Full wwPDB EM Validation Report ⓘ

Dec 13, 2023 – 02:34 PM EST

PDB ID	:	8FCM
EMDB ID	:	EMD-28983
Title	:	Cryo-EM structure of p97:UBXD1 open state
Authors	:	Braxton, J.R.; Tucker, M.R.; Tse, E.; Southworth, D.R.
Deposited on	:	2022-12-01
Resolution	:	3.27 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

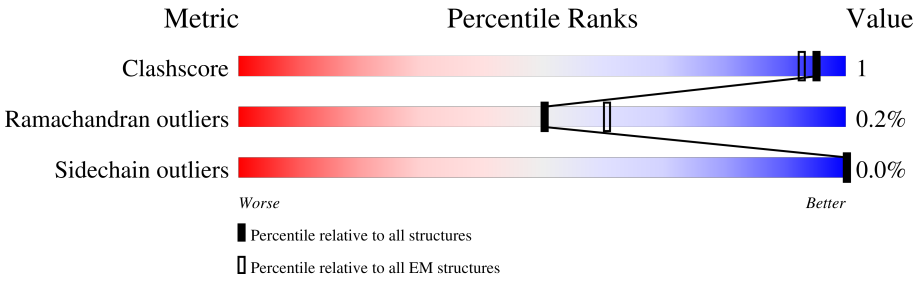
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.27 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	806	29% 87% · 11%
1	B	806	14% 87% · 11%
1	C	806	· 87% · 11%
1	D	806	· 88% · 11%
1	E	806	8% 86% · 11%
1	F	806	8% 86% · 12%
2	G	441	60% 77% · 23%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 36829 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.

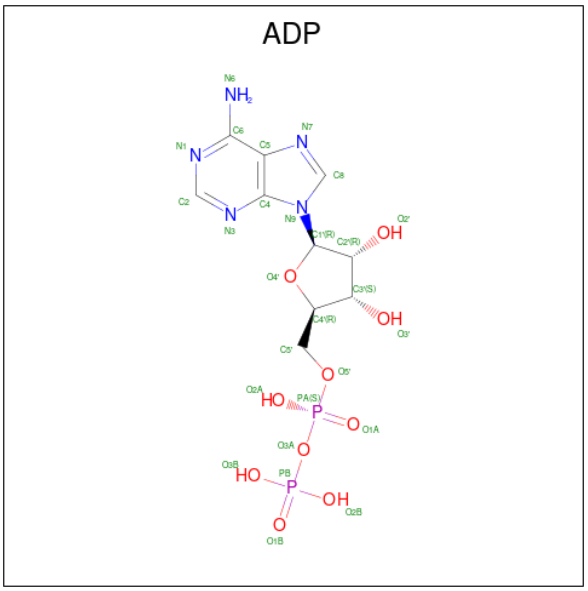
- Molecule 1 is a protein called Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	721	Total	C	N	O	S	0	0
			5640	3551	990	1069	30		
1	E	721	Total	C	N	O	S	0	0
			5640	3551	990	1069	30		
1	D	721	Total	C	N	O	S	0	0
			5640	3551	990	1069	30		
1	C	721	Total	C	N	O	S	0	0
			5640	3551	990	1069	30		
1	A	721	Total	C	N	O	S	0	0
			5640	3551	990	1069	30		
1	F	712	Total	C	N	O	S	0	0
			5565	3499	979	1058	29		

- Molecule 2 is a protein called UBX domain-containing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	341	Total	C	N	O	S	0	0
			2740	1736	477	518	9		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

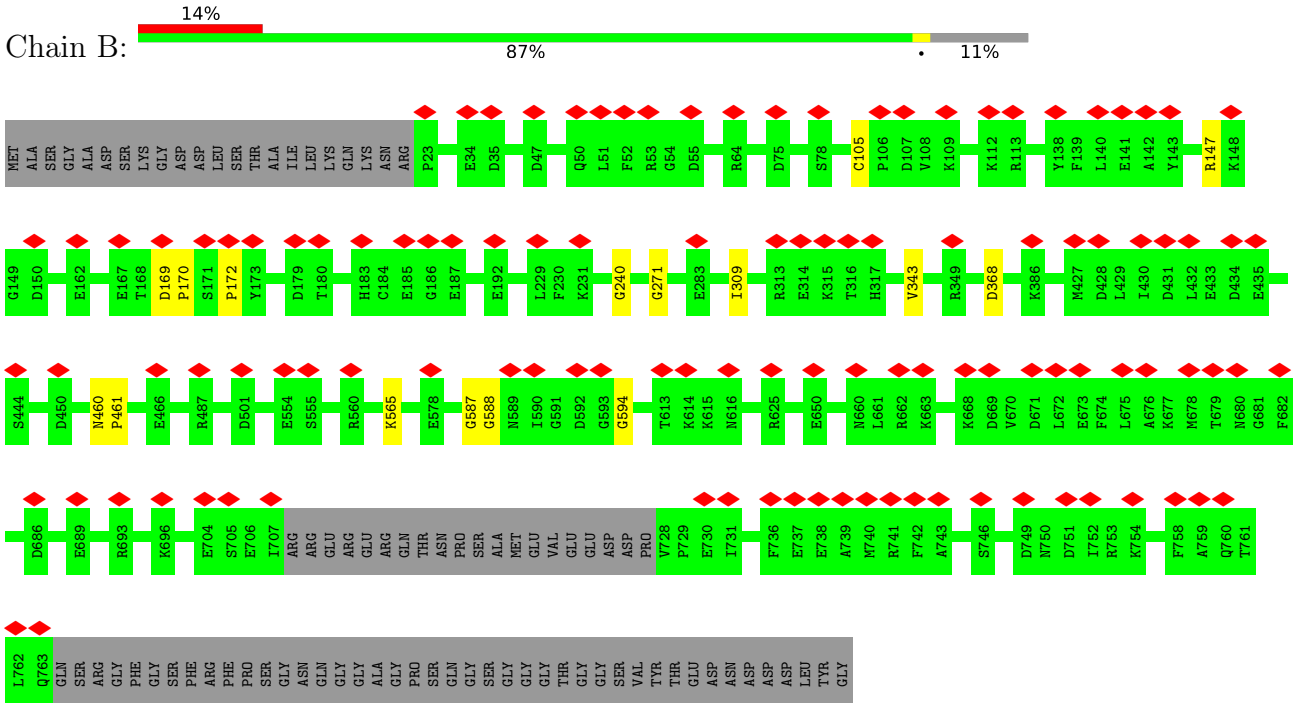


Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

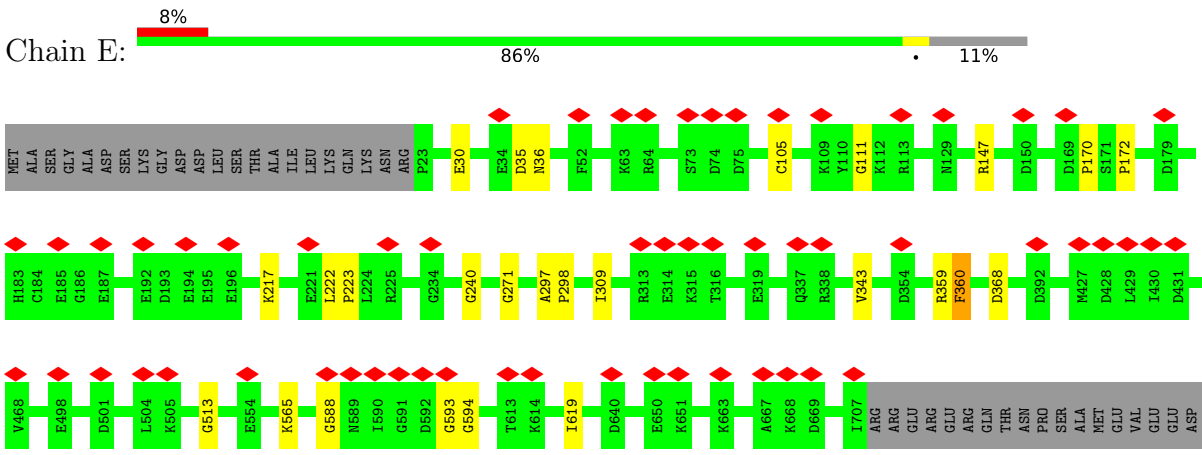
3 Residue-property plots (i)

