wwPDB EM Validation Summary Report (i)

Nov 12, 2022 – 09:48 AM EST

PDB ID	:	6UQO
EMDB ID	:	EMD-20851
Title	:	ClpA/ClpP Engaged State bound to RepA-GFP
Authors	:	Lopez, K.L.; Rizo, A.N.; Southworth, D.R.
Deposited on	:	2019-10-21
Resolution	:	3.10 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:

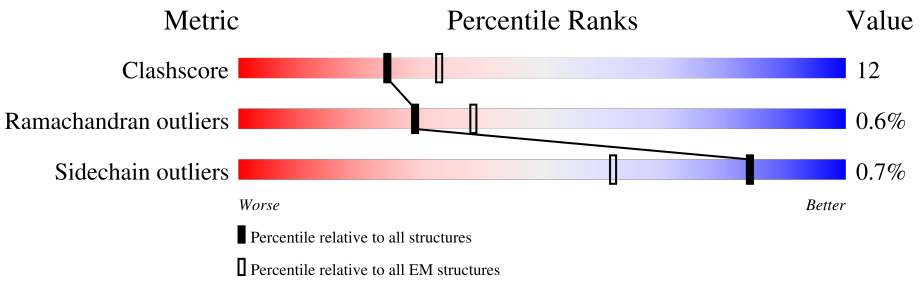
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	578	26% 84% 15% •
1	B	578	8% 84% 14% •
1	C	578	5% 87% 12% •
1	D	578	9% 90% 10%
1	E	578	52% 93% 6% •
1	F	578	87% 88% 11% •
2	G	192	• 91% 8% •
2	H	192	• 88% 10% ••

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	192	91% 8%
2	J	192	90% 9%
2	K	192	90% 10%
2	L	192	85% 12%
2	M	192	88% 8%
2	N	192	5% 91% 9%
2	O	192	89% 10%
2	P	192	90% 9%
2	Q	192	5% 89% 10%
2	R	192	90% 10%
2	S	192	88% 11%
2	T	192	5% 90% 9%
3	X	9	33% 33% 67%
3	Y	9	11% 89%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ADP	A	801	X	-	-	-
4	ADP	A	802	X	-	-	-
4	ADP	E	801	X	-	X	-
4	ADP	F	801	X	-	X	-
4	ADP	F	802	X	-	-	-
5	AGS	B	801	X	-	-	-
5	AGS	B	802	X	-	-	-
5	AGS	C	801	X	-	-	-
5	AGS	C	802	X	-	-	-
5	AGS	D	801	X	-	-	-
5	AGS	D	802	X	-	-	-
5	AGS	E	802	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 48522 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 ATP-dependent Clp protease ATP-binding subunit ClpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	578	4511	2841	805	851	14	0	0
1	B	578	4511	2841	805	851	14	0	0
1	C	578	4511	2841	805	851	14	0	0
1	D	578	4511	2841	805	851	14	0	0
1	E	578	4511	2841	805	851	14	0	0
1	F	578	4511	2841	805	851	14	0	0

- Molecule 2 is a protein called ATP-dependent Clp endopeptidase proteolytic subunit ClpP.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	192	1501	946	260	283	12	0	0
2	H	192	1501	946	260	283	12	0	0
2	I	192	1501	946	260	283	12	0	0
2	J	192	1501	946	260	283	12	0	0
2	K	192	1501	946	260	283	12	0	0
2	L	192	1501	946	260	283	12	0	0
2	M	192	1501	946	260	283	12	0	0
2	N	192	1501	946	260	283	12	0	0
2	O	192	1501	946	260	283	12	0	0

Continued on next page...

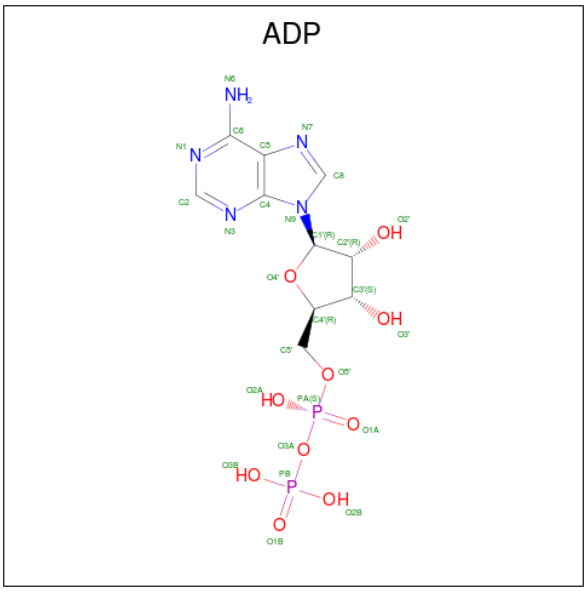
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	P	192	1501	946	260	283	12	0	0
2	Q	192	1501	946	260	283	12	0	0
2	R	192	1501	946	260	283	12	0	0
2	S	192	1501	946	260	283	12	0	0
2	T	192	1501	946	260	283	12	0	0

- Molecule 3 is a protein called RepA-GFP.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	X	9	45	27	9	9	0	0
3	Y	9	45	27	9	9	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



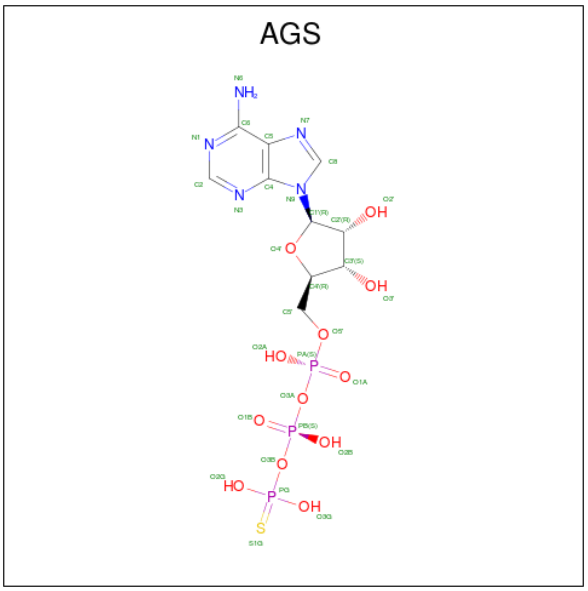
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	A	1	54	20	10	20	4	0
4	A	1	54	20	10	20	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	E	1	27	10	5	10	2	0
			Total	C	N	O	P	
4	F	1	54	20	10	20	4	0
			Total	C	N	O	P	
4	F	1	54	20	10	20	4	0

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



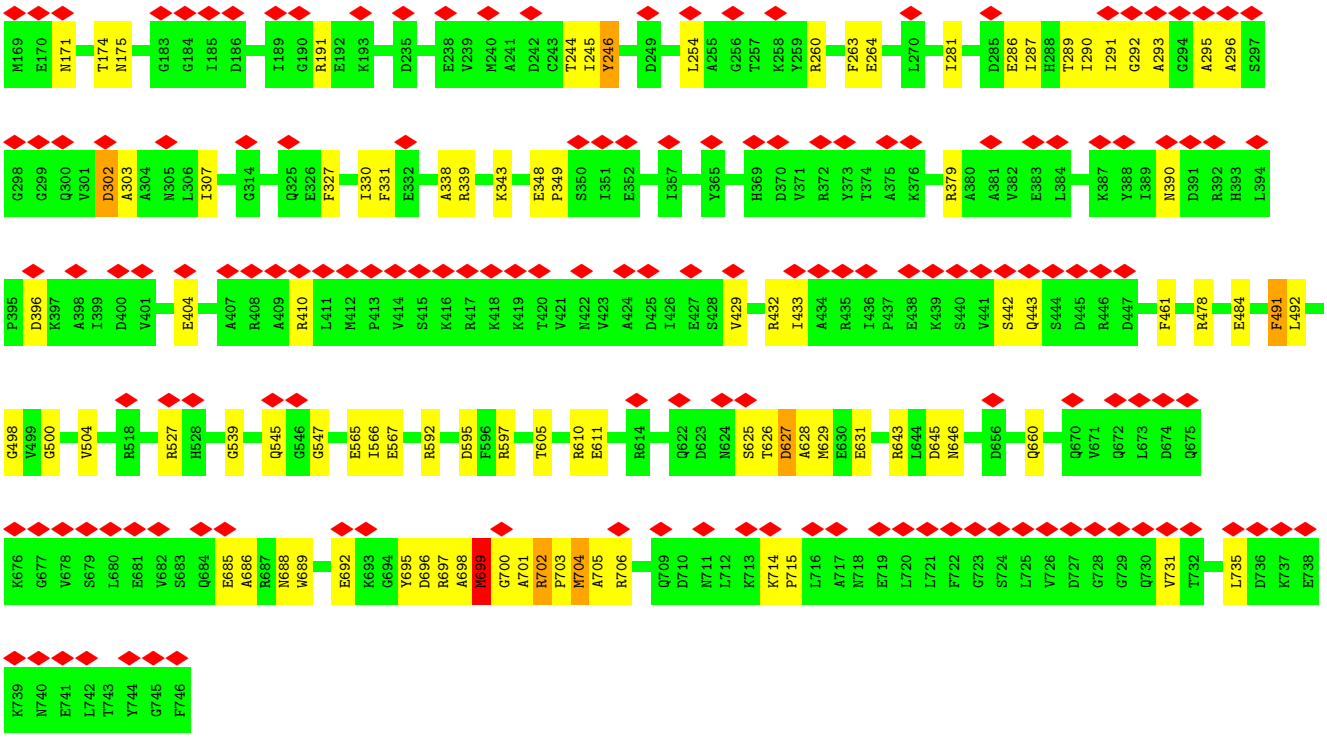
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
5	B	1	62	20	10	24	6	2	0
			Total	C	N	O	P	S	
5	B	1	62	20	10	24	6	2	0
			Total	C	N	O	P	S	
5	C	1	62	20	10	24	6	2	0
			Total	C	N	O	P	S	
5	C	1	62	20	10	24	6	2	0
			Total	C	N	O	P	S	
5	D	1	62	20	10	24	6	2	0
			Total	C	N	O	P	S	
5	D	1	62	20	10	24	6	2	0
			Total	C	N	O	P	S	
5	E	1	31	10	5	12	3	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.

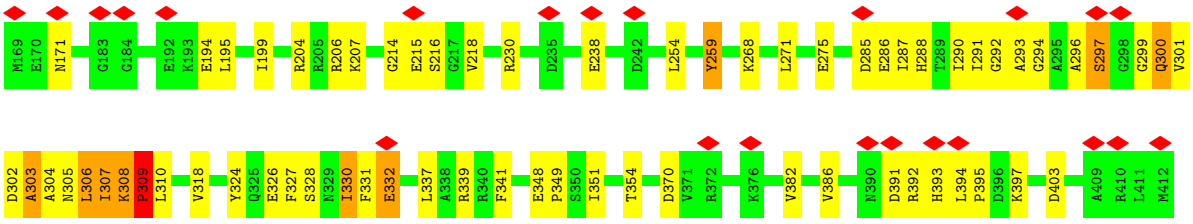
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA

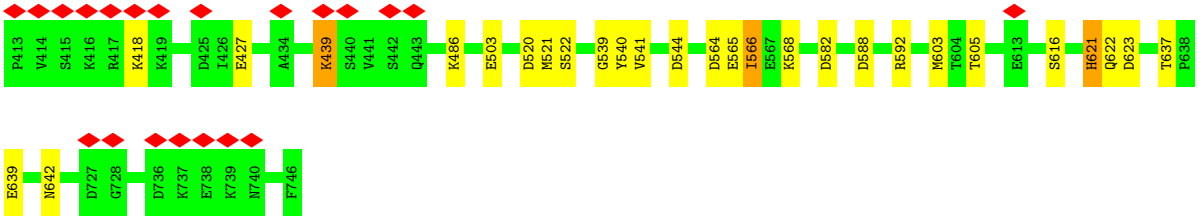
Chain A: 26% 84% 15%



• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA

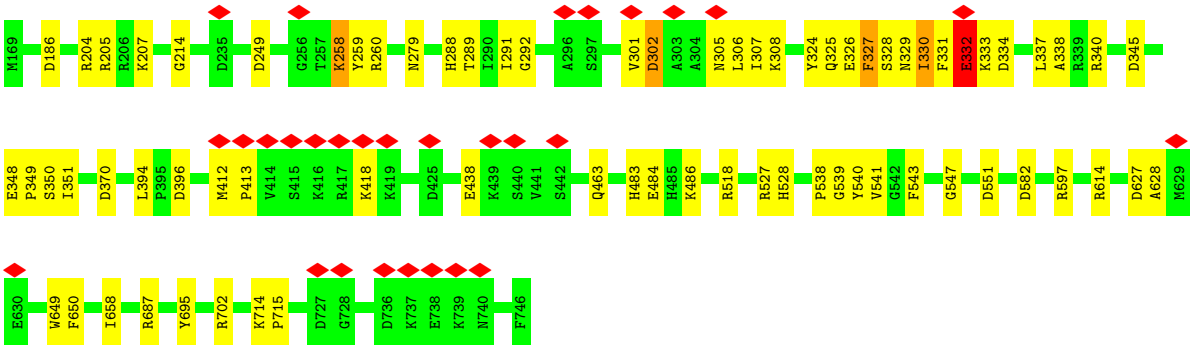
Chain B: 8% 84% 14%





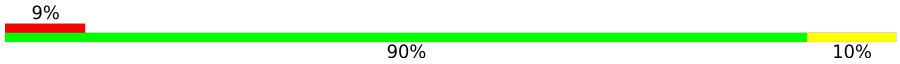
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA

