405:ASN:HD21	1.70	0.54
1:B:343:VAL:HA	1:B:347:GLY:HA2	1.90	0.54
1:G:166:THR:HG22	1:G:168:ASN:H	1.72	0.54
2:M:319:GLN:O	2:M:364:SER:OG	2.25	0.54
1:D:295:ILE:HD11	1:D:317:ILE:HG22	1.89	0.54
2:P:417:VAL:HG11	2:P:460:ILE:HG13	1.89	0.54
1:L:126:THR:HG22	1:L:129:GLN:HB2	1.90	0.53
1:D:194:ARG:HG2	1:D:242:GLU:HB3	1.90	0.53
2:Q:389:ARG:HG3	2:R:499:ARG:HH22	1.73	0.53
1:A:255:ASP:O	1:A:259:LYS:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:103:ASP:OD1	1:K:104:GLU:N	2.41	0.53
2:R:330:ARG:HE	2:R:353:PHE:HE1	1.57	0.53
1:E:116:TYR:HA	1:E:119:VAL:HG22	1.92	0.52
1:H:262:PHE:O	1:H:266:GLN:NE2	2.42	0.52
2:R:177:GLY:HA3	2:R:535:LEU:HB2	1.90	0.52
2:R:192:ARG:O	2:R:195:SER:OG	2.21	0.52
1:A:343:VAL:HG21	1:A:356:VAL:HG11	1.92	0.51
2:P:255:LYS:NZ	2:P:392:SER:O	2.43	0.51
1:D:190:GLY:O	1:D:194:ARG:NE	2.35	0.51
1:C:129:GLN:OE1	1:C:138:LYS:NZ	2.42	0.51
1:D:238:LEU:HD23	1:D:238:LEU:O	2.11	0.51
1:I:47:ASP:HA	1:I:50:LYS:HG2	1.93	0.51
2:R:342:PRO:O	2:R:345:SER:OG	2.21	0.51
2:N:7:THR:HG22	2:N:9:ILE:H	1.75	0.51
1:L:295:ILE:HD12	1:L:321:ALA:HB2	1.92	0.51
2:P:322:LEU:HD22	2:P:325:TRP:CE3	2.40	0.51
1:C:131:ARG:NH1	1:C:250:ASP:OD1	2.45	0.50
2:O:248:GLU:O	2:O:249:GLU:HG3	2.11	0.50
1:G:197:TYR:HB2	1:G:200:ASN:OD1	2.11	0.50
1:A:238:LEU:HD12	1:A:279:THR:HG21	1.93	0.50
2:P:153:ASP:OD2	2:P:156:THR:OG1	2.30	0.50
2:R:497:TYR:CE1	2:R:525:VAL:HG22	2.47	0.49
2:R:504:GLY:HA2	2:R:509:CYS:HB2	1.94	0.49
2:M:424:GLU:OE1	2:M:424:GLU:N	2.46	0.49
2:N:413:MET:HG2	2:N:460:ILE:HD11	1.94	0.49
2:P:204:VAL:HB	2:P:474:LEU:HD23	1.95	0.49
2:R:396:LEU:HD23	2:R:396:LEU:H	1.77	0.49
2:M:471:PRO:HA	2:M:508:LYS:HB3	1.95	0.49
2:P:308:PHE:CG	2:P:321:LYS:HG3	2.48	0.49
2:R:550:MET:HE3	2:R:558:LEU:HD11	1.94	0.49
1:J:194:ARG:HB2	1:J:242:GLU:H	1.77	0.49
2:N:134:ASN:O	2:N:138:SER:OG	2.27	0.49
1:H:249:TYR:HA	1:H:253:ILE:HG12	1.94	0.49
2:M:471:PRO:HB3	2:M:508:LYS:HG2	1.94	0.49
2:R:115:ASP:N	2:R:115:ASP:OD1	2.46	0.49
1:D:12:GLU:OE2	1:D:16:ARG:NH1	2.46	0.48
2:M:594:SER:OG	2:M:595:ASP:N	2.45	0.48
2:R:319:GLN:HE22	2:R:322:LEU:HD23	1.78	0.48
1:H:313:HIS:CE1	1:H:317:ILE:HD11	2.48	0.48
1:C:142:LYS:NZ	1:C:146:GLU:OE2	2.44	0.48
2:N:202:ARG:HG2	2:N:472:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:301:GLU:OE2	2:P:307:THR:OG1	2.30	0.48
1:I:145:LYS:HB3	1:I:180:LEU:HD11	1.94	0.48
2:Q:417:VAL:HG21	2:Q:460:ILE:HG13	1.95	0.48
2:R:310:LEU:HD22	2:R:352:GLU:HG3	1.94	0.48
1:C:289:ARG:NH1	1:C:293:GLU:OE2	2.46	0.48
2:P:499:ARG:O	2:P:503:GLU:HG3	2.13	0.48
2:R:52:ILE:HG13	2:R:63:ALA:HB3	1.95	0.48
1:C:104:GLU:OE2	1:D:99:ARG:NH2	2.46	0.48
2:O:504:GLY:HA2	2:O:509:CYS:HB3	1.95	0.48
2:R:147:ALA:HB1	2:R:162:PHE:HB3	1.94	0.48
1:C:150:LYS:NZ	1:C:384:LEU:O	2.37	0.47
1:A:243:VAL:CG1	1:A:247:GLN:HB3	2.44	0.47
1:E:312:TYR:HE1	1:G:406:LEU:HB3	1.80	0.47
2:Q:274:ASP:OD2	2:Q:277:GLN:NE2	2.48	0.47
2:M:417:VAL:HG21	2:M:460:ILE:HD12	1.95	0.47
2:P:323:ALA:C	2:P:325:TRP:N	2.71	0.47
2:M:105:GLU:HG2	2:M:106:LEU:N	2.30	0.47
1:I:116:TYR:HA	1:I:119:VAL:HG22	1.97	0.47
1:C:218:HIS:O	1:C:218:HIS:ND1	2.47	0.47
2:P:8:GLU:HG3	2:P:9:ILE:HD12	1.97	0.47
1:L:65:ASP:OD1	1:L:66:LYS:N	2.48	0.46
2:O:165:VAL:HG13	2:O:169:LEU:HD12	1.97	0.46
1:G:146:GLU:O	1:G:150:LYS:HG2	2.15	0.46
2:P:550:MET:SD	2:P:558:LEU:HD13	2.56	0.46
1:C:201:PHE:CE1	1:C:224:TYR:HE1	2.33	0.46
2:O:259:GLN:HG2	2:O:340:TRP:CE2	2.51	0.46
2:Q:27:LEU:HD21	2:Q:94:ILE:HD12	1.98	0.46
2:R:499:ARG:O	2:R:502:LYS:HG2	2.16	0.46
1:B:194:ARG:HH11	1:C:191:LEU:HD13	1.80	0.46
1:D:249:TYR:HA	1:D:253:ILE:HB	1.98	0.46
1:G:286:GLU:HA	1:G:289:ARG:HG2	1.97	0.46
1:I:338:GLU:OE1	1:I:338:GLU:N	2.45	0.46
1:F:395:ILE:O	1:F:399:LEU:HD23	2.15	0.46
1:G:109:ARG:O	1:G:113:SER:OG	2.23	0.46
2:P:439:LYS:O	2:Q:506:LYS:NZ	2.34	0.46
1:D:97:LYS:NZ	1:D:105:GLU:OE2	2.48	0.46
2:N:547:ARG:HA	2:N:550:MET:HE3	1.98	0.46
2:Q:185:ASN:ND2	4:Q:701:ADP:N7	2.62	0.46
1:J:295:ILE:HD12	1:J:321:ALA:HB2	1.98	0.45
2:R:424:GLU:OE1	2:R:424:GLU:N	2.50	0.45
2:N:517:ARG:HH21	2:O:551:GLU:HG3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:231:THR:HG22	1:I:243:VAL:H	1.82	0.45
2:O:321:LYS:O	2:O:321:LYS:HG3	2.17	0.45
1:K:116:TYR:HA	1:K:119:VAL:HG12	1.97	0.45
1:E:352:GLU:OE1	1:E:352:GLU:N	2.49	0.45
1:I:90:THR:HG21	1:I:273:ALA:HB1	1.99	0.44
2:P:105:GLU:HG3	2:P:106:LEU:H	1.82	0.44
1:A:282:PHE:HE1	1:B:313:HIS:CD2	2.35	0.44
1:K:358:LEU:HA	1:K:361:MET:SD	2.57	0.44
1:D:3:ILE:HG23	1:D:369:VAL:HG22	1.99	0.44
1:G:352:GLU:HA	1:G:355:ILE:HG22	1.99	0.44
2:P:181:TYR:N	4:P:701:ADP:O1B	2.50	0.44
1:H:26:ASP:O	1:H:155:ARG:NH2	2.50	0.44
2:O:35:LEU:HD12	2:O:44:SER:HB3	2.00	0.44
2:O:550:MET:SD	2:O:558:LEU:HD11	2.58	0.44
1:H:194:ARG:NE	1:H:242:GLU:OE1	2.50	0.44
2:O:301:GLU:OE1	2:O:335:LYS:NZ	2.44	0.44
2:O:402:LEU:O	2:O:402:LEU:HD23	2.17	0.44
2:P:462:PHE:CZ	2:P:499:ARG:HD3	2.52	0.44
1:B:188:PHE:HB2	1:B:194:ARG:HH21	1.83	0.43
1:F:103:ASP:O	1:F:107:GLU:HG3	2.18	0.43
2:M:401:GLU:OE1	2:M:401:GLU:N	2.50	0.43
2:P:417:VAL:HG21	2:P:460:ILE:HG13	1.99	0.43
1:A:103:ASP:OD1	1:A:103:ASP:N	2.51	0.43
2:O:259:GLN:HG2	2:O:340:TRP:CD2	2.52	0.43
1:G:295:ILE:HD11	1:G:302:LEU:HD22	2.00	0.43
2:P:323:ALA:C	2:P:325:TRP:H	2.25	0.43
2:N:140:ASP:O	2:N:142:GLU:N	2.51	0.43
2:R:50:ASP:OD1	2:R:51:LEU:N	2.52	0.43
2:R:109:TYR:HB2	2:R:135:ILE:HG12	2.00	0.43
2:R:277:GLN:HG2	2:R:377:LEU:HD22	2.00	0.43
1:G:280:ILE:O	1:G:283:VAL:HG12	2.19	0.43
1:H:238:LEU:HD13	1:H:280:ILE:HD11	2.00	0.43
1:F:97:LYS:NZ	1:F:105:GLU:OE2	2.52	0.43
1:H:403:ILE:HG12	1:J:402:ALA:HA	2.00	0.43
2:R:496:ALA:O	2:R:499:ARG:HG2	2.19	0.43
2:P:298:ILE:O	2:P:310:LEU:HB3	2.19	0.43
1:A:27:ASN:HB2	1:A:300:THR:HG23	2.02	0.42
1:B:145:LYS:HB3	1:B:180:LEU:HD11	2.00	0.42
2:Q:321:LYS:O	2:Q:324:GLU:HG3	2.19	0.42
1:B:227:HIS:CD2	1:B:275:LYS:HE2	2.54	0.42
1:E:337:LYS:O	1:E:341:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:379:SER:O	1:E:383:HIS:ND1	2.50	0.42
1:J:338:GLU:OE1	1:J:338:GLU:N	2.50	0.42
2:P:447:PRO:HA	2:P:482:TYR:HB3	2.00	0.42
1:D:86:ILE:O	1:D:90:THR:HG23	2.19	0.42
1:K:53:LYS:HB2	1:K:60:LEU:HD11	2.00	0.42
2:O:539:ASN:OD1	2:O:540:GLU:N	2.52	0.42
2:Q:516:GLN:HG3	2:Q:517:ARG:HG2	2.02	0.42
2:R:64:ARG:HB2	2:R:99:ILE:HD11	2.02	0.42
1:E:336:LEU:HD11	1:E:368:VAL:HG12	2.02	0.42
2:R:182:GLY:O	2:R:186:PHE:N	2.38	0.42
1:C:73:ILE:HG13	1:C:74:ASP:N	2.34	0.42
1:D:234:GLN:HG2	1:D:236:ASP:H	1.85	0.42
2:P:375:LEU:N	2:P:376:PRO:HD2	2.35	0.42
2:P:418:ASP:OD1	2:P:419:TYR:N	2.49	0.42
2:Q:54:PHE:CD2	2:Q:119:PRO:HG3	2.55	0.42
1:I:398:GLU:OE1	1:I:398:GLU:N	2.49	0.42
1:L:197:TYR:HB2	1:L:200:ASN:OD1	2.19	0.42
2:N:166:ASP:O	2:N:170:SER:HB3	2.20	0.42
2:Q:323:ALA:O	2:Q:326:LEU:HG	2.20	0.42
2:M:105:GLU:HG2	2:M:106:LEU:H	1.84	0.41
2:M:424:GLU:HG2	2:M:464:ARG:HG2	2.02	0.41
1:D:349:SER:OG	1:D:350:GLU:N	2.53	0.41
2:N:478:GLU:HB3	2:N:481:HIS:ND1	2.35	0.41
2:O:391:LYS:HG2	2:O:396:LEU:HD21	2.02	0.41
2:P:482:TYR:O	2:P:483:LEU:HD23	2.20	0.41
1:A:295:ILE:HD11	1:A:317:ILE:HG22	2.03	0.41
1:C:333:TYR:HD2	1:C:355:ILE:HG12	1.86	0.41
1:D:400:VAL:O	1:D:403:ILE:HG12	2.20	0.41
1:F:209:ASN:OD1	1:F:209:ASN:N	2.54	0.41
2:Q:526:LEU:HD22	2:Q:532:TRP:CZ3	2.56	0.41
2:O:192:ARG:CZ	2:O:219:ILE:HD11	2.50	0.41
1:B:255:ASP:O	1:B:259:LYS:HB2	2.21	0.41
2:M:114:GLU:HB3	2:M:116:TRP:CD1	2.55	0.41
2:R:471:PRO:HG3	2:R:508:LYS:HD2	2.02	0.41
2:M:34:ARG:HB2	2:M:46:THR:OG1	2.21	0.41
2:P:320:SER:C	2:P:322:LEU:H	2.28	0.41
2:Q:47:GLN:NE2	2:R:116:TRP:O	2.53	0.41
1:G:54:GLN:NE2	1:G:55:ASN:OD1	2.53	0.41
1:A:207:ASN:OD1	1:A:208:VAL:N	2.54	0.41
1:I:145:LYS:HG2	1:I:176:ALA:HB1	2.03	0.41
2:M:192:ARG:NH1	2:M:215:ALA:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:212:TYR:OH	2:N:477:GLU:OE2	2.24	0.41
2:P:599:SER:OG	2:Q:166:ASP:OD1	2.29	0.41
2:Q:300:LEU:HD11	2:Q:310:LEU:HD11	2.03	0.41
2:R:257:PRO:HD2	2:R:416:GLU:OE2	2.21	0.41
1:B:407:SER:OG	1:D:405:ASN:ND2	2.53	0.41
1:F:244:SER:OG	1:F:245:ALA:N	2.54	0.41
1:H:249:TYR:HA	1:H:253:ILE:CG1	2.50	0.41
2:M:546:LEU:HD12	2:M:546:LEU:HA	1.94	0.41
2:Q:389:ARG:HE	2:R:499:ARG:NH2	2.19	0.41
1:F:49:TRP:CE2	1:F:80:VAL:HG11	2.56	0.40
1:J:311:ASP:O	1:J:315:ASN:ND2	2.55	0.40
2:O:313:ASP:OD2	2:O:315:ARG:NH2	2.53	0.40
2:O:321:LYS:HG3	2:O:325:TRP:CD1	2.56	0.40
1:H:406:LEU:HA	1:H:406:LEU:HD23	1.86	0.40
2:N:252:CYS:SG	2:N:253:TYR:N	2.94	0.40
2:P:462:PHE:HZ	2:P:499:ARG:HD3	1.85	0.40
1:C:407:SER:O	1:C:407:SER:OG	2.35	0.40
2:R:467:GLU:CD	2:R:468:ARG:HG2	2.46	0.40
1:B:249:TYR:HA	1:B:253:ILE:HB	2.03	0.40
1:B:253:ILE:O	1:B:257:ILE:HG12	2.21	0.40
2:N:304:ASP:OD1	2:N:305:GLY:N	2.55	0.40
2:R:350:VAL:HG11	2:R:377:LEU:HD23	2.04	0.40
1:B:268:LEU:HD23	1:B:268:LEU:H	1.87	0.40
1:L:312:TYR:O	1:L:316:ARG:HG2	2.20	0.40
2:M:6:LEU:HD23	2:M:7:THR:HG23	2.02	0.40
2:P:430:ASP:OD1	2:P:431:TRP:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
4	ADP	P	701	-	28,29,29	1.39	4 (14%)	43,45,45	1.84	9 (20%)
3	AR6	C	501	-	39,39,39	1.28	2 (5%)	56,60,60	0.70	0
3	AR6	G	501	-	39,39,39	1.27	2 (5%)	56,60,60	0.72	1 (1%)
3	AR6	H	501	-	39,39,39	1.22	2 (5%)	56,60,60	0.70	0
3	AR6	E	501	-	39,39,39	1.31	2 (5%)	56,60,60	0.67	0
3	AR6	K	501	-	39,39,39	1.33	2 (5%)	56,60,60	0.72	0
4	ADP	O	701	5	28,29,29	1.39	4 (14%)	43,45,45	1.84	8 (18%)
4	ADP	Q	701	5	28,29,29	1.39	4 (14%)	43,45,45	1.86	10 (23%)
4	ADP	N	701	5	28,29,29	1.39	4 (14%)	43,45,45	1.83	9 (20%)
3	AR6	F	501	-	39,39,39	1.28	2 (5%)	56,60,60	0.70	0
3	AR6	L	501	-	39,39,39	1.25	2 (5%)	56,60,60	0.67	0
3	AR6	D	501	-	39,39,39	1.16	2 (5%)	56,60,60	0.70	0
3	AR6	J	501	-	39,39,39	1.31	2 (5%)	56,60,60	0.68	0
4	ADP	M	701	5	28,29,29	1.39	4 (14%)	43,45,45	1.84	10 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AR6	I	501	-	39,39,39	1.31	2 (5%)	56,60,60	0.71	0
3	AR6	B	501	-	39,39,39	1.30	2 (5%)	56,60,60	0.65	0
3	AR6	A	501	-	39,39,39	1.26	2 (5%)	56,60,60	0.68	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
4	ADP	P	701	-	-	3/16/32/32	0/3/3/3
3	AR6	C	501	-	-	11/22/54/54	0/4/4/4
3	AR6	G	501	-	-	7/22/54/54	0/4/4/4
3	AR6	H	501	-	-	9/22/54/54	0/4/4/4
3	AR6	E	501	-	-	11/22/54/54	0/4/4/4
3	AR6	K	501	-	-	15/22/54/54	0/4/4/4
4	ADP	O	701	5	-	3/16/32/32	0/3/3/3
4	ADP	Q	701	5	-	2/16/32/32	0/3/3/3
4	ADP	N	701	5	-	4/16/32/32	0/3/3/3
3	AR6	F	501	-	-	11/22/54/54	0/4/4/4
3	AR6	L	501	-	-	10/22/54/54	0/4/4/4
3	AR6	D	501	-	-	9/22/54/54	0/4/4/4
3	AR6	J	501	-	-	11/22/54/54	0/4/4/4
4	ADP	M	701	5	-	5/16/32/32	0/3/3/3
3	AR6	I	501	-	-	14/22/54/54	0/4/4/4
3	AR6	B	501	-	-	12/22/54/54	0/4/4/4
3	AR6	A	501	-	-	13/22/54/54	0/4/4/4

