wwPDB EM Validation Summary Report (i)

Aug 17, 2026 – 04:50 PM JST

PDB ID	:	9WIE / pdb_00009wie
EMDB ID	:	EMD-65991
Title	:	AMP-PNP bound E.coli CnoX-GroEL/ES complex, state IV
Authors	:	Kim, J.; Roh, S.H.
Deposited on	:	2025-08-27
Resolution	:	2.79 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

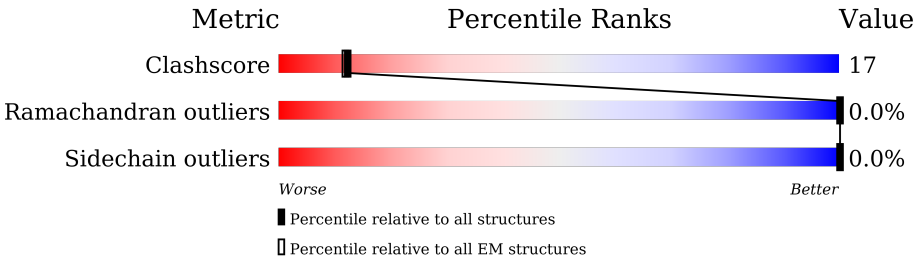
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

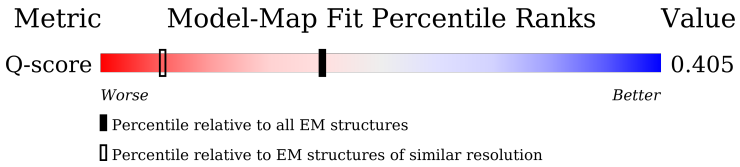
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.79 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	10811 (2.29 - 3.29)

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 <=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	548	78% 18% •
1	B	548	76% 21% •
1	C	548	78% 18% •
1	D	548	76% 20% •

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Mol	Chain	Length	Quality of chain
1	E	548	70% 26%
1	F	548	80% 17%
1	G	548	76% 20%
1	P	548	68% 28%
1	R	548	68% 28%
1	S	548	70% 26%
1	T	548	69% 27%
1	U	548	68% 28%
1	V	548	69% 27%
1	W	548	69% 27%
2	H	97	64% 35%
2	I	97	58% 41%
2	J	97	61% 38%
2	K	97	57% 42%
2	L	97	67% 31%
2	M	97	65% 34%
2	N	97	62% 37%
3	d	284	13% 18% 69%
3	e	284	14% 17% 69%
3	f	284	13% 18% 69%
3	g	284	13% 18% 69%
3	h	284	13% 18% 69%
3	i	284	13% 18% 69%
3	j	284	13% 18% 69%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 64638 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 Chaperonin GroEL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	527	3880	2412	670	777	21	0	0
1	B	527	3880	2412	670	777	21	0	0
1	C	527	3880	2412	670	777	21	0	0
1	D	527	3880	2412	670	777	21	0	0
1	E	527	3880	2412	670	777	21	0	0
1	F	527	3880	2412	670	777	21	0	0
1	G	527	3880	2412	670	777	21	0	0
1	P	527	3880	2412	670	777	21	0	0
1	R	527	3880	2412	670	777	21	0	0
1	S	527	3880	2412	670	777	21	0	0
1	T	527	3880	2412	670	777	21	0	0
1	U	527	3880	2412	670	777	21	0	0
1	V	527	3880	2412	670	777	21	0	0
1	W	527	3880	2412	670	777	21	0	0

- Molecule 2 is a protein called Co-chaperonin GroES.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	96	720	449	126	144	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	I	96	720	449	126	144	1	0	0
2	J	96	720	449	126	144	1	0	0
2	K	96	720	449	126	144	1	0	0
2	L	96	720	449	126	144	1	0	0
2	M	96	720	449	126	144	1	0	0
2	N	96	720	449	126	144	1	0	0

- Molecule 3 is a protein called Chaperedoxin.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	d	88	689	430	123	136	0	0
3	e	88	689	430	123	136	0	0
3	f	88	689	430	123	136	0	0
3	g	88	689	430	123	136	0	0
3	h	88	689	430	123	136	0	0
3	i	88	689	430	123	136	0	0
3	j	88	689	430	123	136	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	A	1	1	1	0
4	B	1	1	1	0
4	C	1	1	1	0
4	D	1	1	1	0

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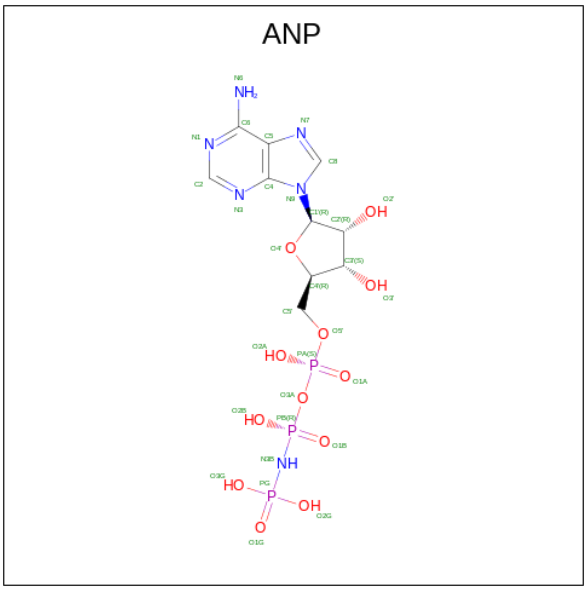
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	E	1	1	1	0
4	F	1	1	1	0
4	G	1	1	1	0
4	P	1	1	1	0
4	R	1	1	1	0
4	S	1	1	1	0
4	T	1	1	1	0
4	U	1	1	1	0
4	V	1	1	1	0
4	W	1	1	1	0

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	A	1	31	10	6	12	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	B	1	31	10	6	12	3	0
5	C	1	31	10	6	12	3	0
5	D	1	31	10	6	12	3	0
5	E	1	31	10	6	12	3	0
5	F	1	31	10	6	12	3	0
5	G	1	31	10	6	12	3	0
5	P	1	31	10	6	12	3	0
5	R	1	31	10	6	12	3	0
5	S	1	31	10	6	12	3	0
5	T	1	31	10	6	12	3	0
5	U	1	31	10	6	12	3	0
5	V	1	31	10	6	12	3	0
5	W	1	31	10	6	12	3	0

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
6	P	1	1	1	0
6	R	1	1	1	0
6	S	1	1	1	0
6	T	1	1	1	0
6	U	1	1	1	0
6	V	1	1	1	0

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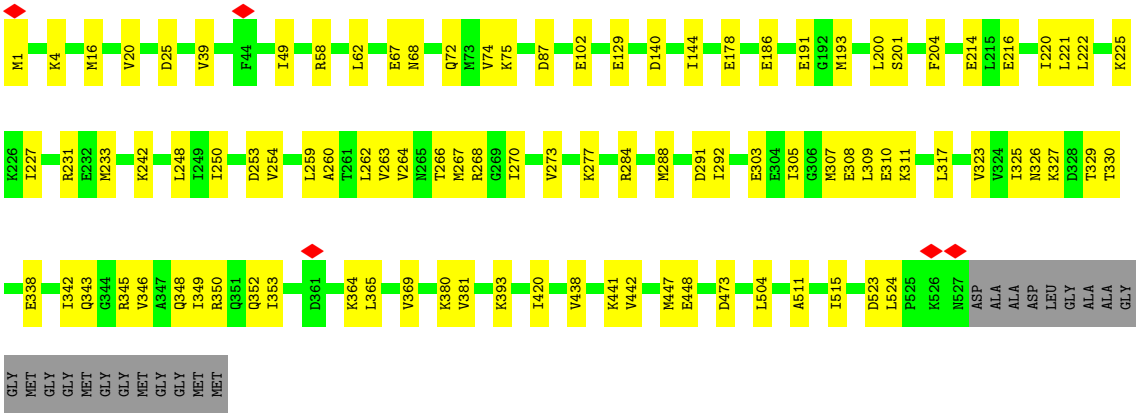
Mol	Chain	Residues	Atoms		AltConf
			Total	K	
6	W	1	1	1	0

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.

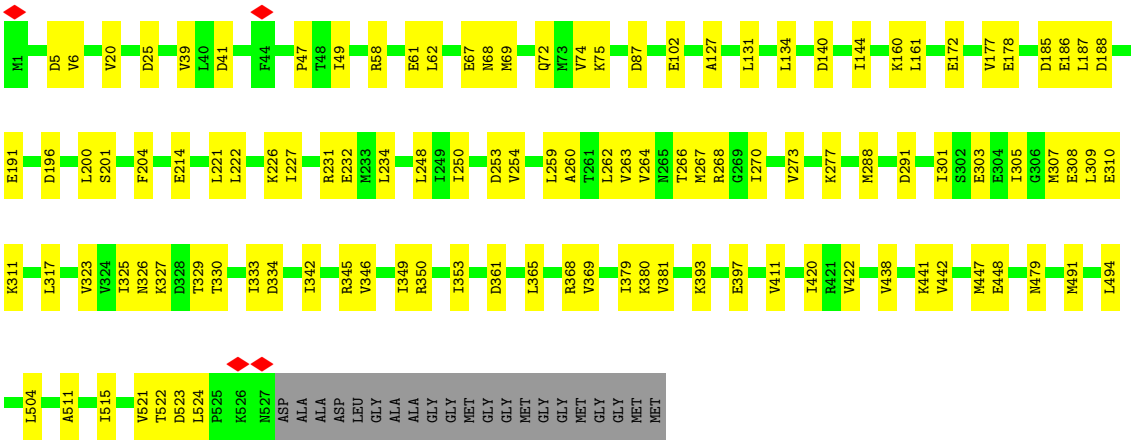
• Molecule 1: Chaperonin GroEL

Chain A:



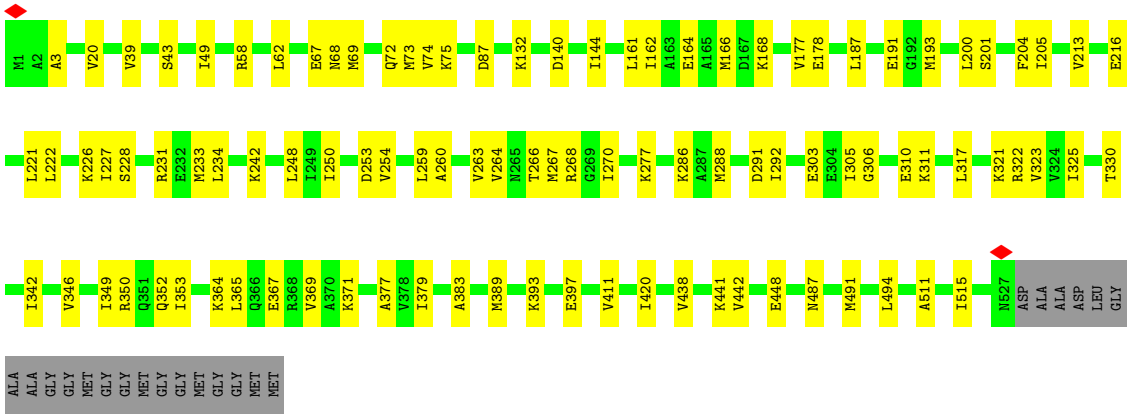
• Molecule 1: Chaperonin GroEL

Chain B:



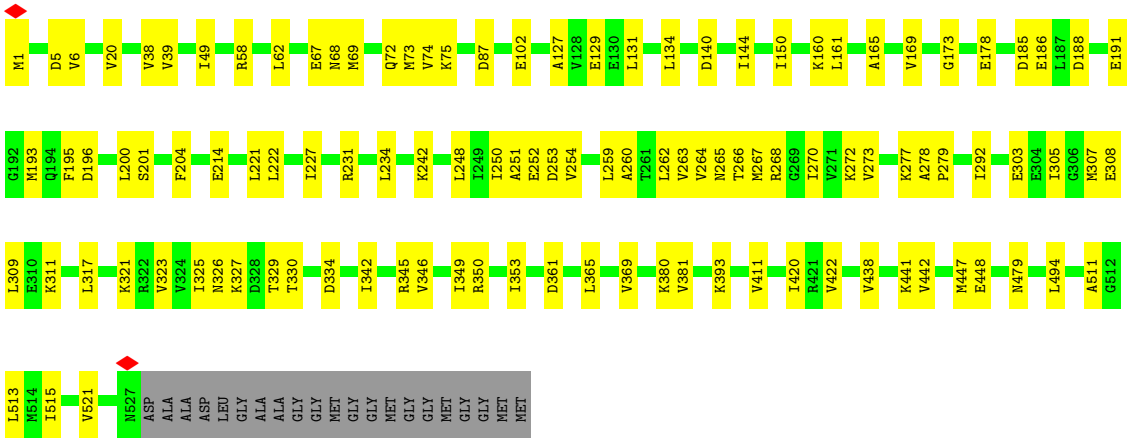
• Molecule 1: Chaperonin GroEL

Chain C:



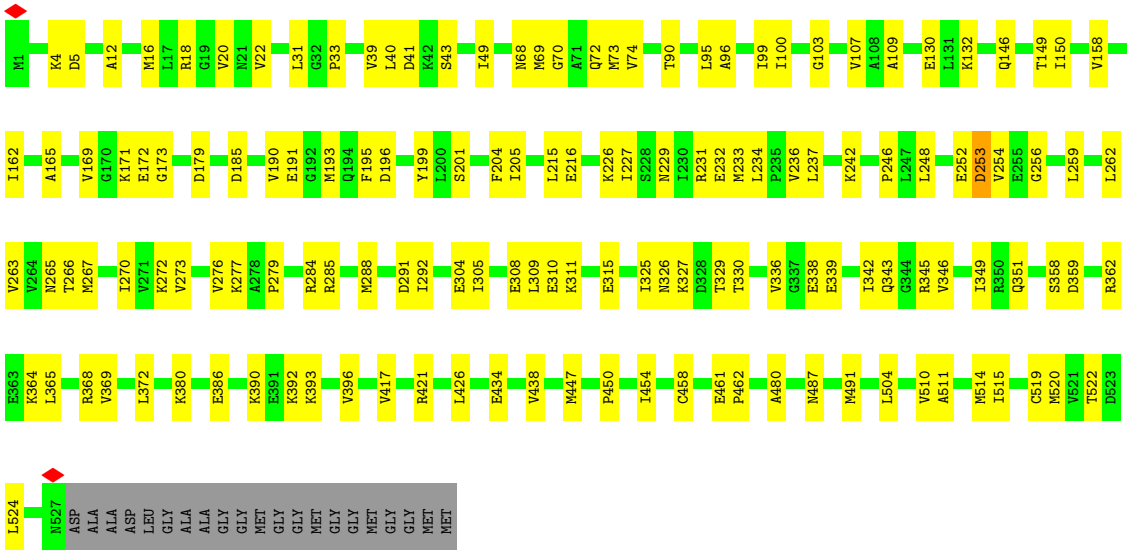
- Molecule 1: Chaperonin GroEL

Chain D: 76% 20% •



- Molecule 1: Chaperonin GroEL

Chain E: 70% 26% •



• Molecule 1: Chaperonin GroEL

Chain F: 80% 17%

M1 K4 V20 V39 L40 D41 I49 R58 L62 E67 N68 M69 Q72 M73 V74 K75 D87 E102 K132 D140 I144 I150 L161 M166 K171 E178 E186 E191 G192 M193 D196 L200 S201 F204 E214

L221 K226 I227 S228 R231 E232 M233 L234 L248 D253 V254 L259 A260 T261 L262 V263 V264 N265 T266 M267 R268 G269 I270 V273 K277 I292 E303 E308 L309 E310 K311 L317 K321 R322 V323 V324 I325 N326 T330 E339 I342 Q343 V346

I349 R350 I353 D361 L365 V369 K380 V407 V411 I420 V438 V442 M447 E448 D473 N487 M491 L494 L504 A511 I515 V521 N527 ASP ALA ALA ASP LEU GLY ALA ALA GLY GLY MET GLY GLY MET GLY GLY MET

GLY GLY MET MET

• Molecule 1: Chaperonin GroEL

Chain G: 76% 20%

M1 D5 V6 M16 L17 R18 G19 V20 D25 V39 I49 R58 L62 E67 N68 M69 Q72 M73 V74 K75 D87 E102 M111 E129 E130 L131 K132 S135 D140 I144 I150 K171 V177 E178 E186 E191 G192 M193

D196 L200 S201 F204 E214 L221 L222 K226 I227 R231 L234 L248 I249 I250 A251 E252 D253 V254 L259 A260 T261 L262 V263 V264 N265 T266 M267 R268 G269 I270 V271 K272 V273 K277 A278 R284 R285 I292 E303 E304 I305 E308 L309 E310 K311

L317 K321 R322 V323 N326 I342 Q343 V346 I349 R350 Q351 Q352 I353 T357 S358 D359 Y360 D361 R362 E363 K364 L365 V369 I379 V411 V412 I420 V438 K441 V442 E448 N487 M491 L494 A511 M514 I515 M520 V521 T522 D523

L524 N527 ASP ALA ALA ASP LEU GLY ALA ALA GLY GLY MET GLY GLY MET GLY GLY MET GLY GLY MET MET

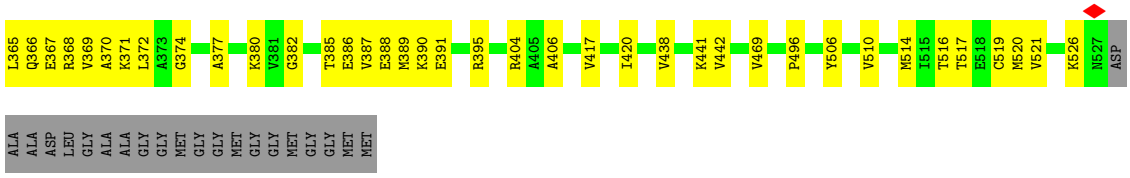
• Molecule 1: Chaperonin GroEL

Chain P: 68% 28%

M1 A2 A3 K7 F8 G9 K15 M16 L17 D25 A26 V27 K28 N37 V38 V39 L40 D41 K42 A46 P47 T48 D52 G53 V54 S55 V56 E63 D64 M69 M73 V77 T90 V94 L104 D140 S141 K142 D155 M166 D167 K168 V169