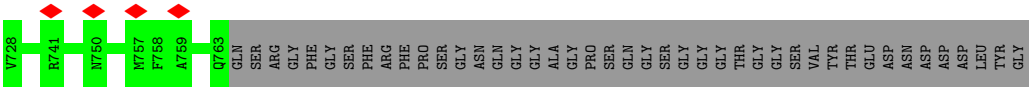
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Transitional endoplasmic reticulum ATPase



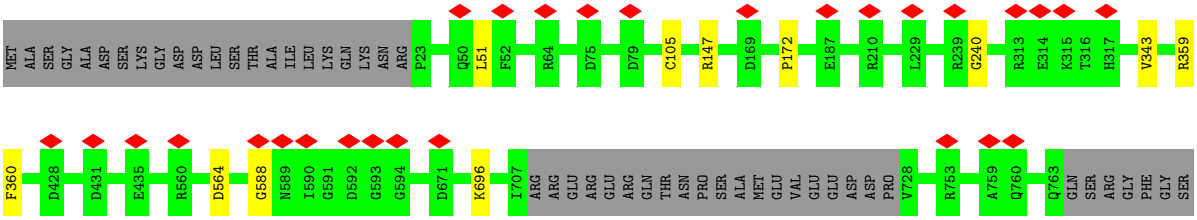
• Molecule 1: Transitional endoplasmic reticulum ATPase





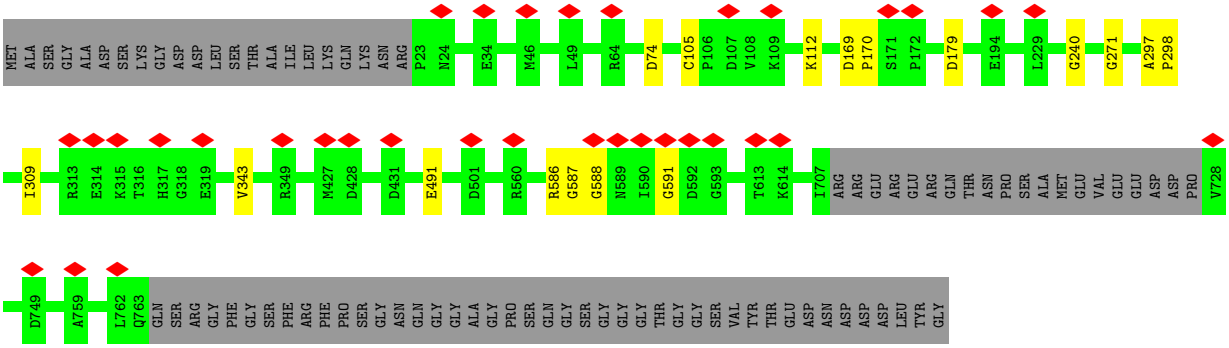
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain D:



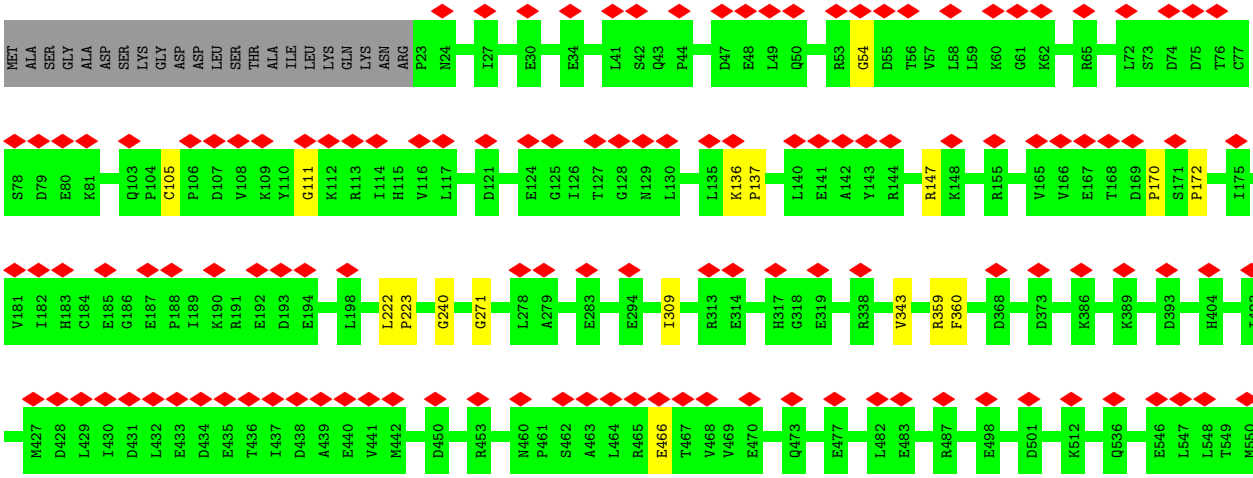
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain C:



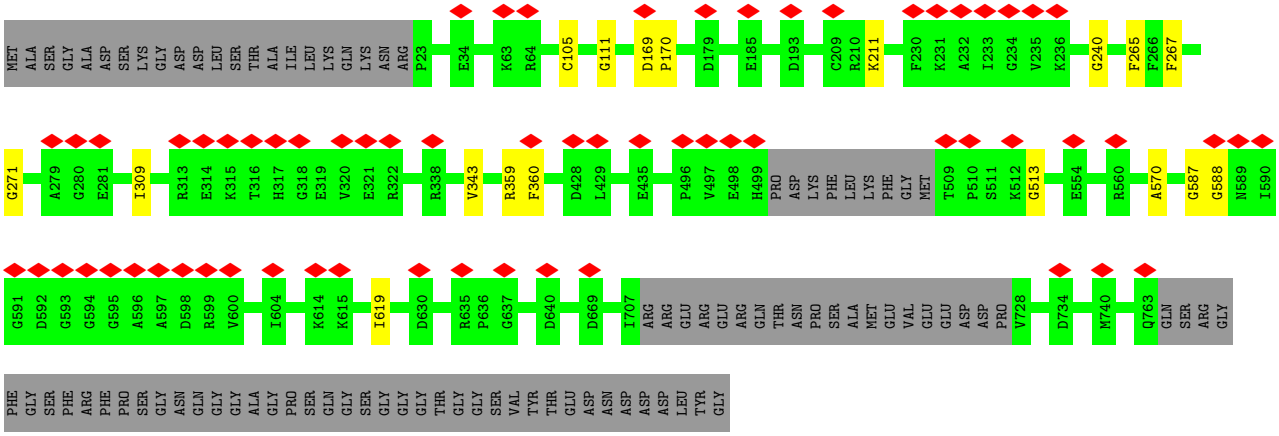
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain A:



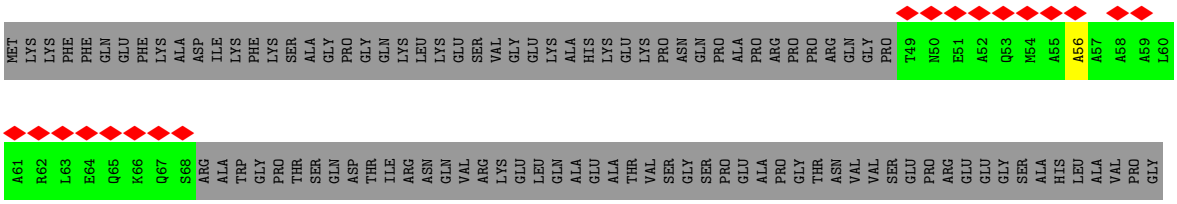
• Molecule 1: Transitional endoplasmic reticulum ATPase

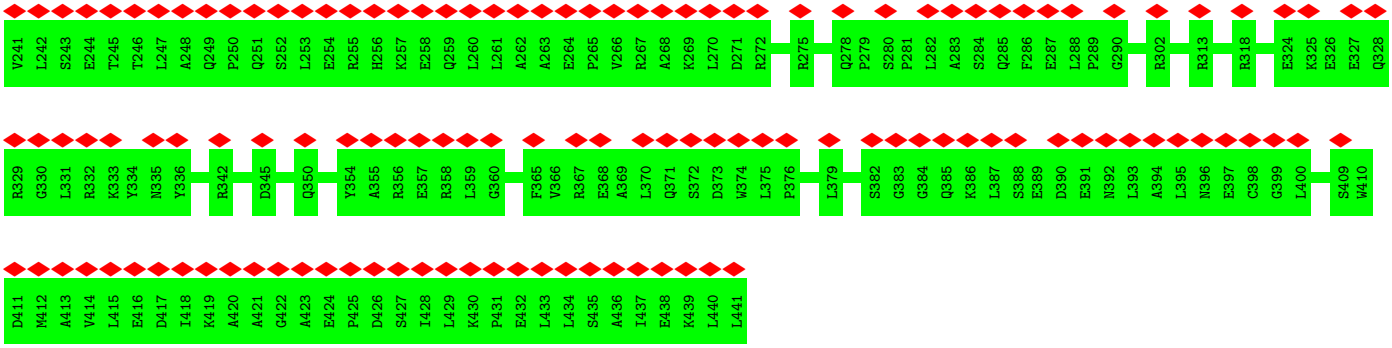
Chain F:



• Molecule 2: UBX domain-containing protein 6

Chain G:




V241 L242 S243 E244 T245 T246 L247 A248 Q249 P250 Q251 S252 L253 E254 R255 H256 K257 E258 Q259 L260 L261 A262 A263 E264 P265 V266 R267 A268 K269 L270 D271 R272 R275 Q278 P279 S280 P281 L282 A283 S284 Q285 F286 E287 L288 P289 G290 R302 R313 R318 E324 K325 E326 E327 Q328
R329 G330 L331 R332 K333 Y334 N335 Y336 R342 D345 Q350 Y354 A355 R356 E357 R358 L359 G360 F365 V366 R367 E368 A369 L370 Q371 S372 D373 W374 L375 P376 L379 S382 G383 G384 Q385 K386 L387 S388 E389 D390 E391 N392 L393 A394 L395 N396 E397 C398 G399 L400 S409 W410
D411 M412 A413 V414 L415 E416 D417 I418 K419 A420 A421 G422 A423 E424 P425 D426 S427 I428 L429 K430 P431 E432 L433 L434 S435 A436 I437 E438 K439 L440 L441

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	563468	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 ($e^-/Å^2$)	43	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	59952	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.155	Depositor
Minimum map value	-1.591	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	333.6, 333.6, 333.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.77	0/5732	0.48	0/7741
1	B	0.77	0/5732	0.46	0/7741
1	C	0.76	0/5732	0.46	0/7741
1	D	0.77	0/5732	0.46	0/7741
1	E	0.77	0/5732	0.46	0/7741
1	F	0.76	0/5653	0.47	0/7635
2	G	0.80	0/2787	0.60	0/3758
All	All	0.77	0/37100	0.47	0/50098

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5640	0	5713	13	0
1	B	5640	0	5713	11	0
1	C	5640	0	5713	16	0
1	D	5640	0	5713	6	0
1	E	5640	0	5713	19	0
1	F	5565	0	5634	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	2740	0	2760	3	0
3	A	54	0	24	0	0
3	B	54	0	24	0	0
3	C	54	0	24	0	0
3	D	54	0	24	0	0
3	E	54	0	24	0	0
3	F	54	0	24	0	0
All	All	36829	0	37103	70	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 1.