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	501	AR6	PB-O3A	4.89	1.64	1.59
3	I	501	AR6	PB-O3A	4.87	1.64	1.59
3	E	501	AR6	PB-O3A	4.87	1.64	1.59
3	K	501	AR6	PB-O3A	4.86	1.64	1.59
3	B	501	AR6	PB-O3A	4.80	1.64	1.59
3	C	501	AR6	PB-O3A	4.79	1.64	1.59
3	G	501	AR6	PB-O3A	4.77	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	501	AR6	PB-O3A	4.76	1.64	1.59
3	K	501	AR6	PA-O3A	4.72	1.64	1.59
3	L	501	AR6	PB-O3A	4.67	1.64	1.59
3	A	501	AR6	PB-O3A	4.62	1.64	1.59
4	Q	701	ADP	C5-C4	4.62	1.47	1.39
3	J	501	AR6	PA-O3A	4.60	1.64	1.59
4	O	701	ADP	C5-C4	4.59	1.47	1.39
3	I	501	AR6	PA-O3A	4.56	1.64	1.59
4	N	701	ADP	C5-C4	4.56	1.47	1.39
3	B	501	AR6	PA-O3A	4.55	1.64	1.59
3	E	501	AR6	PA-O3A	4.55	1.64	1.59
4	M	701	ADP	C5-C4	4.55	1.47	1.39
4	P	701	ADP	C5-C4	4.53	1.47	1.39
3	G	501	AR6	PA-O3A	4.39	1.64	1.59
3	H	501	AR6	PB-O3A	4.38	1.64	1.59
3	A	501	AR6	PA-O3A	4.38	1.64	1.59
3	C	501	AR6	PA-O3A	4.33	1.64	1.59
3	F	501	AR6	PA-O3A	4.29	1.64	1.59
3	L	501	AR6	PA-O3A	4.23	1.64	1.59
3	H	501	AR6	PA-O3A	4.03	1.63	1.59
3	D	501	AR6	PB-O3A	3.99	1.63	1.59
3	D	501	AR6	PA-O3A	3.77	1.63	1.59
4	N	701	ADP	C5-C6	2.68	1.48	1.41
4	O	701	ADP	C5-C6	2.67	1.48	1.41
4	M	701	ADP	C5-C6	2.65	1.48	1.41
4	Q	701	ADP	C5-C6	2.65	1.48	1.41
4	P	701	ADP	C5-C6	2.60	1.48	1.41
4	P	701	ADP	C5-N7	-2.42	1.34	1.39
4	M	701	ADP	C5-N7	-2.34	1.34	1.39
4	N	701	ADP	C5-N7	-2.33	1.34	1.39
4	O	701	ADP	C5-N7	-2.32	1.34	1.39
4	N	701	ADP	C8-N7	2.31	1.36	1.31
4	Q	701	ADP	C8-N7	2.31	1.36	1.31
4	O	701	ADP	C8-N7	2.30	1.36	1.31
4	Q	701	ADP	C5-N7	-2.29	1.34	1.39
4	M	701	ADP	C8-N7	2.27	1.36	1.31
4	P	701	ADP	C8-N7	2.19	1.35	1.31

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	701	ADP	C5-C4-N3	-5.94	118.54	126.72

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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	-5.82	118.70	126.72
4	N	701	ADP	C5-C4-N3	-5.81	118.71	126.72
4	Q	701	ADP	C5-C4-N3	-5.78	118.75	126.72
4	P	701	ADP	N3-C4-N9	4.67	135.11	127.17
4	O	701	ADP	N3-C4-N9	4.64	135.06	127.17
4	M	701	ADP	N3-C4-N9	4.60	135.00	127.17
4	Q	701	ADP	N3-C4-N9	4.55	134.91	127.17
4	N	701	ADP	N3-C4-N9	4.52	134.86	127.17
4	M	701	ADP	C2-N3-C4	3.71	120.89	111.83
4	N	701	ADP	C2-N3-C4	3.70	120.86	111.83
4	P	701	ADP	C2-N3-C4	3.69	120.85	111.83
4	Q	701	ADP	C2-N3-C4	3.68	120.83	111.83
4	O	701	ADP	C2-N3-C4	3.66	120.78	111.83
4	N	701	ADP	C4-C5-N7	-3.54	106.54	110.58
4	P	701	ADP	C4-C5-N7	-3.46	106.63	110.58
4	M	701	ADP	C4-C5-N7	-3.45	106.64	110.58
4	Q	701	ADP	C4-C5-N7	-3.45	106.64	110.58
4	O	701	ADP	C4-C5-N7	-3.42	106.67	110.58
4	M	701	ADP	N3-C2-N1	-3.24	123.67	128.58
4	Q	701	ADP	N3-C2-N1	-3.21	123.73	128.58
4	N	701	ADP	N3-C2-N1	-3.19	123.75	128.58
4	O	701	ADP	N3-C2-N1	-3.15	123.81	128.58
4	P	701	ADP	N3-C2-N1	-3.15	123.82	128.58
4	M	701	ADP	C4-N9-C8	2.67	108.54	105.74
4	O	701	ADP	C4-N9-C8	2.66	108.53	105.74
4	Q	701	ADP	C4-N9-C8	2.61	108.47	105.74
4	N	701	ADP	C4-N9-C8	2.60	108.47	105.74
4	Q	701	ADP	C3'-C2'-C1'	2.60	106.37	101.46
4	N	701	ADP	C5-N7-C8	2.55	107.45	103.45
4	P	701	ADP	C4-N9-C8	2.54	108.40	105.74
4	M	701	ADP	C5-N7-C8	2.54	107.44	103.45
4	P	701	ADP	C5-N7-C8	2.53	107.42	103.45
4	Q	701	ADP	C5-N7-C8	2.51	107.39	103.45
4	O	701	ADP	C5-N7-C8	2.50	107.38	103.45
4	P	701	ADP	C3'-C2'-C1'	2.39	105.98	101.46
3	G	501	AR6	C1D-C2D-C3D	-2.34	99.42	102.29
4	O	701	ADP	C3'-C2'-C1'	2.34	105.88	101.46
4	M	701	ADP	C3'-C2'-C1'	2.32	105.86	101.46
4	Q	701	ADP	C2'-C1'-N9	-2.14	107.98	113.30
4	N	701	ADP	C6-C5-N7	2.14	136.21	132.09
4	M	701	ADP	C6-C5-N7	2.09	136.11	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	701	ADP	C6-C5-N7	2.08	136.10	132.09
4	P	701	ADP	C2'-C3'-C4'	2.06	106.60	102.61
4	N	701	ADP	C3'-C2'-C1'	2.05	105.34	101.46
4	M	701	ADP	N9-C8-N7	-2.02	111.08	113.94

There are no chirality outliers.

All (150) 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-O3A
3	A	501	AR6	C5D-O5D-PB-O3A
3	B	501	AR6	C5'-O5'-PA-O1A
3	B	501	AR6	C5'-O5'-PA-O2A
3	B	501	AR6	C5'-O5'-PA-O3A
3	B	501	AR6	C5D-O5D-PB-O1B
3	B	501	AR6	C5D-O5D-PB-O2B
3	B	501	AR6	C5D-O5D-PB-O3A
3	C	501	AR6	C5'-O5'-PA-O1A
3	C	501	AR6	C5'-O5'-PA-O3A
3	C	501	AR6	C5D-O5D-PB-O2B
3	D	501	AR6	C5D-O5D-PB-O1B
3	D	501	AR6	C3D-C4D-C5D-O5D
3	D	501	AR6	O4D-C4D-C5D-O5D
3	F	501	AR6	C5D-O5D-PB-O1B
3	F	501	AR6	C5D-O5D-PB-O2B
3	F	501	AR6	C5D-O5D-PB-O3A
3	G	501	AR6	C5D-O5D-PB-O1B
3	G	501	AR6	C5D-O5D-PB-O3A
3	H	501	AR6	C5'-O5'-PA-O1A
3	H	501	AR6	O4D-C4D-C5D-O5D
3	I	501	AR6	C2'-C1'-N9-C8
3	I	501	AR6	C5'-O5'-PA-O2A
3	I	501	AR6	C5D-O5D-PB-O1B
3	I	501	AR6	C5D-O5D-PB-O3A
3	I	501	AR6	C4D-C5D-O5D-PB
3	J	501	AR6	C5'-O5'-PA-O1A
3	J	501	AR6	C5'-O5'-PA-O2A
3	J	501	AR6	C5'-O5'-PA-O3A
3	J	501	AR6	C5D-O5D-PB-O1B
3	J	501	AR6	C5D-O5D-PB-O2B
3	J	501	AR6	C5D-O5D-PB-O3A

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Mol	Chain	Res	Type	Atoms
3	K	501	AR6	C5'-O5'-PA-O2A
3	K	501	AR6	C5'-O5'-PA-O3A
3	K	501	AR6	C5D-O5D-PB-O1B
3	K	501	AR6	C5D-O5D-PB-O3A
3	K	501	AR6	C4D-C5D-O5D-PB
3	L	501	AR6	C5D-O5D-PB-O1B
3	L	501	AR6	C5D-O5D-PB-O2B
3	L	501	AR6	C5D-O5D-PB-O3A
4	M	701	ADP	C5'-O5'-PA-O1A
4	M	701	ADP	C5'-O5'-PA-O2A
4	M	701	ADP	C5'-O5'-PA-O3A
4	M	701	ADP	O4'-C4'-C5'-O5'
4	N	701	ADP	C5'-O5'-PA-O3A
4	N	701	ADP	O4'-C4'-C5'-O5'
4	Q	701	ADP	C5'-O5'-PA-O1A
3	G	501	AR6	C3D-C4D-C5D-O5D
3	G	501	AR6	O4D-C4D-C5D-O5D
4	N	701	ADP	C3'-C4'-C5'-O5'
3	A	501	AR6	O4'-C4'-C5'-O5'
3	B	501	AR6	C3D-C4D-C5D-O5D
3	B	501	AR6	O4D-C4D-C5D-O5D
3	E	501	AR6	O4'-C4'-C5'-O5'
3	F	501	AR6	O4D-C4D-C5D-O5D
3	I	501	AR6	C3D-C4D-C5D-O5D
3	K	501	AR6	O4'-C4'-C5'-O5'
4	M	701	ADP	C3'-C4'-C5'-O5'
3	I	501	AR6	C2'-C1'-N9-C4
3	A	501	AR6	C3'-C4'-C5'-O5'
3	E	501	AR6	C3'-C4'-C5'-O5'
3	H	501	AR6	C3D-C4D-C5D-O5D
3	K	501	AR6	C3'-C4'-C5'-O5'
3	G	501	AR6	C4D-C5D-O5D-PB
3	E	501	AR6	C3D-C4D-C5D-O5D
4	P	701	ADP	O4'-C4'-C5'-O5'
3	A	501	AR6	C3D-C4D-C5D-O5D
3	A	501	AR6	O4D-C4D-C5D-O5D
3	E	501	AR6	O4D-C4D-C5D-O5D
3	I	501	AR6	O4D-C4D-C5D-O5D
3	D	501	AR6	C2'-C1'-N9-C8
3	J	501	AR6	C2'-C1'-N9-C8
3	C	501	AR6	O4'-C4'-C5'-O5'
3	I	501	AR6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	L	501	AR6	O4D-C4D-C5D-O5D
4	O	701	ADP	C3'-C4'-C5'-O5'
3	F	501	AR6	C2'-C1'-N9-C8
3	H	501	AR6	C2'-C1'-N9-C8
3	L	501	AR6	C2'-C1'-N9-C8
3	F	501	AR6	C3D-C4D-C5D-O5D
3	I	501	AR6	C3'-C4'-C5'-O5'
3	L	501	AR6	C3D-C4D-C5D-O5D
3	K	501	AR6	PB-O3A-PA-O2A
3	A	501	AR6	C4D-C5D-O5D-PB
3	C	501	AR6	C4D-C5D-O5D-PB
3	E	501	AR6	C4D-C5D-O5D-PB
3	C	501	AR6	C3'-C4'-C5'-O5'
4	O	701	ADP	O4'-C4'-C5'-O5'
3	K	501	AR6	C2'-C1'-N9-C8
3	D	501	AR6	C4D-C5D-O5D-PB
3	J	501	AR6	C4D-C5D-O5D-PB
3	L	501	AR6	C4D-C5D-O5D-PB
3	F	501	AR6	PA-O3A-PB-O5D
3	J	501	AR6	C2'-C1'-N9-C4
3	A	501	AR6	C2'-C1'-N9-C8
3	B	501	AR6	C2'-C1'-N9-C8
3	C	501	AR6	C2'-C1'-N9-C8
3	E	501	AR6	C2'-C1'-N9-C8
3	A	501	AR6	PA-O3A-PB-O2B
3	E	501	AR6	PA-O3A-PB-O2B
3	I	501	AR6	PB-O3A-PA-O1A
4	Q	701	ADP	C3'-C4'-C5'-O5'
3	D	501	AR6	C5D-O5D-PB-O3A
3	E	501	AR6	C5D-O5D-PB-O2B
3	H	501	AR6	C5'-O5'-PA-O2A
3	H	501	AR6	C5'-O5'-PA-O3A
3	I	501	AR6	C5'-O5'-PA-O1A
3	I	501	AR6	C5'-O5'-PA-O3A
3	K	501	AR6	C5'-O5'-PA-O1A
4	N	701	ADP	C5'-O5'-PA-O1A
4	O	701	ADP	C5'-O5'-PA-O1A
3	H	501	AR6	C4D-C5D-O5D-PB
3	K	501	AR6	PB-O3A-PA-O1A
3	K	501	AR6	PA-O3A-PB-O1B
3	K	501	AR6	PA-O3A-PB-O2B
3	A	501	AR6	C2'-C1'-N9-C4