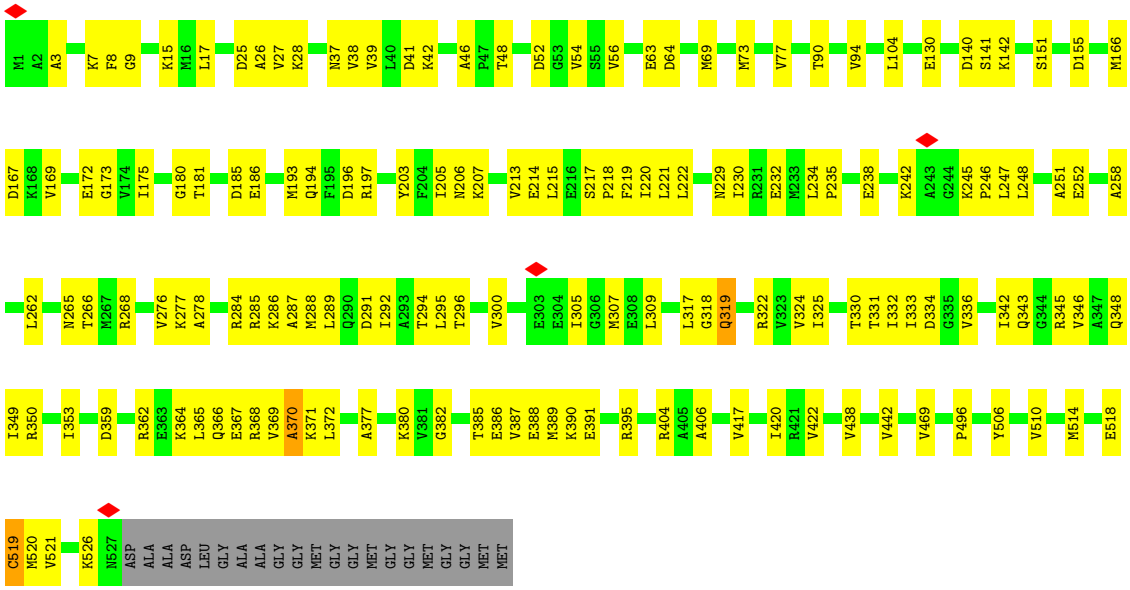
E172 G173 V174 I175 G180 T181 D185 E186 L187 D188 M193 Q194 F195 D196 R197 Y203 F204 I205 N206 K207 V213 E214 I305 L215 E216 S217 P218 F219 I220 L221 L222 N229 I230 R231 E232 M233 L234 E238 K242 K245 P246 A251 E252 E257 A258 L262 N265 T266

M267 R268 A275 V276 K277 A278 R284 R285 K286 A287 M288 L289 Q290 D291 I292 A293 T294 L295 T296 V300 E303 E304 I305 G306 M307 E308 L309 L317 G318 Q319 A320 K321 R322 V323 V324 I325 T330 T331 I332 I333 D334 I342 Q343 G344 R345 V346 A347 Q348 I349 R350 I353



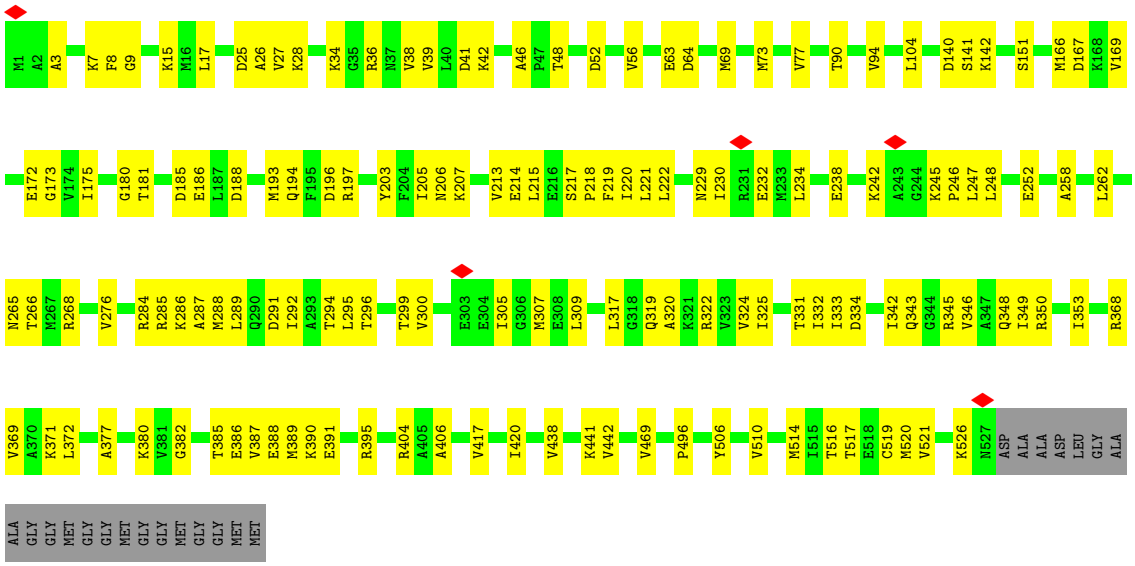
• Molecule 1: Chaperonin GroEL

Chain R:



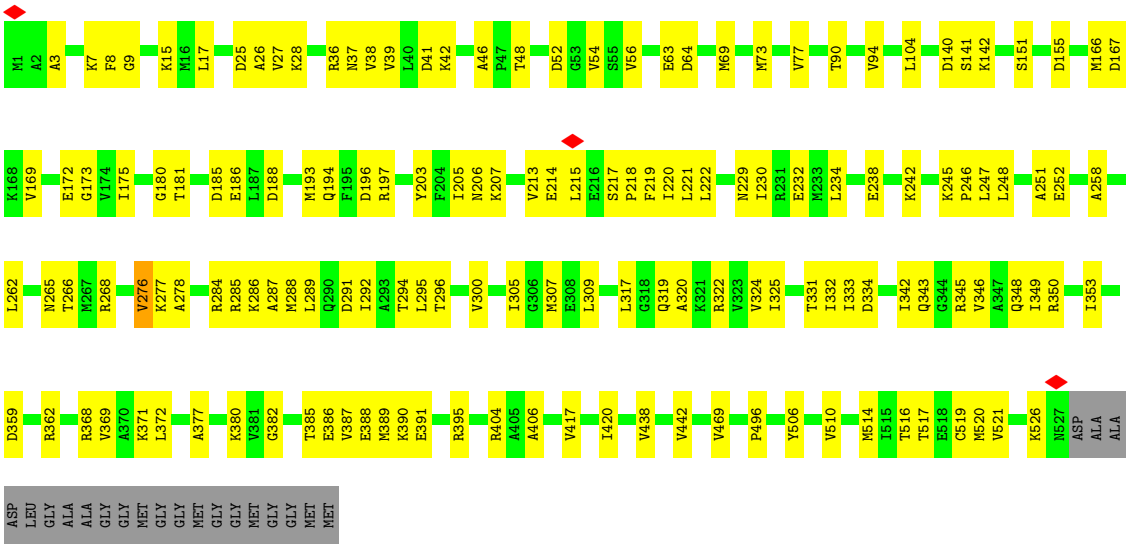
• Molecule 1: Chaperonin GroEL

Chain S:



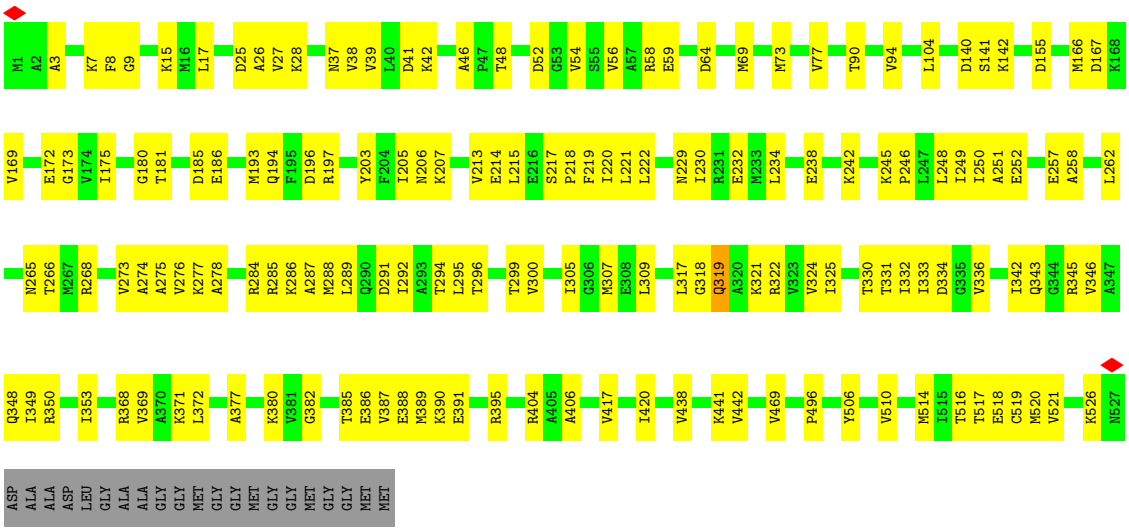
• Molecule 1: Chaperonin GroEL

Chain T:



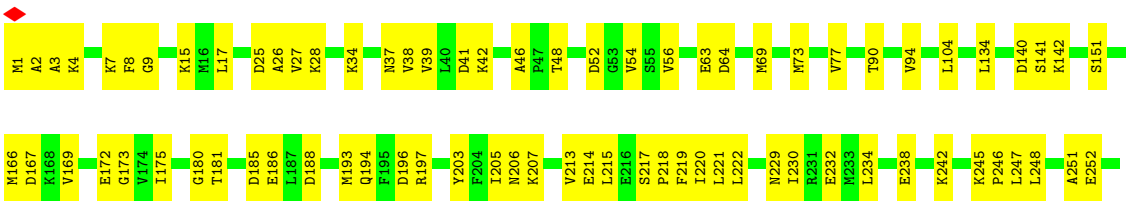
- Molecule 1: Chaperonin GroEL

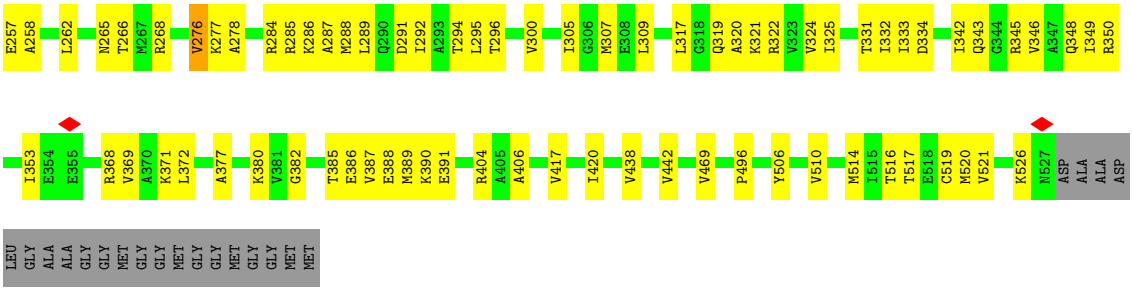
Chain U:



- Molecule 1: Chaperonin GroEL

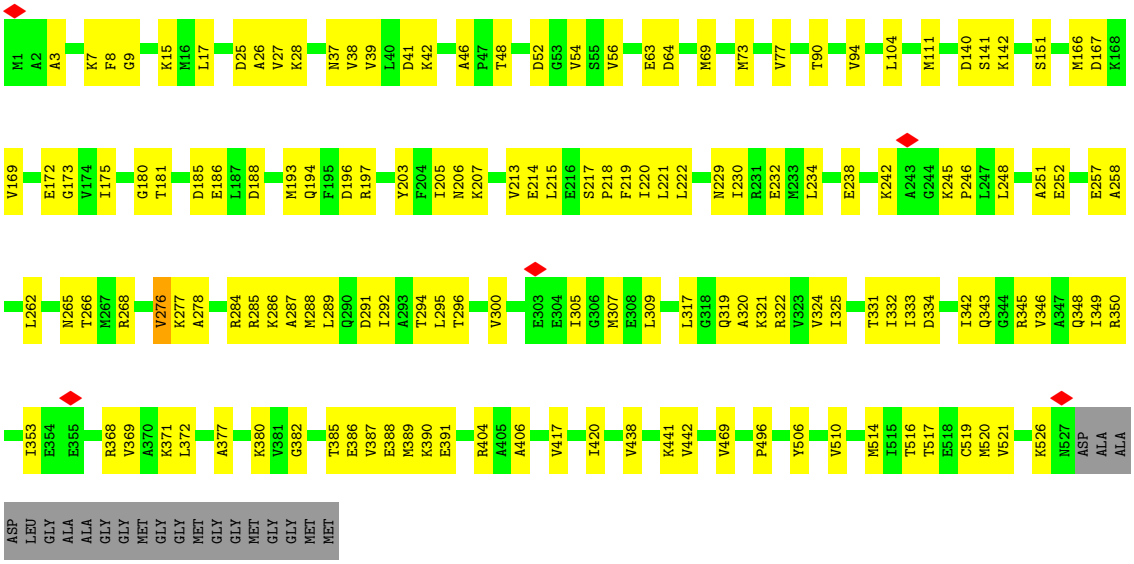
Chain V:





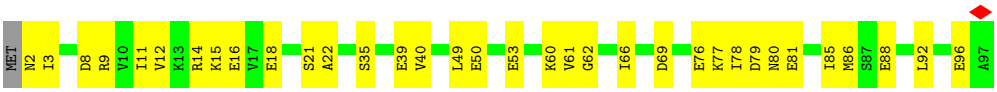
• Molecule 1: Chaperonin GroEL

Chain W:



• Molecule 2: Co-chaperonin GroES

Chain H:

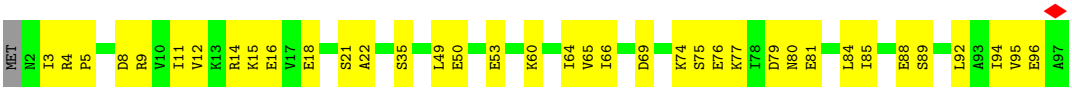


• Molecule 2: Co-chaperonin GroES

Chain I:

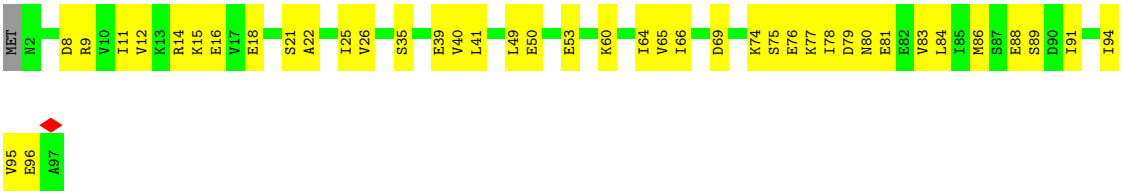
• Molecule 2: Co-chaperonin GroES

Chain J:



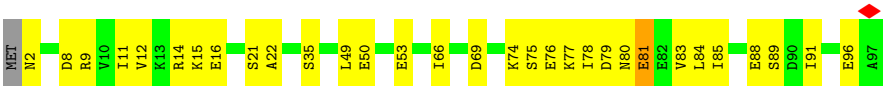
• Molecule 2: Co-chaperonin GroES

Chain K:



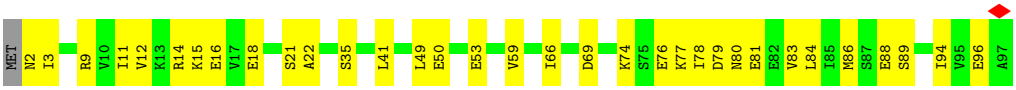
• Molecule 2: Co-chaperonin GroES

Chain L:



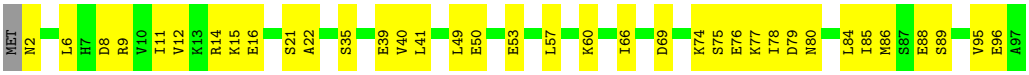
• Molecule 2: Co-chaperonin GroES

Chain M:



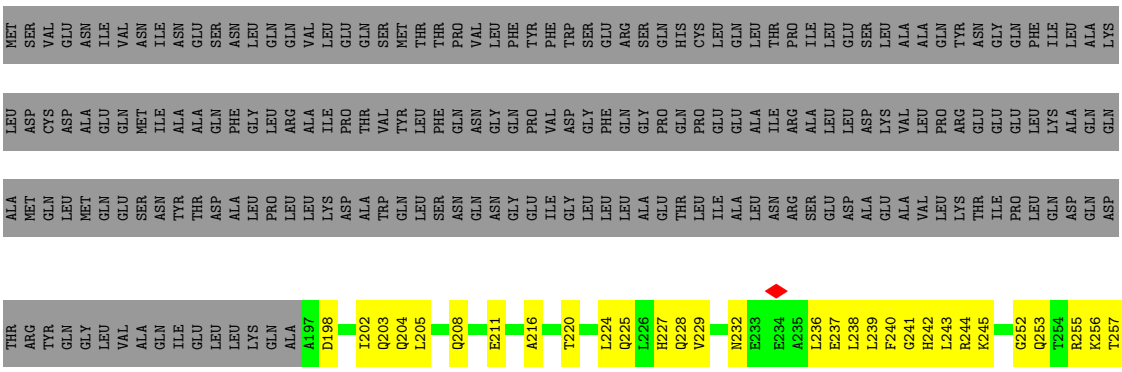
• Molecule 2: Co-chaperonin GroES

Chain N:



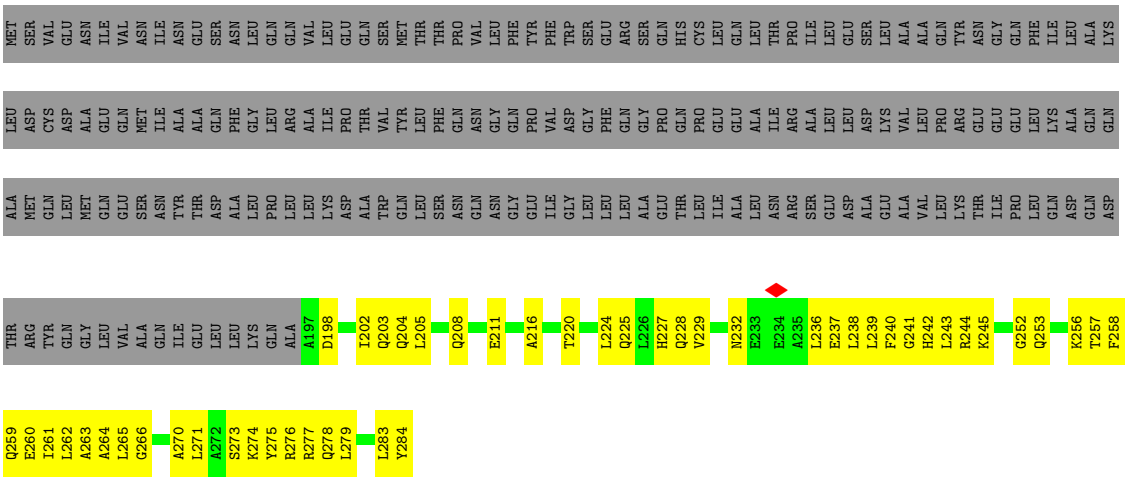
• Molecule 3: Chaperedoxin

Chain d:



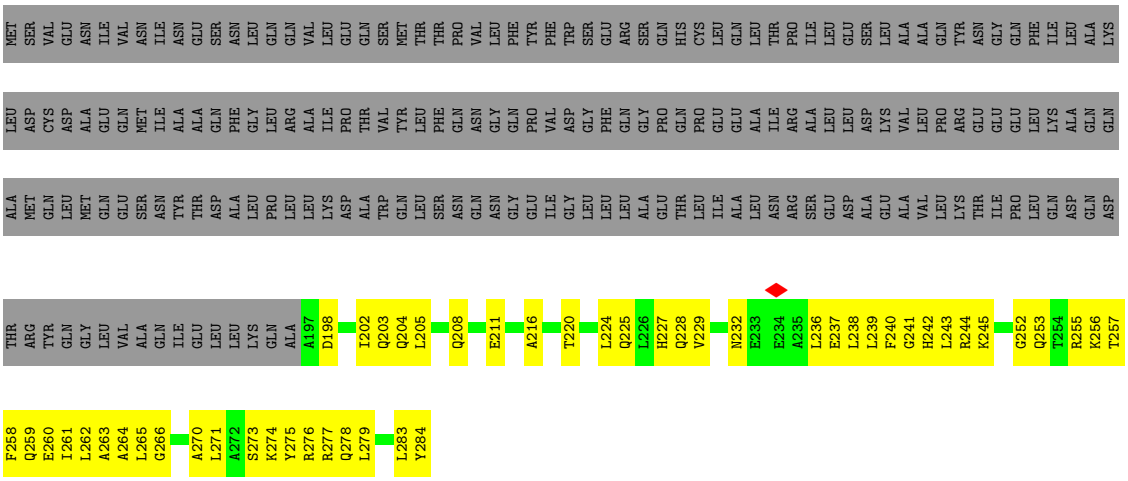
• Molecule 3: Chaperedoxin

Chain e:



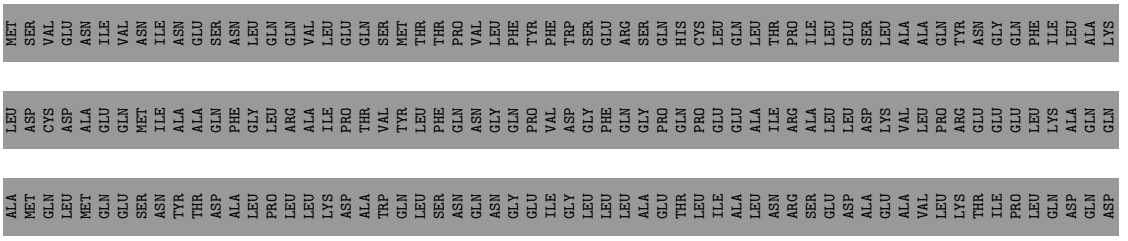
• Molecule 3: Chaperedoxin

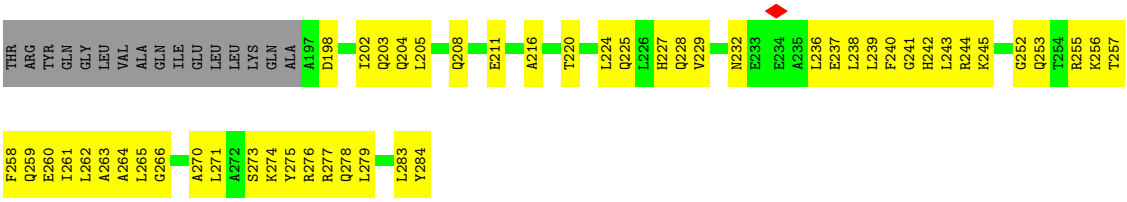
Chain f:



• Molecule 3: Chaperedoxin

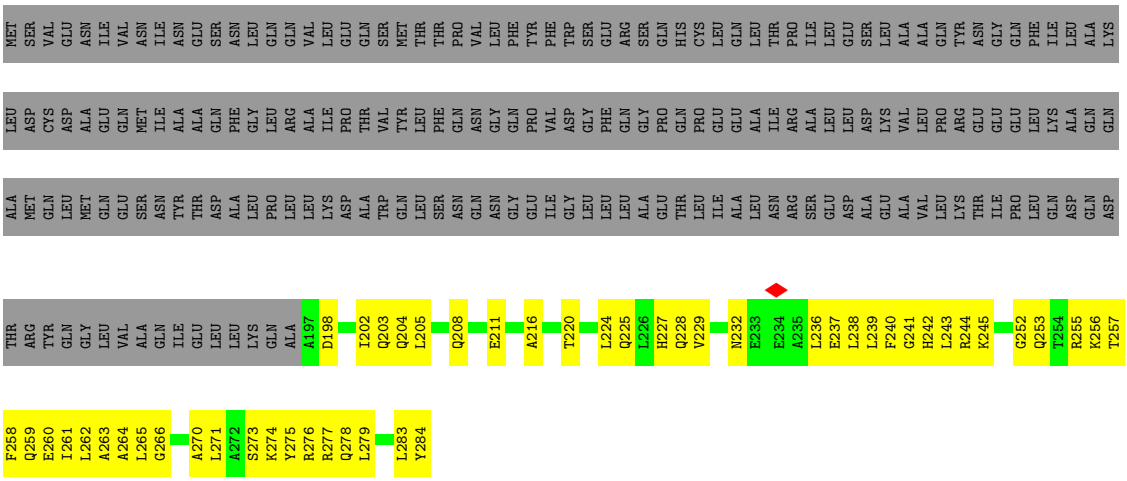
Chain g:





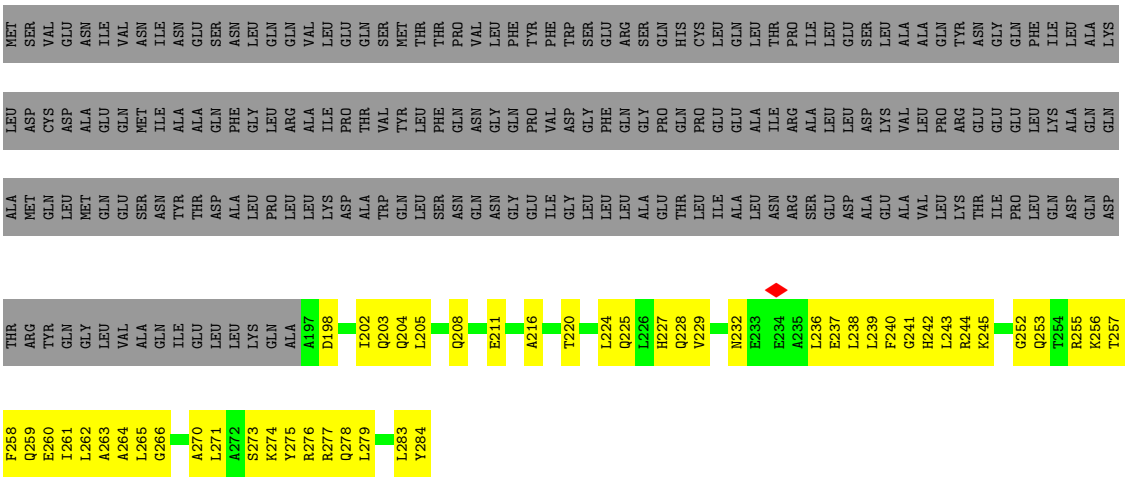
- Molecule 3: Chaperedoxin

Chain h: 13% 18% 69%



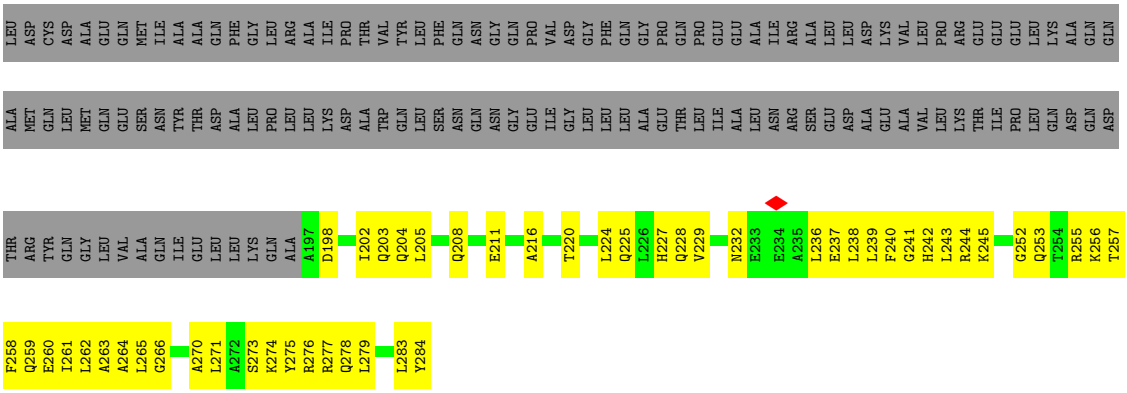
- Molecule 3: Chaperedoxin

Chain i: 13% 18% 69%



- Molecule 3: Chaperedoxin

Chain j: 13% 18% 69%


LEU ASP CYS ASP ALA GLU GLN MET ILE ALA ALA GLN PHE GLY LEU ARG ALA ILE PRO THR VAL TYR LEU PHE GLN ASN GLY GLN PRO VAL ASP GLY PHE GLN GLY PRO GLN PRO GLU GLU ALA ILE ARG ALA LEU LEU ASP LYS VAL LEU PRO ARG GLU GLU GLU LEU LYS ALA GLN GLN
ALA MET GLN LEU MET GLN GLU SER ASN TYR THR ASP ALA LEU PRO LEU LEU LYS ASP ALA TRP GLN LEU SER ASN GLN ASN GLY GLU ILE GLY LEU LEU LEU ALA GLU THR LEU ILE ALA ALA LEU ASN ARG SER GLU ASP ALA GLU ALA VAL LEU LYS THR ILE PRO LEU GLN ASP GLN ASP
THR ARG TYR GLN GLY LEU VAL ALA GLN ILE GLU LEU LEU LYS GLN ALA A197 D198 I202 Q203 Q204 L205 Q208 E211 A216 T220 L224 Q225 L226 H227 Q228 V229 N232 E233 E234 A235 L236 E237 L238 L239 F240 G241 H242 L243 R244 K245 G252 Q253 T254 R255 K256 T257
F258 Q259 E260 I261 L262 A263 A264 L265 G266 A270 L271 A272 S273 K274 Y275 R276 R277 Q278 L279 L283 Y284

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133737	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.983	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	528.0, 528.0, 528.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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: MG, ANP, K

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	0.23	0/3908	0.45	0/5275
1	B	0.28	2/3908 (0.1%)	0.46	0/5275
1	C	0.24	0/3908	0.44	0/5275
1	D	0.21	0/3908	0.46	0/5275
1	E	0.30	1/3908 (0.0%)	0.60	0/5275
1	F	0.24	0/3908	0.48	0/5275
1	G	0.22	0/3908	0.44	0/5275
1	P	0.31	3/3908 (0.1%)	0.53	0/5275
1	R	0.33	3/3908 (0.1%)	0.52	0/5275
1	S	0.25	0/3908	0.50	0/5275
1	T	0.27	1/3908 (0.0%)	0.51	0/5275
1	U	0.34	2/3908 (0.1%)	0.54	0/5275
1	V	0.30	1/3908 (0.0%)	0.55	0/5275
1	W	0.28	1/3908 (0.0%)	0.52	0/5275
2	H	0.39	0/724	0.62	0/973
2	I	0.19	0/724	0.54	0/973
2	J	0.18	0/724	0.52	0/973
2	K	0.27	0/724	0.54	0/973
2	L	0.36	1/724 (0.1%)	0.58	0/973
2	M	0.21	0/724	0.56	0/973
2	N	0.24	0/724	0.51	0/973
3	d	0.39	0/697	0.93	0/942
3	e	0.41	0/697	0.91	0/942
3	f	0.39	0/697	0.93	0/942
3	g	0.40	0/697	0.92	0/942
3	h	0.39	0/697	0.93	0/942
3	i	0.39	0/697	0.93	0/942
3	j	0.39	0/697	0.94	0/942
All	All	0.29	15/64659 (0.0%)	0.55	0/87255

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	186	GLU	C-N	8.18	1.44	1.33
1	R	319	GLN	C-N	8.05	1.42	1.33
1	U	319	GLN	C-N	8.03	1.42	1.33
1	P	277	LYS	C-N	7.55	1.44	1.33
1	P	275	ALA	C-N	7.15	1.43	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3880	0	4007	77	0
1	B	3880	0	4007	91	0
1	C	3880	0	4007	76	0
1	D	3880	0	4007	93	0
1	E	3880	0	4007	114	0
1	F	3880	0	4007	75	0
1	G	3880	0	4007	82	0
1	P	3880	0	4007	148	0
1	R	3880	0	4007	145	0
1	S	3880	0	4007	136	0
1	T	3880	0	4007	141	0
1	U	3880	0	4007	156	0
1	V	3880	0	4007	150	0
1	W	3880	0	4007	143	0
2	H	720	0	750	34	0
2	I	720	0	750	39	0
2	J	720	0	750	34	0
2	K	720	0	750	38	0
2	L	720	0	750	27	0
2	M	720	0	750	35	0
2	N	720	0	750	35	0
3	d	689	0	686	71	0
3	e	689	0	686	72	0
3	f	689	0	686	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	g	689	0	686	73	0
3	h	689	0	686	72	0
3	i	689	0	686	74	0
3	j	689	0	686	68	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	P	1	0	0	0	0
4	R	1	0	0	0	0
4	S	1	0	0	0	0
4	T	1	0	0	0	0
4	U	1	0	0	0	0
4	V	1	0	0	0	0
4	W	1	0	0	0	0
5	A	31	0	13	2	0
5	B	31	0	13	2	0
5	C	31	0	13	2	0
5	D	31	0	13	3	0
5	E	31	0	13	2	0
5	F	31	0	13	2	0
5	G	31	0	13	2	0
5	P	31	0	13	0	0
5	R	31	0	13	0	0
5	S	31	0	13	0	0
5	T	31	0	13	0	0
5	U	31	0	13	0	0
5	V	31	0	13	0	0
5	W	31	0	13	0	0
6	P	1	0	0	0	0
6	R	1	0	0	0	0
6	S	1	0	0	0	0
6	T	1	0	0	0	0
6	U	1	0	0	0	0
6	V	1	0	0	0	0
6	W	1	0	0	0	0
All	All	64638	0	66332	2222	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 17.

The worst 5 of 2222 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:420:ILE:CD1	1:V:469:VAL:HG11	1.89	1.03
1:U:420:ILE:CD1	1:U:469:VAL:HG11	1.89	1.03
1:W:420:ILE:CD1	1:W:469:VAL:HG11	1.89	1.03
1:T:420:ILE:CD1	1:T:469:VAL:HG11	1.89	1.02
1:S:420:ILE:CD1	1:S:469:VAL:HG11	1.89	1.02

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	525/548 (96%)	514 (98%)	11 (2%)	0	100	100
1	B	525/548 (96%)	517 (98%)	8 (2%)	0	100	100
1	C	525/548 (96%)	515 (98%)	10 (2%)	0	100	100
1	D	525/548 (96%)	517 (98%)	8 (2%)	0	100	100
1	E	525/548 (96%)	502 (96%)	22 (4%)	1 (0%)	43	72
1	F	525/548 (96%)	513 (98%)	12 (2%)	0	100	100
1	G	525/548 (96%)	516 (98%)	9 (2%)	0	100	100
1	P	525/548 (96%)	497 (95%)	28 (5%)	0	100	100
1	R	525/548 (96%)	495 (94%)	29 (6%)	1 (0%)	43	72
1	S	525/548 (96%)	496 (94%)	29 (6%)	0	100	100
1	T	525/548 (96%)	497 (95%)	28 (5%)	0	100	100
1	U	525/548 (96%)	495 (94%)	30 (6%)	0	100	100
1	V	525/548 (96%)	497 (95%)	28 (5%)	0	100	100
1	W	525/548 (96%)	495 (94%)	30 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	94/97 (97%)	86 (92%)	8 (8%)	0	100	100
2	I	94/97 (97%)	88 (94%)	6 (6%)	0	100	100
2	J	94/97 (97%)	89 (95%)	5 (5%)	0	100	100
2	K	94/97 (97%)	86 (92%)	8 (8%)	0	100	100
2	L	94/97 (97%)	86 (92%)	8 (8%)	0	100	100
2	M	94/97 (97%)	88 (94%)	6 (6%)	0	100	100
2	N	94/97 (97%)	87 (93%)	7 (7%)	0	100	100
3	d	86/284 (30%)	81 (94%)	5 (6%)	0	100	100
3	e	86/284 (30%)	80 (93%)	6 (7%)	0	100	100
3	f	86/284 (30%)	81 (94%)	5 (6%)	0	100	100
3	g	86/284 (30%)	81 (94%)	5 (6%)	0	100	100
3	h	86/284 (30%)	81 (94%)	5 (6%)	0	100	100
3	i	86/284 (30%)	81 (94%)	5 (6%)	0	100	100
3	j	86/284 (30%)	80 (93%)	6 (7%)	0	100	100
All	All	8610/10339 (83%)	8241 (96%)	367 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	253	ASP
1	R	370	ALA