All (70) 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:A:240:GLY:HA2	1:A:343:VAL:O	1.86	0.76
1:B:240:GLY:HA2	1:B:343:VAL:O	1.87	0.74
1:E:271:GLY:HA2	1:E:309:ILE:HD11	1.72	0.70
1:C:586:ARG:O	1:C:591:GLY:HA2	1.95	0.66
1:E:240:GLY:HA2	1:E:343:VAL:O	1.96	0.66
1:F:240:GLY:HA2	1:F:343:VAL:O	1.98	0.63
1:E:271:GLY:HA2	1:E:309:ILE:CD1	2.30	0.62
1:E:513:GLY:HA2	1:E:619:ILE:O	2.02	0.60
1:B:594:GLY:HA2	1:C:587:GLY:CA	2.33	0.59
1:F:211:LYS:NZ	1:F:570:ALA:O	2.38	0.57
1:B:368:ASP:OD2	1:B:565:LYS:NZ	2.39	0.56
1:F:513:GLY:HA2	1:F:619:ILE:O	2.06	0.55
1:B:271:GLY:HA2	1:B:309:ILE:HG13	1.89	0.55
1:A:271:GLY:HA2	1:A:309:ILE:HB	1.89	0.54
1:C:240:GLY:HA2	1:C:343:VAL:O	2.07	0.53
1:E:593:GLY:O	1:F:587:GLY:HA2	2.08	0.53
1:E:368:ASP:OD2	1:E:565:LYS:NZ	2.41	0.53
1:A:147:ARG:HG3	1:A:172:PRO:O	2.10	0.52
2:G:176:ASP:OD2	2:G:180:LYS:NZ	2.43	0.52
1:E:147:ARG:HG3	1:E:172:PRO:O	2.09	0.52
1:E:111:GLY:HA2	1:E:170:PRO:HG3	1.92	0.51
1:E:594:GLY:HA2	1:F:587:GLY:HA2	1.93	0.51
1:C:271:GLY:HA2	1:C:309:ILE:HG13	1.92	0.51
1:D:240:GLY:HA2	1:D:343:VAL:O	2.12	0.50
1:C:587:GLY:HA3	1:C:591:GLY:HA2	1.95	0.48
1:E:35:ASP:OD1	1:E:36:ASN:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:GLY:HA2	1:C:587:GLY:HA2	1.95	0.48
1:A:111:GLY:HA2	1:A:170:PRO:HG3	1.96	0.48
1:B:147:ARG:HG3	1:B:172:PRO:O	2.14	0.47
1:F:111:GLY:HA2	1:F:170:PRO:HG3	1.95	0.47
1:E:105:CYS:SG	1:E:105:CYS:O	2.71	0.47
1:A:105:CYS:SG	1:A:105:CYS:O	2.73	0.46
1:C:169:ASP:CB	1:C:170:PRO:HD3	2.47	0.45
1:A:136:LYS:HB3	1:A:137:PRO:HD3	1.98	0.45
1:C:169:ASP:CB	1:C:170:PRO:CD	2.95	0.45
1:E:359:ARG:O	1:E:360:PHE:C	2.54	0.45
1:E:594:GLY:HA2	1:F:587:GLY:CA	2.47	0.45
1:A:54:GLY:HA2	2:G:56:ALA:HB2	1.98	0.44
1:B:587:GLY:CA	1:A:594:GLY:HA2	2.46	0.44
1:F:105:CYS:SG	1:F:105:CYS:O	2.75	0.44
1:C:74:ASP:OD1	1:C:74:ASP:C	2.56	0.44
1:D:105:CYS:SG	1:D:105:CYS:O	2.76	0.44
1:A:54:GLY:HA2	2:G:56:ALA:CB	2.48	0.44
1:F:169:ASP:HB3	1:F:170:PRO:CD	2.48	0.44
1:C:169:ASP:HB2	1:C:170:PRO:CD	2.47	0.43
1:C:105:CYS:O	1:C:105:CYS:SG	2.77	0.43
1:B:105:CYS:SG	1:B:105:CYS:O	2.76	0.43
1:B:271:GLY:HA2	1:B:309:ILE:CG1	2.48	0.43
1:F:359:ARG:O	1:F:360:PHE:C	2.57	0.43
1:A:359:ARG:O	1:A:360:PHE:C	2.58	0.42
1:A:587:GLY:HA3	1:A:591:GLY:HA2	2.01	0.42
1:E:593:GLY:O	1:F:587:GLY:CA	2.68	0.42
1:B:460:ASN:HA	1:B:461:PRO:HD2	1.88	0.42
1:F:265:PHE:CD2	1:F:267:PHE:CE1	3.07	0.42
1:E:465:ARG:NH2	1:D:564:ASP:OD2	2.52	0.41
1:A:466:GLU:OE1	1:A:466:GLU:N	2.53	0.41
1:D:359:ARG:O	1:D:360:PHE:C	2.59	0.41
1:C:297:ALA:HA	1:C:298:PRO:C	2.40	0.41
1:E:30:GLU:OE2	1:E:217:LYS:NZ	2.44	0.41
1:E:222:LEU:HB3	1:E:223:PRO:HD3	2.03	0.41
1:B:169:ASP:HB3	1:B:170:PRO:CD	2.50	0.41
1:A:222:LEU:HB3	1:A:223:PRO:HD3	2.03	0.41
1:E:594:GLY:HA2	1:F:587:GLY:N	2.35	0.41
1:D:147:ARG:HG3	1:D:172:PRO:O	2.21	0.41
1:F:271:GLY:HA2	1:F:309:ILE:HB	2.03	0.41
1:E:297:ALA:HA	1:E:298:PRO:C	2.42	0.40
1:D:696:LYS:NZ	1:C:491:GLU:OE1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:LYS:NZ	1:C:179:ASP:OD2	2.54	0.40
1:C:169:ASP:HB2	1:C:170:PRO:HD3	2.03	0.40
1:C:271:GLY:HA2	1:C:309:ILE:CG1	2.51	0.40

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	717/806 (89%)	698 (97%)	18 (2%)	1 (0%)	51	82
1	B	717/806 (89%)	701 (98%)	15 (2%)	1 (0%)	51	82
1	C	717/806 (89%)	704 (98%)	12 (2%)	1 (0%)	51	82
1	D	717/806 (89%)	705 (98%)	11 (2%)	1 (0%)	51	82
1	E	717/806 (89%)	704 (98%)	11 (2%)	2 (0%)	41	72
1	F	706/806 (88%)	691 (98%)	14 (2%)	1 (0%)	51	82
2	G	337/441 (76%)	336 (100%)	1 (0%)	0	100	100
All	All	4628/5277 (88%)	4539 (98%)	82 (2%)	7 (0%)	50	77

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	588	GLY
1	C	588	GLY
1	A	588	GLY
1	F	588	GLY
1	E	360	PHE
1	D	588	GLY
1	E	588	GLY

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	613/678 (90%)	613 (100%)	0	100 100
1	B	613/678 (90%)	613 (100%)	0	100 100
1	C	613/678 (90%)	613 (100%)	0	100 100
1	D	613/678 (90%)	612 (100%)	1 (0%)	93 97
1	E	613/678 (90%)	613 (100%)	0	100 100
1	F	605/678 (89%)	605 (100%)	0	100 100
2	G	293/374 (78%)	293 (100%)	0	100 100
All	All	3963/4442 (89%)	3962 (100%)	1 (0%)	100 100

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

Mol	Chain	Res	Type
1	D	51	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	660	ASN
1	F	103	GLN
1	F	660	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	$\#\|Z\| > 2$
3	ADP	C	902	-	24,29,29	0.93	1 (4%)	29,45,45	1.48	4 (13%)
3	ADP	A	901	-	24,29,29	0.71	1 (4%)	29,45,45	0.71	1 (3%)
3	ADP	F	902	-	24,29,29	0.92	1 (4%)	29,45,45	1.47	4 (13%)
3	ADP	C	901	-	24,29,29	0.67	1 (4%)	29,45,45	0.70	1 (3%)
3	ADP	F	901	-	24,29,29	0.66	0	29,45,45	0.72	1 (3%)
3	ADP	B	902	-	24,29,29	0.94	1 (4%)	29,45,45	1.48	4 (13%)
3	ADP	D	901	-	24,29,29	0.68	1 (4%)	29,45,45	0.71	1 (3%)
3	ADP	A	902	-	24,29,29	0.93	1 (4%)	29,45,45	1.48	4 (13%)
3	ADP	D	902	-	24,29,29	0.93	1 (4%)	29,45,45	1.49	4 (13%)
3	ADP	E	901	-	24,29,29	0.68	1 (4%)	29,45,45	0.70	0
3	ADP	B	901	-	24,29,29	0.66	0	29,45,45	0.70	1 (3%)
3	ADP	E	902	-	24,29,29	0.93	1 (4%)	29,45,45	1.49	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	C	902	-	-	0/12/32/32	0/3/3/3
3	ADP	A	901	-	-	6/12/32/32	0/3/3/3
3	ADP	F	902	-	-	0/12/32/32	0/3/3/3
3	ADP	C	901	-	-	6/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	F	901	-	-	7/12/32/32	0/3/3/3
3	ADP	B	902	-	-	1/12/32/32	0/3/3/3
3	ADP	D	901	-	-	6/12/32/32	0/3/3/3
3	ADP	A	902	-	-	3/12/32/32	0/3/3/3
3	ADP	D	902	-	-	0/12/32/32	0/3/3/3
3	ADP	E	901	-	-	7/12/32/32	0/3/3/3
3	ADP	B	901	-	-	6/12/32/32	0/3/3/3
3	ADP	E	902	-	-	0/12/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	902	ADP	C5-C4	2.44	1.47	1.40
3	E	902	ADP	C5-C4	2.43	1.47	1.40
3	D	902	ADP	C5-C4	2.41	1.47	1.40
3	B	902	ADP	C5-C4	2.41	1.47	1.40
3	A	902	ADP	C5-C4	2.39	1.47	1.40
3	F	902	ADP	C5-C4	2.37	1.47	1.40
3	A	901	ADP	C8-N7	-2.05	1.31	1.34
3	C	901	ADP	C8-N7	-2.03	1.31	1.34
3	E	901	ADP	C8-N7	-2.02	1.31	1.34
3	D	901	ADP	C8-N7	-2.01	1.31	1.34