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Mol	Chain	Res	Type	Atoms
3	B	501	AR6	C2'-C1'-N9-C4
3	D	501	AR6	C2'-C1'-N9-C4
3	F	501	AR6	C2'-C1'-N9-C4
3	H	501	AR6	C2'-C1'-N9-C4
3	K	501	AR6	C2'-C1'-N9-C4
3	L	501	AR6	C2'-C1'-N9-C4
4	P	701	ADP	C3'-C4'-C5'-O5'
3	J	501	AR6	O4'-C4'-C5'-O5'
3	I	501	AR6	PB-O3A-PA-O2A
3	A	501	AR6	O4'-C1'-N9-C8
3	C	501	AR6	O4'-C1'-N9-C8
3	F	501	AR6	C4D-C5D-O5D-PB
3	E	501	AR6	O4'-C1'-N9-C8
3	H	501	AR6	O4'-C1'-N9-C8
3	K	501	AR6	O4'-C1'-N9-C8
3	L	501	AR6	O4'-C1'-N9-C8
3	C	501	AR6	C2'-C1'-N9-C4
3	B	501	AR6	O4'-C1'-N9-C8
3	F	501	AR6	O4'-C1'-N9-C8
3	G	501	AR6	C2'-C1'-N9-C8
3	A	501	AR6	PA-O3A-PB-O1B
3	C	501	AR6	PB-O3A-PA-O2A
3	D	501	AR6	PB-O3A-PA-O1A
3	E	501	AR6	PA-O3A-PB-O1B
4	P	701	ADP	PB-O3A-PA-O2A
3	E	501	AR6	C2'-C1'-N9-C4
3	D	501	AR6	O4'-C1'-N9-C8
3	J	501	AR6	O4'-C1'-N9-C8
3	B	501	AR6	PB-O3A-PA-O1A
3	C	501	AR6	PB-O3A-PA-O1A
3	F	501	AR6	PA-O3A-PB-O1B
3	G	501	AR6	O4'-C4'-C5'-O5'
3	L	501	AR6	O4'-C4'-C5'-O5'

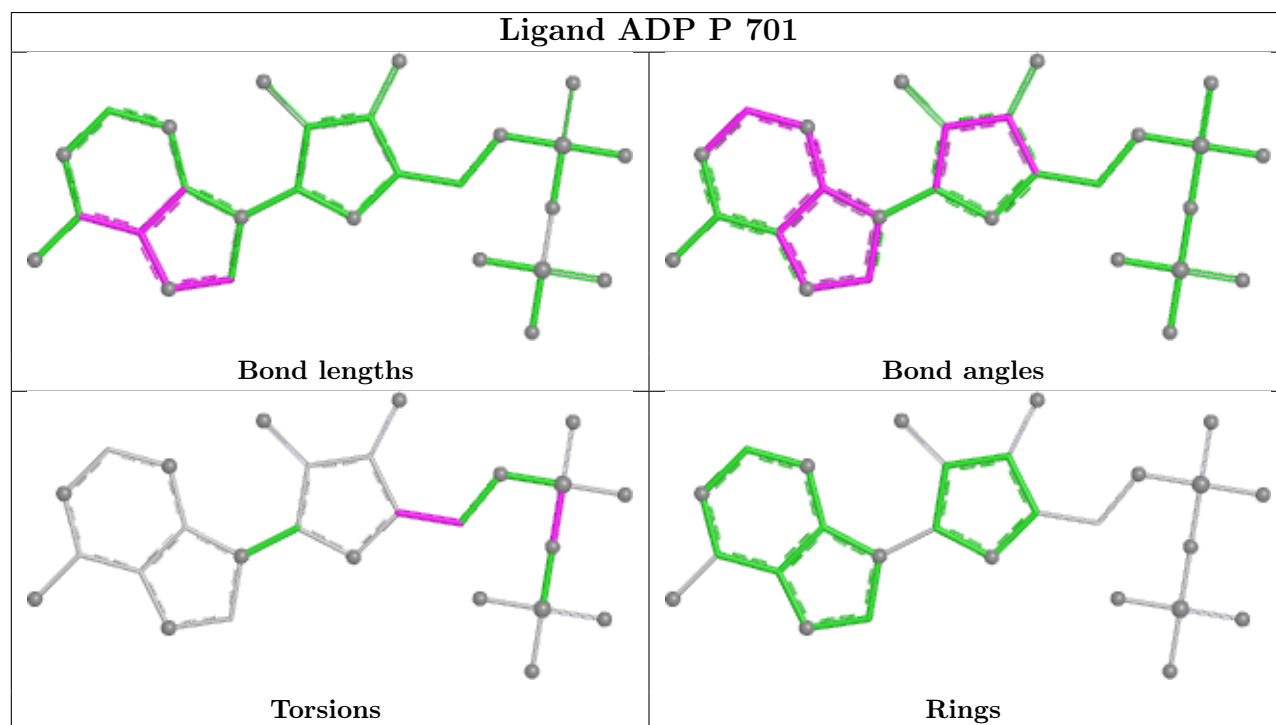
There are no ring outliers.

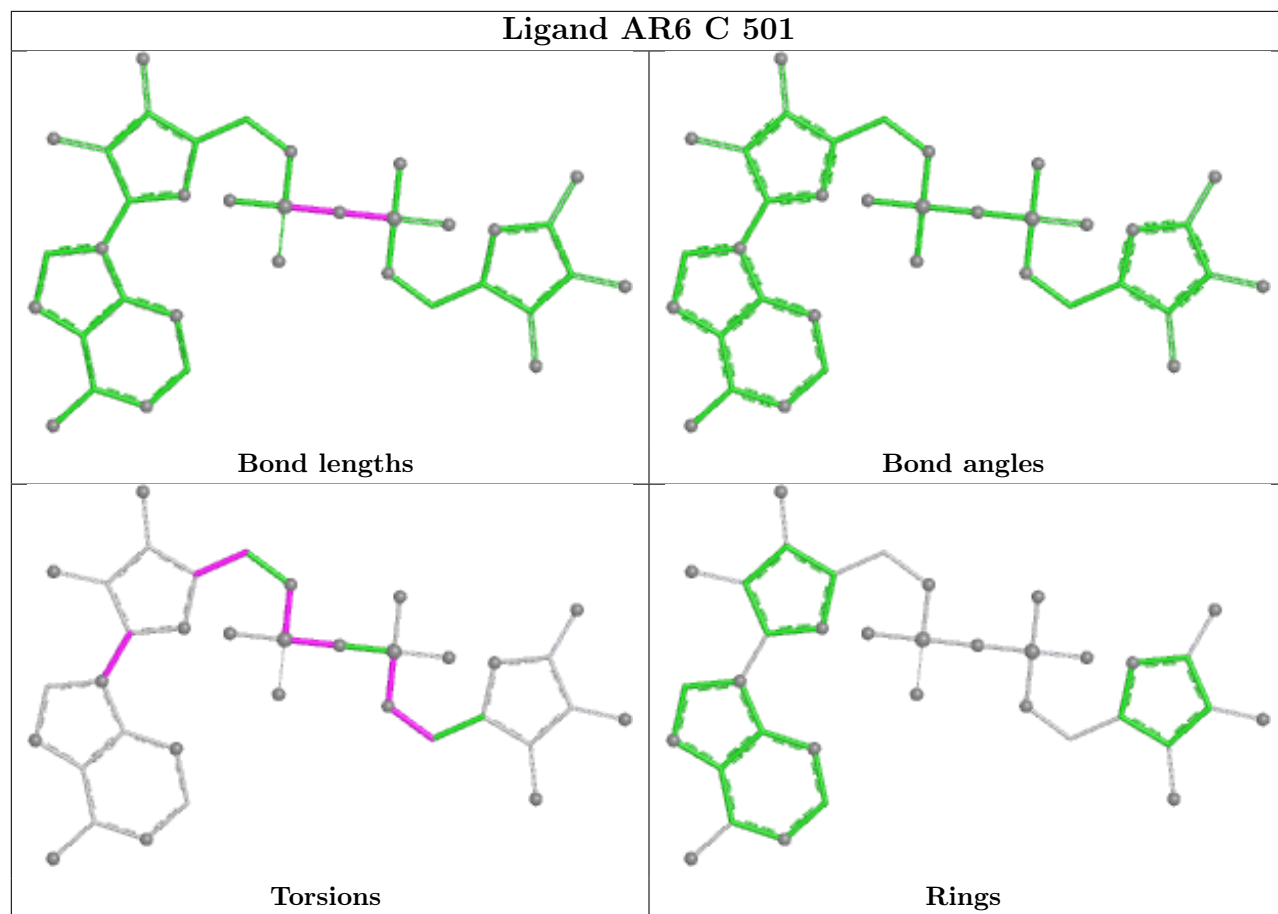
2 monomers are involved in 2 short contacts:

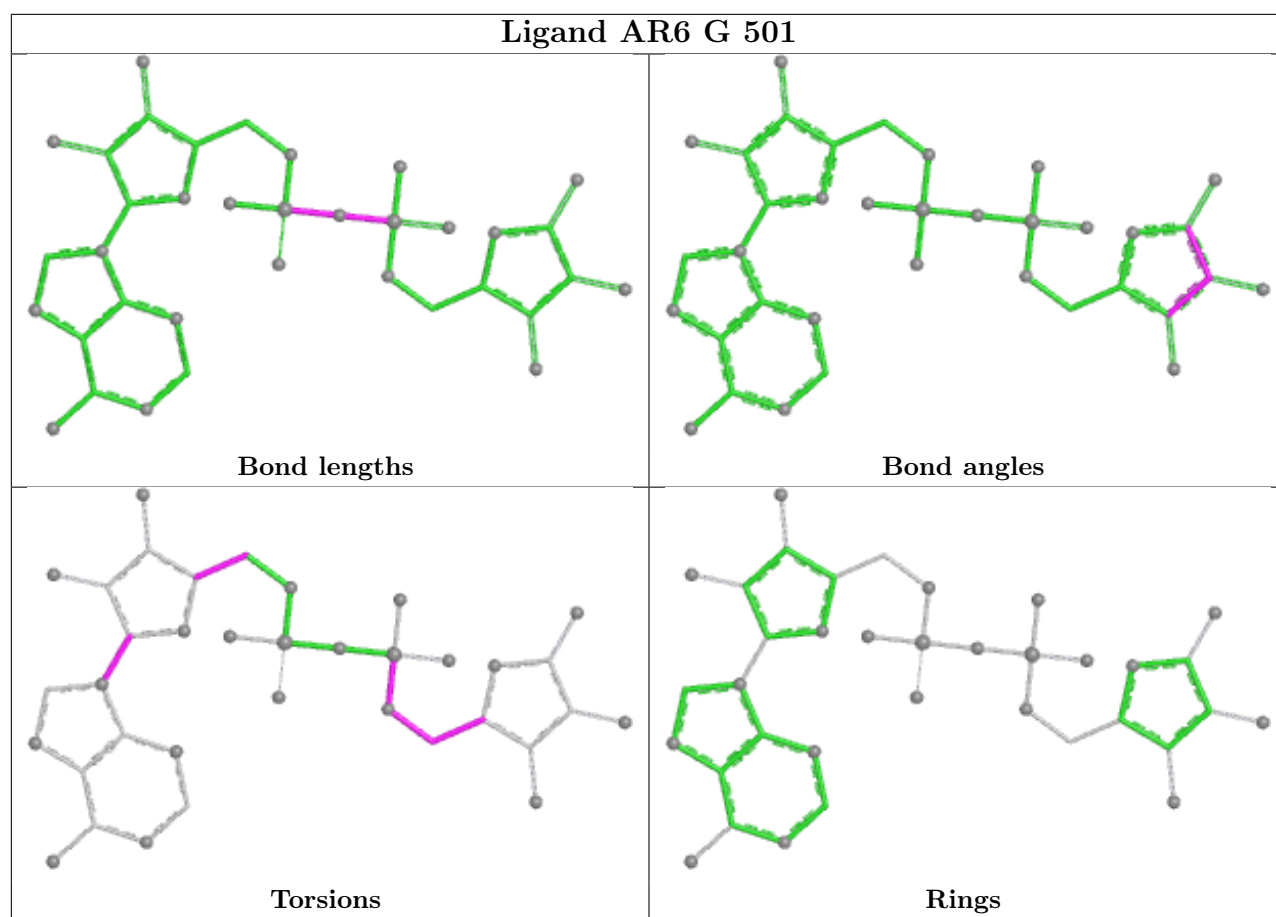
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	701	ADP	1	0
4	Q	701	ADP	1	0

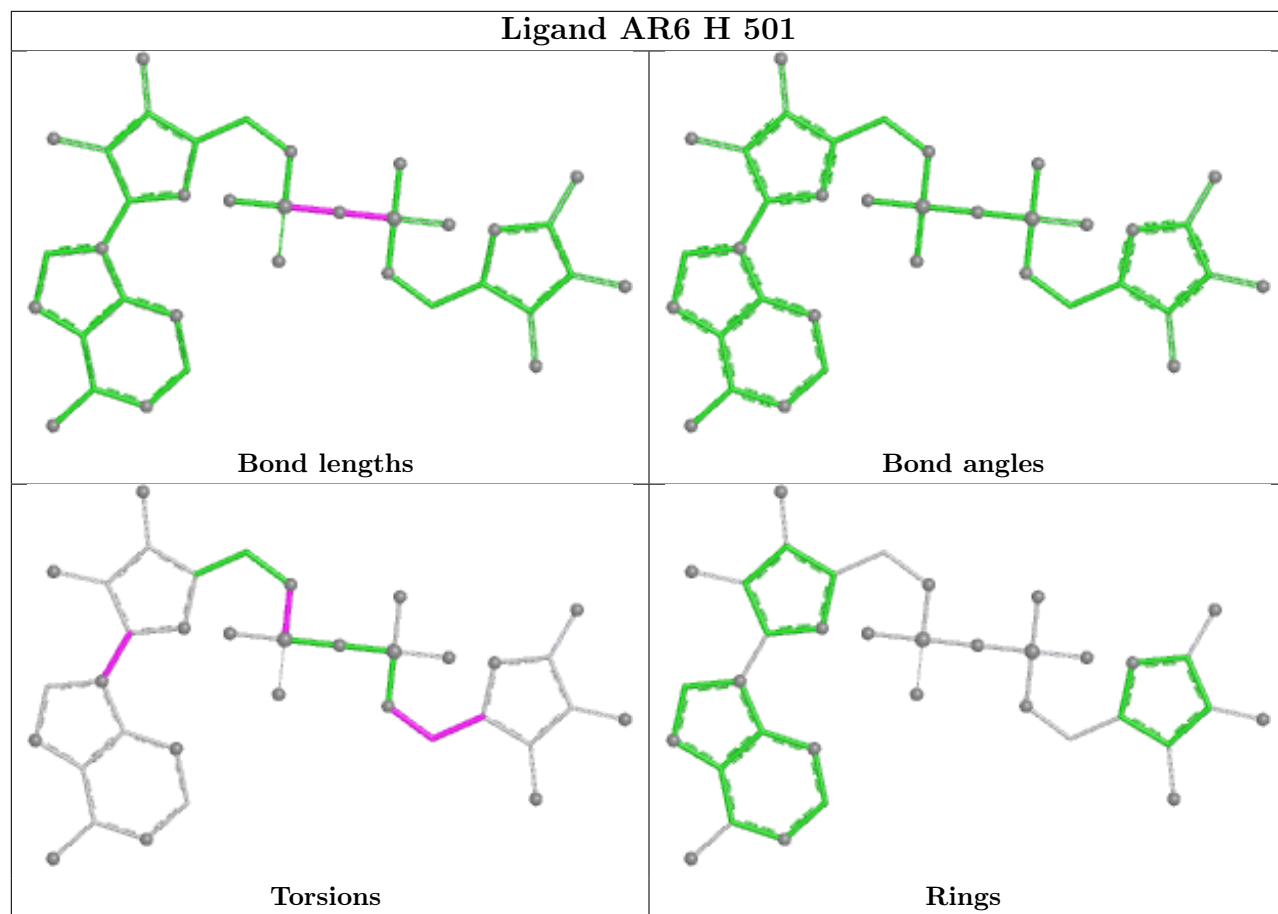
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