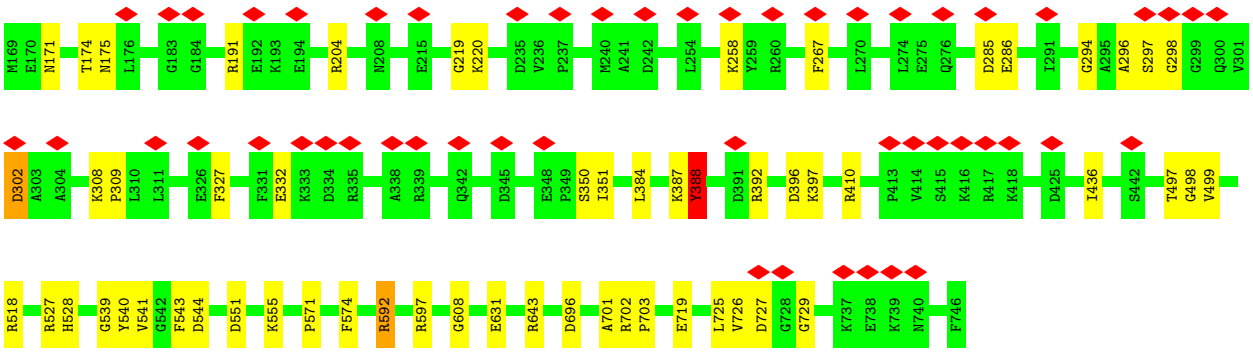
Chain C:



• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA

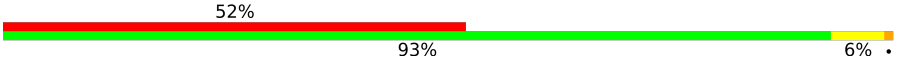
Chain D:

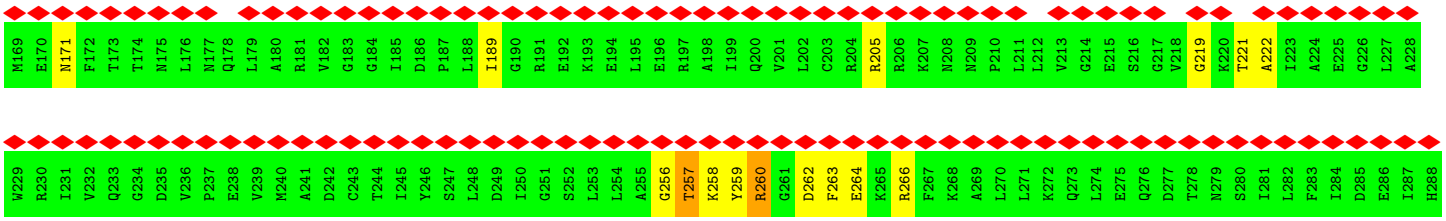




• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA

Chain E:





T289 I290 I291 G292 A293 G294 A295 A296 S297 G298 G299 Q300 V301 D302 A303 A304 N305 L306 I307 K308 P309 L310 L311 S312 S313 G314 K315 I316 R317 V318 I319 G320 S321 T322 T323 Y324 Q325 E326 F327 S328 N329 I330 F331 E332 K333 D334 R335 A336 L337 A338 R339 R340 F341 Q342 K343 I344 D345 I346 T347 E348

P349 S350 I351 E352 E353 T354 V355 Q356 I357 I358 L361 Y365 E366 A367 H368 H369 D370 V371 R372 Y373 T374 A375 K376 A377 V378 R379 A380 A381 V382 E383 L384 A385 V386 K387 Y388 I389 N390 D391 R392 H393 L394 P395 D396 K397 A398 I399 D400 V401 I402 D403 E404 R408 L411 M412 P413 V414

S415 K416 R417 K418 K419 T420 V421 N422 V423 A424 D425 I426 E427 S428 V429 V430 A431 R432 I433 A434 R435 I436 P437 E438 K439 S440 V441 S442 Q443 S444 D445 R446 D447 R455 I474 R478 A479 G480 L481 G482 H483 E484 F491 S531 R532 A536 P537 P538 G539 Y540 V541 G542 F543 D544

Q545 G546 L586 T587 D588 N589 N590 G591 R592 K593 A594 D595 G608 V609 R610 E611 T612 E613 R614 N624 S625 T626 D627 A628 M629 E630 E631 E639 R643 D651 S654 D696 R702 P703 R706 D727 T732 D736 K737 E738 K739 Y744 G745 F746

- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA

Chain F: 87% 88% 11%

M169 E170 N171 F172 T173 T174 N175 L176 N177 Q178 L179 A180 R181 V182 G183 G184 I185 D186 P187 L188 I189 G190 R191 E192 K193 E194 L195 E196 R197 A198 I199 Q200 V201 L202 C203 R204 R205 R206 K207 N208 N209 P210 L211 L212 V213 G214 E215 S216 G217 V218 G219 K220 T221 A222 I223 A224 E225 G226 L227 A228

W229 R230 I231 V232 Q233 G234 D235 V236 P237 E238 V239 M240 A241 D242 C243 T244 I245 Y246 S247 L248 D249 I250 G251 S252 L253 L254 A255 G256 T257 K258 Y259 R260 G261 D262 F263 E264 K265 R266 F267 K268 A269 L270 L271 K272 Q273 L274 E275 Q276 D277 T278 N279 S280 I281 L282 F283 I284 D285 E286 I287 H288

T289 I290 I291 G292 A293 G294 A295 A296 S297 G298 G299 Q300 V301 D302 A303 A304 N305 L306 I307 K308 P309 L310 L311 S312 S313 G314 K315 I316 R317 V318 I319 G320 S321 T322 T323 Y324 Q325 E326 F327 S328 N329 I330 F331 E332 K333 D334 R335 A336 L337 A338 R339 R340 F341 Q342 K343 I344 D345 I346 T347 E348

P349 S350 I351 E352 E353 T354 V355 Q356 I357 I358 N359 G360 L361 K362 P363 K364 Y365 E366 A367 H368 H369 D370 V371 R372 Y373 T374 A375 K376 A377 V378 R379 A380 A381 V382 E383 L384 A385 V386 K387 Y388 I389 N390 D391 R392 H393 L394 P395 D396 K397 A398 I399 D400 V401 I402 D403 E404 A405 G406 A407 R408

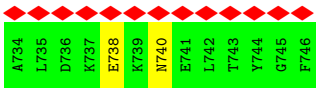
A409 R410 L411 M412 P413 V414 S415 K416 R417 K418 K419 T420 V421 N422 V423 A424 D425 I426 E427 S428 V429 V430 A431 R432 I433 A434 R435 I436 P437 E438 K439 S440 V441 S442 Q443 S444 D445 R446 D447 T448 L449 K450 N451 L452 G453 D454 R455 L456 K457 M458 L459 V460 F461 Q462 Q463 D464 K465 A466 I467 E468

A469 L470 T471 E472 A473 I474 K475 M476 A477 R478 A479 G480 L481 G482 H483 E484 H485 K486 P487 V488 G489 S490 F491 L492 T497 G500 K501 T502 E503 V504 T505 A511 L512 G513 I514 E515 L516 L517 R518 F519 D520 M521 S522 E523 Y524 M525 E526 R527 H528 T529 V530 S531 R532 L533 I534 G535 A536

P537 P538 G539 Y540 V541 G542 F543 D544 Q545 G546 G547 L548 L549 T550 D551 A552 V553 I554 K555 H556 P557 H558 L561 L562 L563 D564 E565 I566 E567 K568 A569 H570 P571 D572 V573 F574 N575 I576 L577 L578 Q579 V580 M581 D582 N583 G584 T585 L586 T587 D588 N589 N590 G591 R592 K593 A594 D595 T596 R597

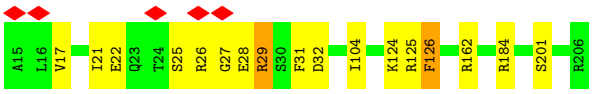
V600 L601 T604 T605 N606 A607 G608 V609 R610 E611 T612 E613 R614 K615 D623 N624 S625 T626 D627 A628 M629 E630 E631 I632 K633 K634 I635 F636 T637 P638 E639 F640 R641 N642 R643 L644 D645 N646 I647 I648 W649 F650 D651 H652 L653 S654 T655 D656 V657 I658 H659 Q660 V661 V662 D663 K664 F665

E668 Q672 L673 D674 Q675 K676 G677 V678 S679 L680 E681 V682 S683 Q684 E685 A686 R687 N688 W689 L690 A691 E692 K693 G694 Y695 D696 R697 A698 M699 G700 A701 R702 P703 M704 A705 R706 L712 K713 K714 A717 N718 E719 L720 L721 F722 G723 S724 L725 V726 D727 G728 G729 Q730 V731 T732 V733



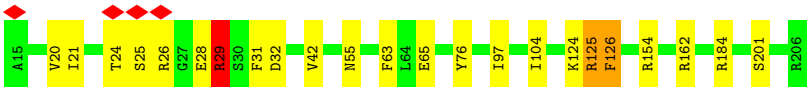
• Molecule 2: ATP-dependent Clp endopeptidase proteolytic subunit ClpP

Chain G:



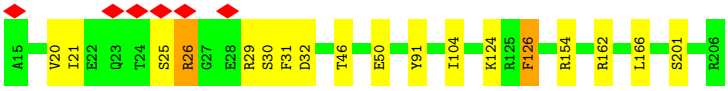
• Molecule 2: ATP-dependent Clp endopeptidase proteolytic subunit ClpP

Chain H:



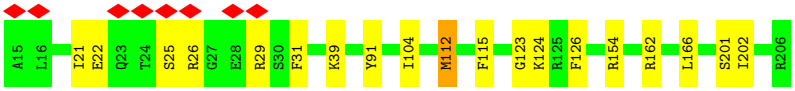
• Molecule 2: ATP-dependent Clp endopeptidase proteolytic subunit ClpP

Chain I:



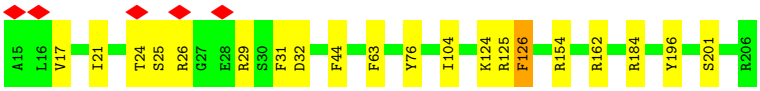
• Molecule 2: ATP-dependent Clp endopeptidase proteolytic subunit ClpP

Chain J:



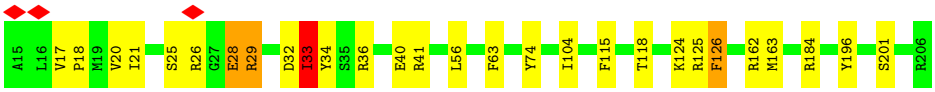
• Molecule 2: ATP-dependent Clp endopeptidase proteolytic subunit ClpP

Chain K:



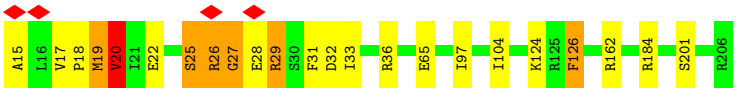
• Molecule 2: ATP-dependent Clp endopeptidase proteolytic subunit ClpP

Chain L:



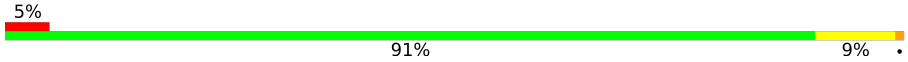
• Molecule 2: ATP-dependent Clp endopeptidase proteolytic subunit ClpP

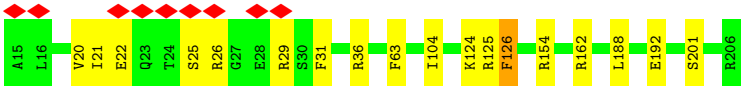
Chain M:



• Molecule 2: ATP-dependent Clp endopeptidase proteolytic subunit ClpP

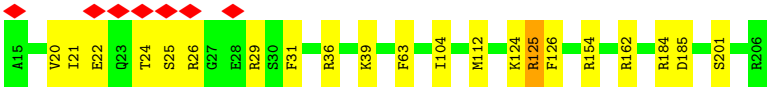
Chain N:





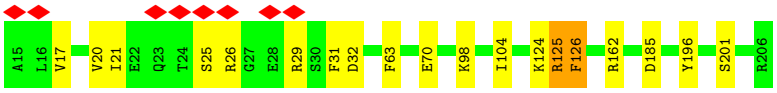
• Molecule 2: ATP-dependent Clp endopeptidase proteolytic subunit ClpP

Chain O:



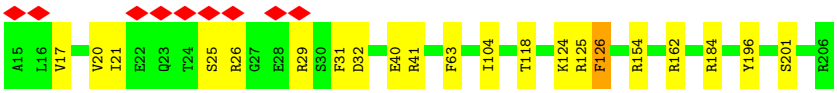
• Molecule 2: ATP-dependent Clp endopeptidase proteolytic subunit ClpP

Chain P:



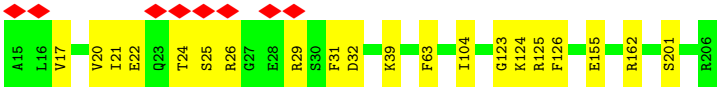
• Molecule 2: ATP-dependent Clp endopeptidase proteolytic subunit ClpP