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	902	ADP	C3'-C2'-C1'	3.72	106.58	100.98
3	B	902	ADP	C3'-C2'-C1'	3.68	106.52	100.98
3	A	902	ADP	C3'-C2'-C1'	3.67	106.50	100.98
3	F	902	ADP	C3'-C2'-C1'	3.63	106.45	100.98
3	C	902	ADP	C3'-C2'-C1'	3.63	106.44	100.98
3	E	902	ADP	C3'-C2'-C1'	3.60	106.40	100.98
3	F	902	ADP	PA-O3A-PB	-3.43	121.06	132.83
3	B	902	ADP	PA-O3A-PB	-3.42	121.08	132.83
3	E	902	ADP	PA-O3A-PB	-3.41	121.13	132.83
3	A	902	ADP	PA-O3A-PB	-3.41	121.13	132.83
3	D	902	ADP	PA-O3A-PB	-3.41	121.13	132.83
3	C	902	ADP	PA-O3A-PB	-3.39	121.19	132.83
3	C	902	ADP	N3-C2-N1	-3.23	123.63	128.68
3	E	902	ADP	N3-C2-N1	-3.19	123.69	128.68
3	B	902	ADP	N3-C2-N1	-3.17	123.72	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	902	ADP	N3-C2-N1	-3.15	123.76	128.68
3	D	902	ADP	N3-C2-N1	-3.13	123.79	128.68
3	F	902	ADP	N3-C2-N1	-2.97	124.04	128.68
3	F	902	ADP	C4-C5-N7	-2.66	106.63	109.40
3	E	902	ADP	C4-C5-N7	-2.65	106.64	109.40
3	C	902	ADP	C4-C5-N7	-2.64	106.65	109.40
3	D	902	ADP	C4-C5-N7	-2.61	106.67	109.40
3	B	902	ADP	C4-C5-N7	-2.58	106.71	109.40
3	A	902	ADP	C4-C5-N7	-2.51	106.78	109.40
3	F	901	ADP	C5-C6-N6	2.09	123.52	120.35
3	D	901	ADP	C5-C6-N6	2.06	123.47	120.35
3	A	901	ADP	C5-C6-N6	2.03	123.43	120.35
3	B	901	ADP	C5-C6-N6	2.02	123.42	120.35
3	C	901	ADP	C5-C6-N6	2.01	123.41	120.35

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	901	ADP	PA-O3A-PB-O2B
3	E	901	ADP	PA-O3A-PB-O2B
3	E	901	ADP	C5'-O5'-PA-O3A
3	D	901	ADP	PA-O3A-PB-O2B
3	C	901	ADP	C5'-O5'-PA-O1A
3	C	901	ADP	C5'-O5'-PA-O2A
3	C	901	ADP	C5'-O5'-PA-O3A
3	A	901	ADP	PA-O3A-PB-O2B
3	A	902	ADP	PA-O3A-PB-O2B
3	F	901	ADP	PA-O3A-PB-O2B
3	B	901	ADP	O4'-C4'-C5'-O5'
3	F	901	ADP	O4'-C4'-C5'-O5'
3	F	901	ADP	C3'-C4'-C5'-O5'
3	B	901	ADP	C3'-C4'-C5'-O5'
3	C	901	ADP	PA-O3A-PB-O1B
3	D	901	ADP	PB-O3A-PA-O1A
3	A	901	ADP	PB-O3A-PA-O1A
3	E	901	ADP	O4'-C4'-C5'-O5'
3	C	901	ADP	PA-O3A-PB-O2B
3	F	901	ADP	PA-O3A-PB-O3B
3	F	901	ADP	C5'-O5'-PA-O3A
3	B	901	ADP	PB-O3A-PA-O2A
3	E	901	ADP	C5'-O5'-PA-O1A

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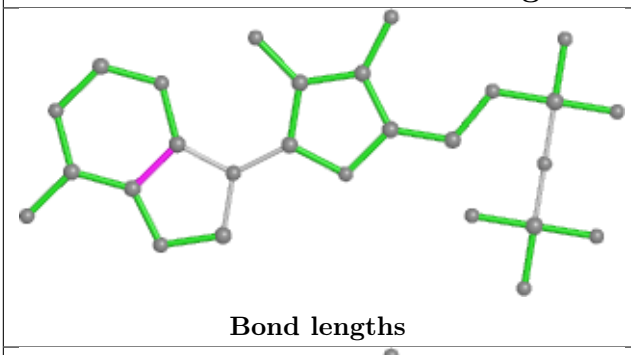
Mol	Chain	Res	Type	Atoms
3	E	901	ADP	C5'-O5'-PA-O2A
3	D	901	ADP	PB-O3A-PA-O2A
3	B	901	ADP	PA-O3A-PB-O1B
3	B	902	ADP	PA-O3A-PB-O1B
3	A	901	ADP	PB-O3A-PA-O2A
3	E	901	ADP	C3'-C4'-C5'-O5'
3	E	901	ADP	PA-O3A-PB-O1B
3	A	902	ADP	PA-O3A-PB-O1B
3	F	901	ADP	PA-O3A-PB-O1B
3	D	901	ADP	PA-O3A-PB-O3B
3	A	902	ADP	PA-O3A-PB-O3B
3	D	901	ADP	O4'-C4'-C5'-O5'
3	C	901	ADP	O4'-C4'-C5'-O5'
3	B	901	ADP	PB-O3A-PA-O1A
3	D	901	ADP	C5'-O5'-PA-O1A
3	A	901	ADP	C5'-O5'-PA-O1A
3	F	901	ADP	C5'-O5'-PA-O1A
3	A	901	ADP	O4'-C4'-C5'-O5'
3	A	901	ADP	PA-O3A-PB-O1B

There are no ring outliers.

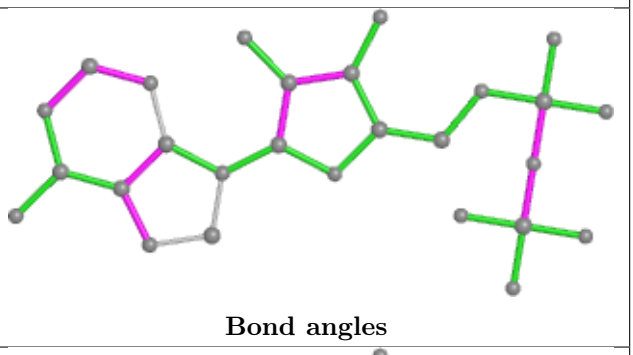
No monomer is involved in short contacts.

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.