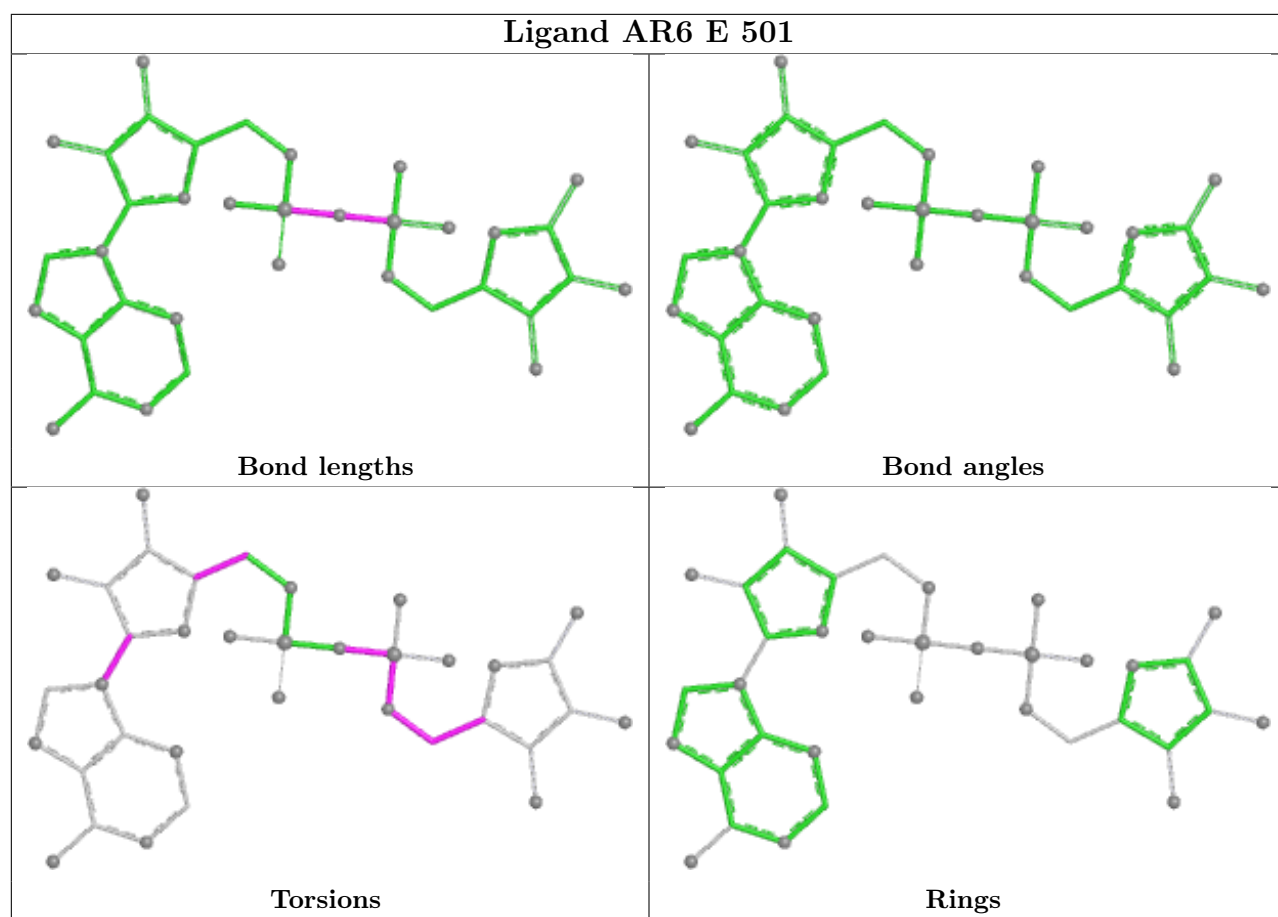
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

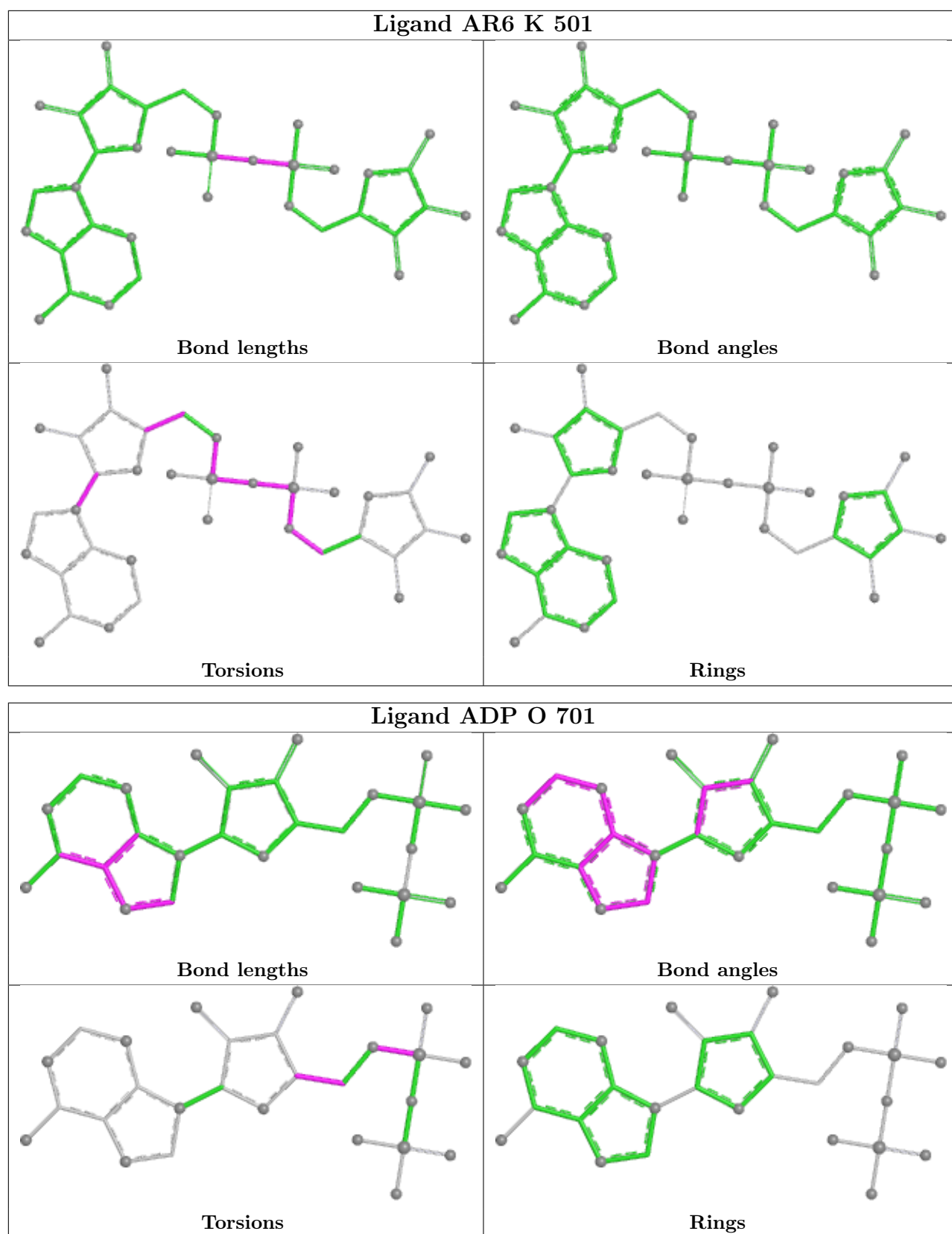


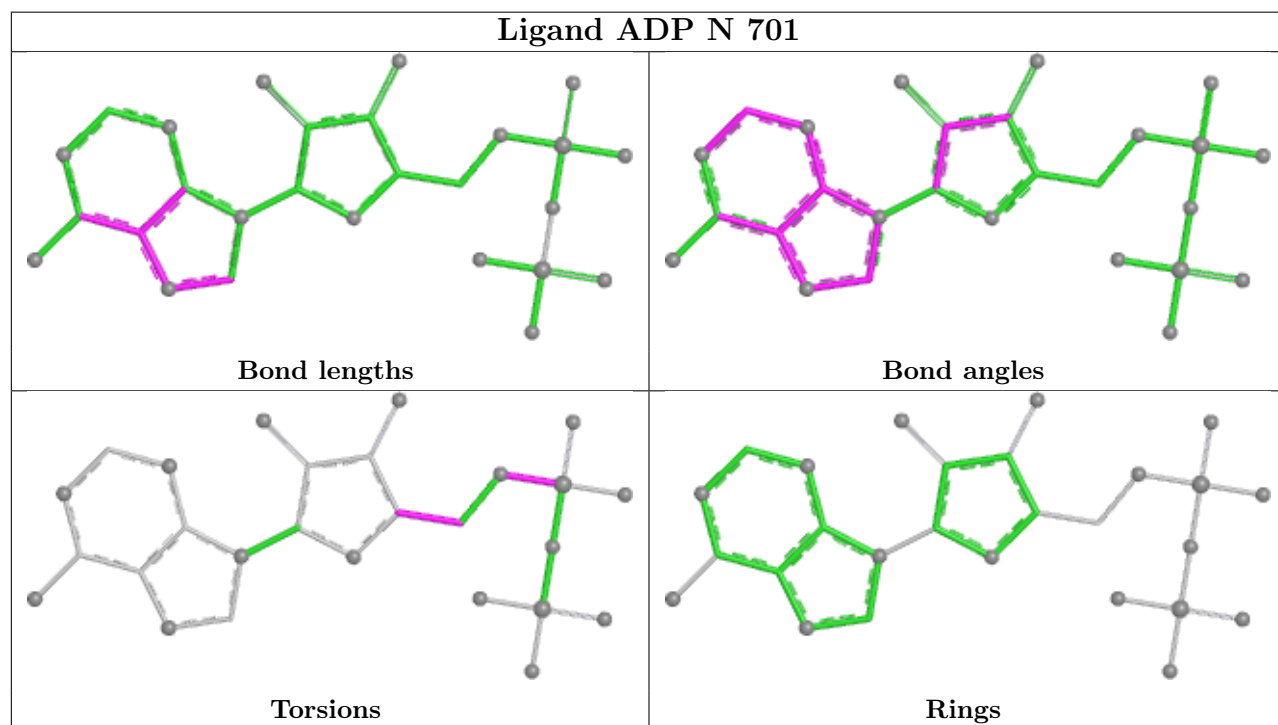
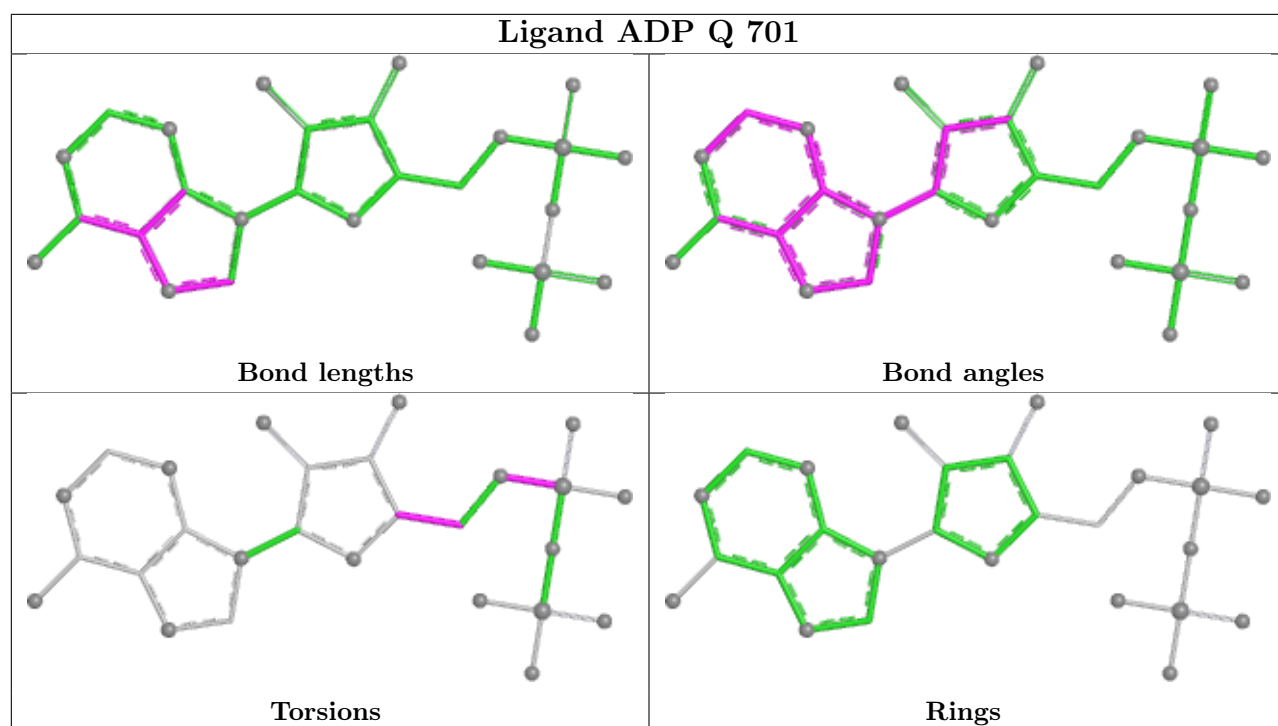