Chain Q:



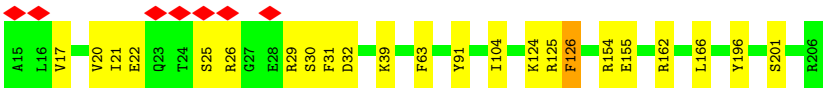
• Molecule 2: ATP-dependent Clp endopeptidase proteolytic subunit ClpP

Chain R:



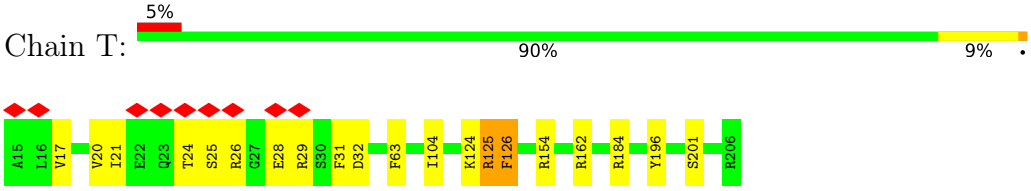
• Molecule 2: ATP-dependent Clp endopeptidase proteolytic subunit ClpP

Chain S:



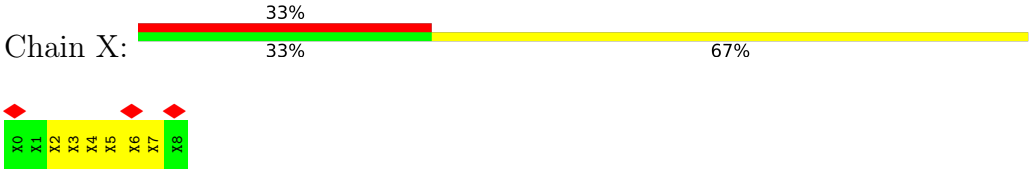
• Molecule 2: ATP-dependent Clp endopeptidase proteolytic subunit ClpP

Chain T:



• Molecule 3: RepA-GFP

Chain X:



• Molecule 3: RepA-GFP

Chain Y:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97000	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 ($e^-/Å^2$)	69	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	58616	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.563	Depositor
Minimum map value	-1.554	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.65	Depositor
Map size (Å)	511.8, 511.8, 511.8	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.853, 0.853, 0.853	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, AGS

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	1.05	0/4577	0.92	9/6175 (0.1%)
1	B	1.11	0/4577	0.91	7/6175 (0.1%)
1	C	1.17	0/4577	0.95	13/6175 (0.2%)
1	D	1.15	0/4577	0.95	14/6175 (0.2%)
1	E	1.02	0/4577	0.95	14/6175 (0.2%)
1	F	0.98	0/4577	0.94	11/6175 (0.2%)
2	G	1.40	0/1525	0.94	4/2054 (0.2%)
2	H	1.25	0/1525	0.96	7/2054 (0.3%)
2	I	1.29	0/1525	0.93	3/2054 (0.1%)
2	J	1.23	0/1525	0.91	4/2054 (0.2%)
2	K	1.32	0/1525	0.95	6/2054 (0.3%)
2	L	1.32	0/1525	0.90	3/2054 (0.1%)
2	M	1.34	0/1525	0.92	4/2054 (0.2%)
2	N	1.27	0/1525	0.92	5/2054 (0.2%)
2	O	1.26	0/1525	0.92	6/2054 (0.3%)
2	P	1.30	0/1525	0.91	4/2054 (0.2%)
2	Q	1.30	0/1525	0.90	4/2054 (0.2%)
2	R	1.31	0/1525	0.92	4/2054 (0.2%)
2	S	1.26	0/1525	0.93	6/2054 (0.3%)
2	T	1.25	0/1525	0.96	8/2054 (0.4%)
All	All	1.18	0/48812	0.93	136/65806 (0.2%)

There are no bond length outliers.

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	204	ARG	NE-CZ-NH2	-10.69	114.96	120.30
1	C	204	ARG	NE-CZ-NH2	-10.42	115.09	120.30
1	D	410	ARG	NE-CZ-NH2	-10.28	115.16	120.30
1	E	643	ARG	NE-CZ-NH2	-10.05	115.27	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	184	ARG	NE-CZ-NH1	9.84	125.22	120.30

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	4511	0	4609	161	0
1	B	4511	0	4608	236	0
1	C	4511	0	4609	143	0
1	D	4511	0	4609	58	0
1	E	4511	0	4608	69	0
1	F	4511	0	4608	81	0
2	G	1501	0	1512	25	0
2	H	1501	0	1512	38	0
2	I	1501	0	1512	36	0
2	J	1501	0	1512	33	0
2	K	1501	0	1512	31	0
2	L	1501	0	1512	55	0
2	M	1501	0	1512	59	0
2	N	1501	0	1512	32	0
2	O	1501	0	1512	31	0
2	P	1501	0	1512	33	0
2	Q	1501	0	1512	28	0
2	R	1501	0	1512	31	0
2	S	1501	0	1512	35	0
2	T	1501	0	1512	36	0
3	X	45	0	14	17	0
3	Y	45	0	17	25	0
4	A	54	0	23	8	0
4	E	27	0	11	27	0
4	F	54	0	22	17	0
5	B	62	0	23	0	0
5	C	62	0	23	2	0
5	D	62	0	22	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	31	0	12	0	0
All	All	48522	0	48986	1149	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 12.

The worst 5 of 1149 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:C:328:SER:CA	1:C:332:GLU:CG	1.76	1.64
1:A:291:ILE:CG2	1:A:330:ILE:CG2	1.78	1.61
1:A:291:ILE:HD11	1:A:331:PHE:CE1	1.35	1.57
1:A:291:ILE:HG21	1:A:330:ILE:CG2	1.17	1.57
1:B:293:ALA:CB	1:B:303:ALA:HB3	1.27	1.57

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	576/578 (100%)	554 (96%)	17 (3%)	5 (1%)	17 52
1	B	576/578 (100%)	554 (96%)	13 (2%)	9 (2%)	9 37
1	C	576/578 (100%)	550 (96%)	20 (4%)	6 (1%)	15 49
1	D	576/578 (100%)	559 (97%)	14 (2%)	3 (0%)	29 64
1	E	576/578 (100%)	564 (98%)	10 (2%)	2 (0%)	41 73
1	F	576/578 (100%)	552 (96%)	19 (3%)	5 (1%)	17 52
2	G	190/192 (99%)	181 (95%)	8 (4%)	1 (0%)	29 64
2	H	190/192 (99%)	180 (95%)	8 (4%)	2 (1%)	14 46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	190/192 (99%)	184 (97%)	6 (3%)	0	100	100
2	J	190/192 (99%)	180 (95%)	10 (5%)	0	100	100
2	K	190/192 (99%)	183 (96%)	7 (4%)	0	100	100
2	L	190/192 (99%)	179 (94%)	8 (4%)	3 (2%)	9	37
2	M	190/192 (99%)	178 (94%)	9 (5%)	3 (2%)	9	37
2	N	190/192 (99%)	183 (96%)	7 (4%)	0	100	100
2	O	190/192 (99%)	182 (96%)	8 (4%)	0	100	100
2	P	190/192 (99%)	182 (96%)	8 (4%)	0	100	100
2	Q	190/192 (99%)	181 (95%)	9 (5%)	0	100	100
2	R	190/192 (99%)	183 (96%)	7 (4%)	0	100	100
2	S	190/192 (99%)	183 (96%)	7 (4%)	0	100	100
2	T	190/192 (99%)	184 (97%)	6 (3%)	0	100	100
All	All	6116/6156 (99%)	5876 (96%)	201 (3%)	39 (1%)	29	59

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	628	ALA
1	A	702	ARG
1	A	704	MET
1	B	297	SER
1	B	303	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	485/485 (100%)	479 (99%)	6 (1%)	71	88
1	B	485/485 (100%)	481 (99%)	4 (1%)	81	92
1	C	485/485 (100%)	483 (100%)	2 (0%)	91	96
1	D	485/485 (100%)	484 (100%)	1 (0%)	93	97

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	485/485 (100%)	483 (100%)	2 (0%)	91	96
1	F	485/485 (100%)	483 (100%)	2 (0%)	91	96
2	G	162/162 (100%)	161 (99%)	1 (1%)	86	94
2	H	162/162 (100%)	160 (99%)	2 (1%)	71	88
2	I	162/162 (100%)	160 (99%)	2 (1%)	71	88
2	J	162/162 (100%)	162 (100%)	0	100	100
2	K	162/162 (100%)	161 (99%)	1 (1%)	86	94
2	L	162/162 (100%)	160 (99%)	2 (1%)	71	88
2	M	162/162 (100%)	159 (98%)	3 (2%)	57	81
2	N	162/162 (100%)	161 (99%)	1 (1%)	86	94
2	O	162/162 (100%)	161 (99%)	1 (1%)	86	94
2	P	162/162 (100%)	160 (99%)	2 (1%)	71	88
2	Q	162/162 (100%)	161 (99%)	1 (1%)	86	94
2	R	162/162 (100%)	162 (100%)	0	100	100
2	S	162/162 (100%)	161 (99%)	1 (1%)	86	94
2	T	162/162 (100%)	160 (99%)	2 (1%)	71	88
All	All	5178/5178 (100%)	5142 (99%)	36 (1%)	84	93

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	126	PHE
2	T	126	PHE
2	O	125	ARG
2	Q	126	PHE
1	D	388	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	273	GLN
1	F	590	ASN
2	R	55	ASN
1	F	740	ASN
1	C	273	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ADP	A	801	-	24,29,29	4.37	10 (41%)	29,45,45	1.77	6 (20%)
4	ADP	F	802	-	24,29,29	4.28	8 (33%)	29,45,45	1.78	6 (20%)
5	AGS	B	801	-	26,33,33	3.84	11 (42%)	26,52,52	2.10	7 (26%)
5	AGS	C	802	-	26,33,33	3.80	11 (42%)	26,52,52	1.95	5 (19%)
5	AGS	D	801	-	26,33,33	3.94	12 (46%)	26,52,52	1.91	6 (23%)
5	AGS	B	802	-	26,33,33	3.71	12 (46%)	26,52,52	1.78	6 (23%)
5	AGS	E	802	-	26,33,33	3.78	11 (42%)	26,52,52	1.89	5 (19%)
5	AGS	C	801	-	26,33,33	3.88	11 (42%)	26,52,52	2.02	5 (19%)
4	ADP	A	802	-	24,29,29	4.40	9 (37%)	29,45,45	1.62	4 (13%)
4	ADP	F	801	1	24,29,29	4.46	4 (16%)	29,45,45	1.53	3 (10%)
4	ADP	E	801	1	24,29,29	4.39	4 (16%)	29,45,45	1.43	4 (13%)
5	AGS	D	802	-	26,33,33	3.85	12 (46%)	26,52,52	1.92	7 (26%)

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	A	801	-	2/2/6/6	6/12/32/32	0/3/3/3
4	ADP	F	802	-	2/2/6/6	0/12/32/32	0/3/3/3
5	AGS	B	801	-	2/2/7/7	1/17/38/38	0/3/3/3
5	AGS	C	802	-	3/3/7/7	0/17/38/38	0/3/3/3
5	AGS	D	801	-	3/3/7/7	3/17/38/38	0/3/3/3
5	AGS	B	802	-	3/3/7/7	4/17/38/38	0/3/3/3
5	AGS	E	802	-	3/3/7/7	0/17/38/38	0/3/3/3
5	AGS	C	801	-	2/2/7/7	3/17/38/38	0/3/3/3
4	ADP	A	802	-	2/2/6/6	1/12/32/32	0/3/3/3
4	ADP	F	801	1	1/1/6/6	4/12/32/32	0/3/3/3
4	ADP	E	801	1	2/2/6/6	6/12/32/32	0/3/3/3
5	AGS	D	802	-	2/2/7/7	2/17/38/38	0/3/3/3

The worst 5 of 115 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	ADP	O4'-C1'	16.81	1.64	1.41
4	F	802	ADP	O4'-C1'	16.30	1.63	1.41
4	A	802	ADP	O4'-C1'	15.96	1.63	1.41
4	F	801	ADP	O4'-C1'	15.19	1.62	1.41
4	E	801	ADP	O4'-C1'	15.10	1.62	1.41

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	802	AGS	PA-O3A-PB	-6.23	111.46	132.83
5	C	801	AGS	PA-O3A-PB	-5.64	113.48	132.83
5	C	801	AGS	N3-C2-N1	-5.01	120.85	128.68
4	F	801	ADP	PA-O3A-PB	-5.00	115.68	132.83
5	D	801	AGS	O4'-C1'-C2'	-4.98	99.65	106.93

5 of 27 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	801	ADP	C1'
4	A	801	ADP	C3'
4	A	802	ADP	C1'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
4	A	802	ADP	C3'
4	E	801	ADP	C3'

5 of 30 torsion outliers are listed below:

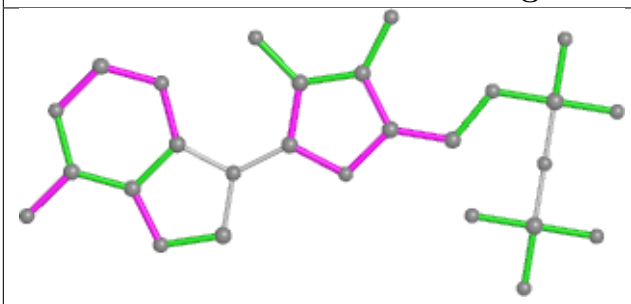
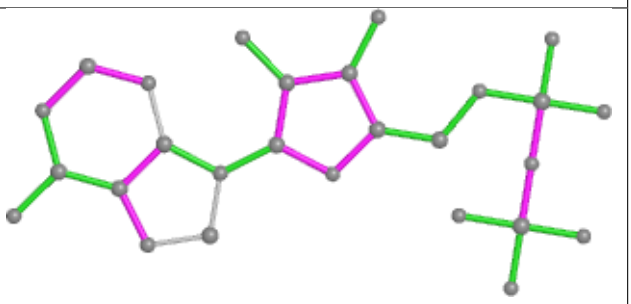
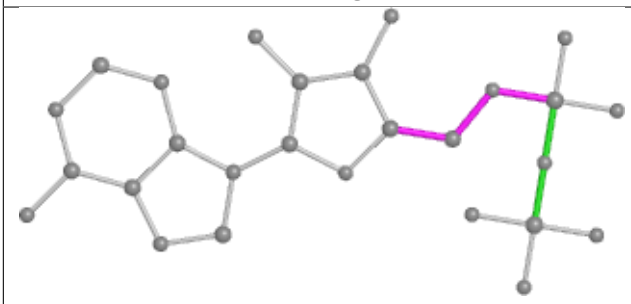
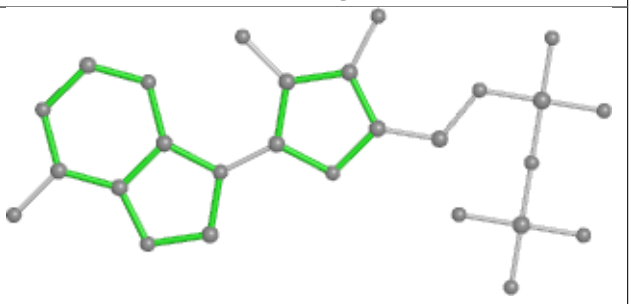
Mol	Chain	Res	Type	Atoms
4	A	801	ADP	C5'-O5'-PA-O1A
4	A	802	ADP	C4'-C5'-O5'-PA
4	E	801	ADP	C5'-O5'-PA-O2A
4	E	801	ADP	C4'-C5'-O5'-PA
4	F	801	ADP	C5'-O5'-PA-O1A

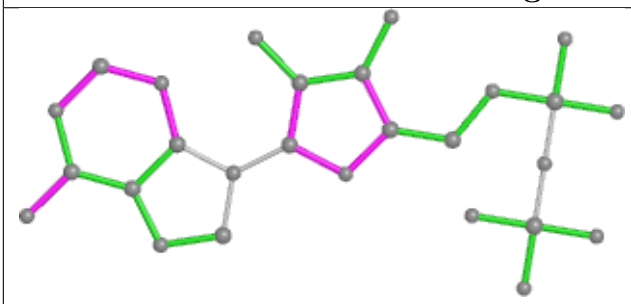
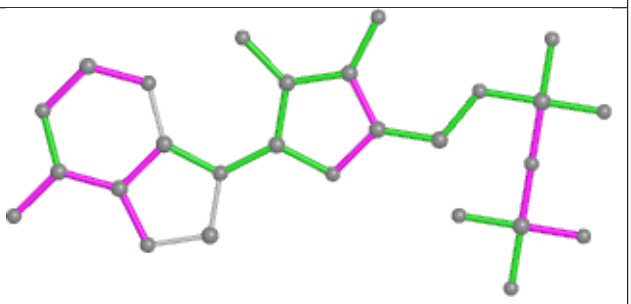
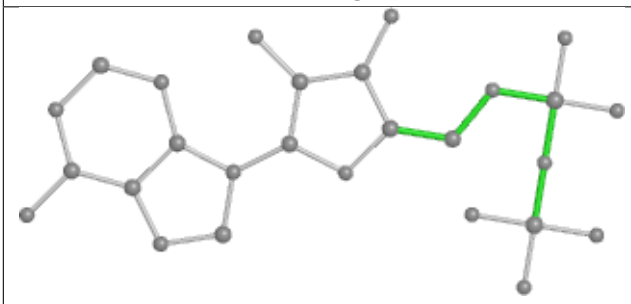
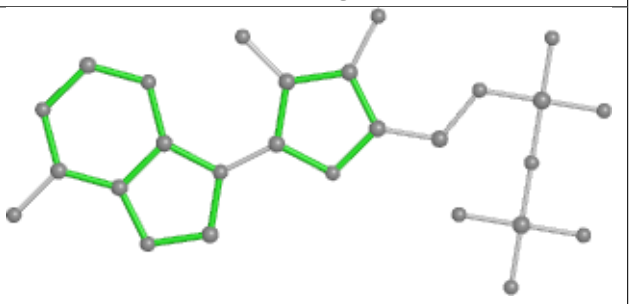
There are no ring outliers.

7 monomers are involved in 54 short contacts:

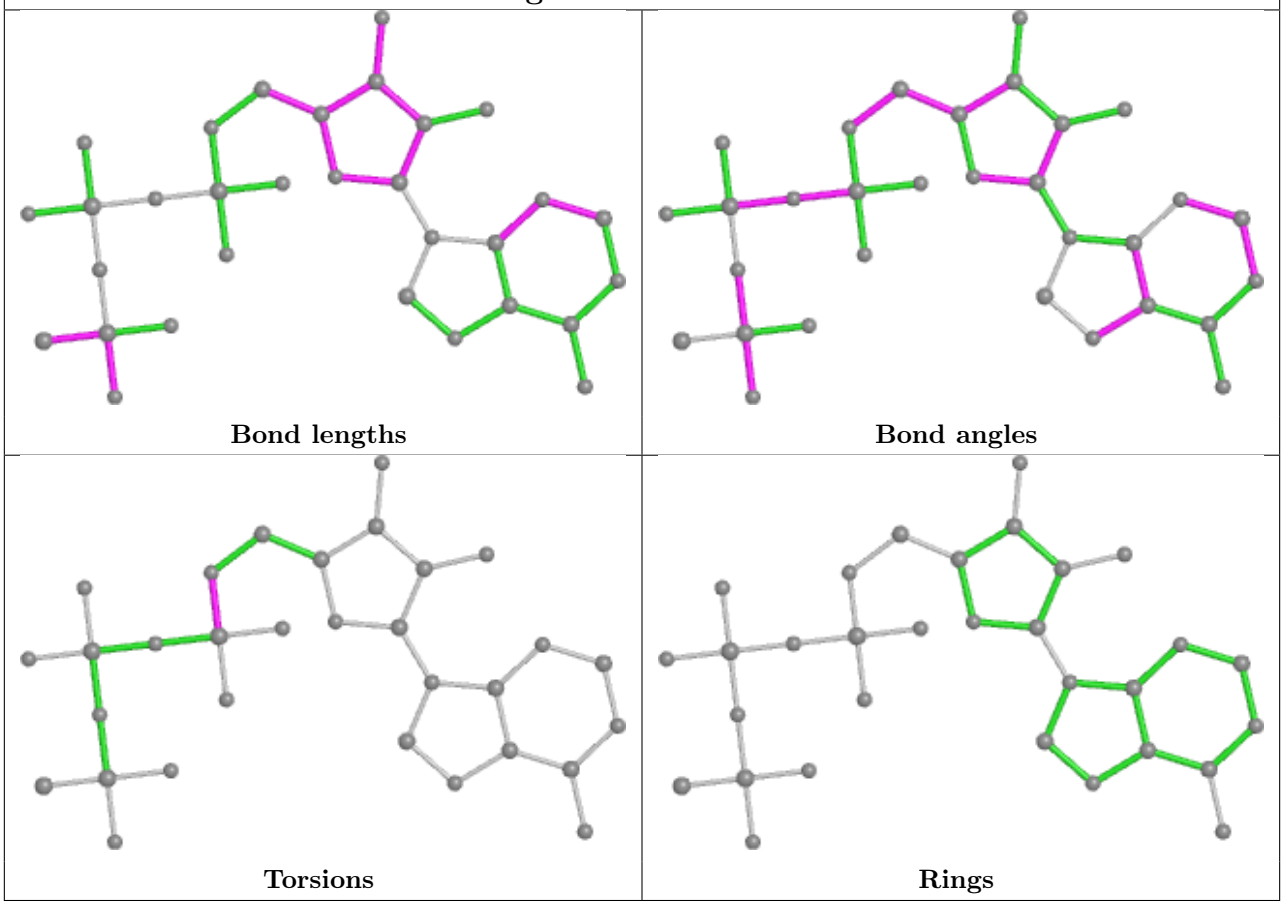
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	ADP	1	0
4	F	802	ADP	2	0
5	C	802	AGS	1	0
5	C	801	AGS	1	0
4	A	802	ADP	7	0
4	F	801	ADP	15	0
4	E	801	ADP	27	0

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.

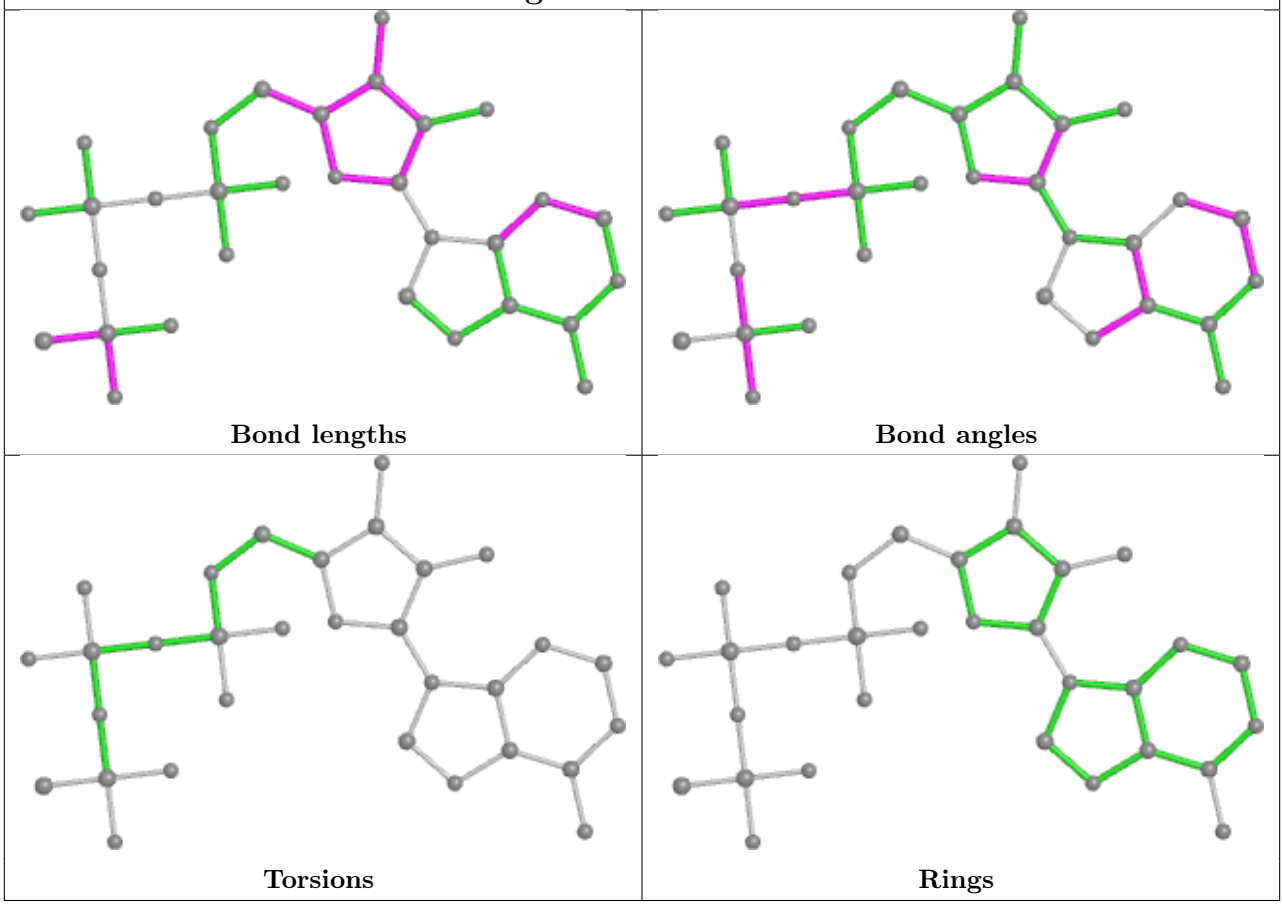
Ligand ADP A 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP F 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