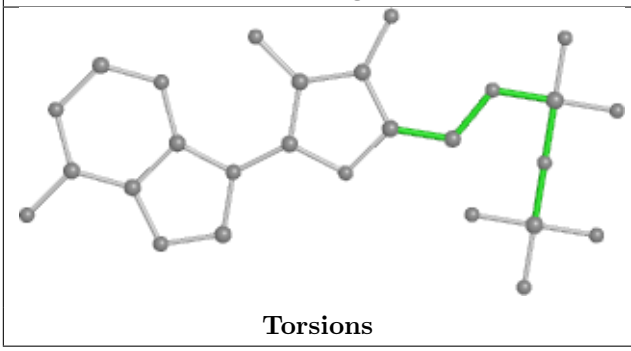
Ligand ADP C 902



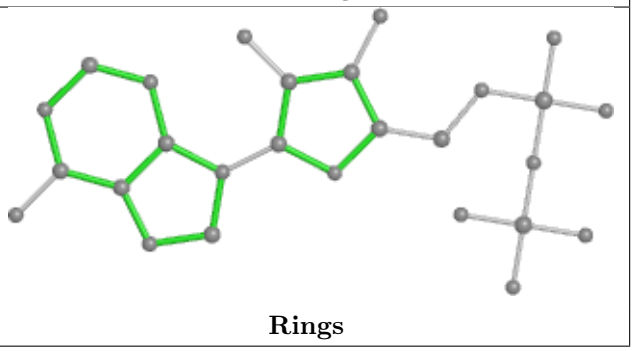
Bond lengths



Bond angles

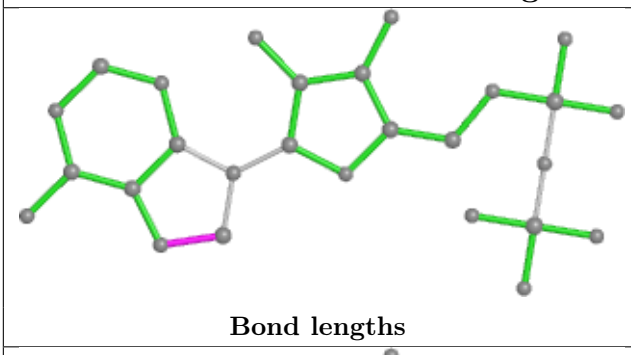


Torsions



Rings

Ligand ADP A 901



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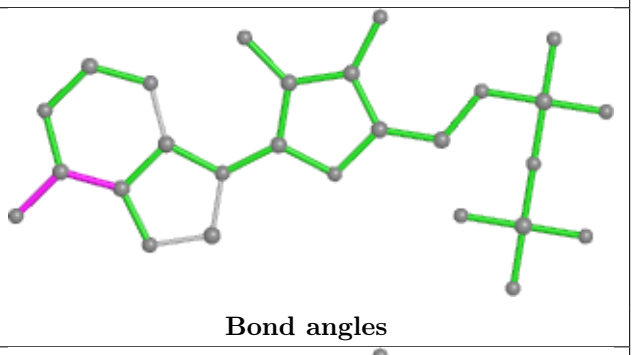
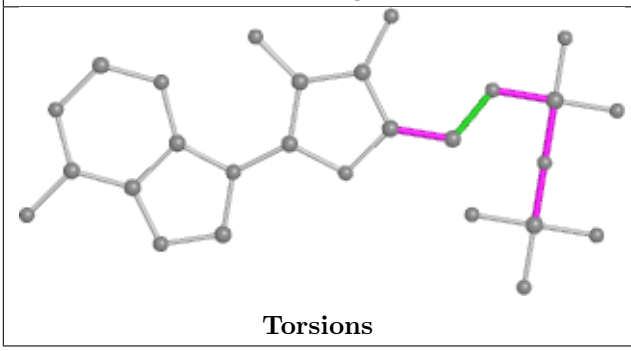
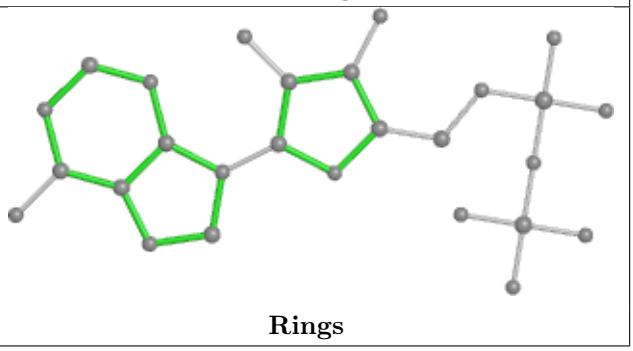


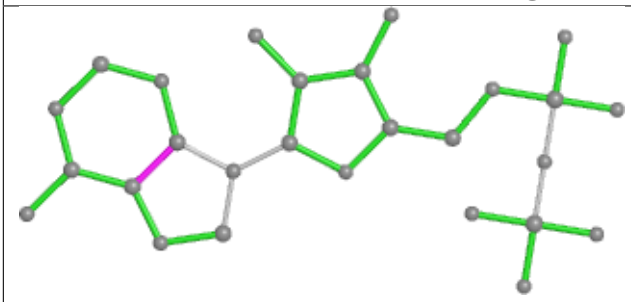
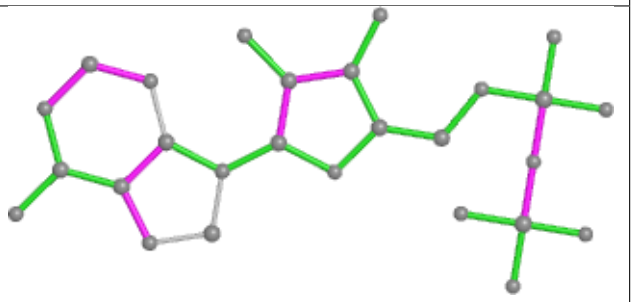
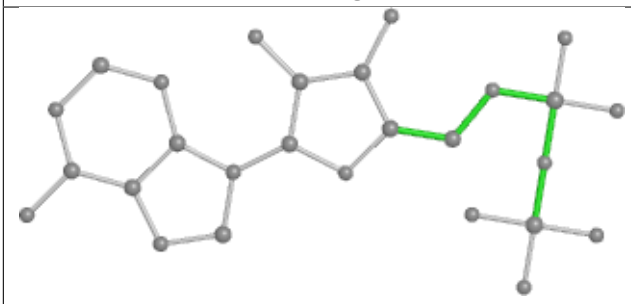
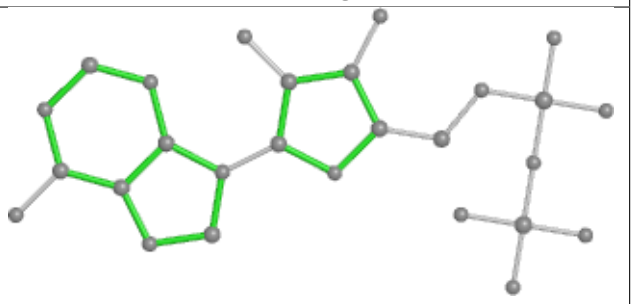
Bond angles