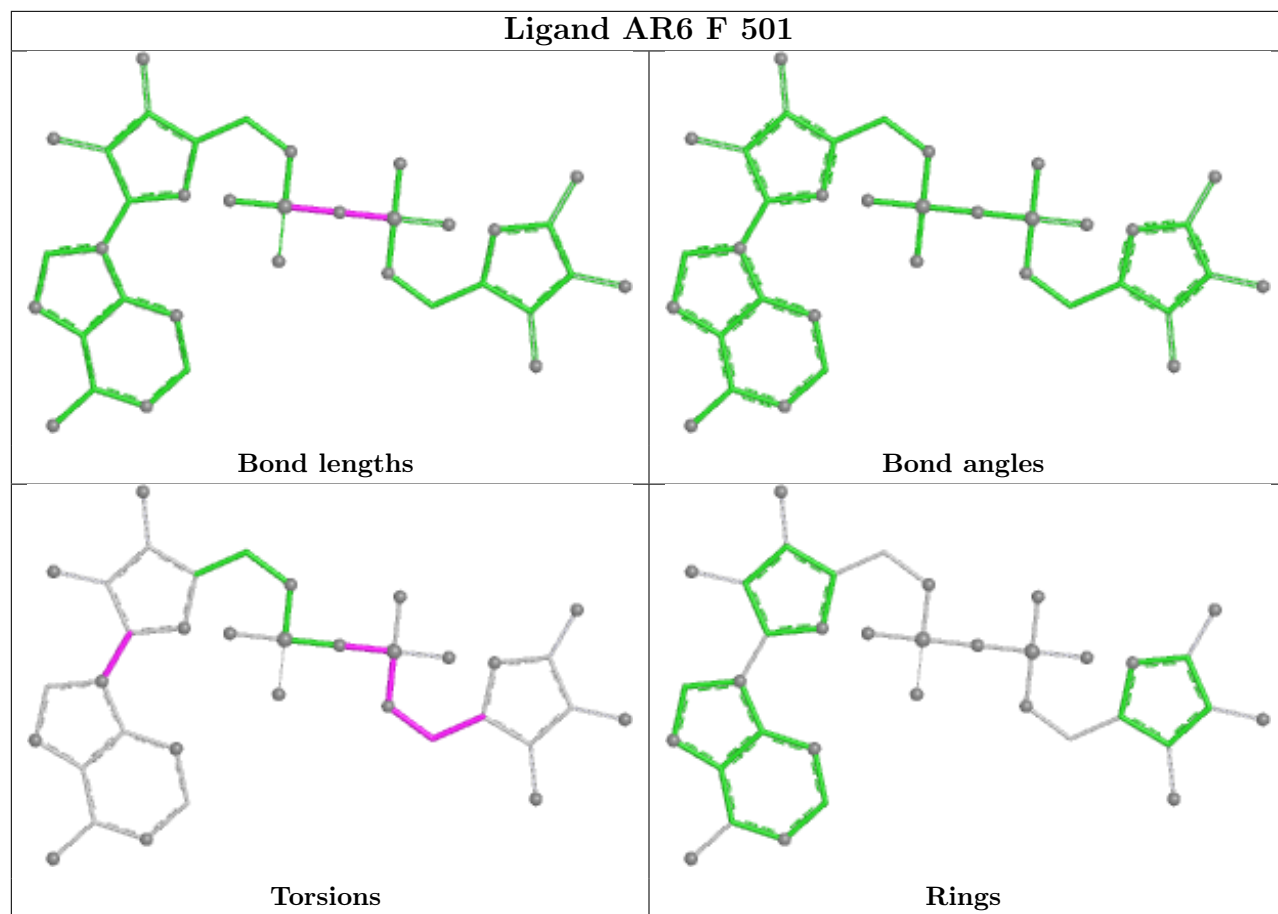


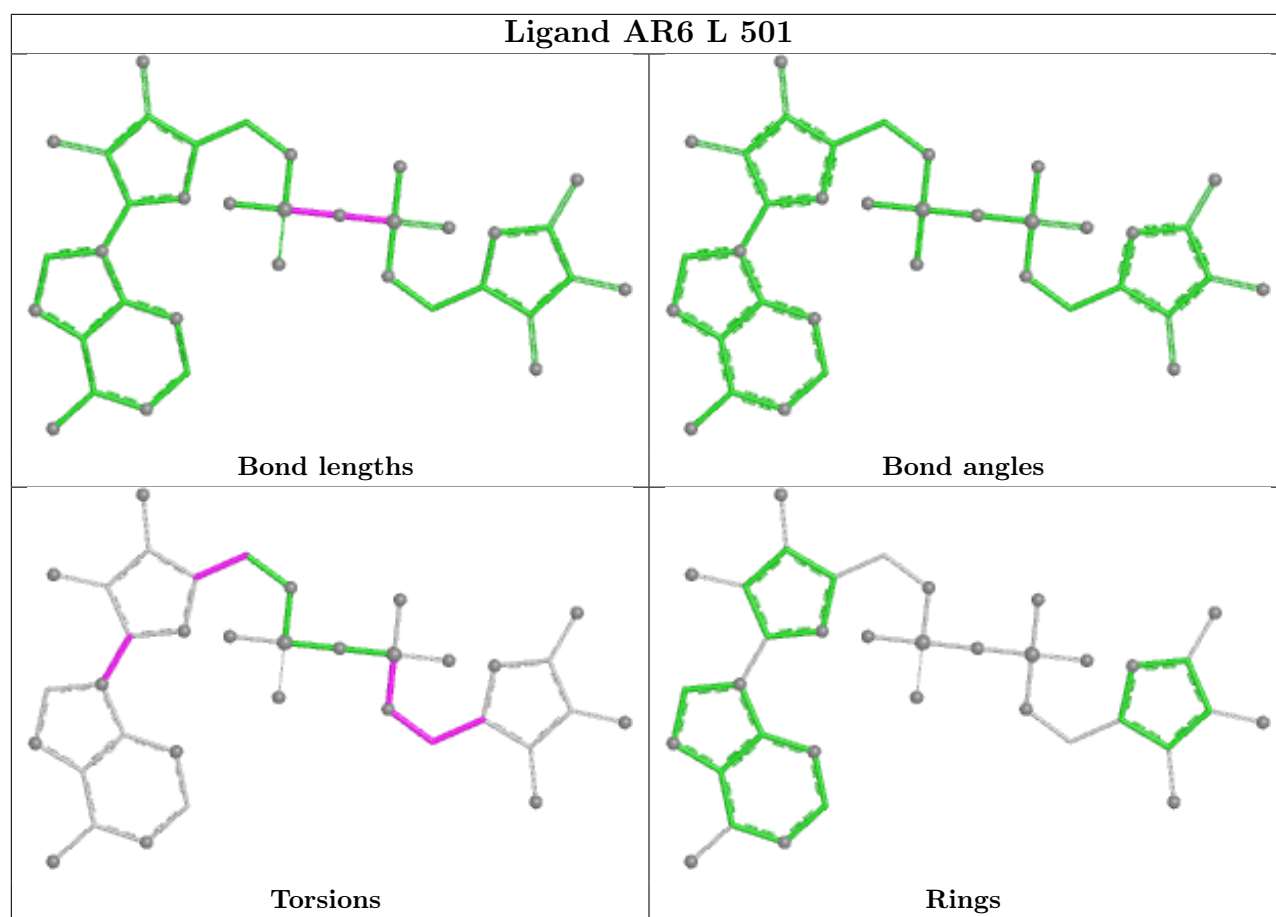


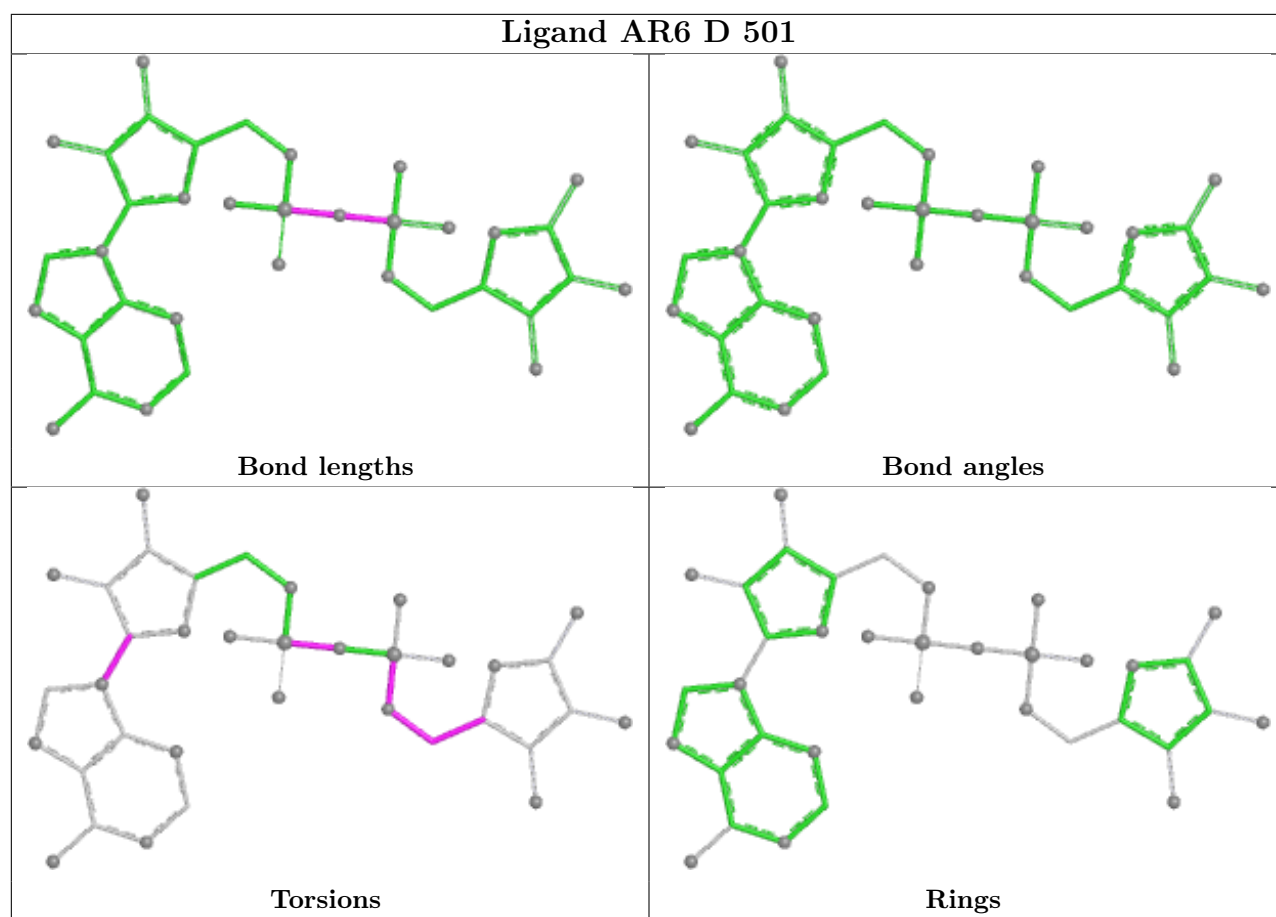




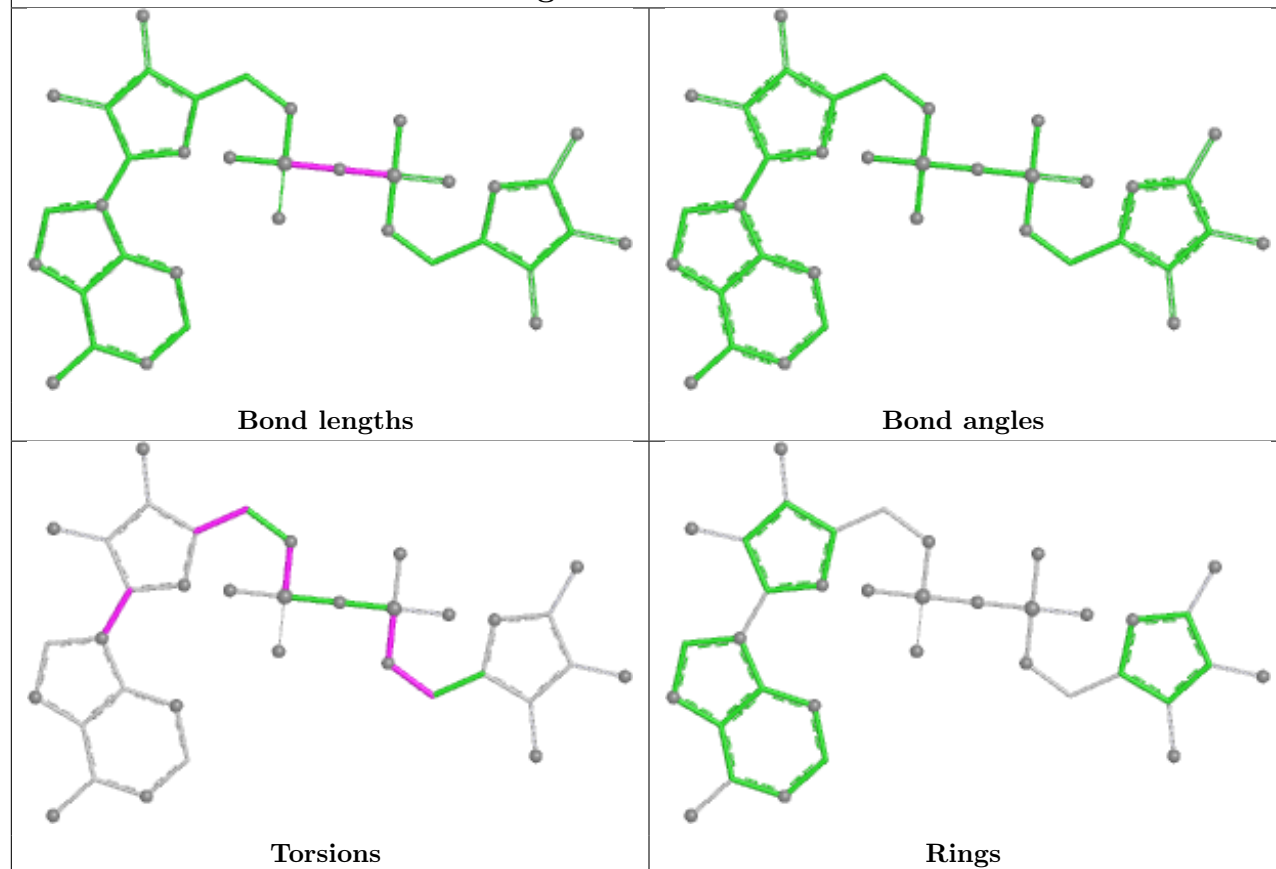




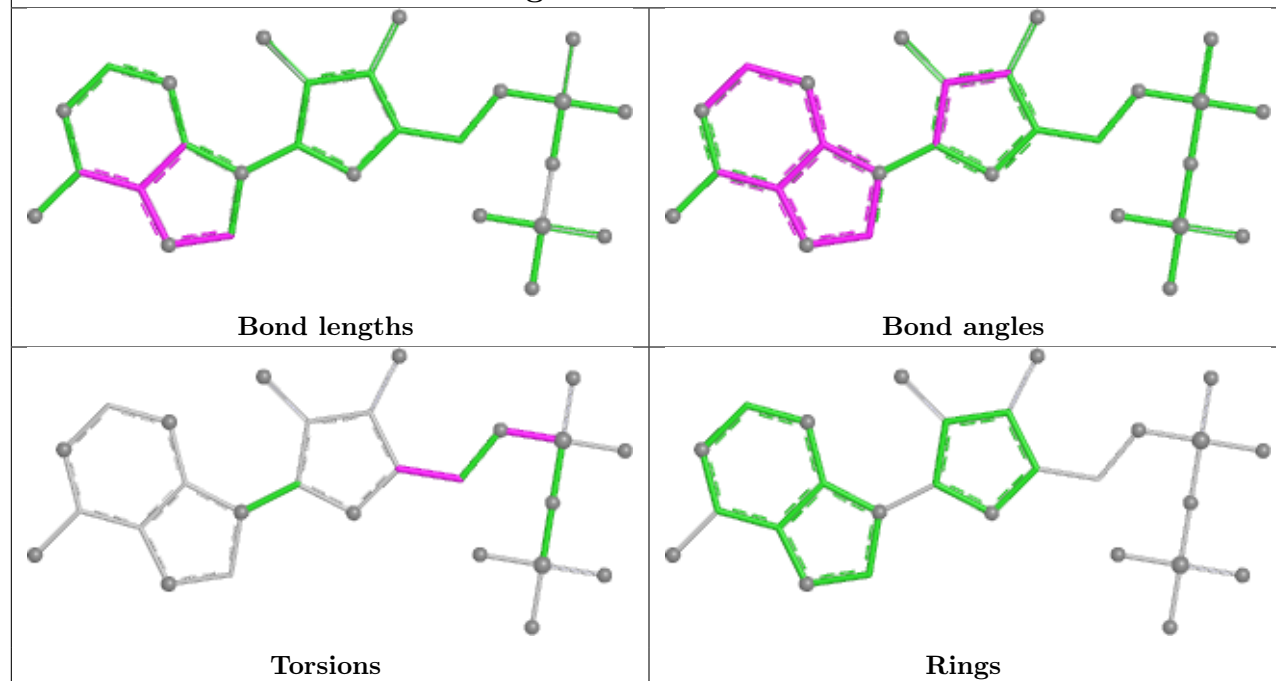


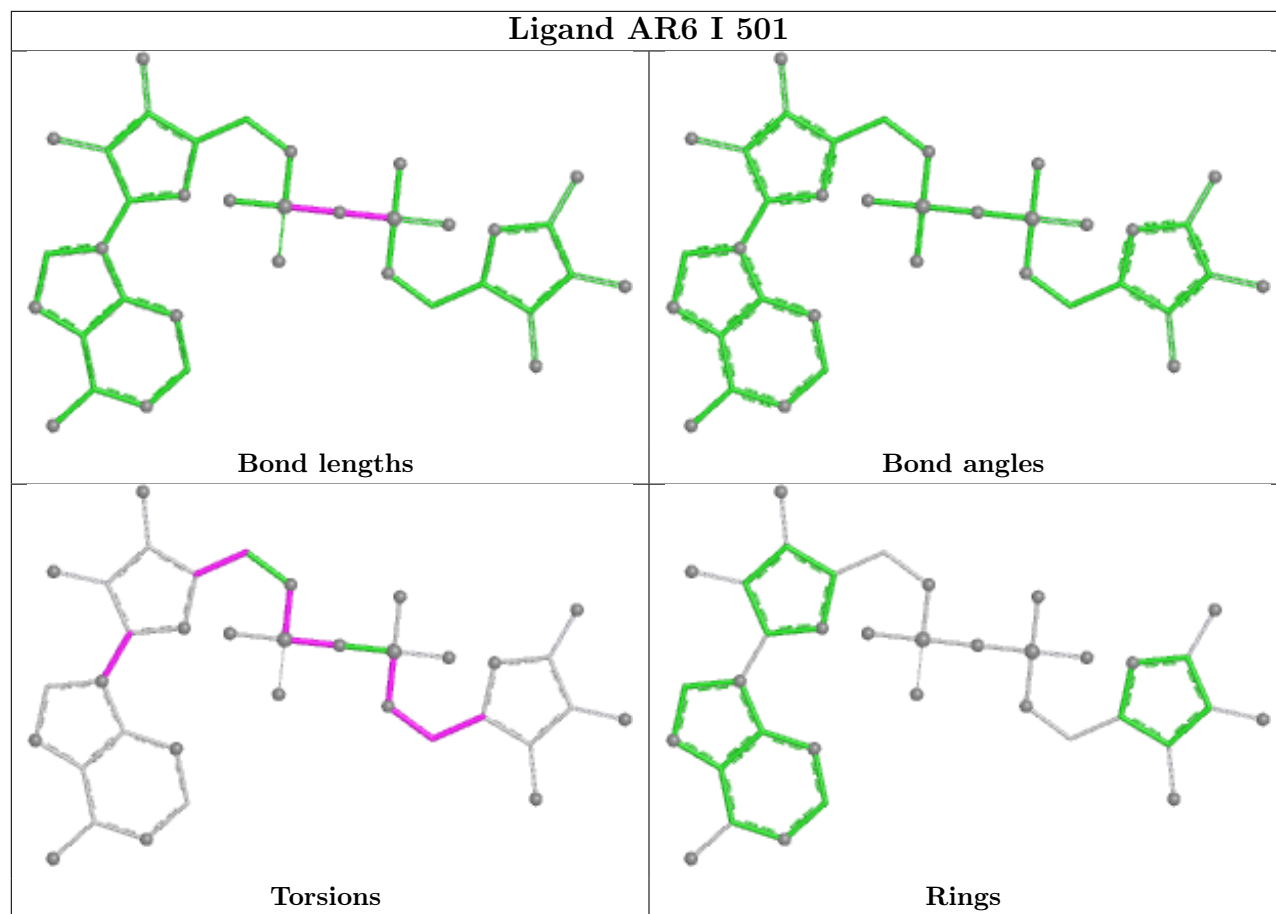


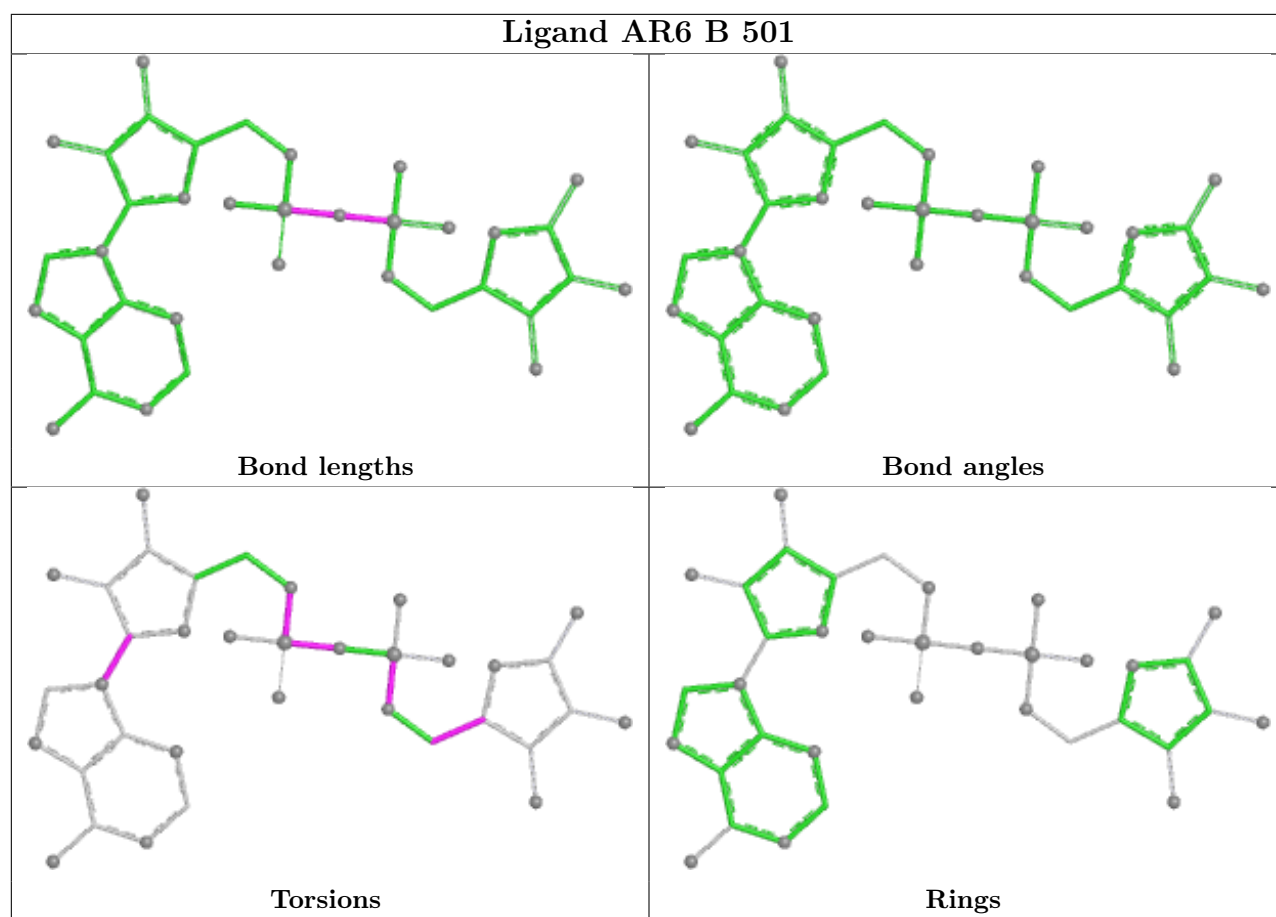
Ligand AR6 J 501

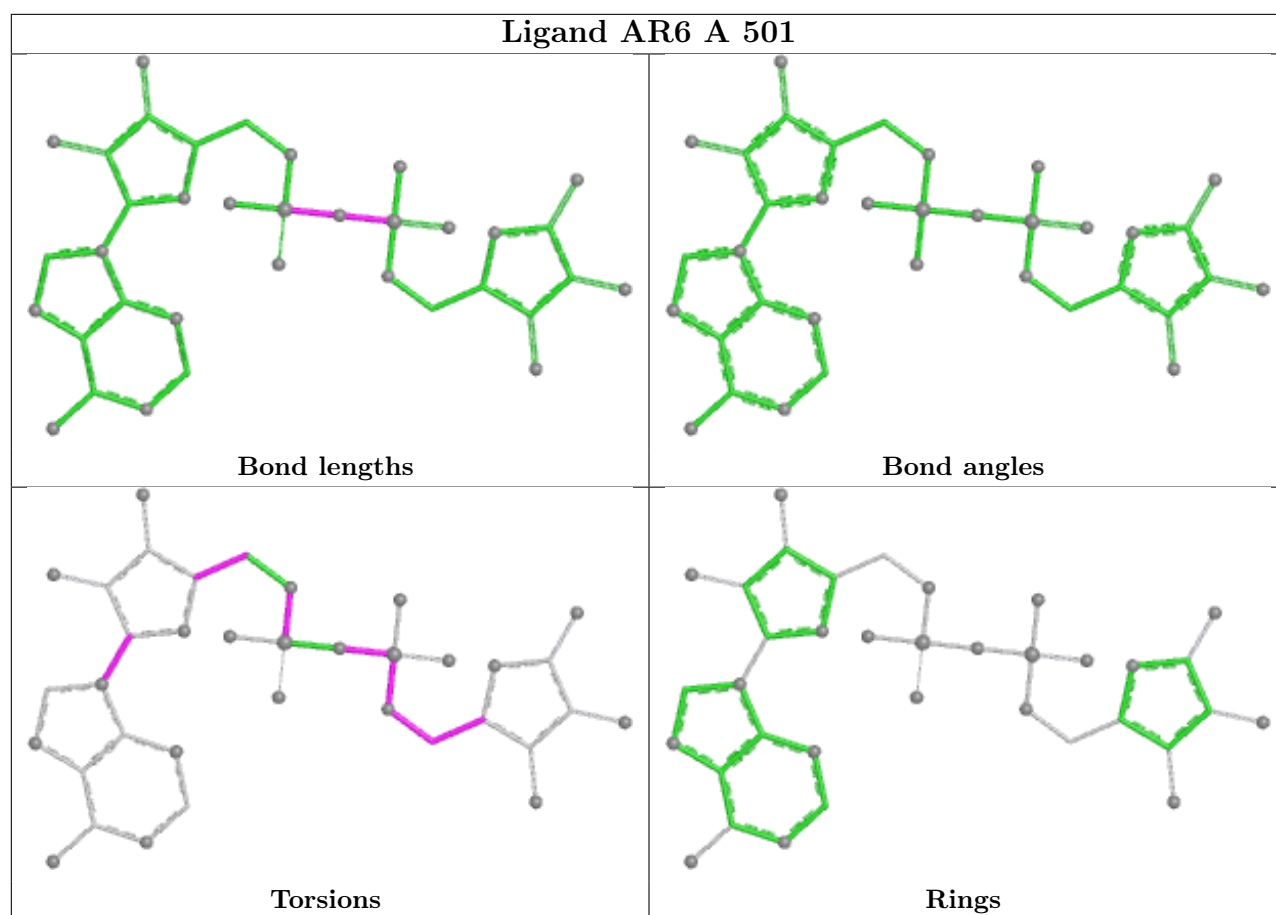


Ligand ADP M 701









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.

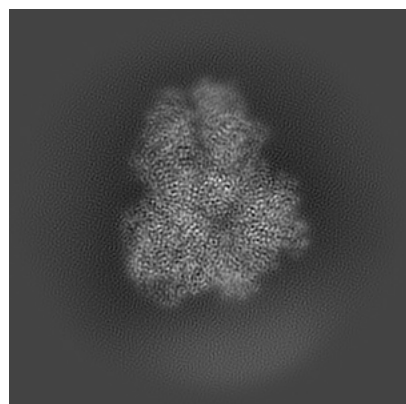
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40762. These allow visual inspection of the internal detail of the map and identification of artifacts.

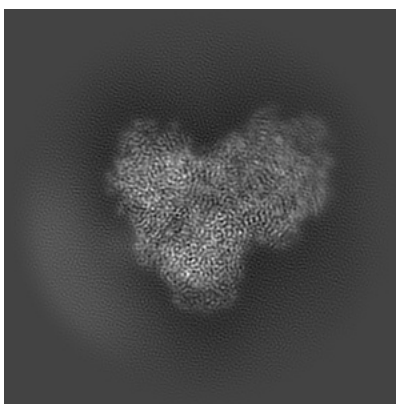
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

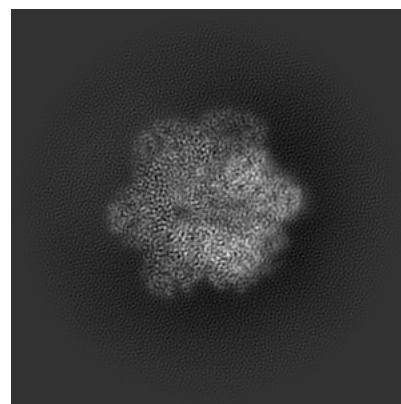