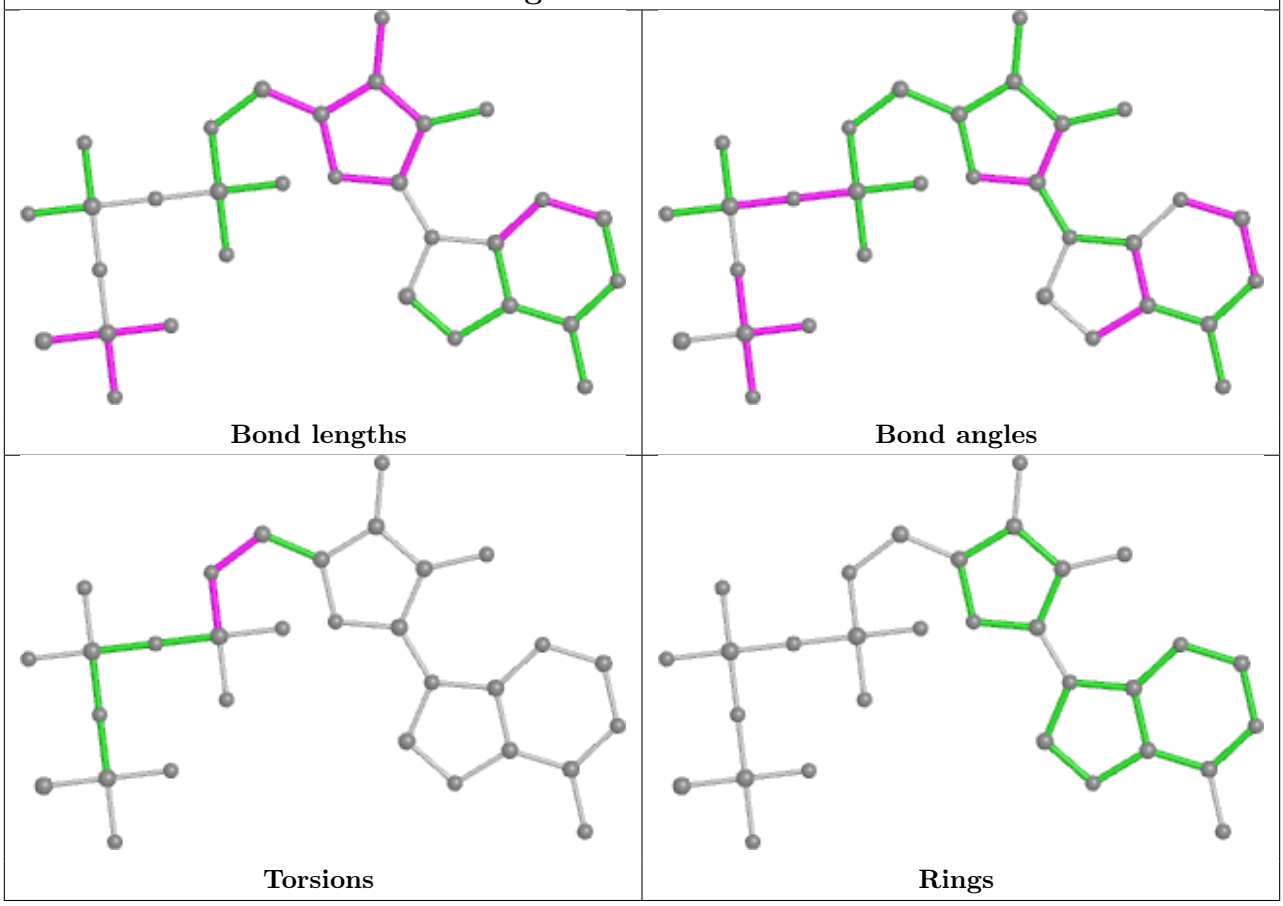
Ligand AGS B 801



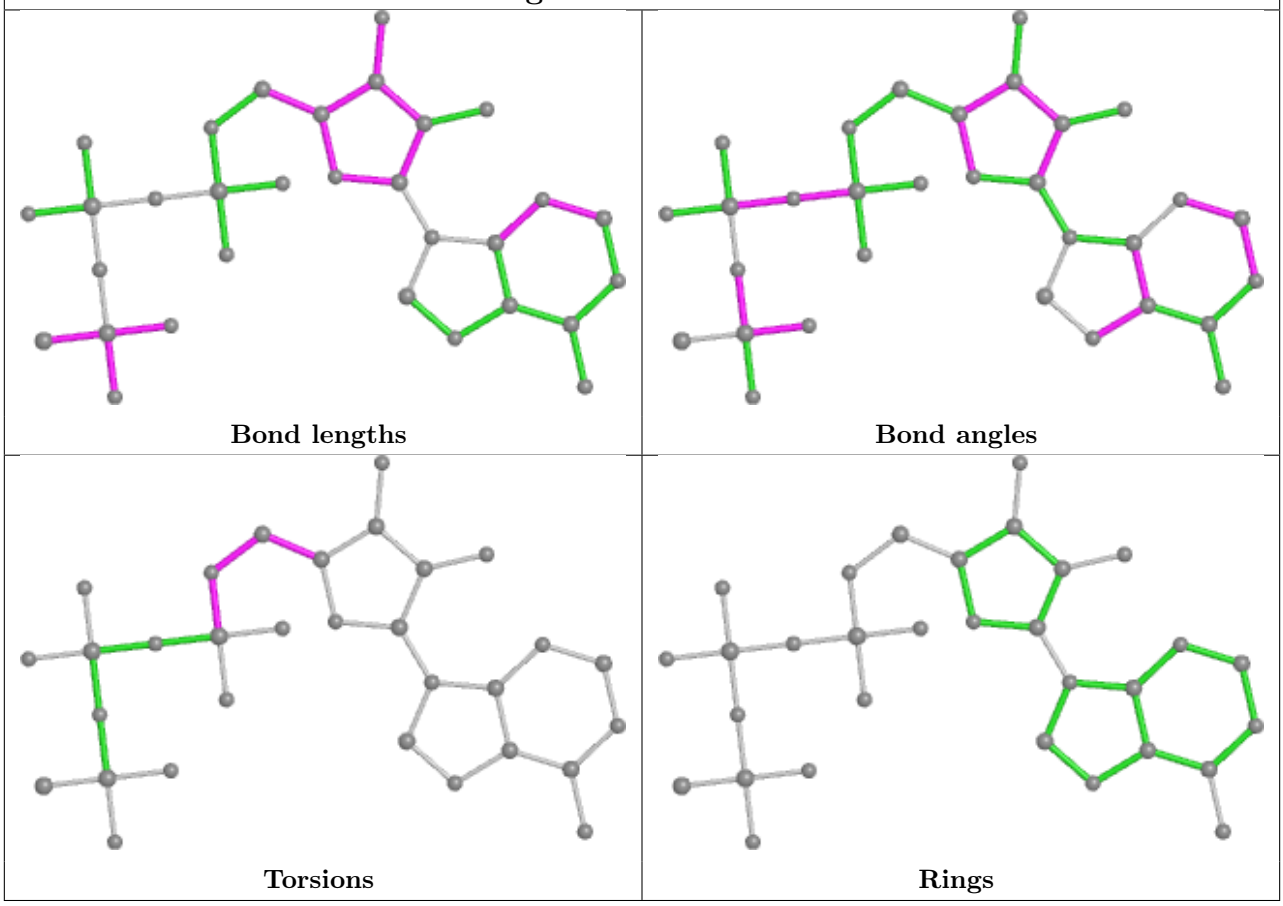
Ligand AGS C 802



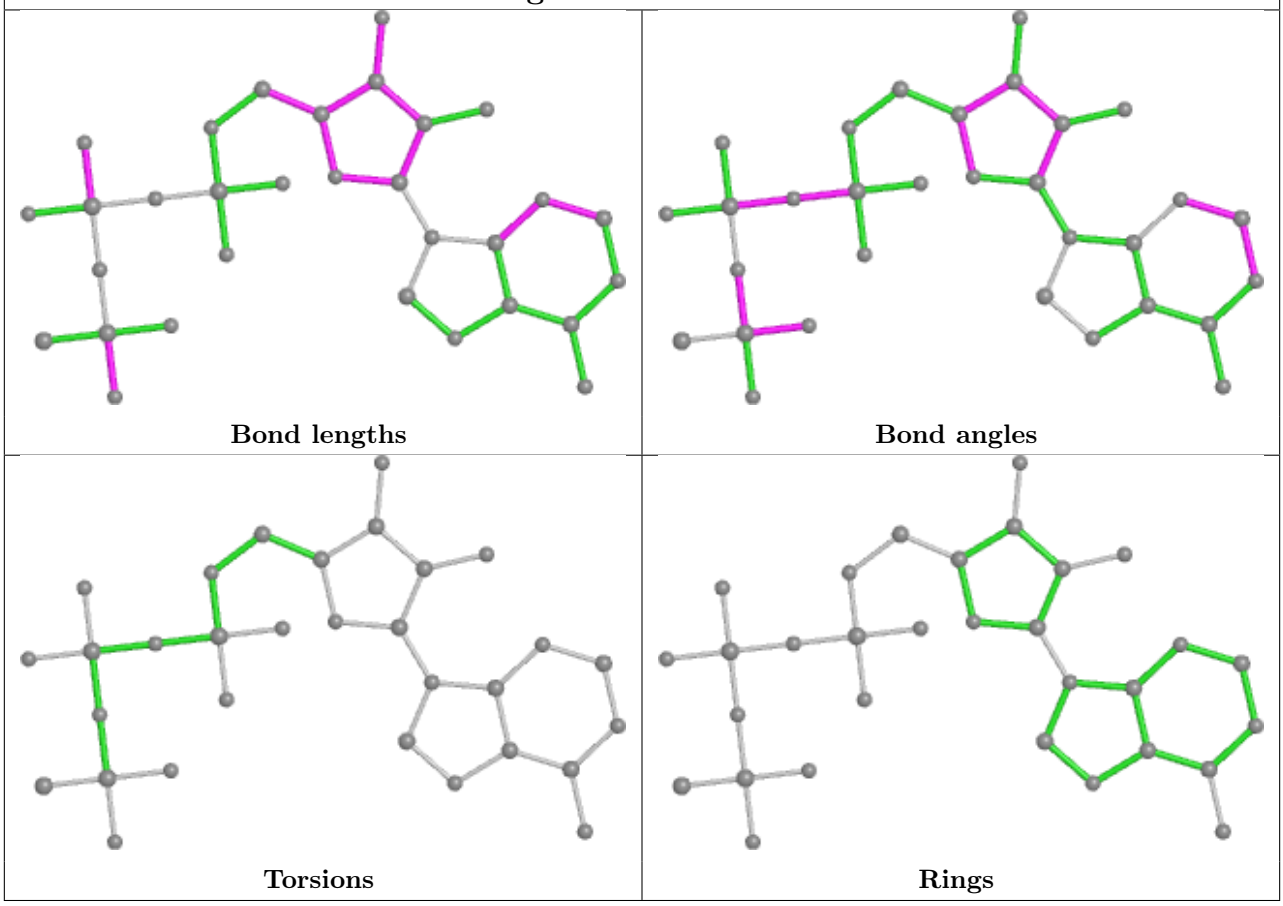
Ligand AGS D 801



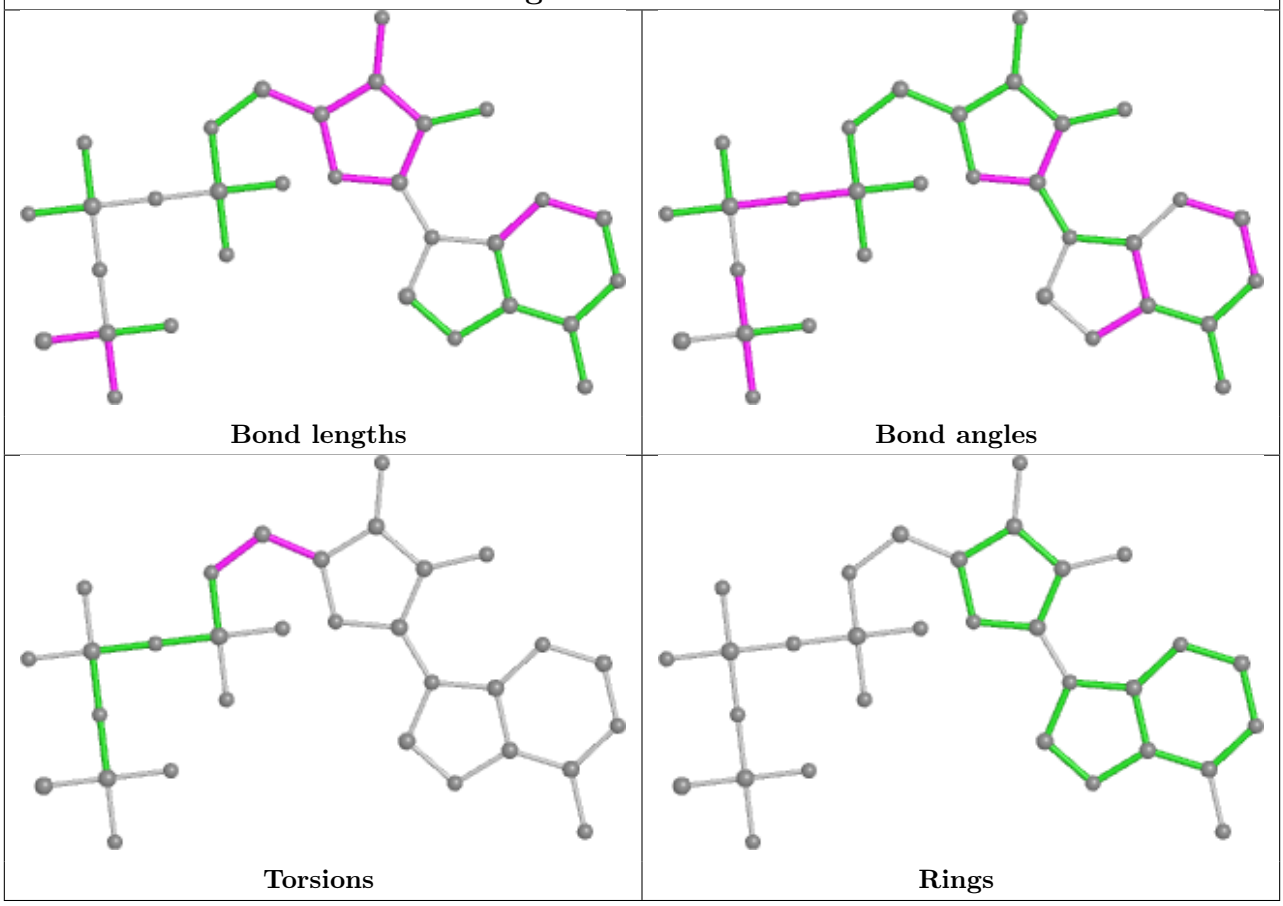
Ligand AGS B 802



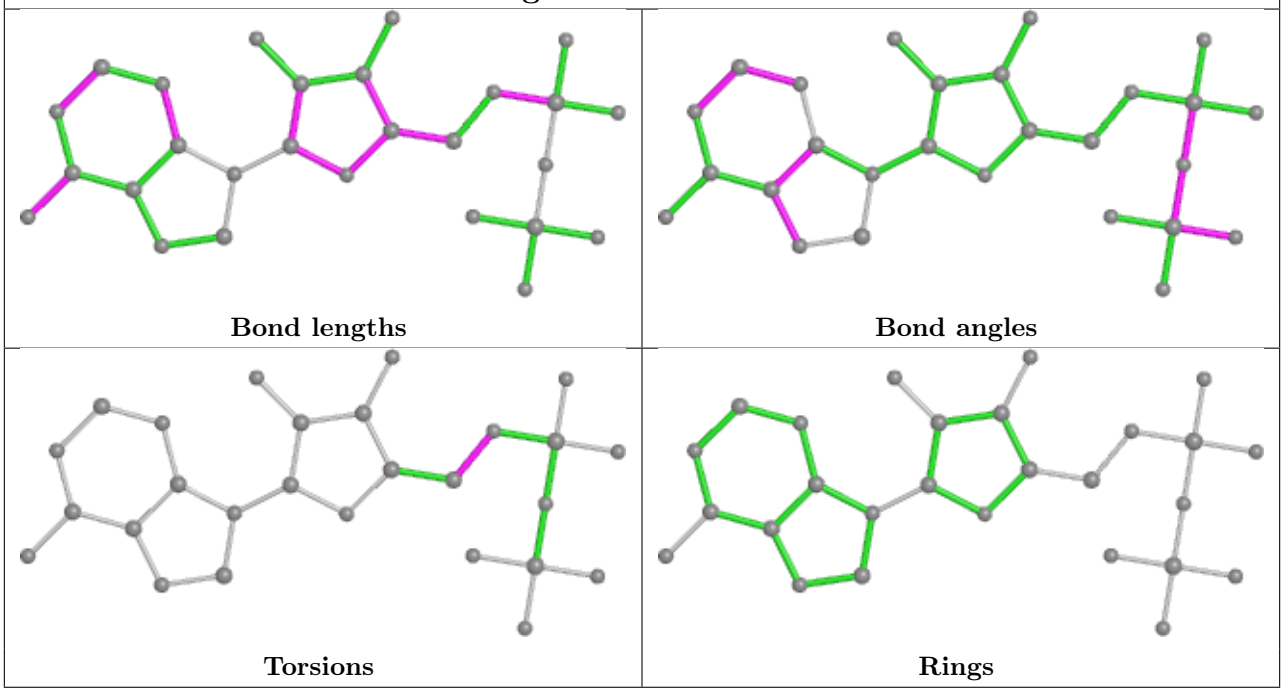