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	407/415 (98%)	407 (100%)	0	100	100
1	B	407/415 (98%)	407 (100%)	0	100	100
1	C	407/415 (98%)	407 (100%)	0	100	100
1	D	407/415 (98%)	407 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	407/415 (98%)	407 (100%)	0	100	100
1	F	407/415 (98%)	407 (100%)	0	100	100
1	G	407/415 (98%)	407 (100%)	0	100	100
1	P	407/415 (98%)	407 (100%)	0	100	100
1	R	407/415 (98%)	406 (100%)	1 (0%)	87	96
1	S	407/415 (98%)	407 (100%)	0	100	100
1	T	407/415 (98%)	407 (100%)	0	100	100
1	U	407/415 (98%)	407 (100%)	0	100	100
1	V	407/415 (98%)	407 (100%)	0	100	100
1	W	407/415 (98%)	407 (100%)	0	100	100
2	H	79/80 (99%)	79 (100%)	0	100	100
2	I	79/80 (99%)	79 (100%)	0	100	100
2	J	79/80 (99%)	79 (100%)	0	100	100
2	K	79/80 (99%)	79 (100%)	0	100	100
2	L	79/80 (99%)	79 (100%)	0	100	100
2	M	79/80 (99%)	79 (100%)	0	100	100
2	N	79/80 (99%)	79 (100%)	0	100	100
3	d	69/238 (29%)	69 (100%)	0	100	100
3	e	69/238 (29%)	69 (100%)	0	100	100
3	f	69/238 (29%)	69 (100%)	0	100	100
3	g	69/238 (29%)	69 (100%)	0	100	100
3	h	69/238 (29%)	69 (100%)	0	100	100
3	i	69/238 (29%)	69 (100%)	0	100	100
3	j	69/238 (29%)	69 (100%)	0	100	100
All	All	6734/8036 (84%)	6733 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	519	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
1	W	487	ASN
3	g	259	GLN
3	d	228	GLN
3	e	259	GLN
3	h	259	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 35 ligands modelled in this entry, 21 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
5	ANP	S	603	4,6	32,33,33	0.92	4 (12%)	44,52,52	0.83	1 (2%)
5	ANP	R	603	4,6	32,33,33	0.93	4 (12%)	44,52,52	0.83	1 (2%)
5	ANP	D	600	4	32,33,33	0.92	4 (12%)	44,52,52	0.77	1 (2%)
5	ANP	W	603	4,6	32,33,33	0.93	4 (12%)	44,52,52	0.83	1 (2%)
5	ANP	G	602	4	32,33,33	0.93	4 (12%)	44,52,52	0.77	1 (2%)
5	ANP	V	602	4,6	32,33,33	0.93	4 (12%)	44,52,52	0.83	1 (2%)
5	ANP	P	602	4,6	32,33,33	0.93	4 (12%)	44,52,52	0.83	1 (2%)
5	ANP	B	602	4	32,33,33	0.93	4 (12%)	44,52,52	0.77	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ANP	T	603	4,6	32,33,33	0.92	4 (12%)	44,52,52	0.83	1 (2%)
5	ANP	F	602	4	32,33,33	0.92	4 (12%)	44,52,52	0.77	1 (2%)
5	ANP	U	603	4,6	32,33,33	0.92	4 (12%)	44,52,52	0.83	1 (2%)
5	ANP	C	602	4	32,33,33	0.94	4 (12%)	44,52,52	0.78	1 (2%)
5	ANP	A	602	4	32,33,33	0.94	4 (12%)	44,52,52	0.77	1 (2%)
5	ANP	E	600	4	32,33,33	0.92	4 (12%)	44,52,52	0.78	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ANP	S	603	4,6	-	7/18/38/38	0/3/3/3
5	ANP	R	603	4,6	-	7/18/38/38	0/3/3/3
5	ANP	D	600	4	-	3/18/38/38	0/3/3/3
5	ANP	W	603	4,6	-	7/18/38/38	0/3/3/3
5	ANP	G	602	4	-	2/18/38/38	0/3/3/3
5	ANP	V	602	4,6	-	7/18/38/38	0/3/3/3
5	ANP	P	602	4,6	-	7/18/38/38	0/3/3/3
5	ANP	B	602	4	-	3/18/38/38	0/3/3/3
5	ANP	T	603	4,6	-	7/18/38/38	0/3/3/3
5	ANP	F	602	4	-	2/18/38/38	0/3/3/3
5	ANP	U	603	4,6	-	7/18/38/38	0/3/3/3
5	ANP	C	602	4	-	2/18/38/38	0/3/3/3
5	ANP	A	602	4	-	2/18/38/38	0/3/3/3
5	ANP	E	600	4	-	2/18/38/38	0/3/3/3

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	ANP	PB-O3A	-2.54	1.55	1.59
5	V	602	ANP	PB-O3A	-2.54	1.55	1.59
5	P	602	ANP	PB-O3A	-2.51	1.55	1.59
5	B	602	ANP	PB-O3A	-2.50	1.55	1.59
5	S	603	ANP	PB-O3A	-2.50	1.55	1.59

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	U	603	ANP	PB-O3A-PA	-3.87	118.97	132.62
5	R	603	ANP	PB-O3A-PA	-3.87	118.99	132.62
5	V	602	ANP	PB-O3A-PA	-3.87	118.99	132.62
5	S	603	ANP	PB-O3A-PA	-3.87	118.99	132.62
5	T	603	ANP	PB-O3A-PA	-3.87	119.00	132.62

There are no chirality outliers.

5 of 65 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	602	ANP	PB-N3B-PG-O1G
5	B	602	ANP	PB-N3B-PG-O1G
5	C	602	ANP	PB-N3B-PG-O1G
5	D	600	ANP	PB-N3B-PG-O1G
5	E	600	ANP	PB-N3B-PG-O1G

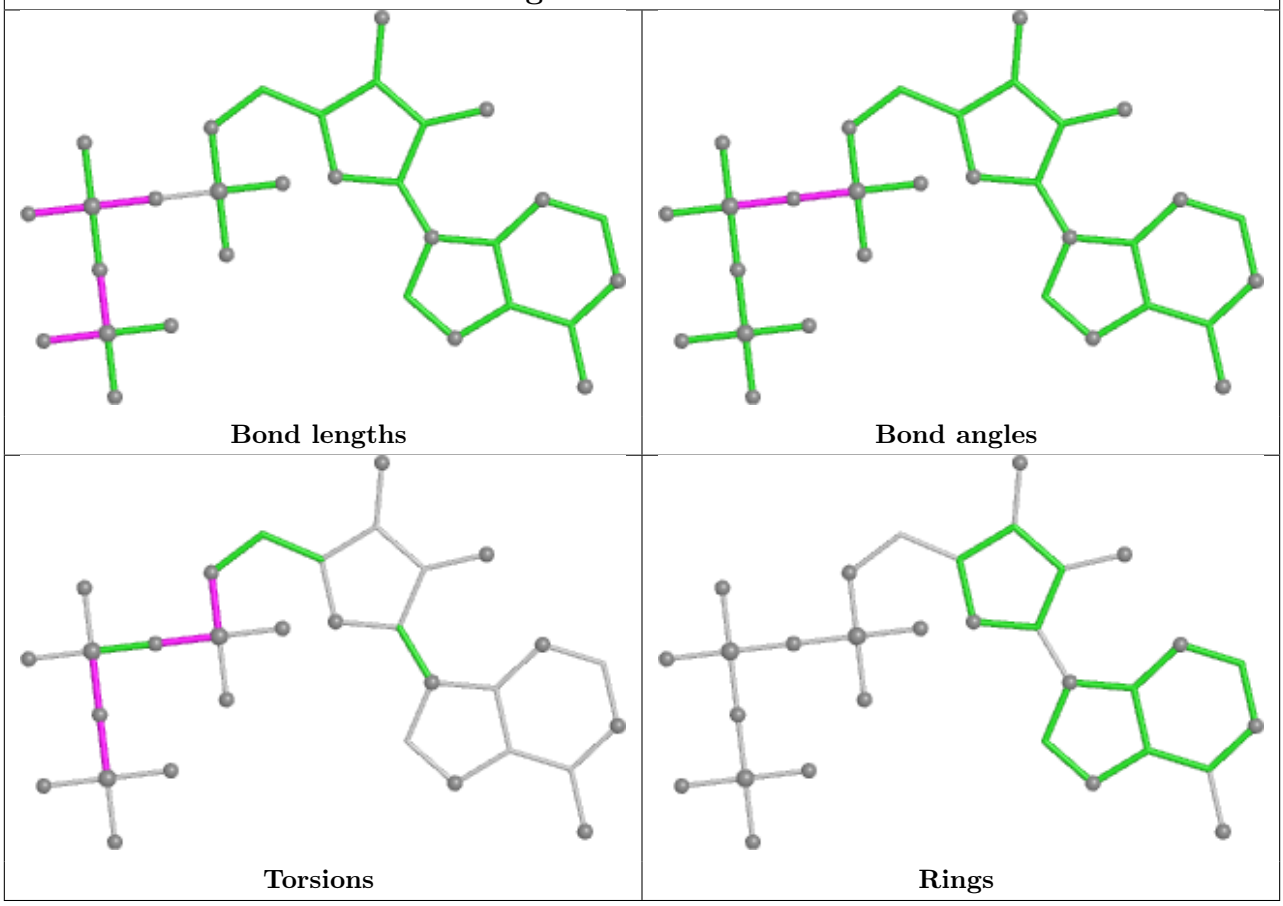
There are no ring outliers.

7 monomers are involved in 15 short contacts:

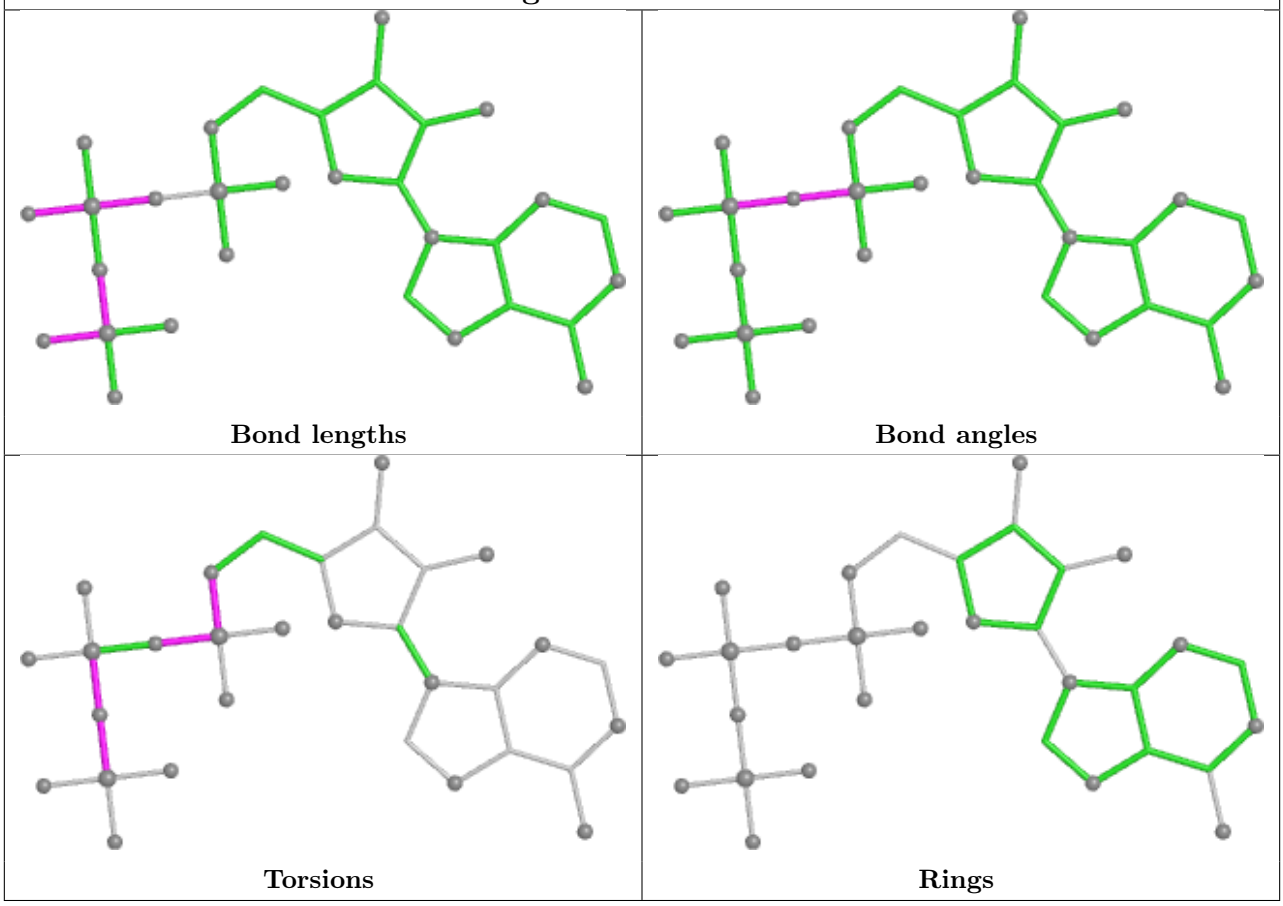
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	600	ANP	3	0
5	G	602	ANP	2	0
5	B	602	ANP	2	0
5	F	602	ANP	2	0
5	C	602	ANP	2	0
5	A	602	ANP	2	0
5	E	600	ANP	2	0

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 then 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.