6.1.1 Primary map



X

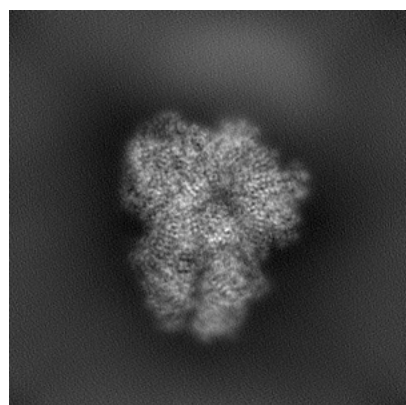


Y

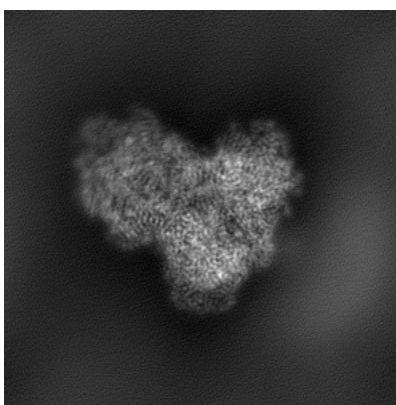


Z

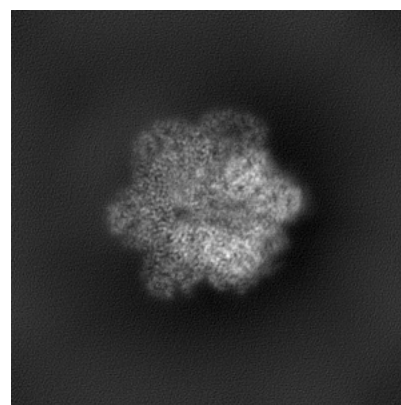
6.1.2 Raw map



X



Y

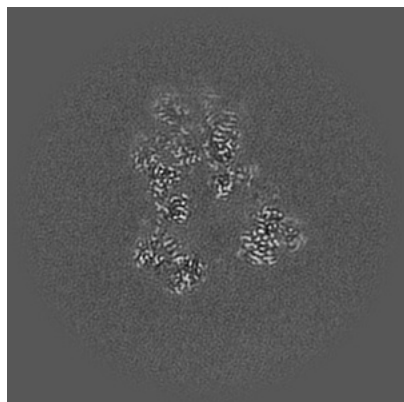


Z

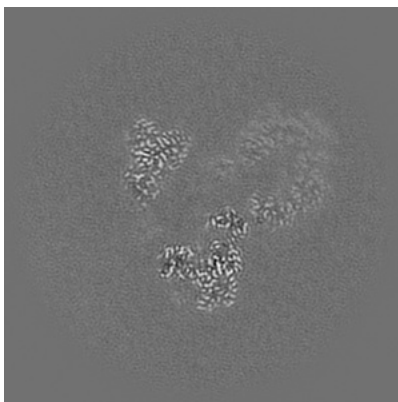
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

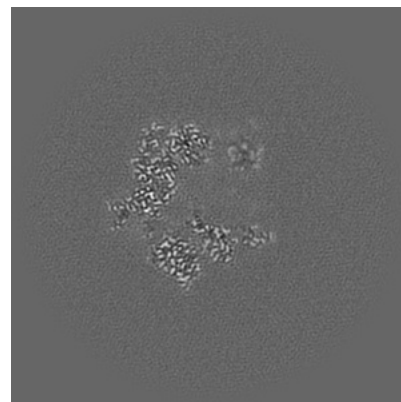
6.2.1 Primary map



X Index: 160

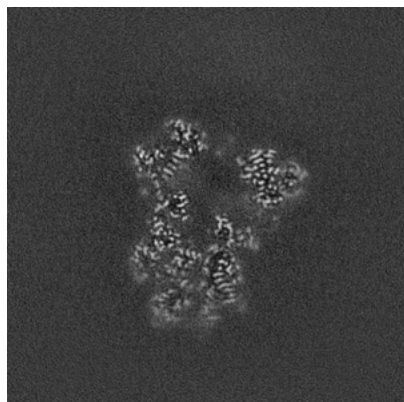


Y Index: 160

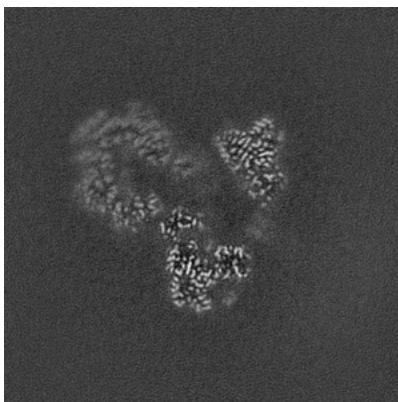


Z Index: 160

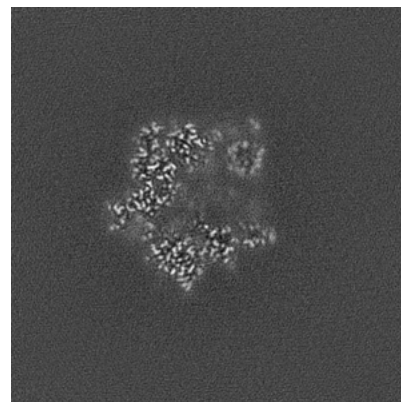
6.2.2 Raw map



X Index: 160



Y Index: 160

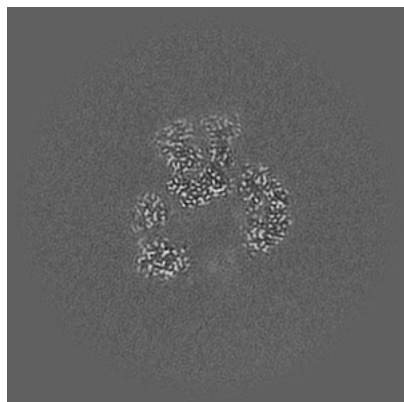


Z Index: 160

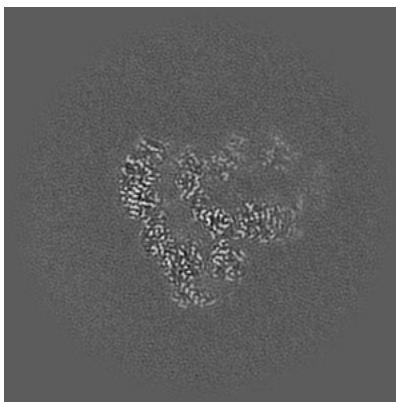
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