Ligand AGS E 802



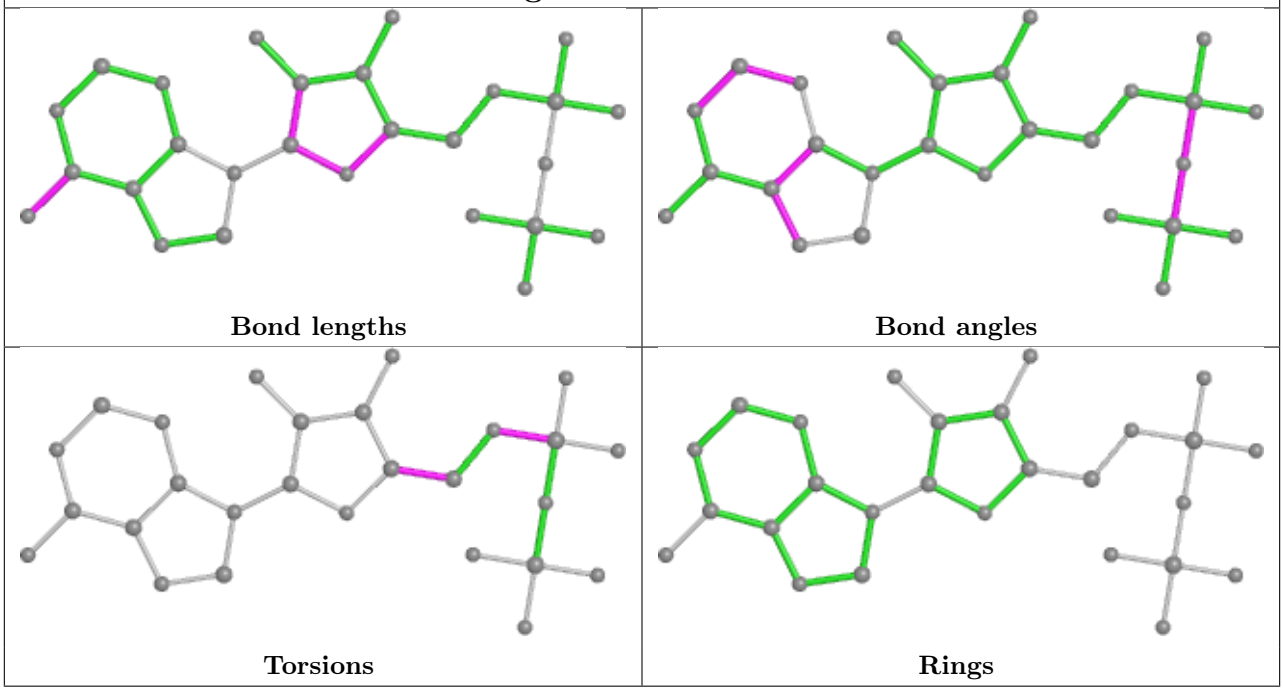
Ligand AGS C 801



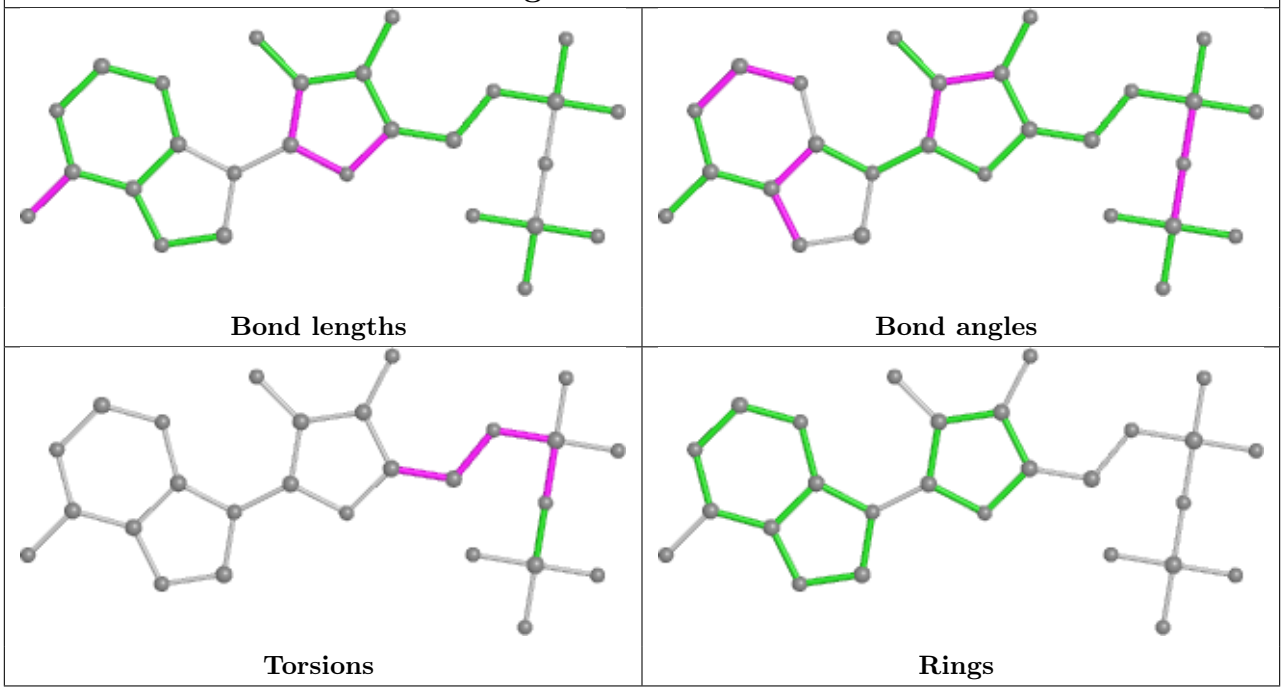
Ligand ADP A 802

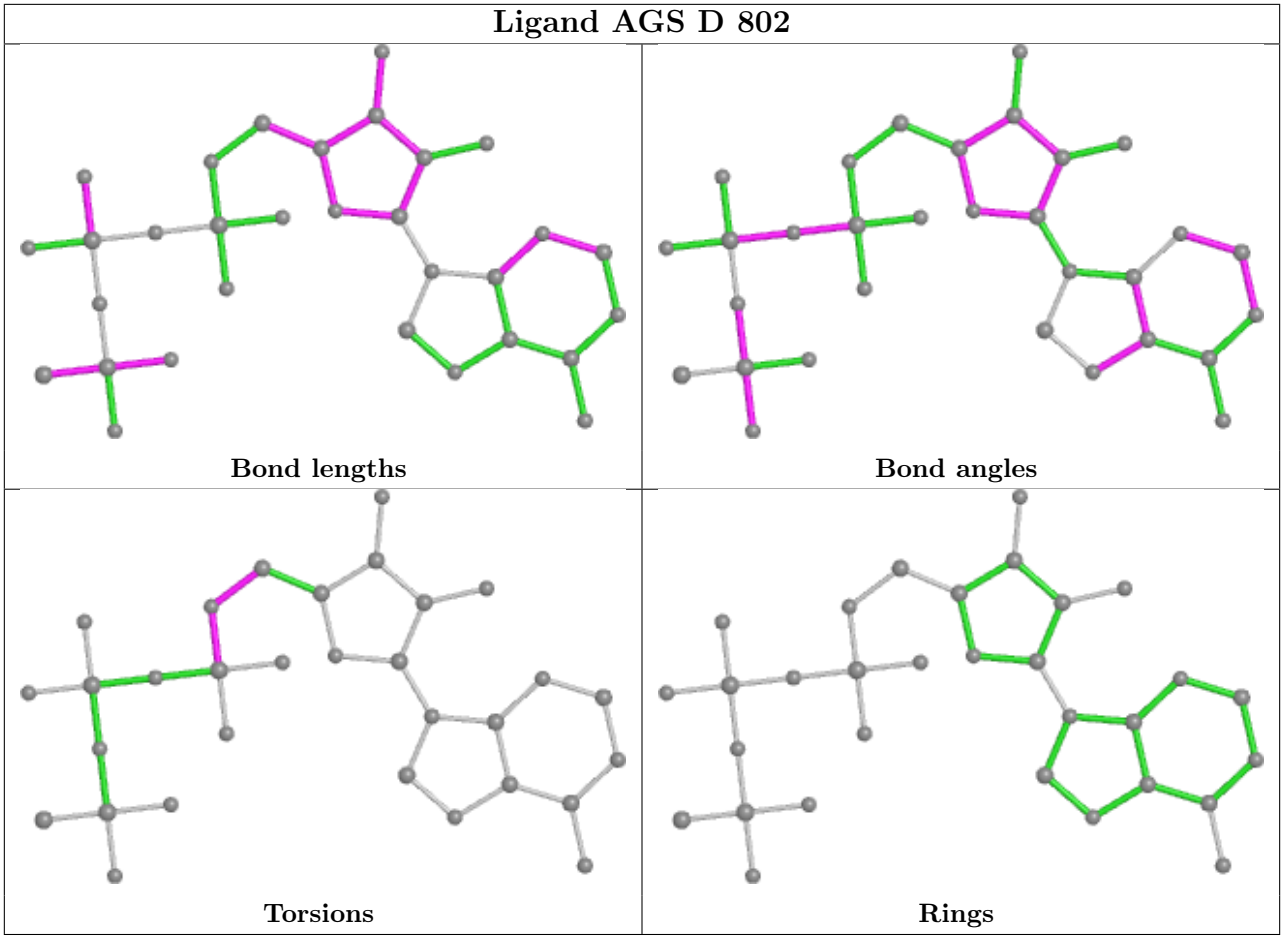


Ligand ADP F 801



Ligand ADP E 801





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.