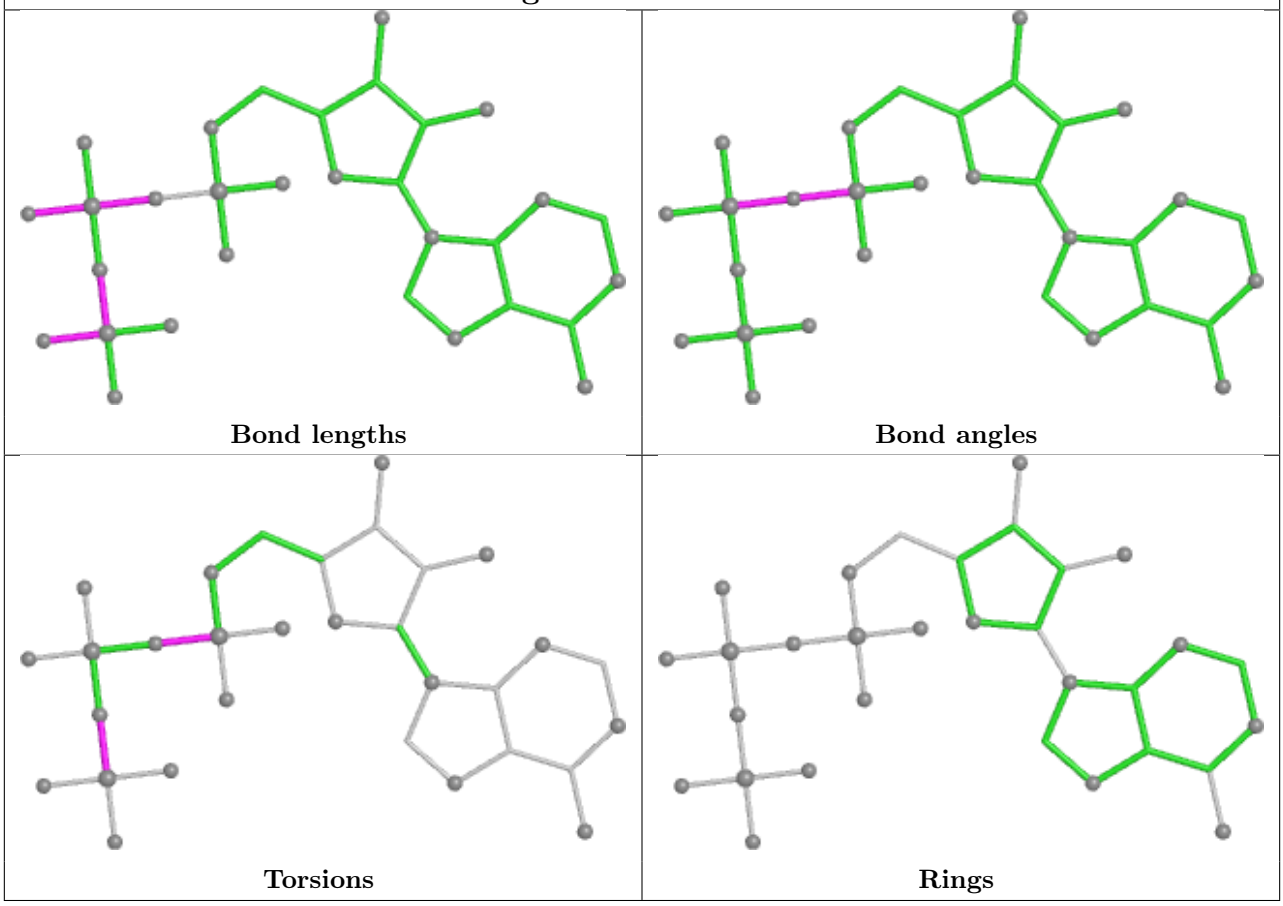
Ligand ANP S 603



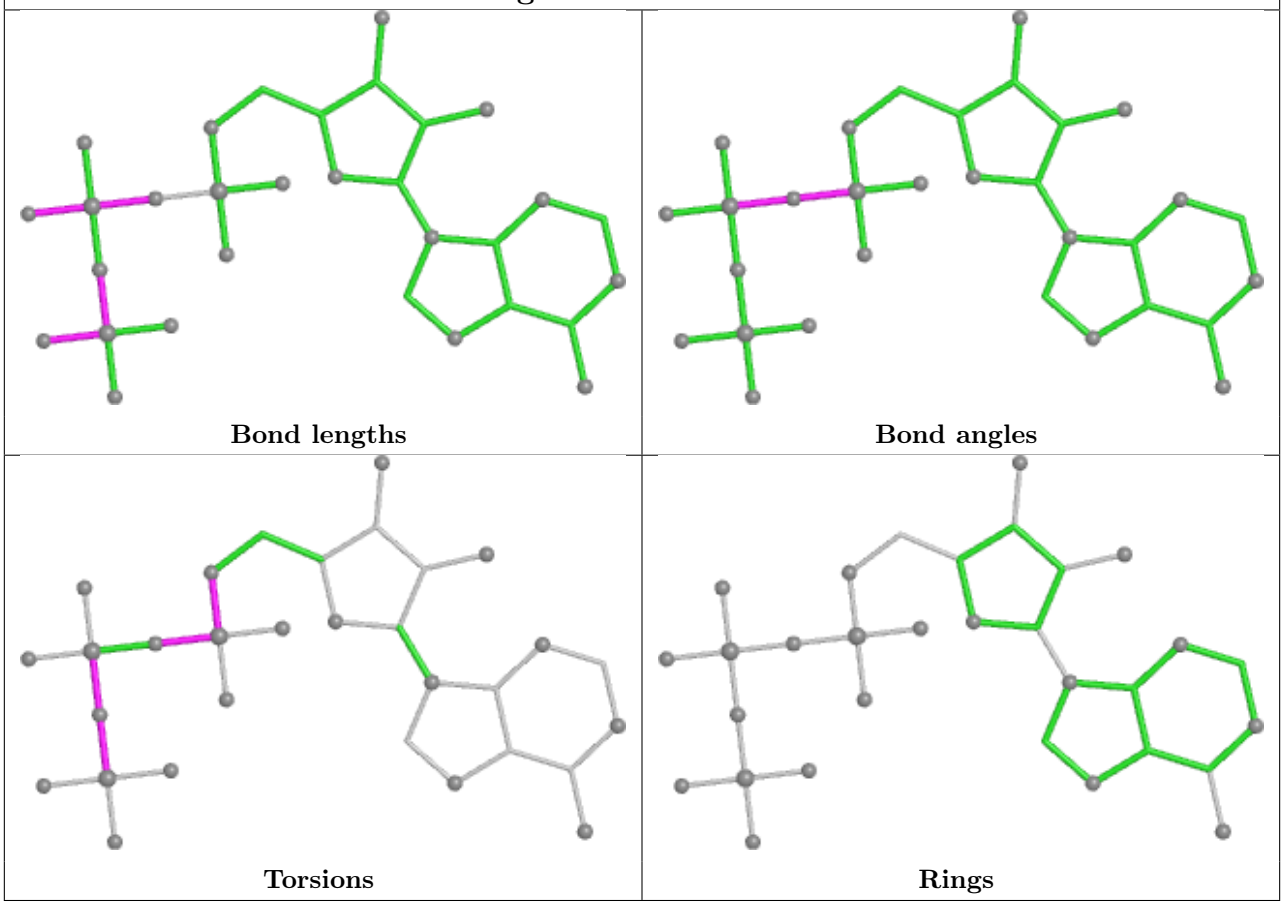
Ligand ANP R 603



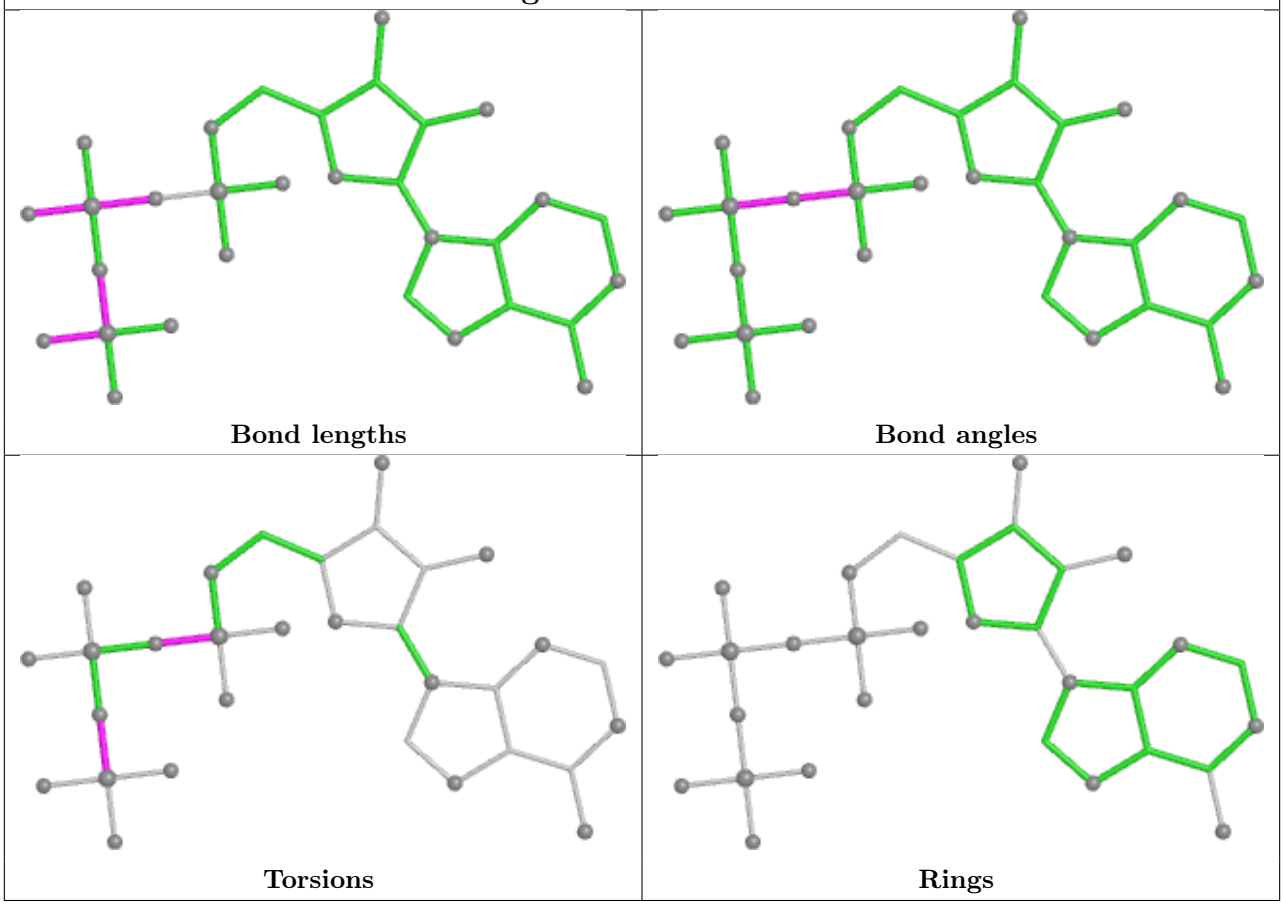
Ligand ANP D 600



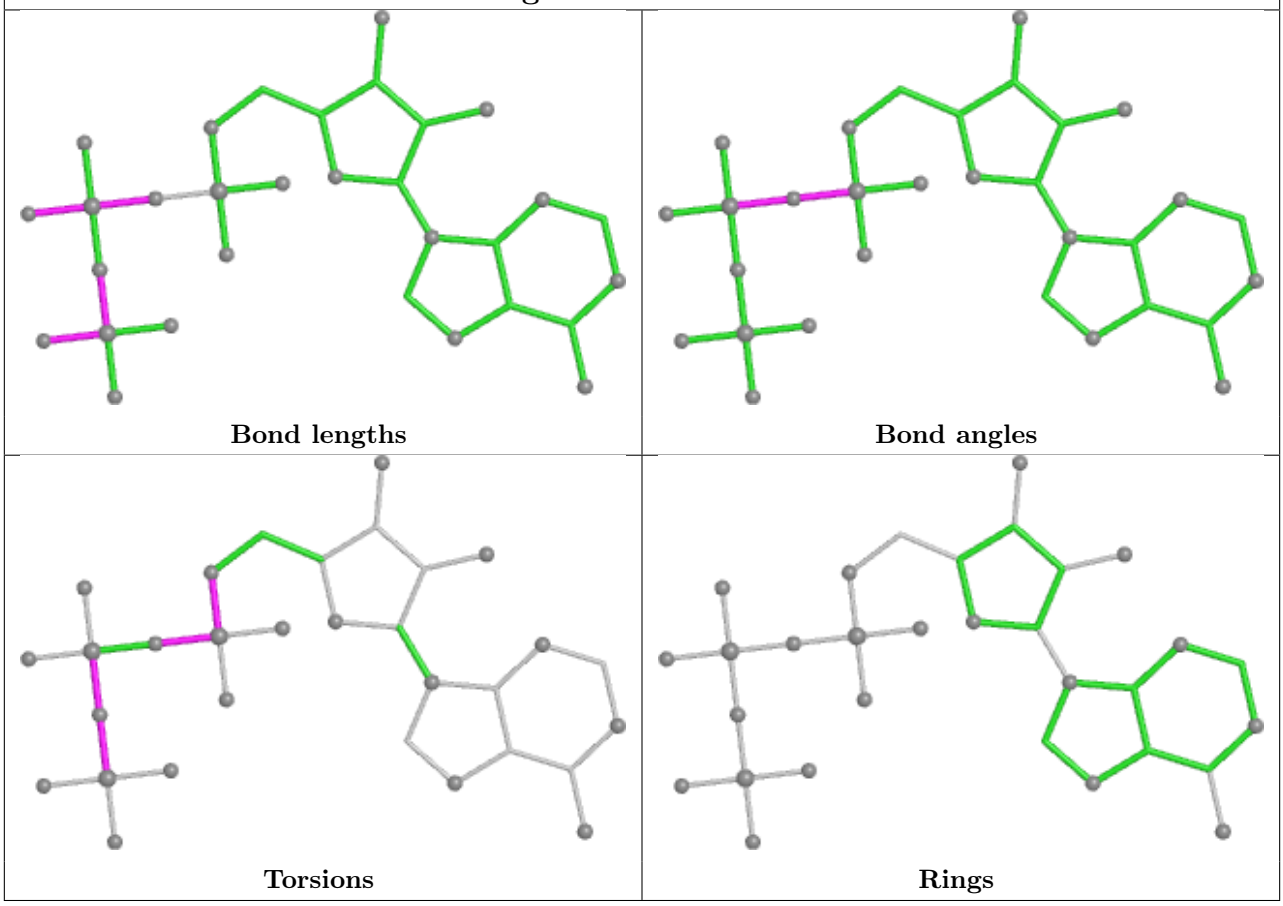
Ligand ANP W 603



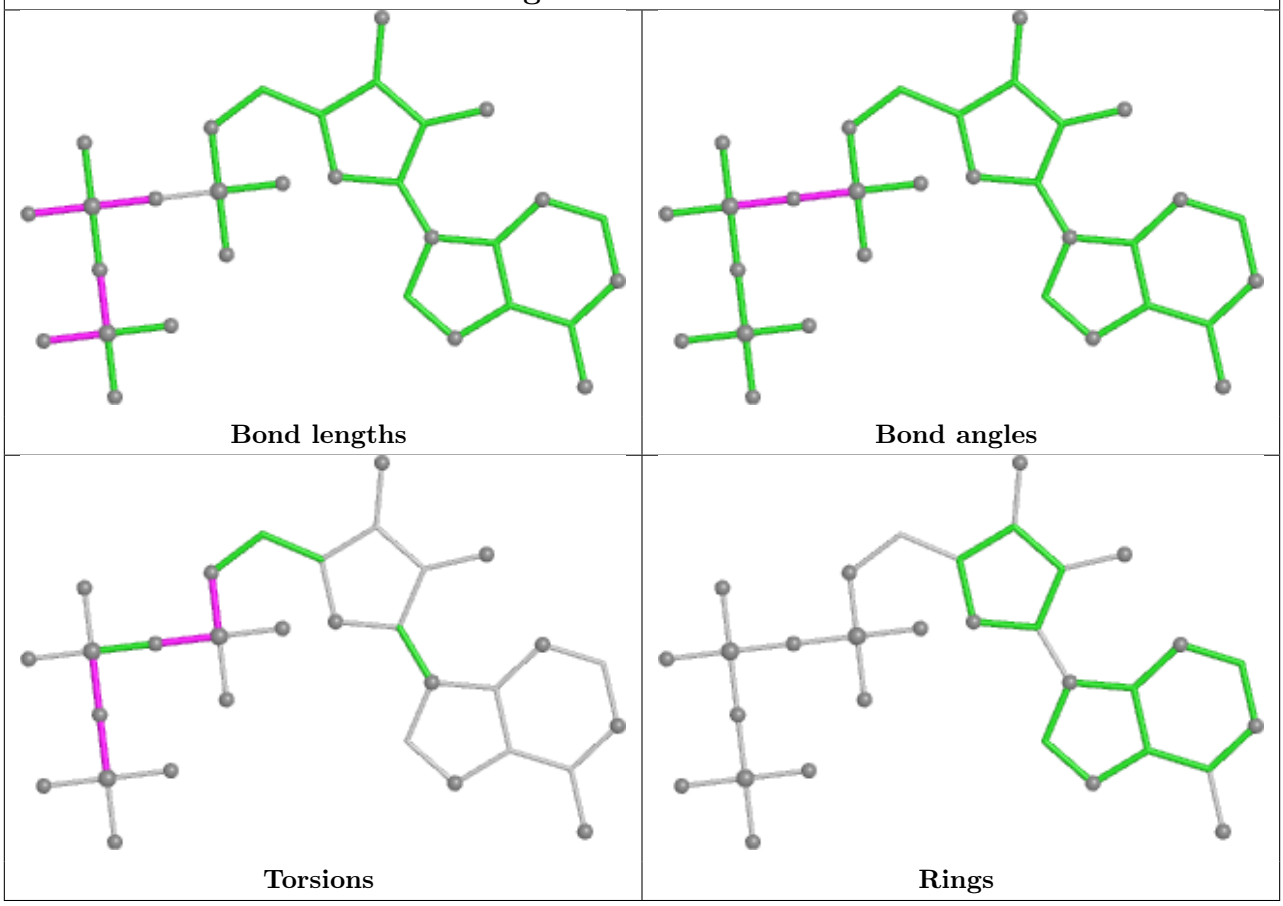
Ligand ANP G 602



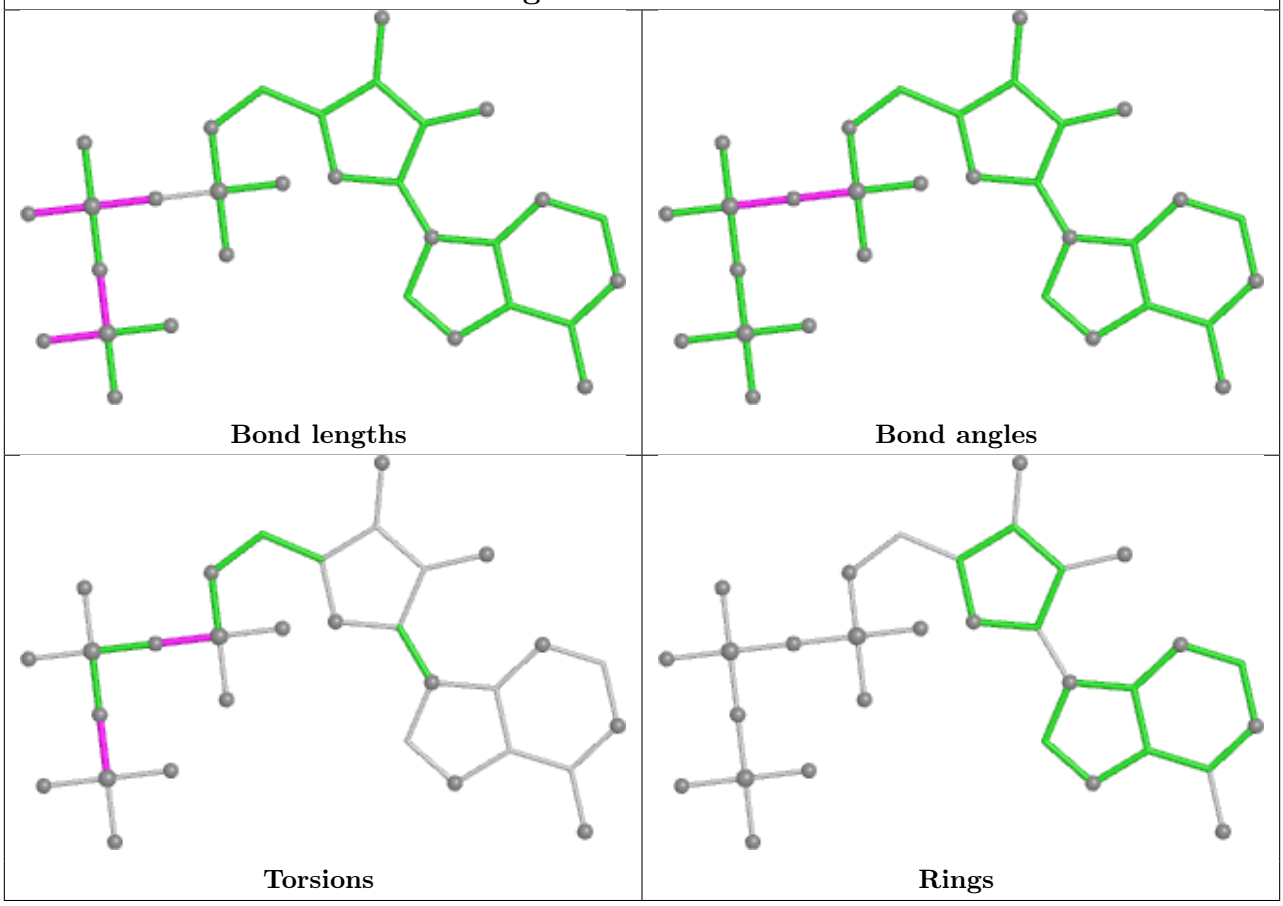
Ligand ANP V 602



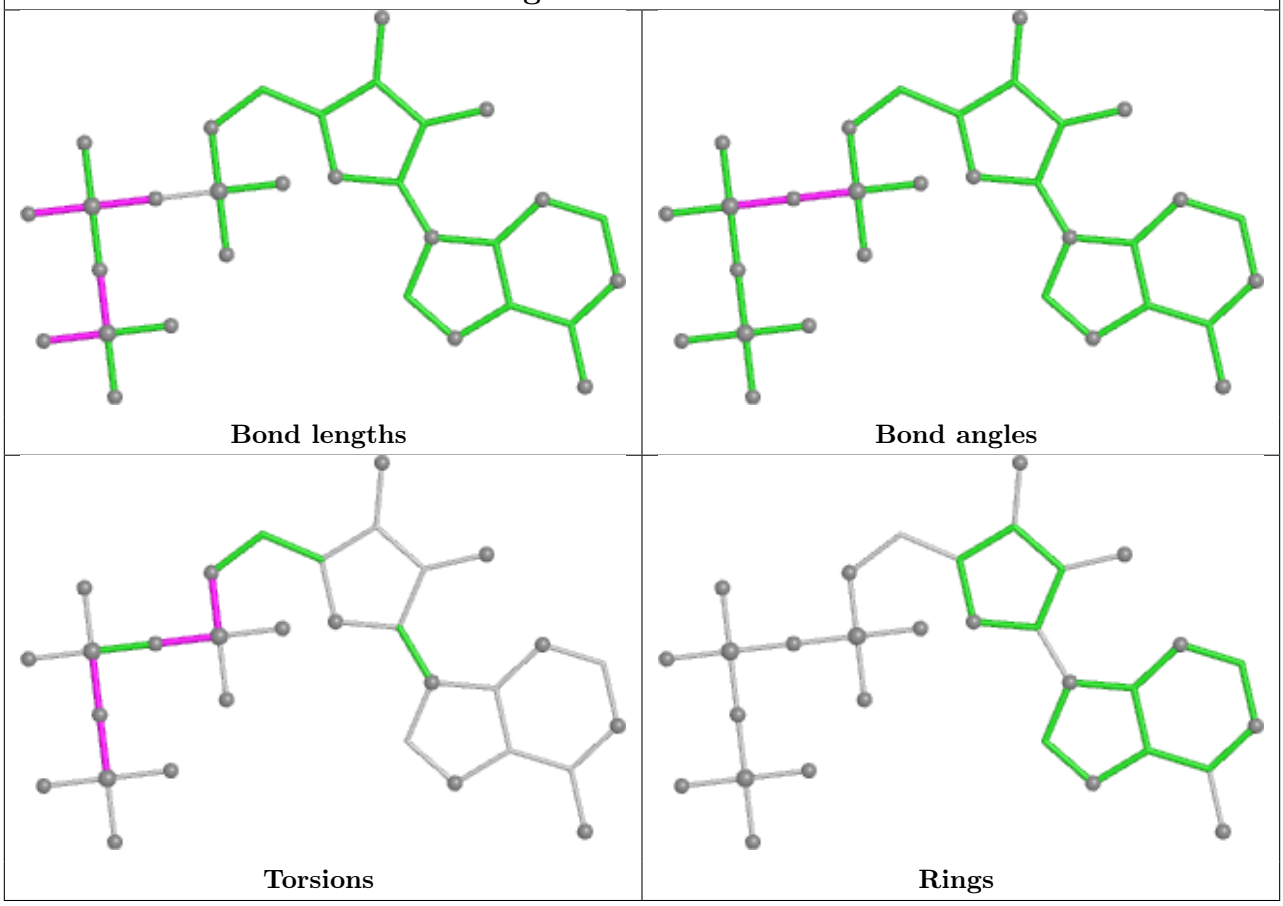