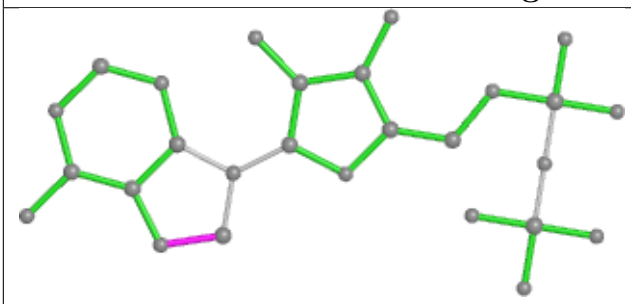
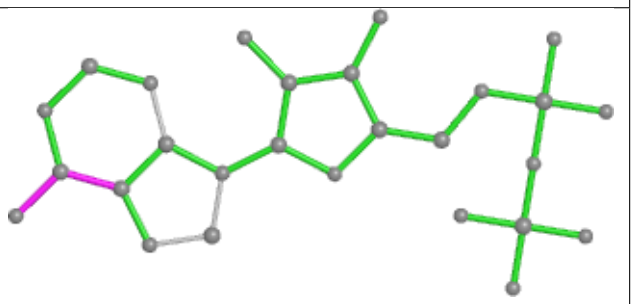
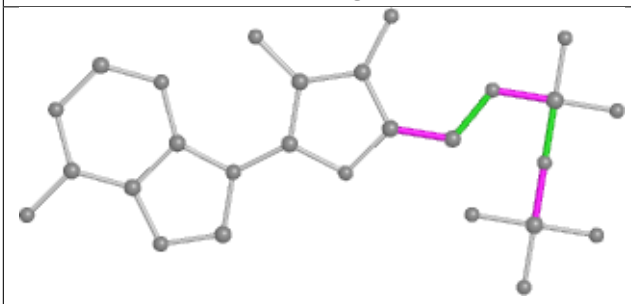
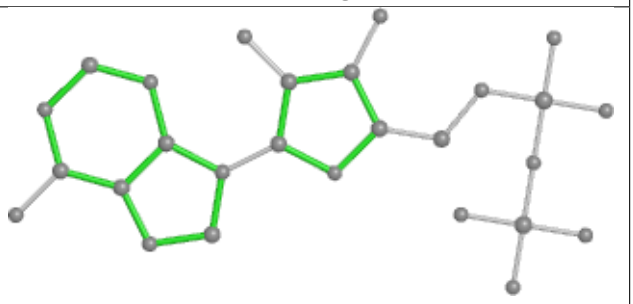


Torsions

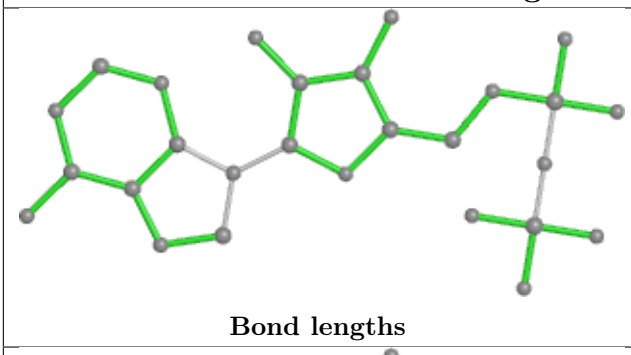


Rings

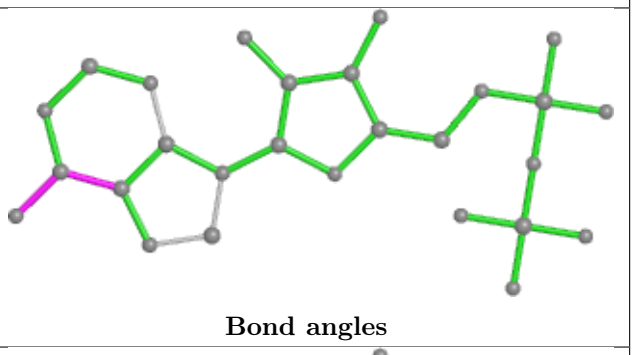
Ligand ADP F 902	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP C 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

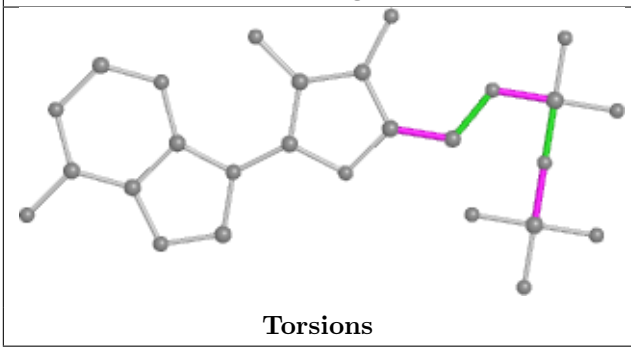
Ligand ADP F 901



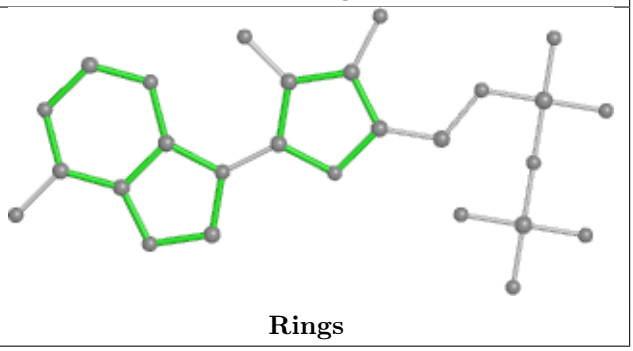
Bond lengths



Bond angles

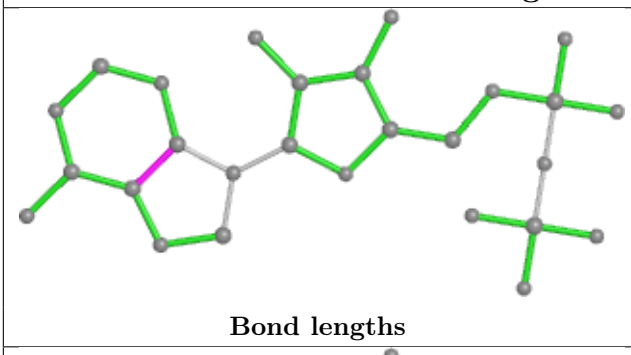


Torsions



Rings

Ligand ADP B 902



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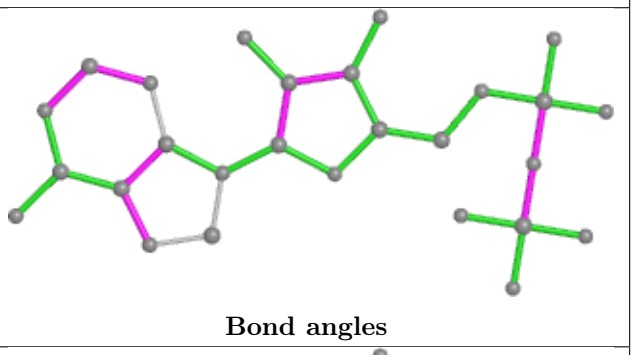

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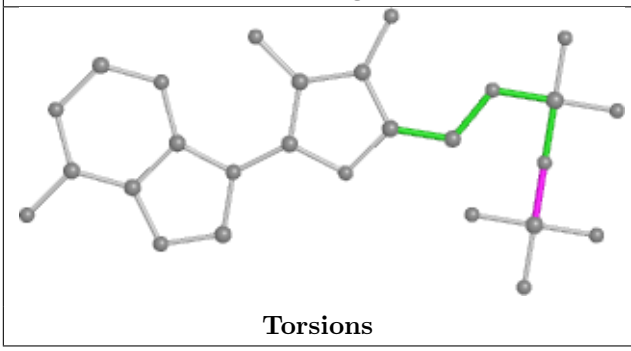