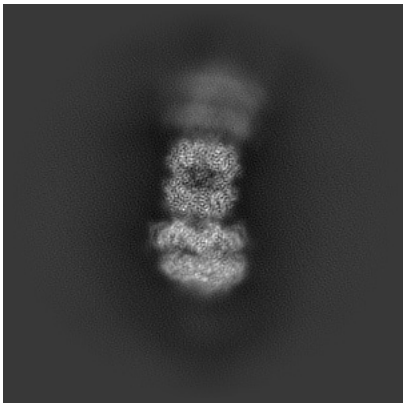
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20851. These allow visual inspection of the internal detail of the map and identification of artifacts.

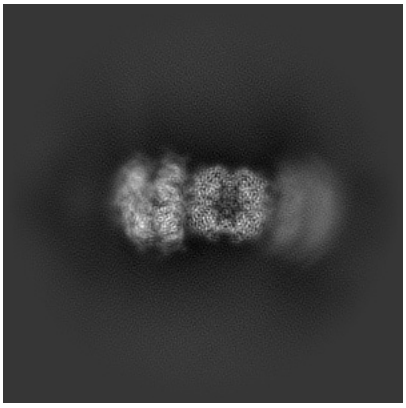
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

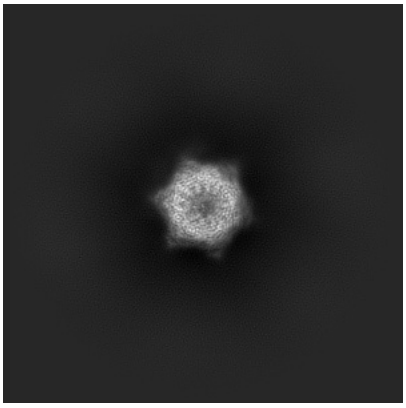
6.1.1 Primary map



X



Y



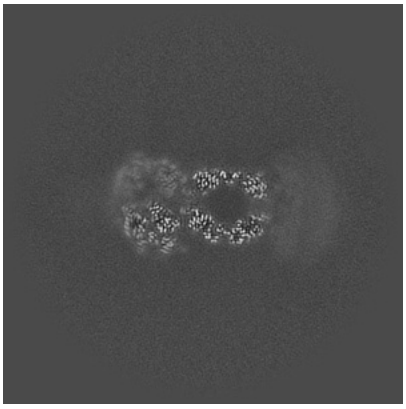
Z

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

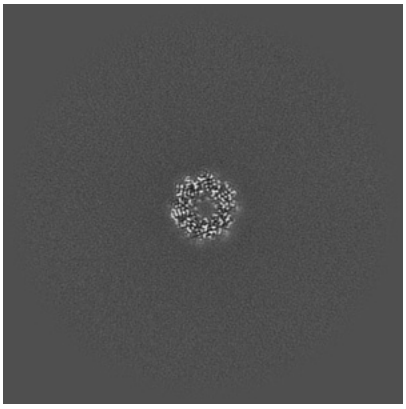
6.2 Central slices (i)

6.2.1 Primary map

X Index: 300



Y Index: 300

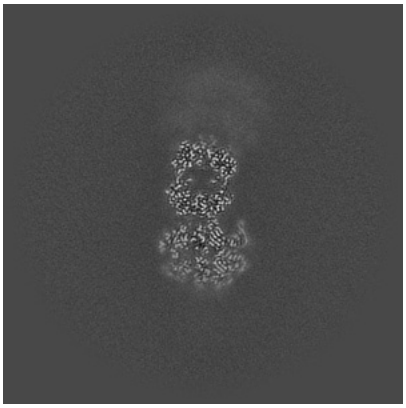


Z Index: 300

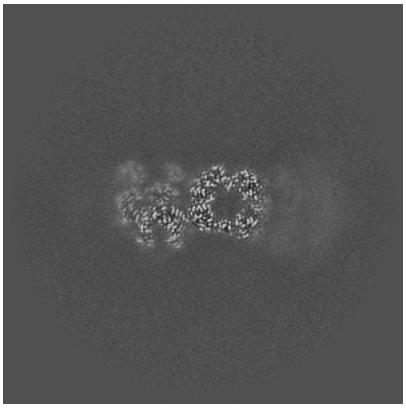
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

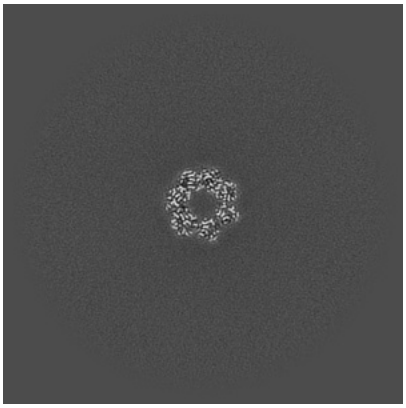
6.3.1 Primary map



X Index: 276



Y Index: 319



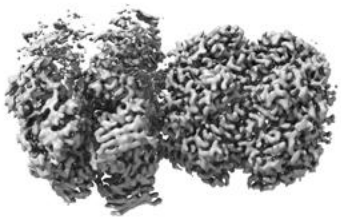
Z Index: 361

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

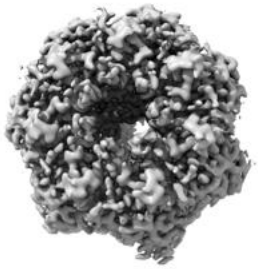
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.65. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

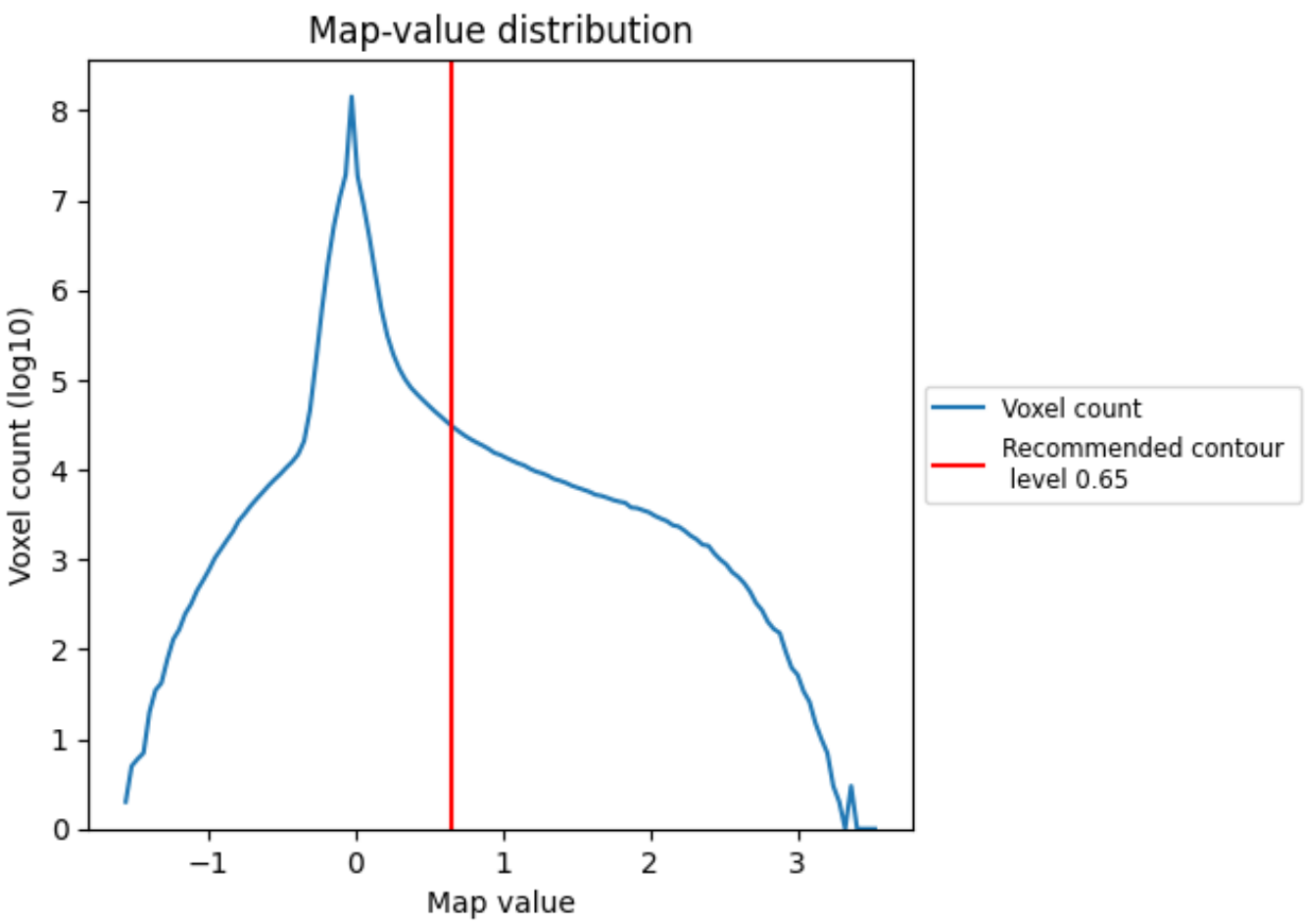
6.5 Mask visualisation (i)

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

7 Map analysis (i)

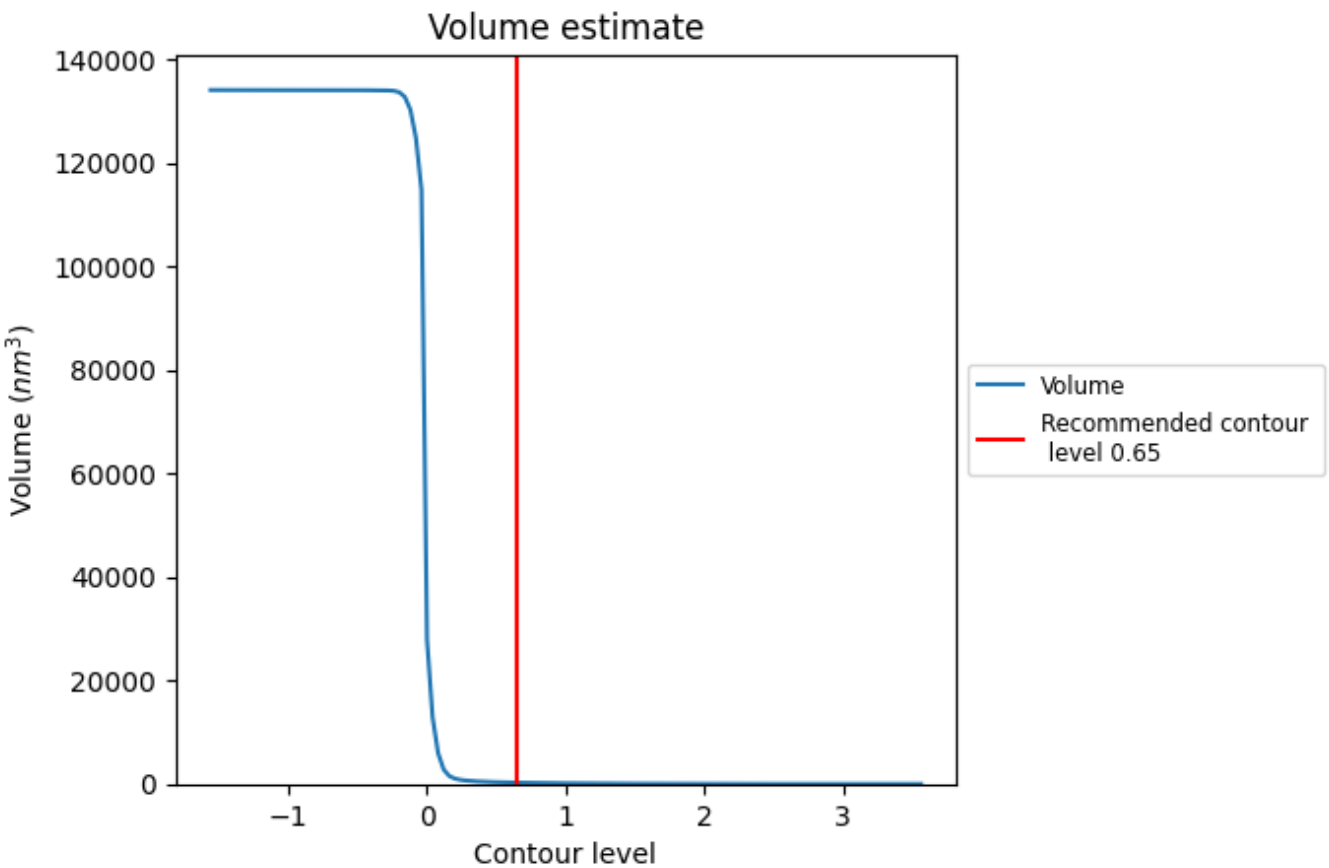
This section contains the results of statistical analysis of the map.

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.