Ligand ANP P 602



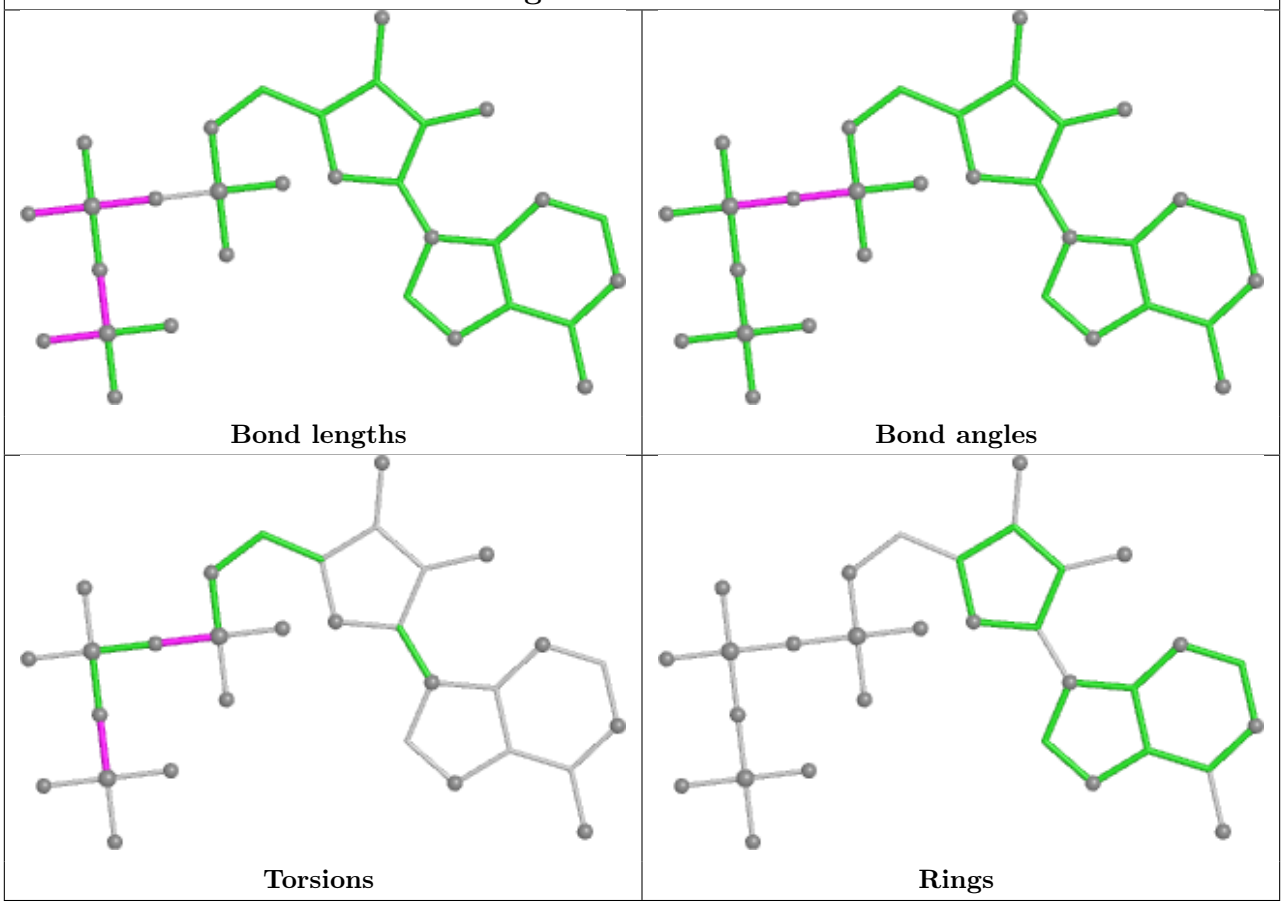
Ligand ANP B 602



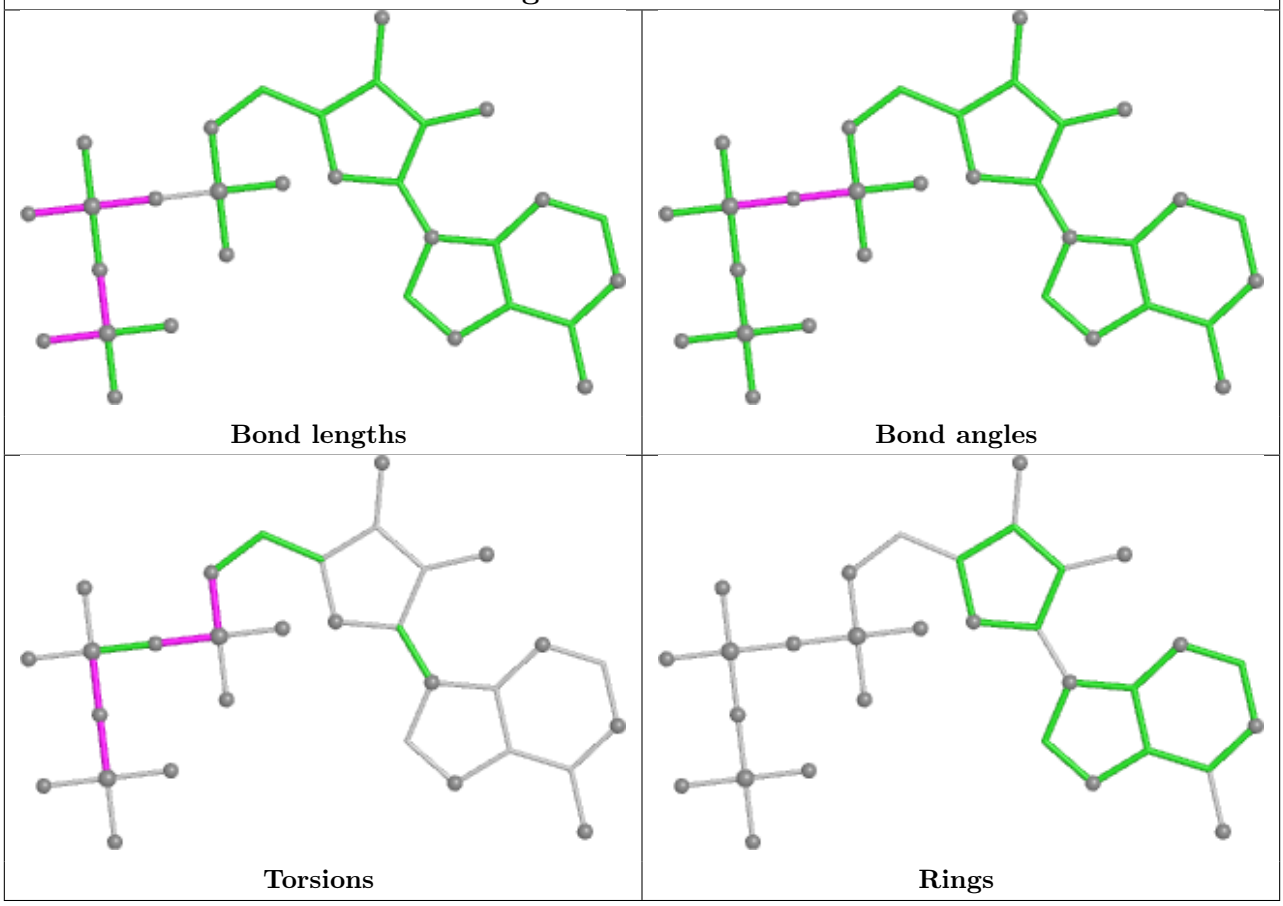
Ligand ANP T 603



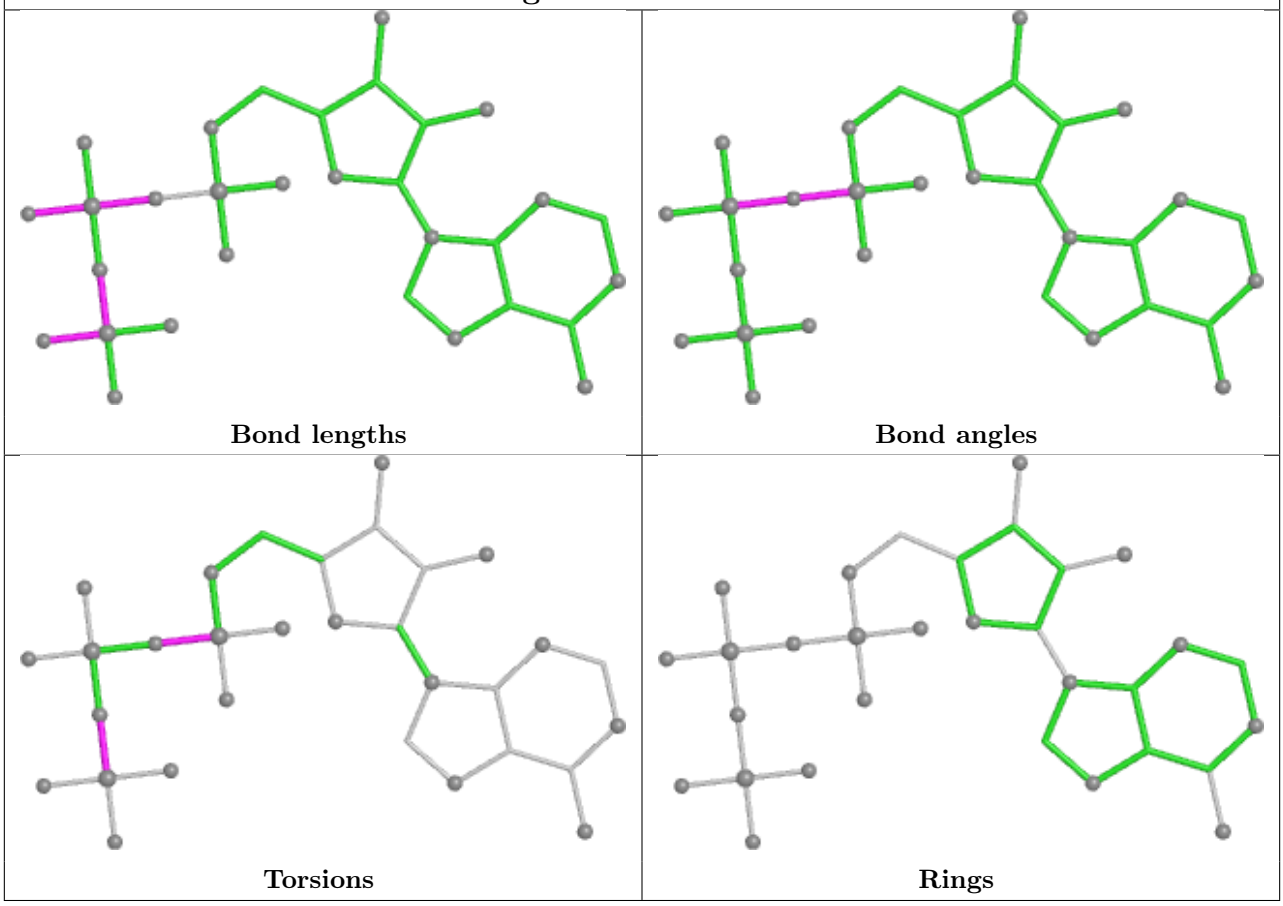
Ligand ANP F 602



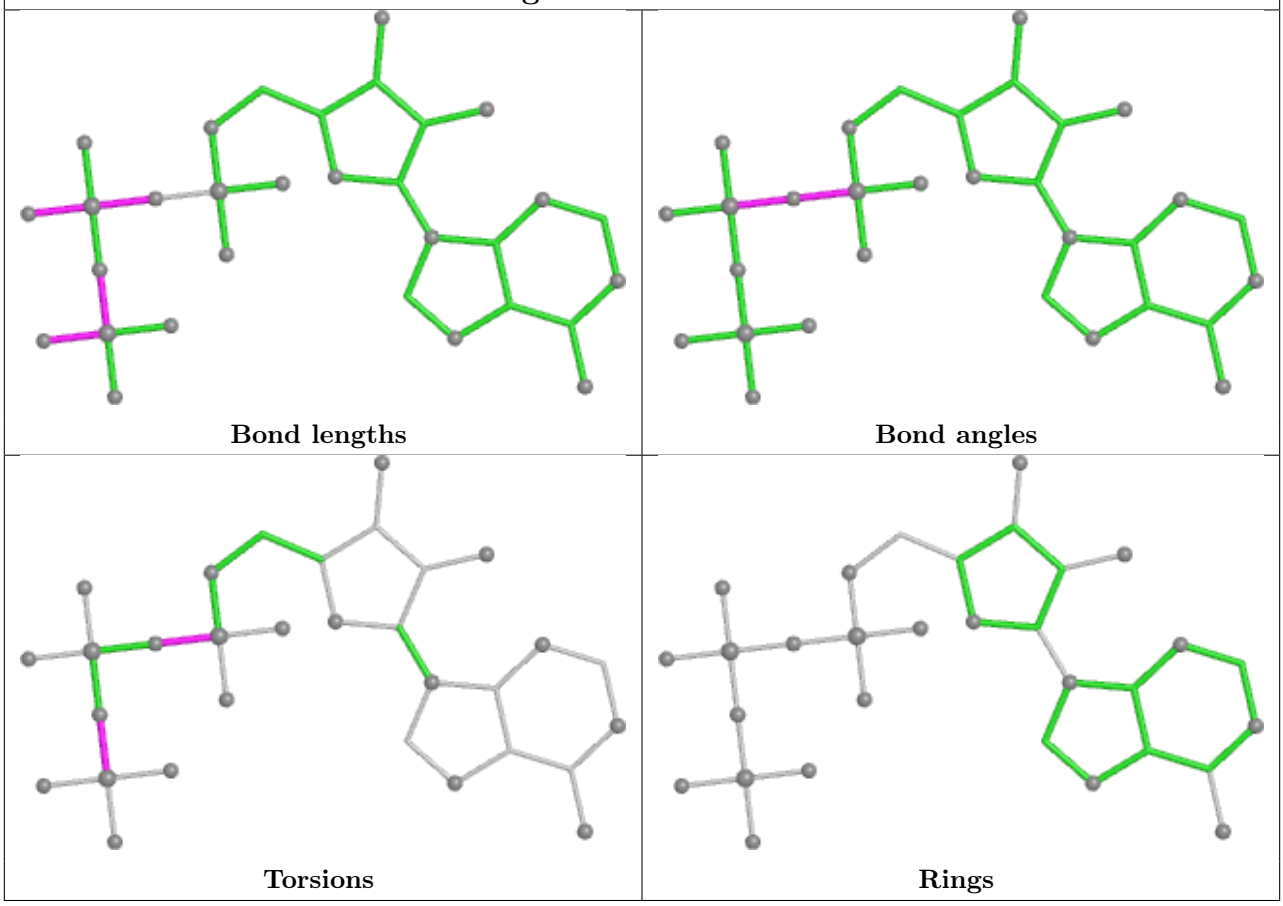
Ligand ANP U 603

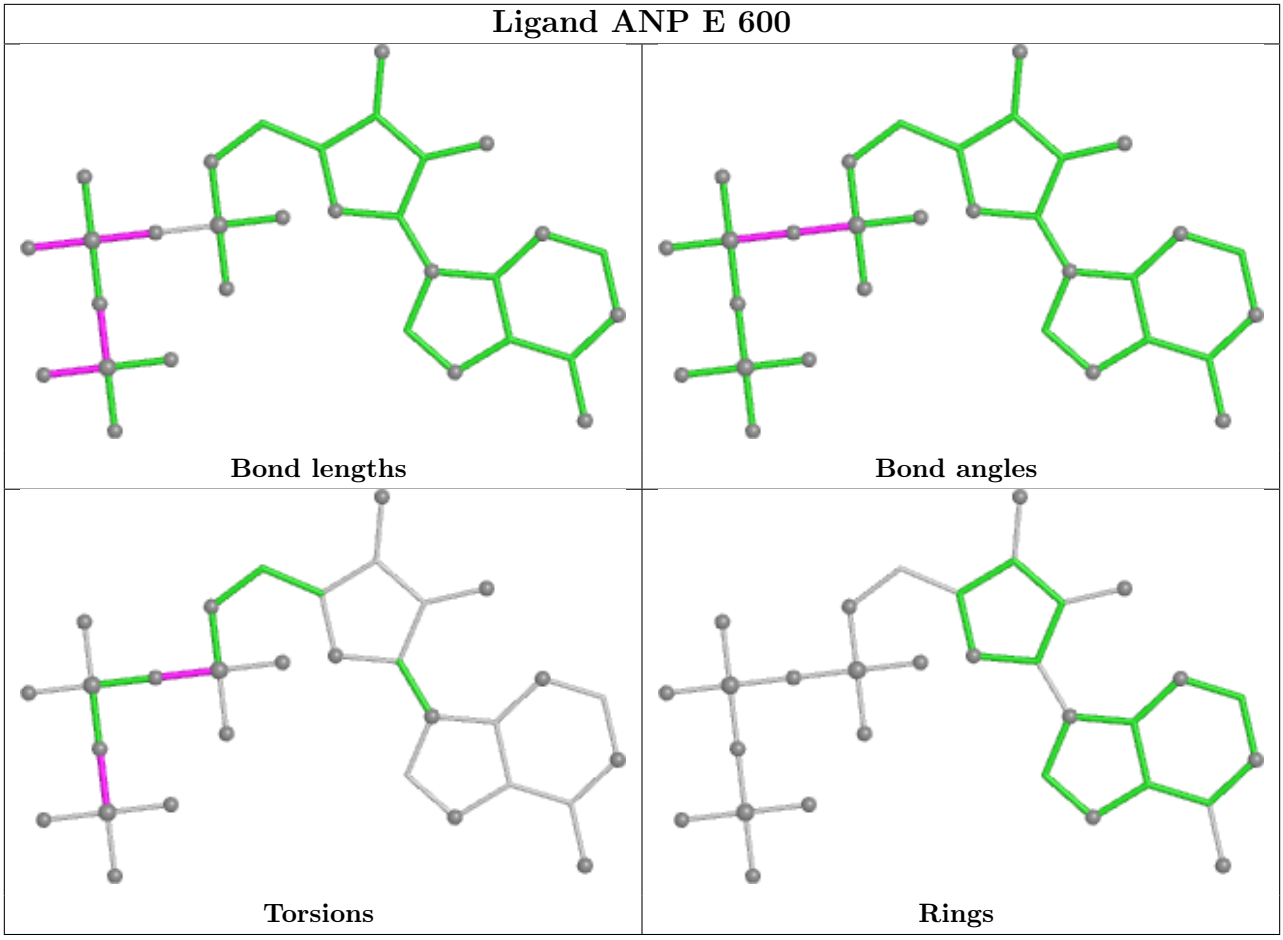


Ligand ANP C 602



Ligand ANP A 602





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.