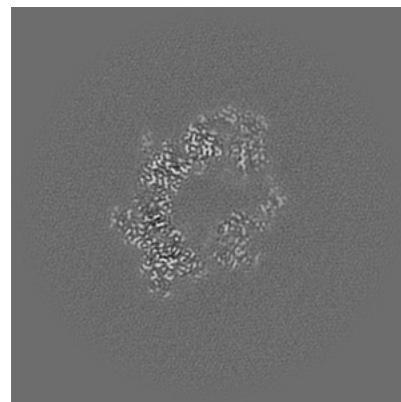
6.3.1 Primary map



X Index: 147

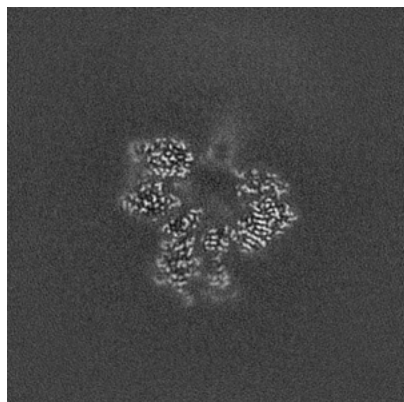


Y Index: 144

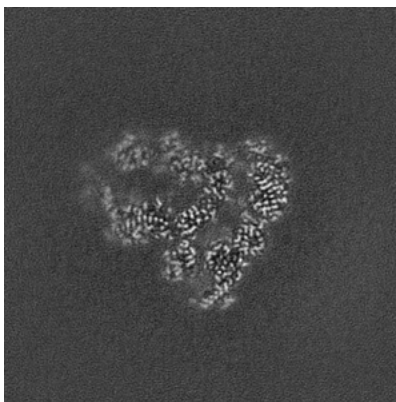


Z Index: 144

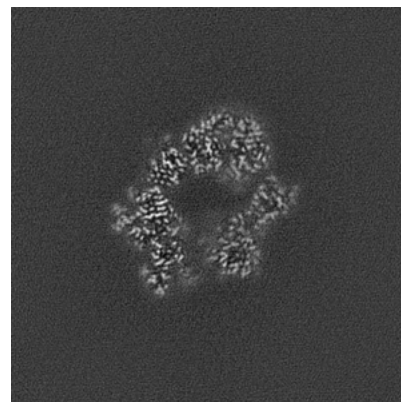
6.3.2 Raw map



X Index: 140



Y Index: 143

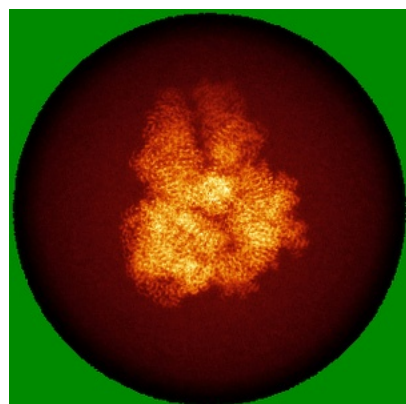


Z Index: 180

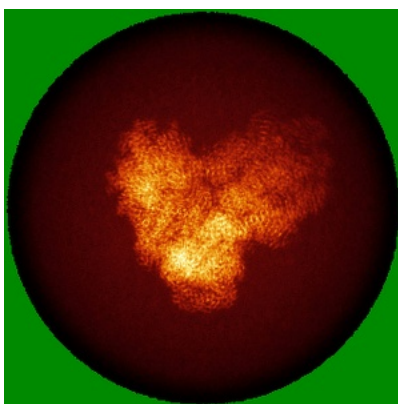
The images above show the largest variance slices of the map in three orthogonal directions.

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

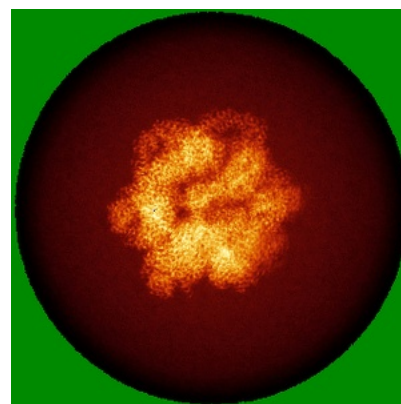
6.4.1 Primary map



X

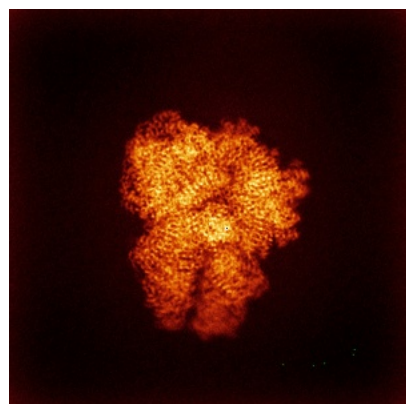


Y

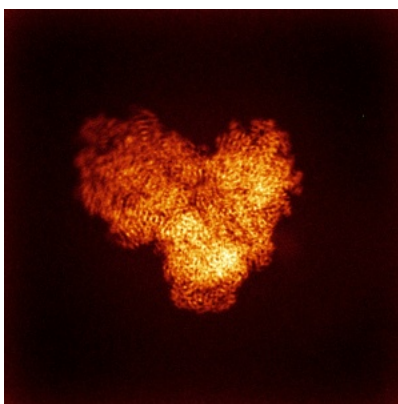


Z

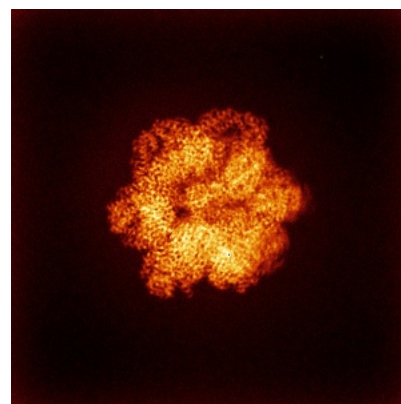
6.4.2 Raw map



X



Y

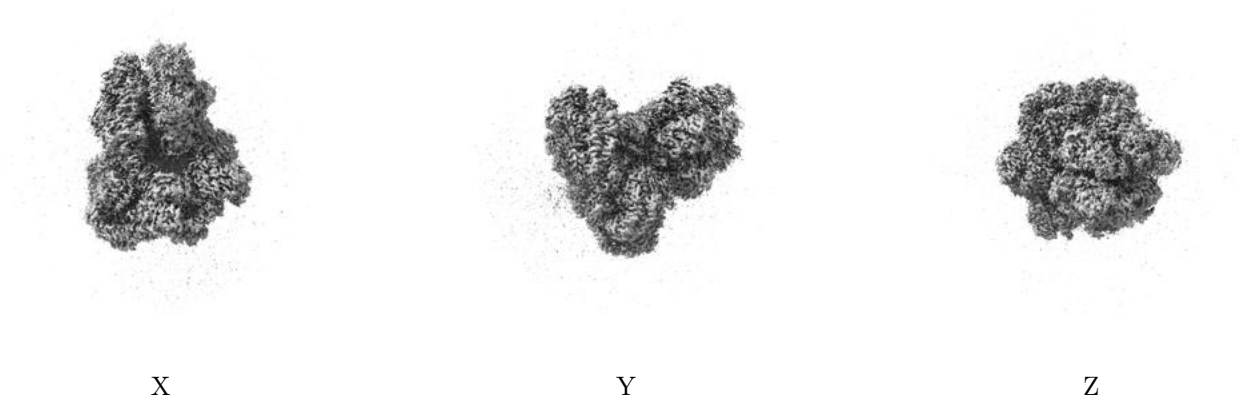


Z

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.

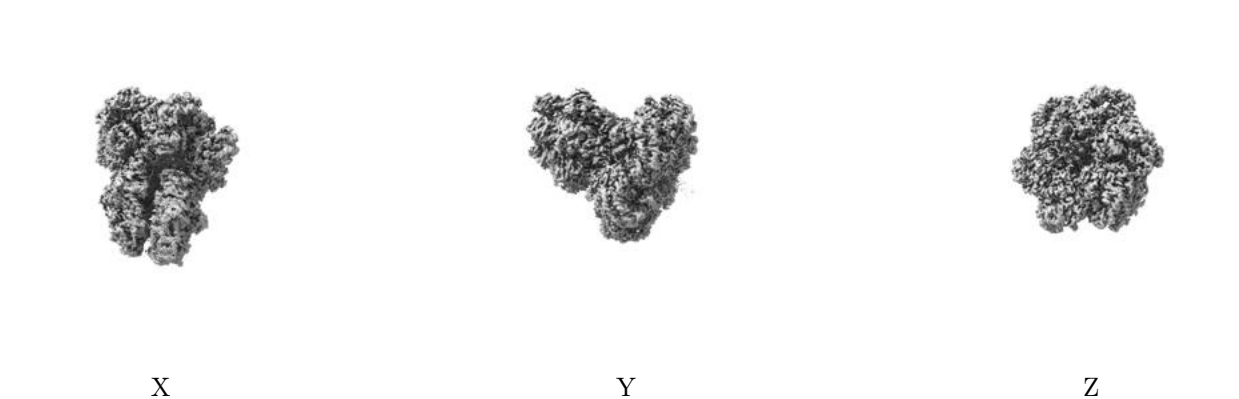
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.286. 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.

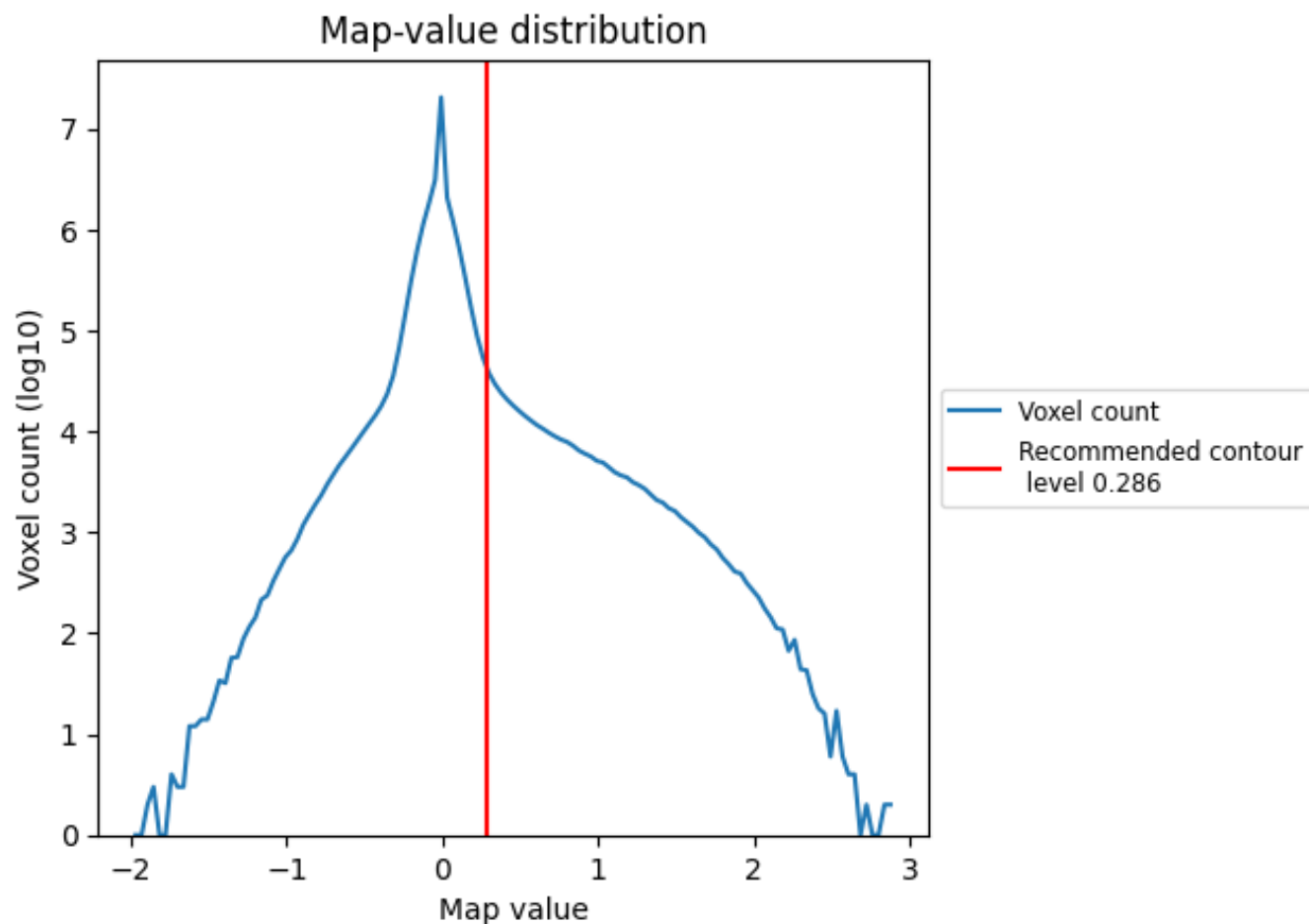
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

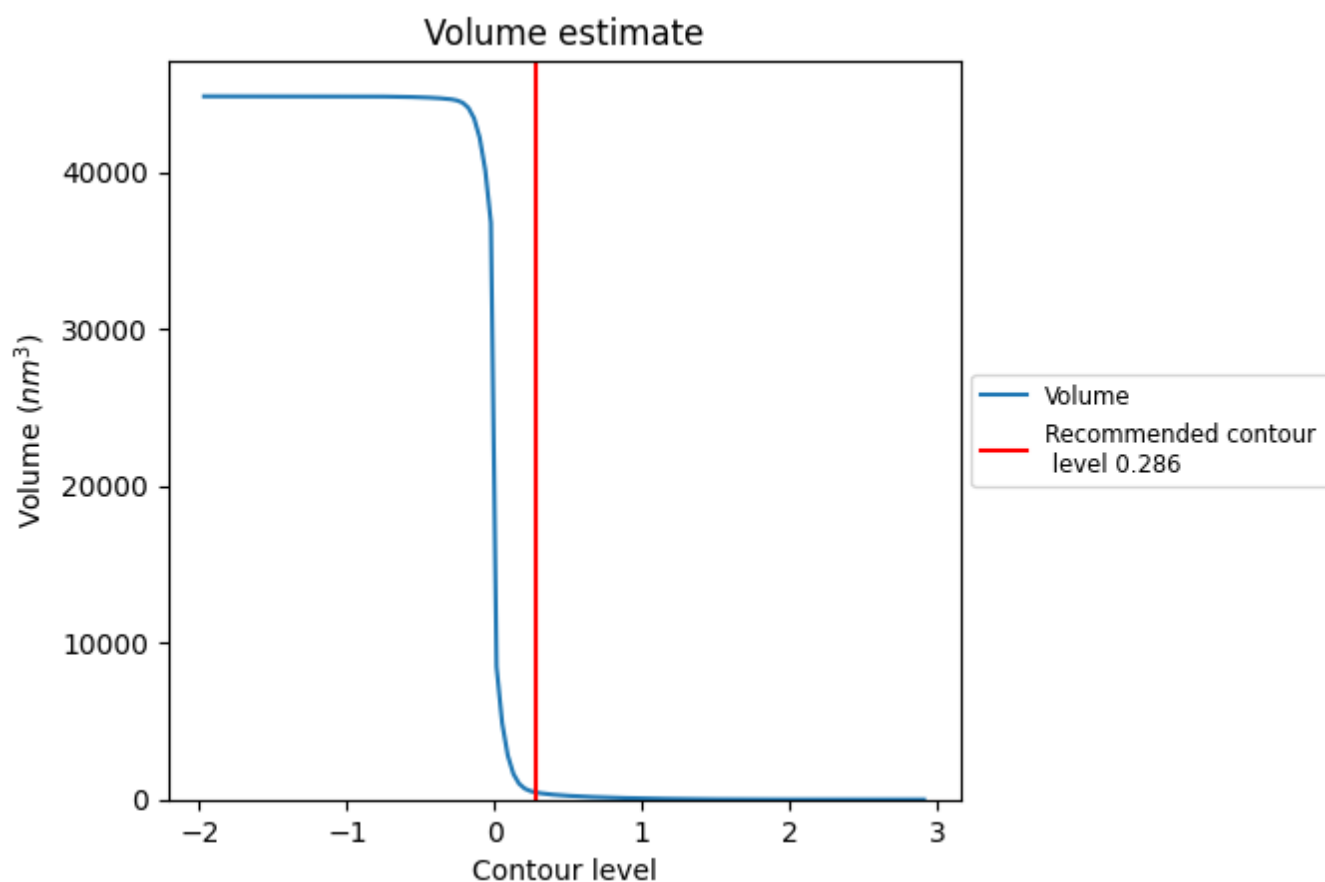
This section contains the results of statistical analysis of the map.

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.