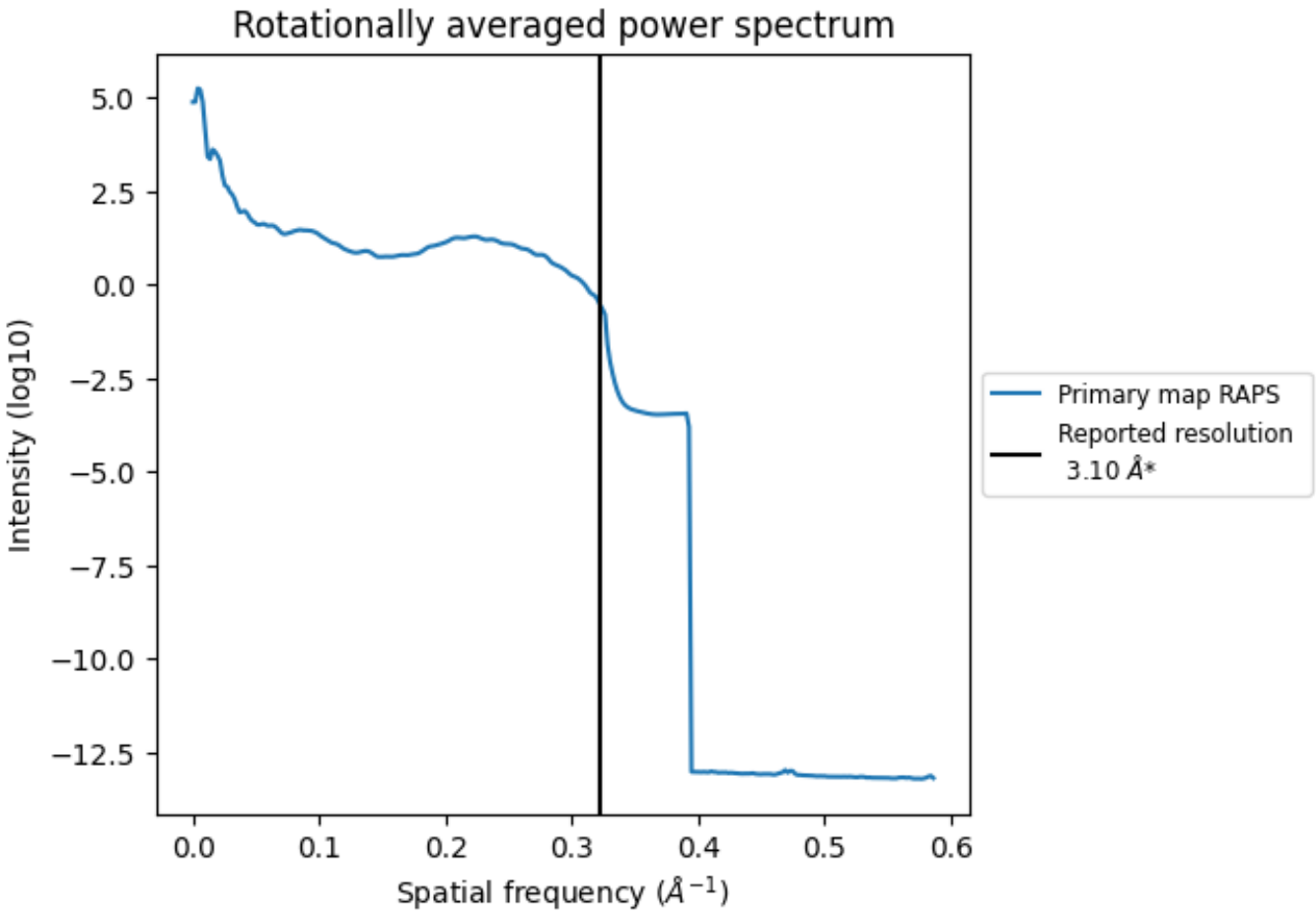
7.2 Volume estimate (i)



The volume at the recommended contour level is 251 nm^3; this corresponds to an approximate mass of 227 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 0.323 Å^{-1}

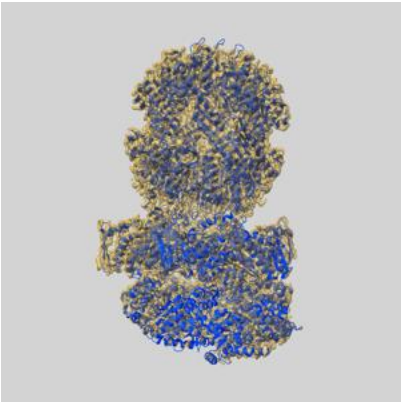
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

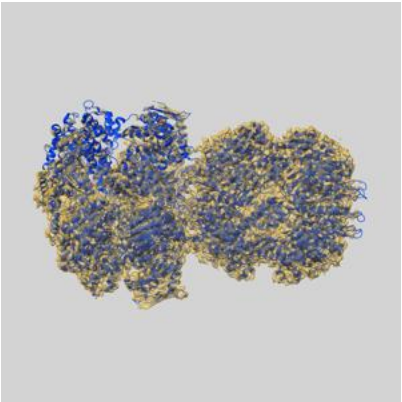
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20851 and PDB model 6UQO. Per-residue inclusion information can be found in section 3 on page 7.

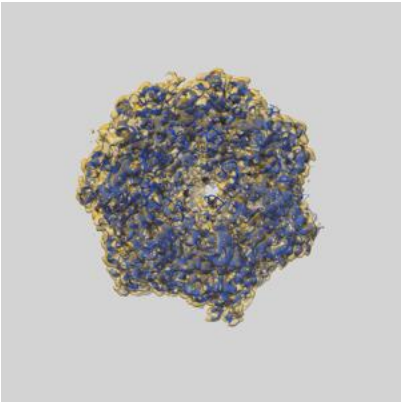
9.1 Map-model overlay (i)



X



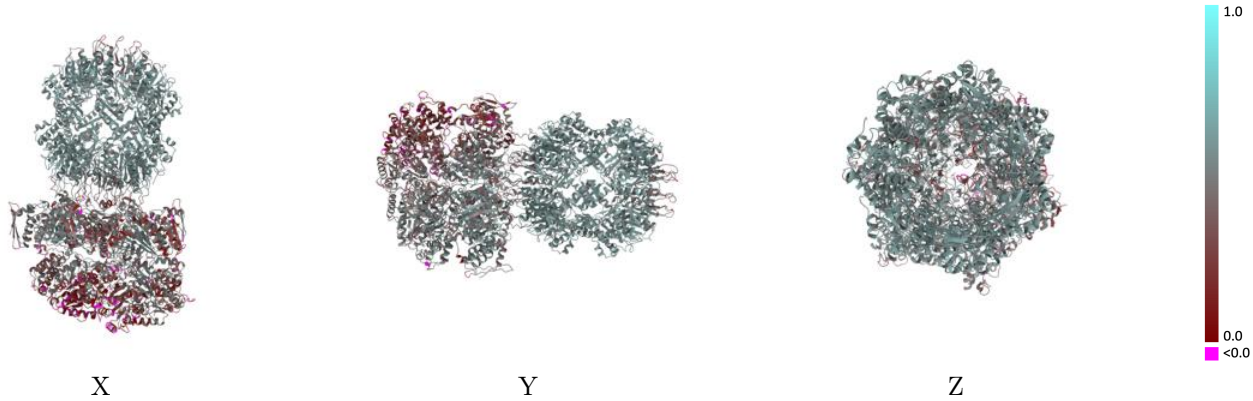
Y



Z

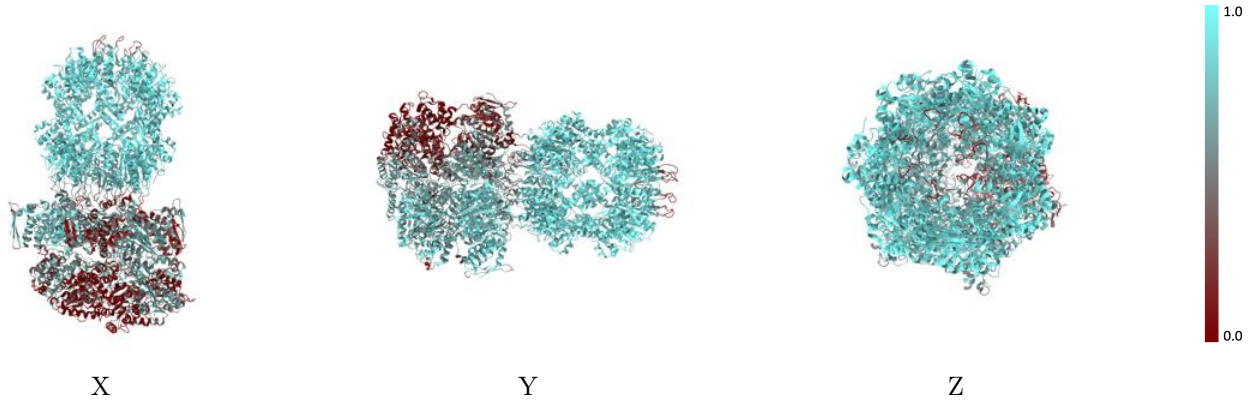
The images above show the 3D surface view of the map at the recommended contour level 0.65 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



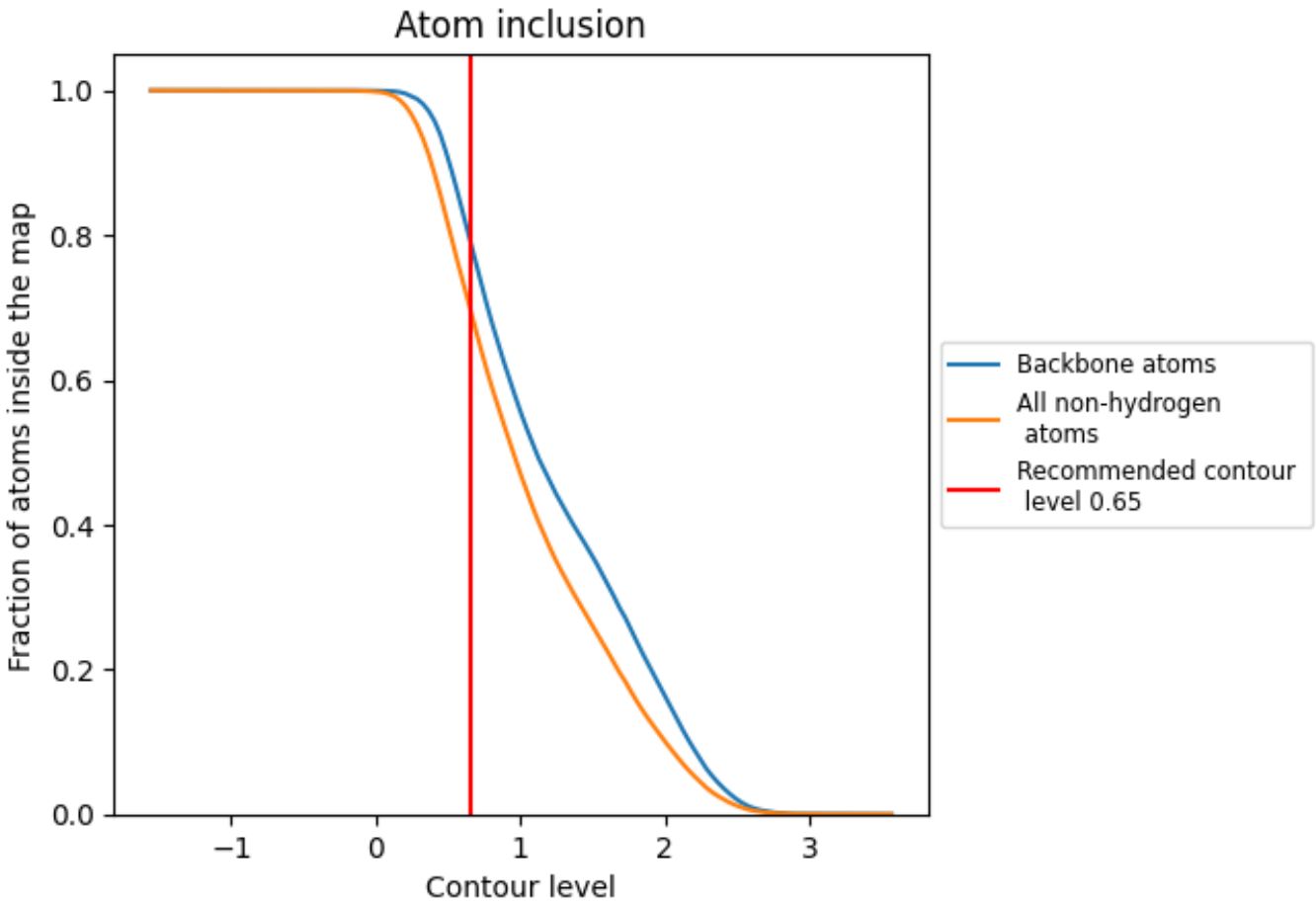
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.65).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 70% 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 (0.65) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6990	0.4690
A	0.5782	0.4130
B	0.7454	0.4810
C	0.7898	0.4980
D	0.7258	0.4700
E	0.3835	0.3490
F	0.1644	0.2470
G	0.8912	0.5490
H	0.8736	0.5490
I	0.8756	0.5490
J	0.8749	0.5480
K	0.8912	0.5500
L	0.8926	0.5540
M	0.8919	0.5480
N	0.8627	0.5400
O	0.8606	0.5430
P	0.8661	0.5400
Q	0.8640	0.5450
R	0.8674	0.5450
S	0.8688	0.5420
T	0.8586	0.5430
X	0.5556	0.4270
Y	0.9111	0.5220