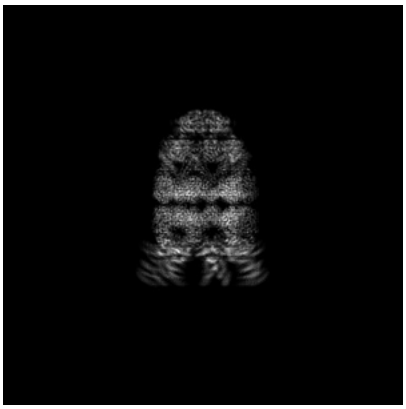
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-65991. These allow visual inspection of the internal detail of the map and identification of artifacts.

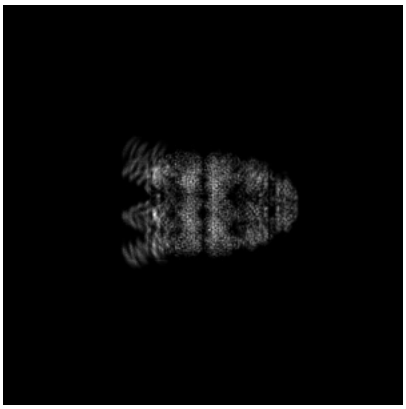
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

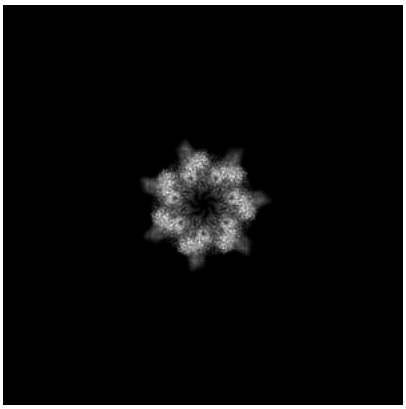
6.1.1 Primary map



X

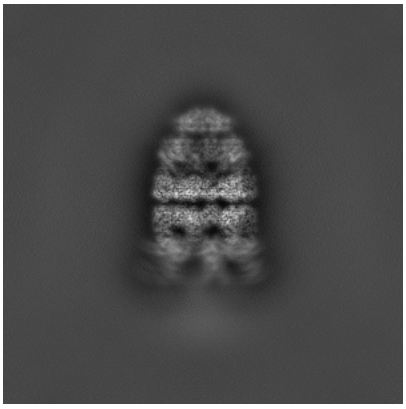


Y

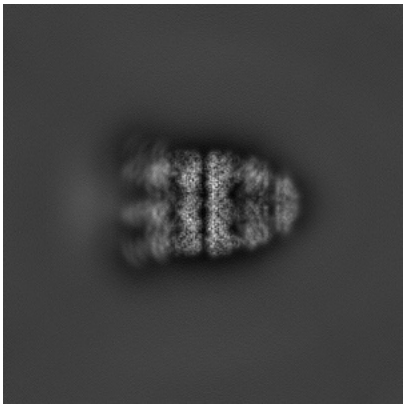


Z

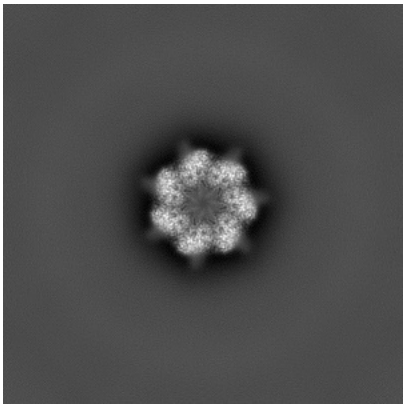
6.1.2 Raw map



X



Y



Z

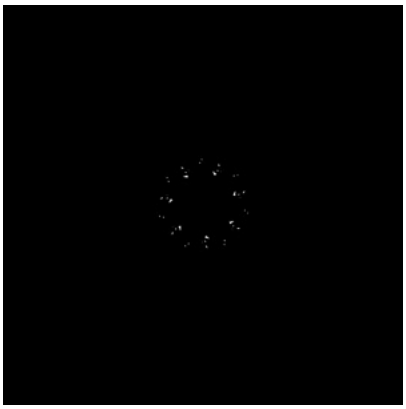
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

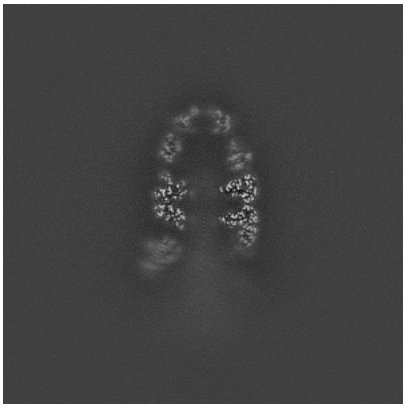
6.2.1 Primary map

X Index: 240

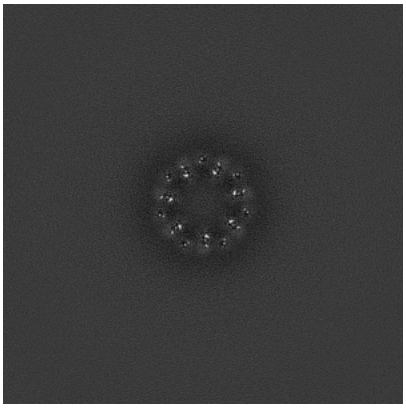
Y Index: 240


Z Index: 240

6.2.2 Raw map


X Index: 240

Y Index: 240


Z Index: 240

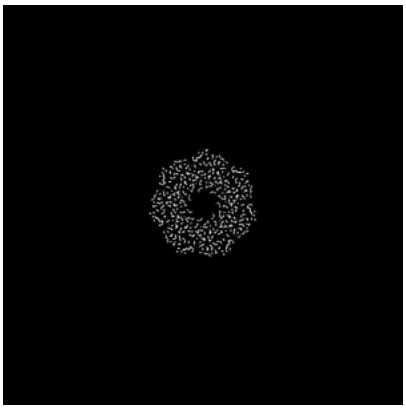
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

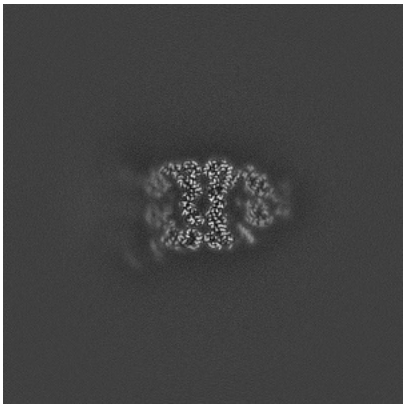
X Index: 273

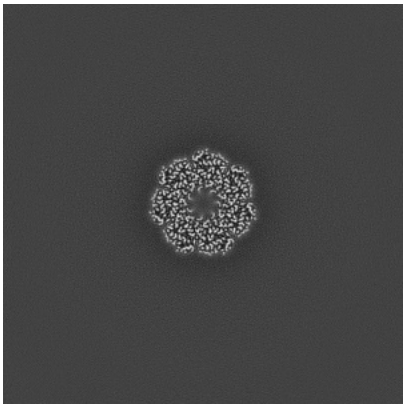
Y Index: 274


Z Index: 252

6.3.2 Raw map

X Index: 273

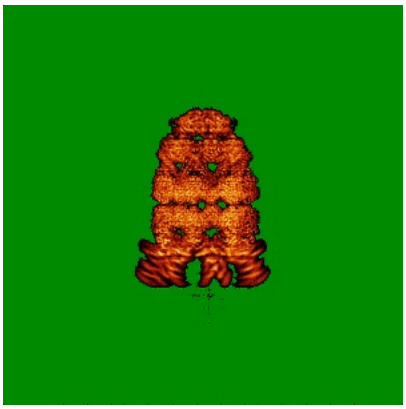

Y Index: 274

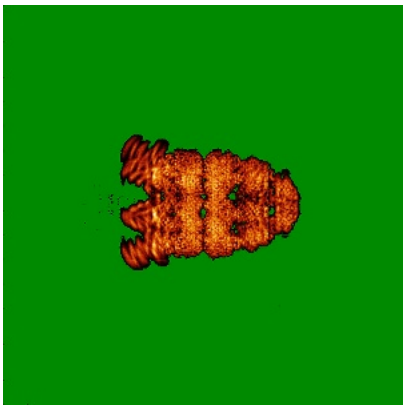

Z Index: 252

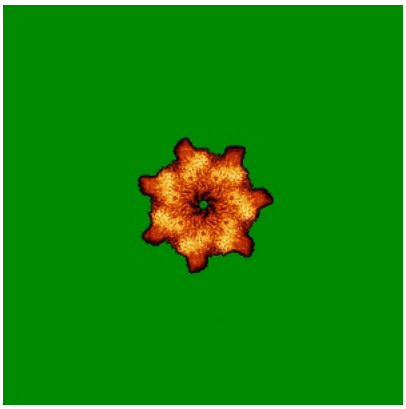
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

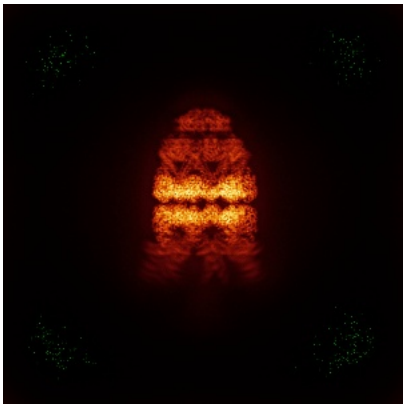
6.4.1 Primary map

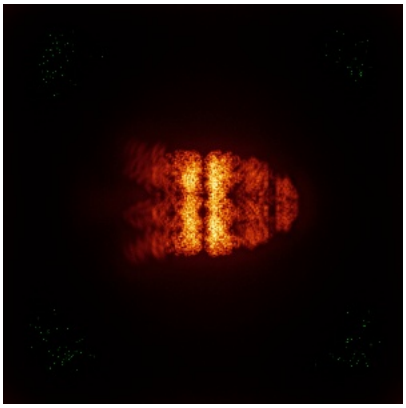

X

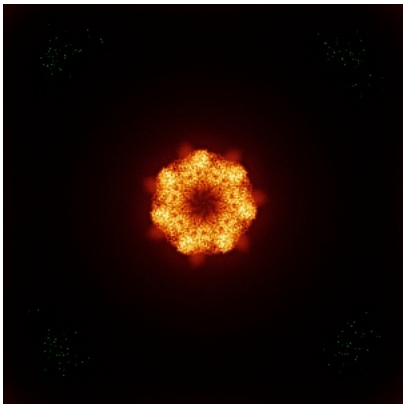

Y


Z

6.4.2 Raw map


X

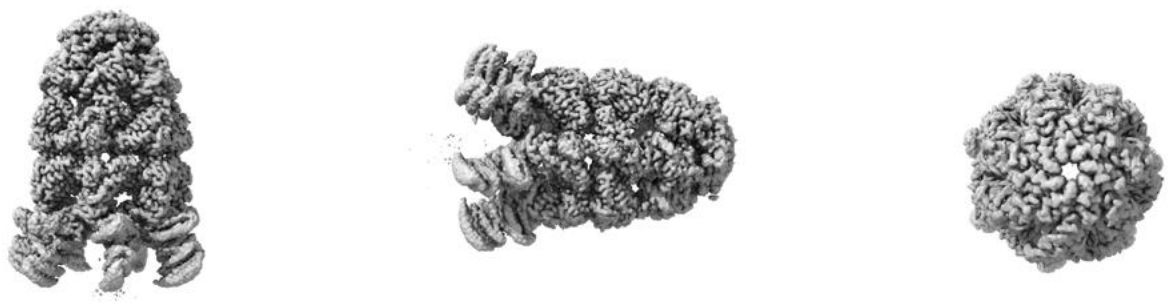

Y


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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. 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

X Y Z

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.

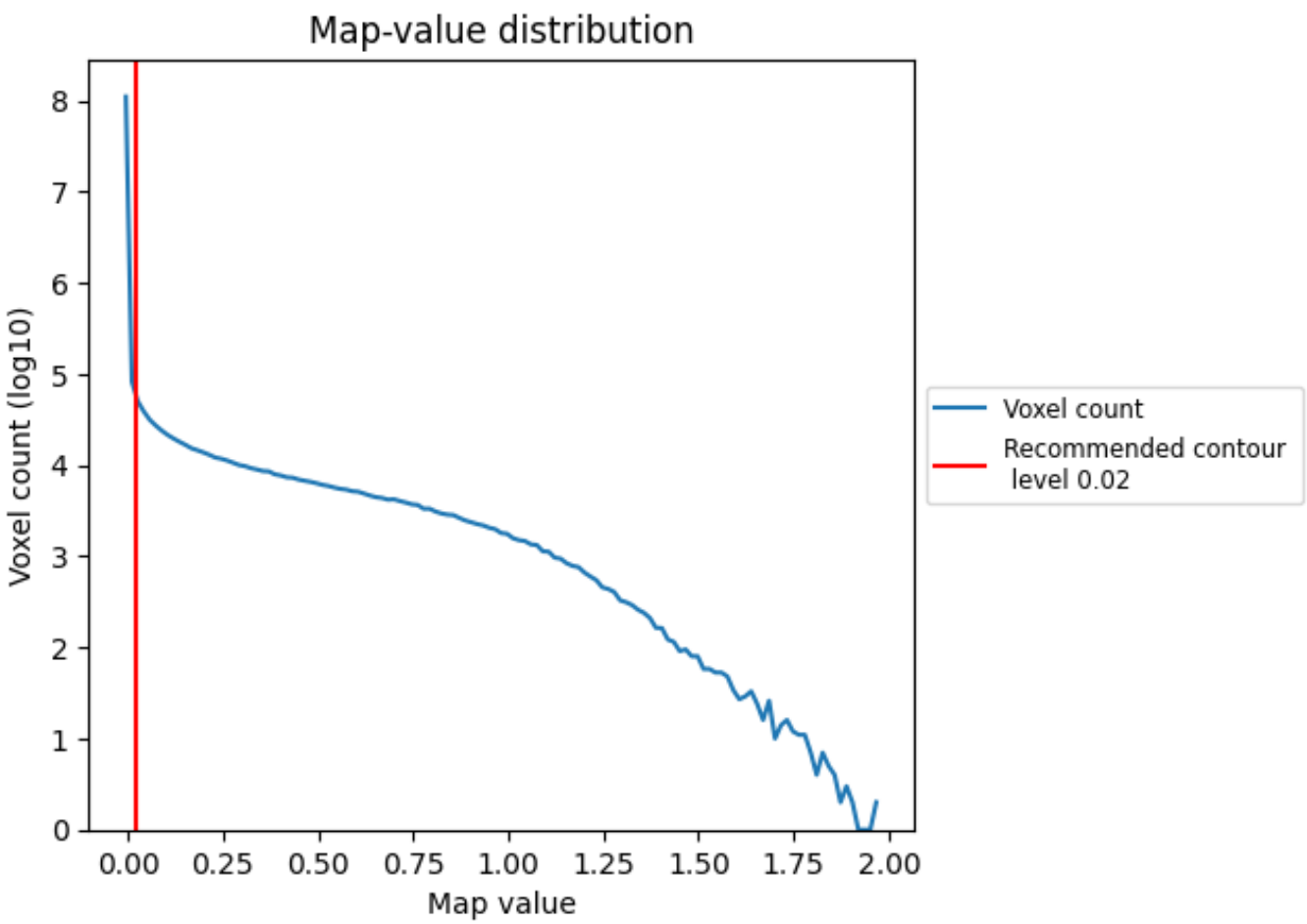
6.6 Mask visualisation (i)

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

7 Map analysis (i)

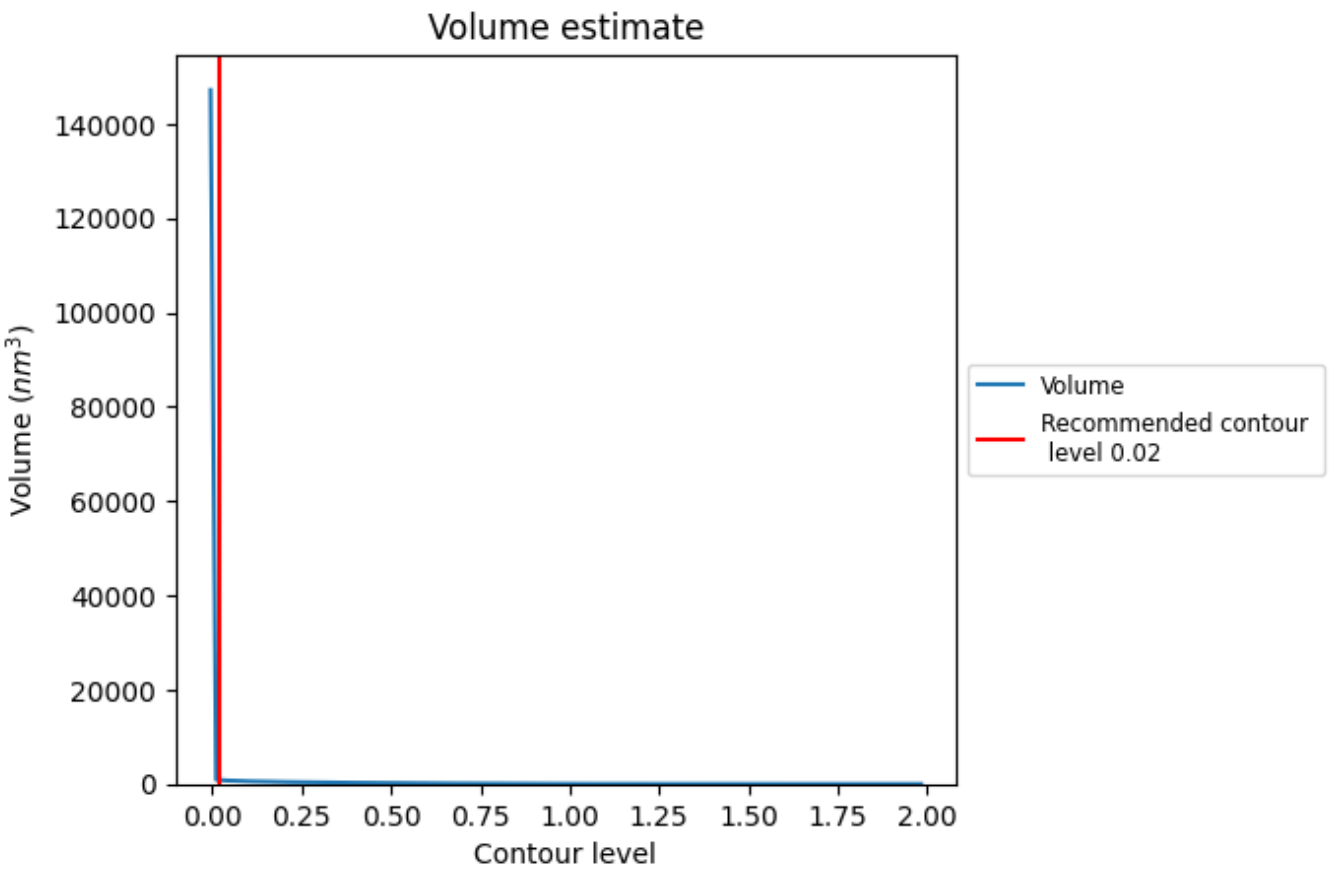
This section contains the results of statistical analysis of the map.