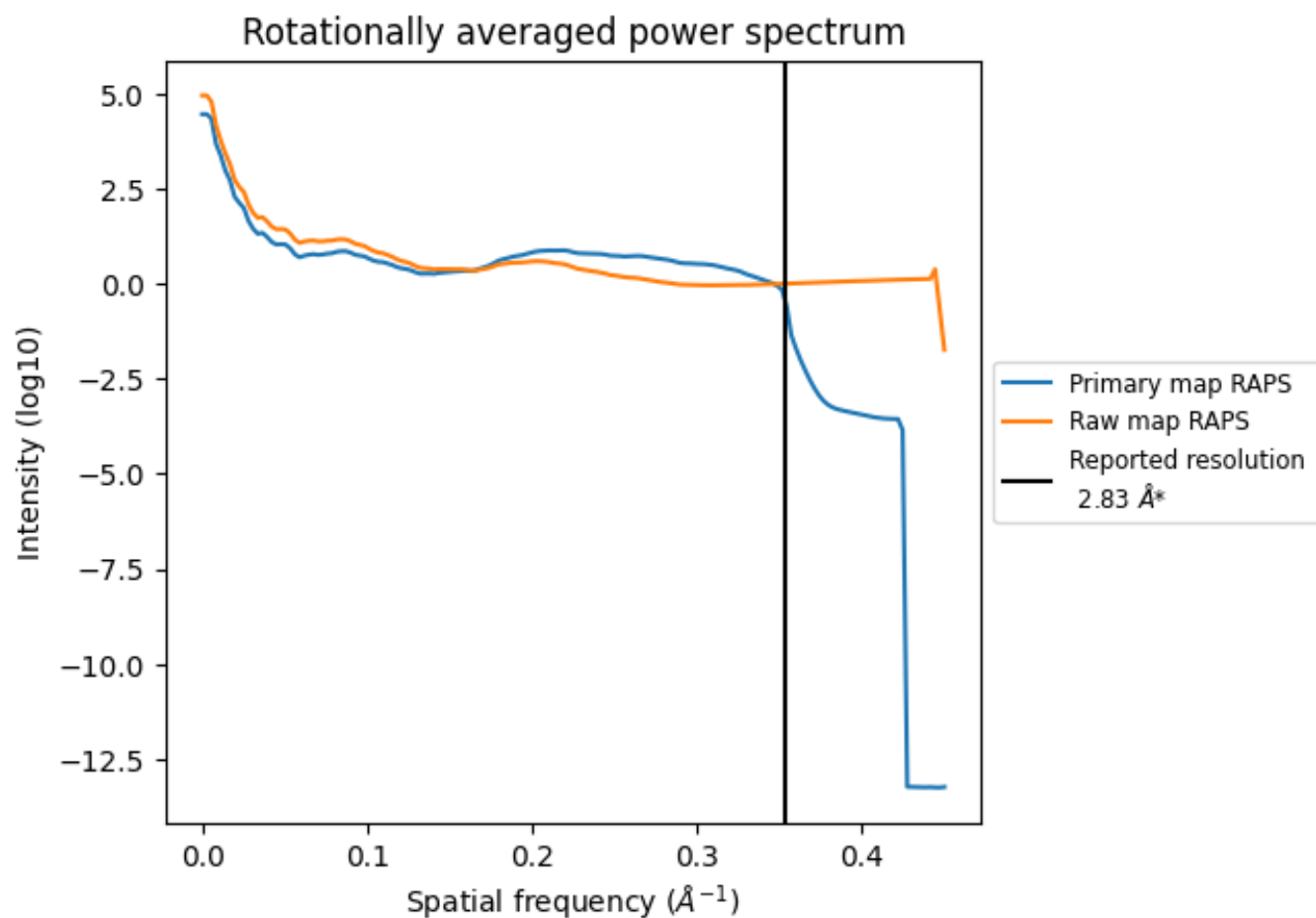
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 447 nm³; this corresponds to an approximate mass of 404 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

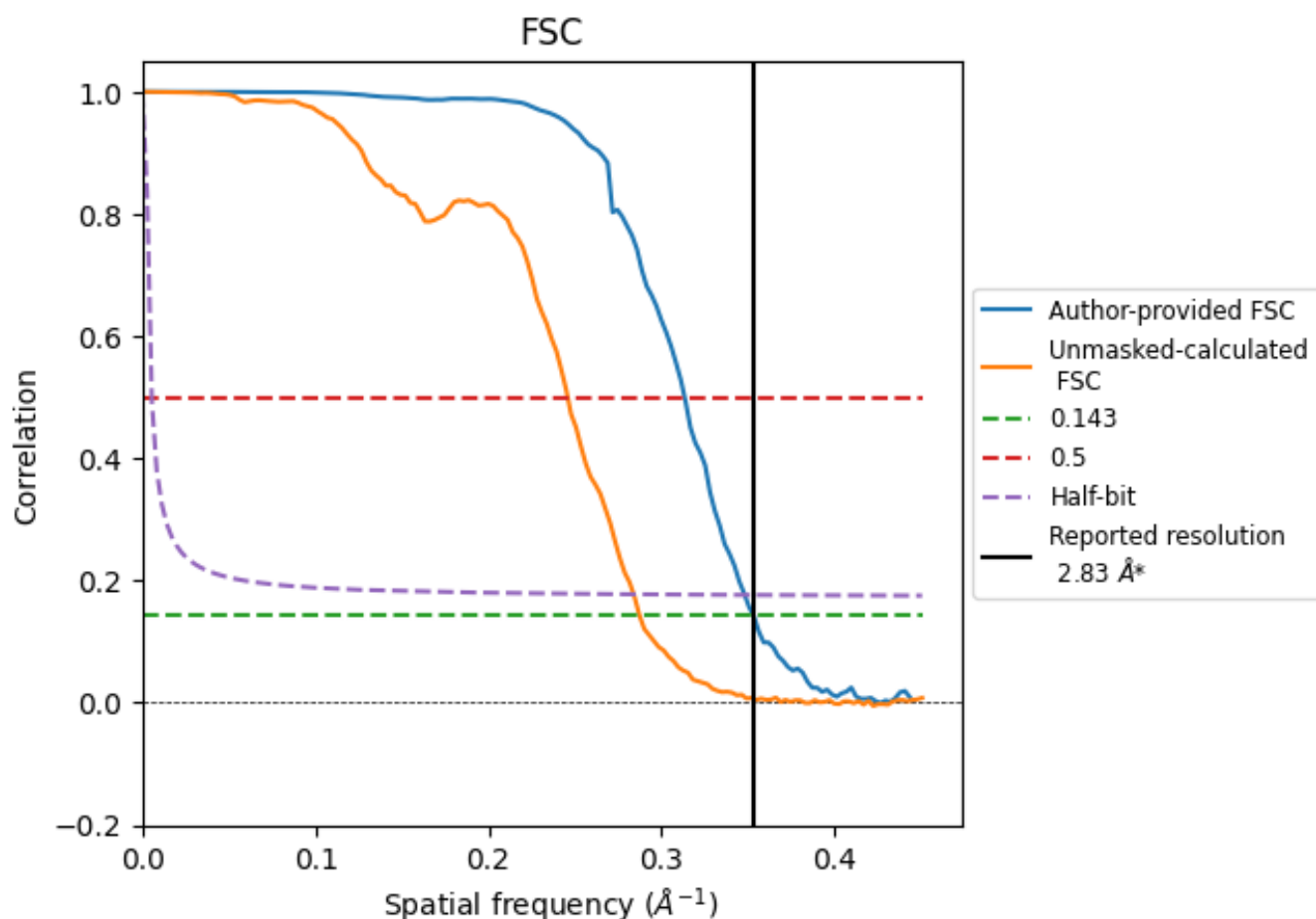


*Reported resolution corresponds to spatial frequency of 0.353 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.353 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

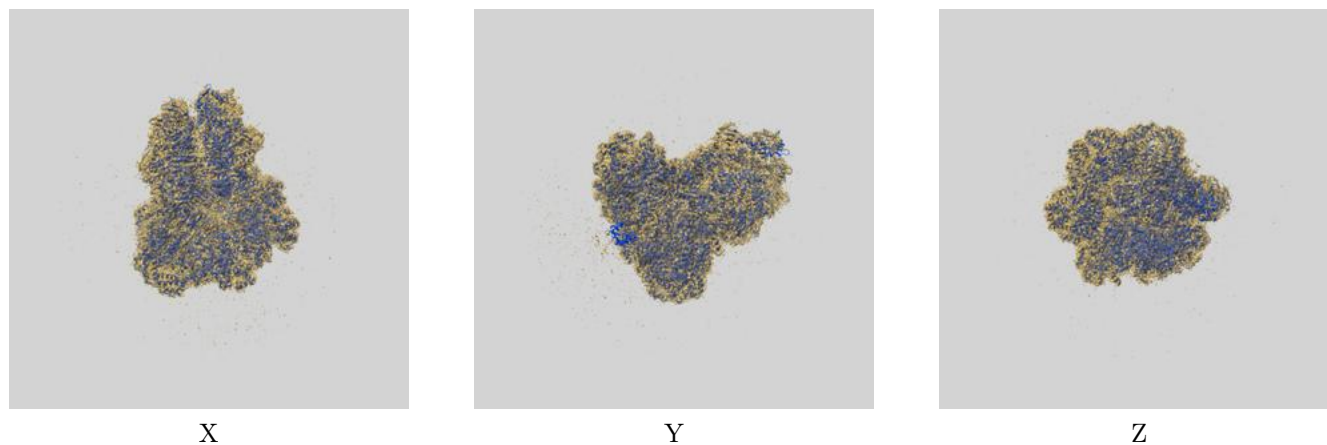
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.83	3.19	2.87
Unmasked-calculated*	3.48	4.07	3.52

*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 3.48 differs from the reported value 2.83 by more than 10 %

9 Map-model fit [i](#)

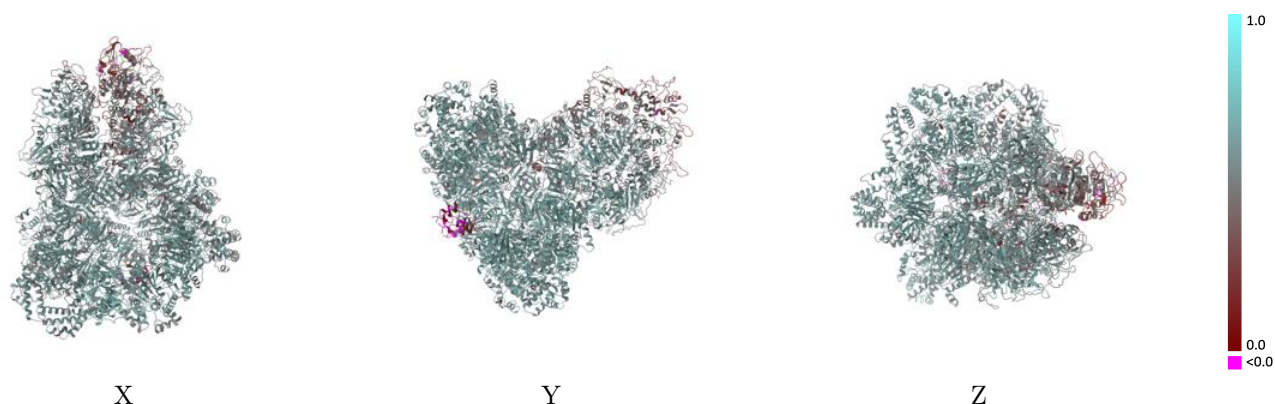
This section contains information regarding the fit between EMDB map EMD-40762 and PDB model 8SU9. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



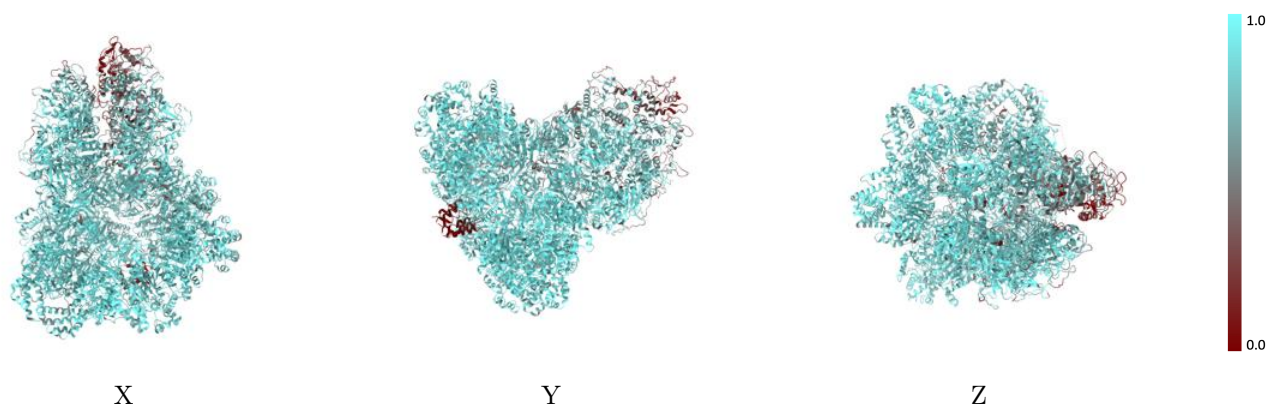
The images above show the 3D surface view of the map at the recommended contour level 0.286 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



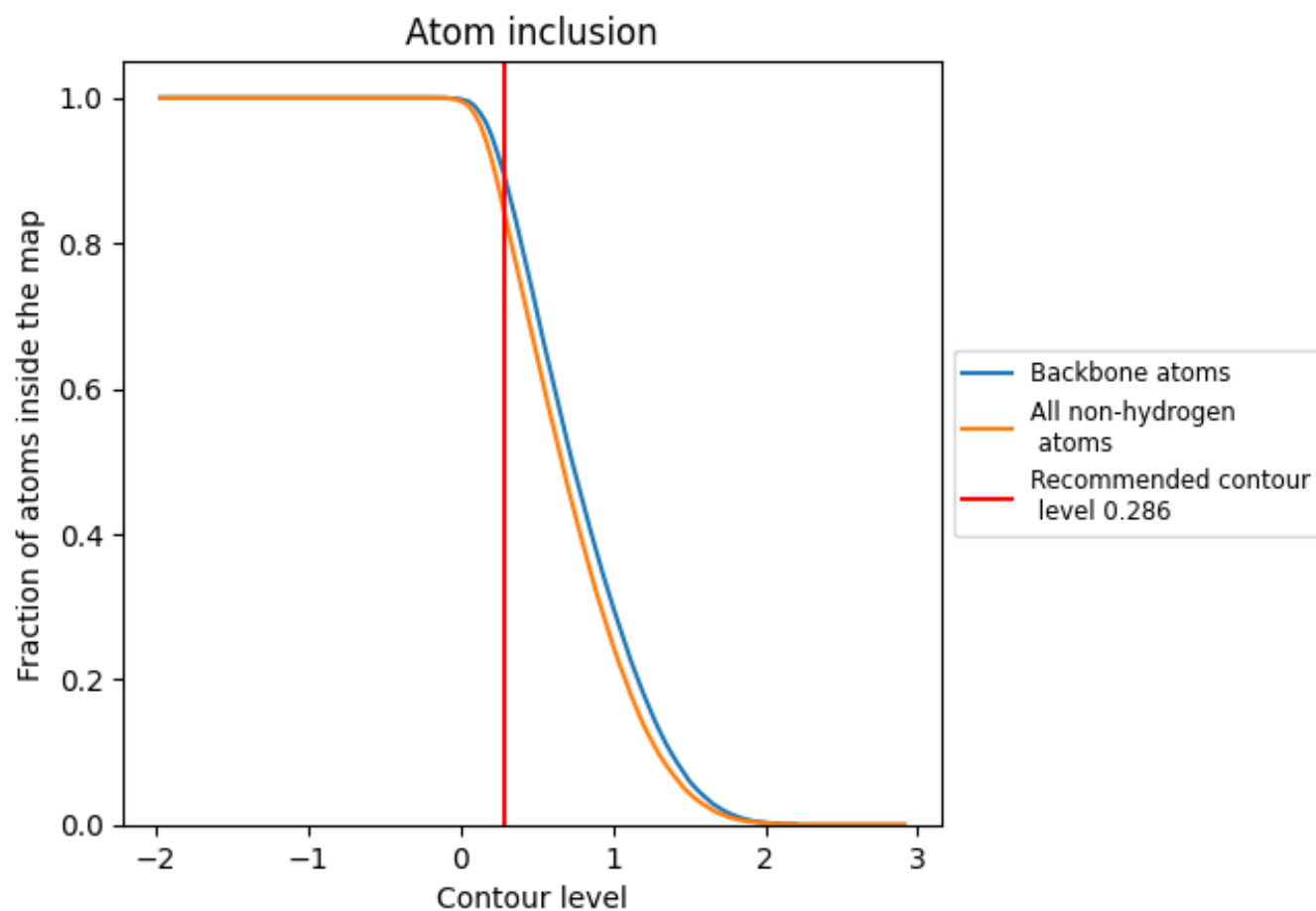
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.286).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 84% 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 (0.286) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8430	 0.5620
A	 0.9260	 0.6050
B	 0.8920	 0.5860
C	 0.8990	 0.5800
D	 0.8680	 0.5720
E	 0.8910	 0.5790
F	 0.8700	 0.5770
G	 0.8460	 0.5550
H	 0.8630	 0.5700
I	 0.9160	 0.5970
J	 0.8910	 0.5900
K	 0.9370	 0.6130
L	 0.8950	 0.5910
M	 0.8090	 0.5400
N	 0.8770	 0.5850
O	 0.8370	 0.5620
P	 0.8110	 0.5420
Q	 0.7650	 0.5230
R	 0.5220	 0.4090