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.

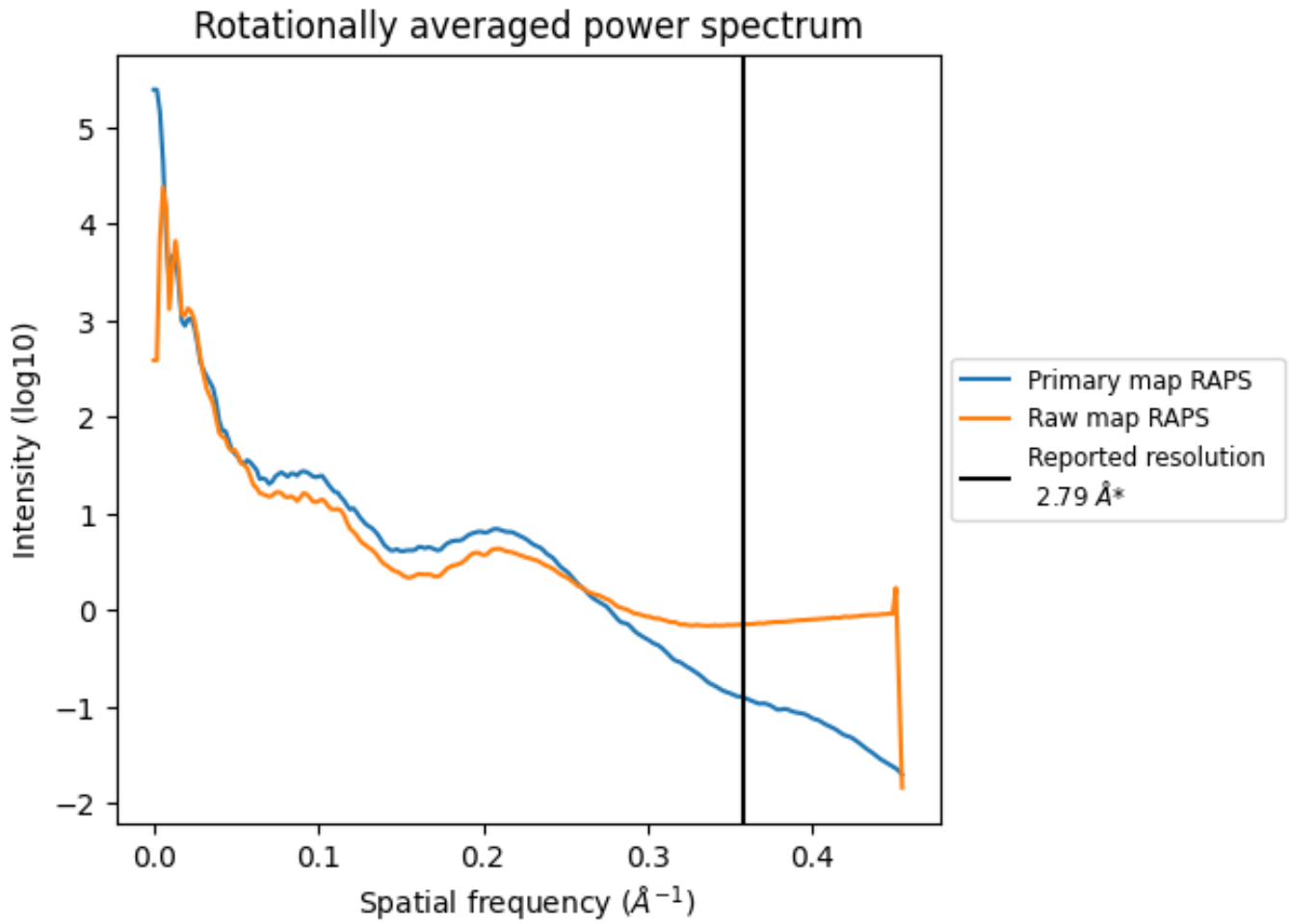
7.2 Volume estimate (i)



The volume at the recommended contour level is 841 nm^3; this corresponds to an approximate mass of 760 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)

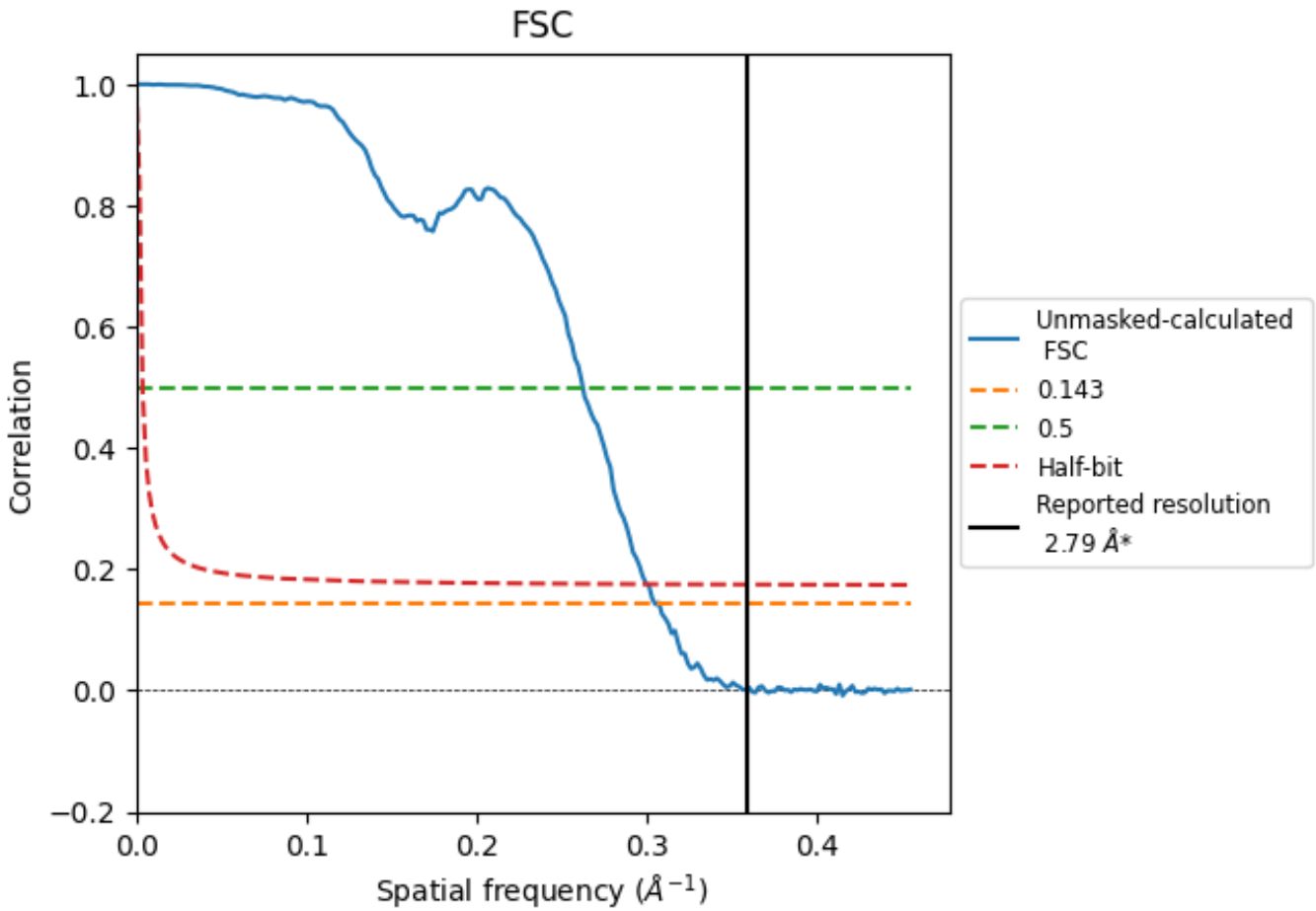


*Reported resolution corresponds to spatial frequency of 0.358 Å^{-1}

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 0.358 Å^{-1}

8.2 Resolution estimates (i)

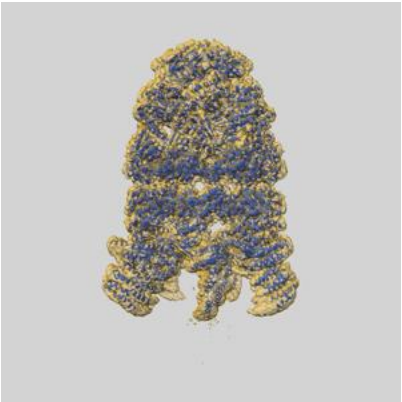
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.28	3.81	3.33

*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 3.28 differs from the reported value 2.79 by more than 10 %

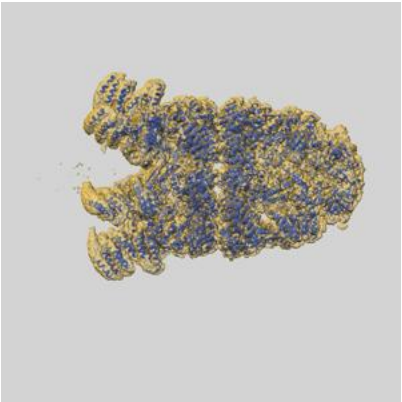
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-65991 and PDB model 9WIE. Per-residue inclusion information can be found in section 3 on page 9.

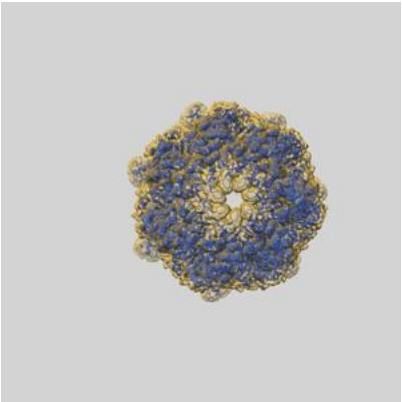
9.1 Map-model overlay (i)



X



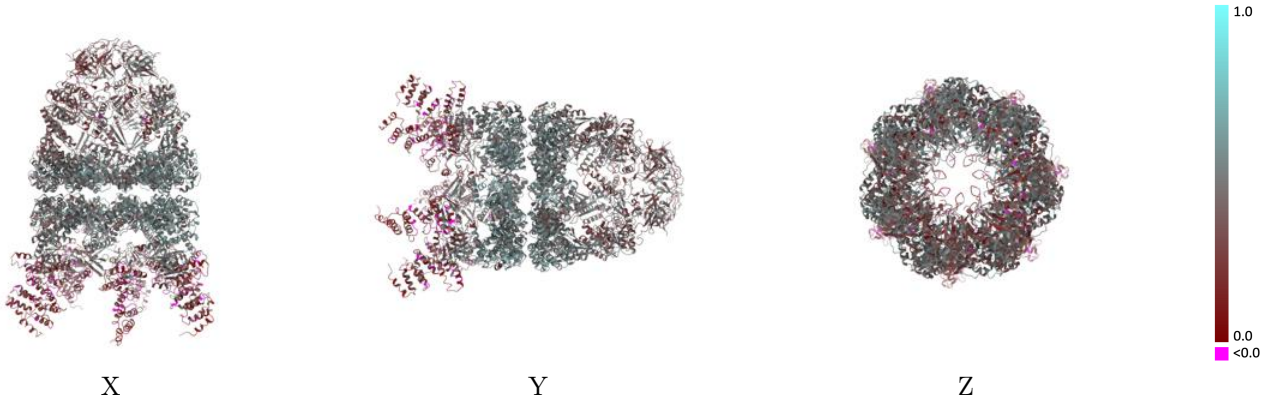
Y



Z

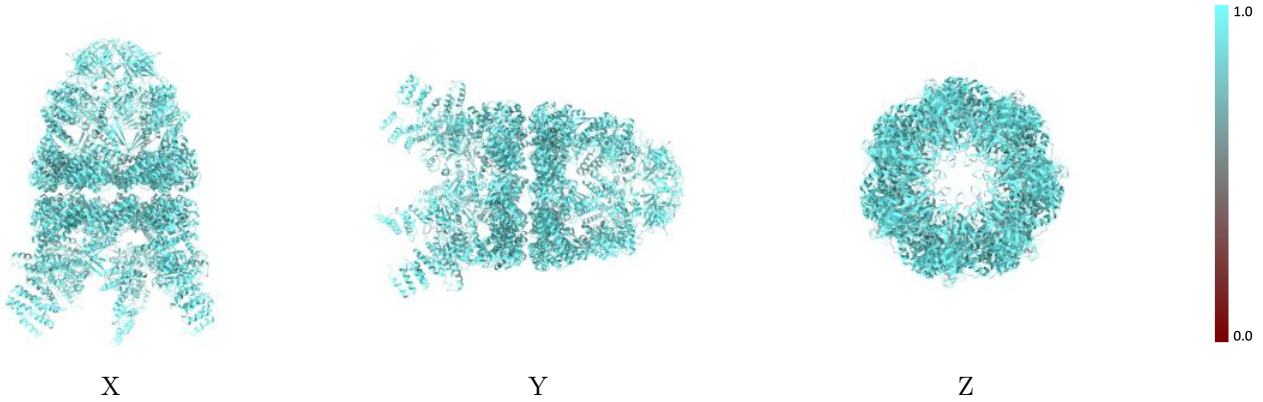
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



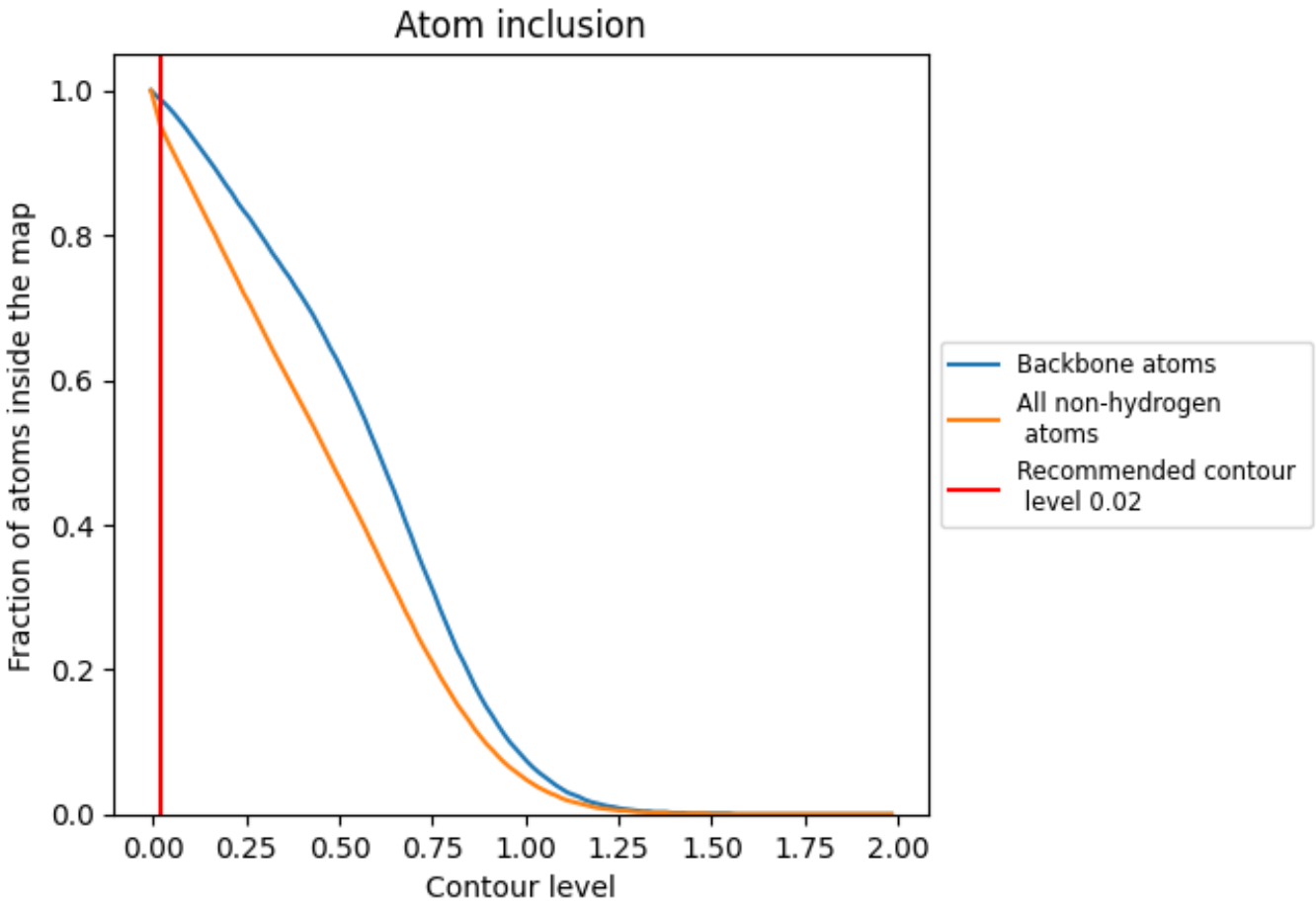
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9520	0.4050
A	0.9550	0.4290
B	0.9540	0.4240
C	0.9550	0.4410
D	0.9610	0.4620
E	0.9610	0.4680
F	0.9620	0.4580
G	0.9590	0.4420
H	0.9380	0.2950
I	0.9490	0.3150
J	0.9690	0.3910
K	0.9770	0.4410
L	0.9760	0.4190
M	0.9650	0.3550
N	0.9540	0.3120
P	0.9430	0.3880
R	0.9450	0.3880
S	0.9460	0.4100
T	0.9480	0.4090
U	0.9480	0.4210
V	0.9510	0.4290
W	0.9470	0.4240
d	0.9270	0.1900
e	0.9470	0.1990
f	0.9500	0.1950
g	0.9260	0.1910
h	0.9390	0.1920
i	0.9250	0.1860
j	0.9270	0.1830