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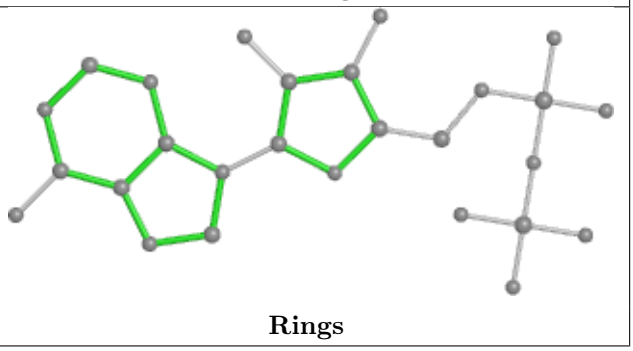
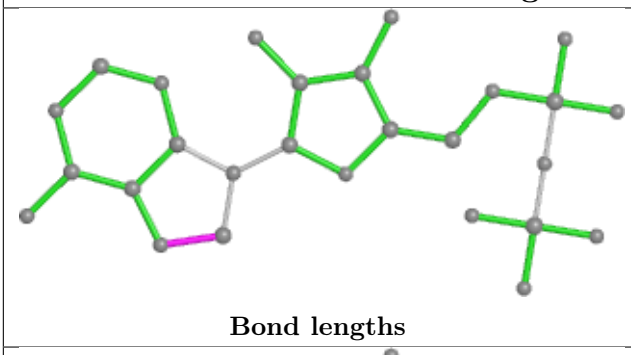
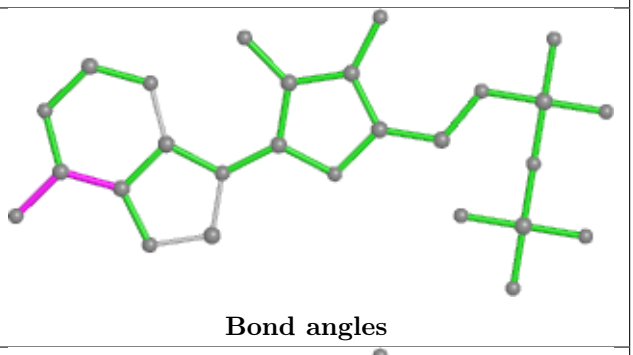


Rings

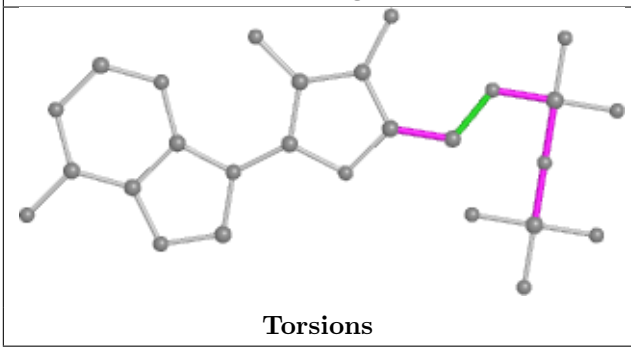
Ligand ADP D 901



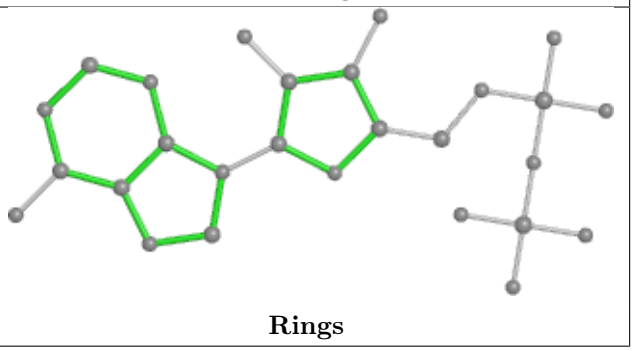
Bond lengths



Bond angles

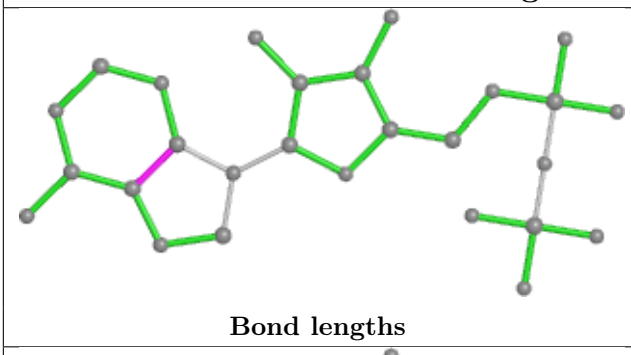


Torsions

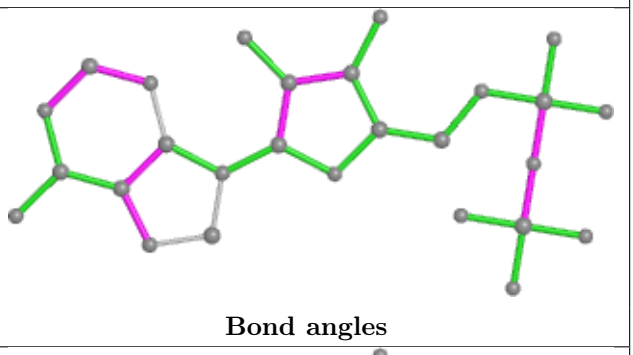


Rings

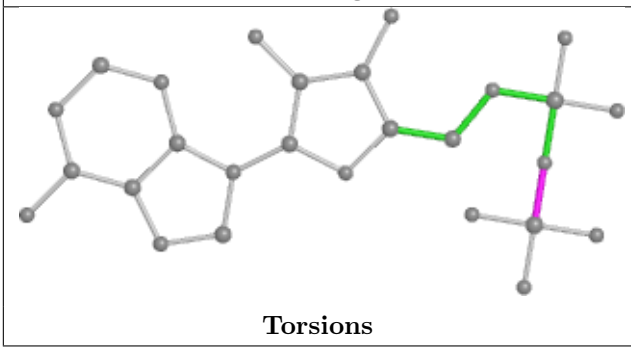
Ligand ADP A 902



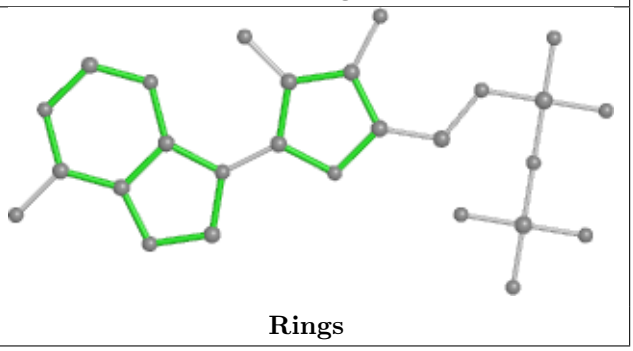
Bond lengths



Bond angles

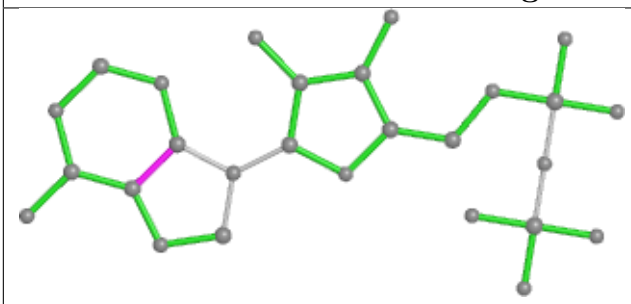


Torsions

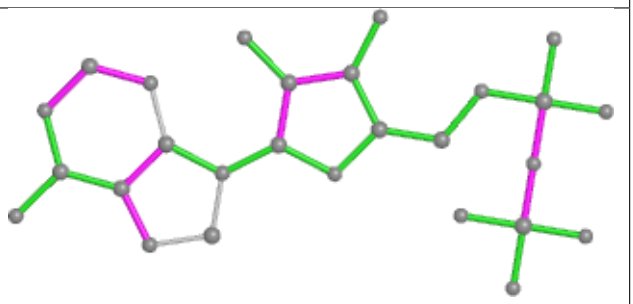


Rings

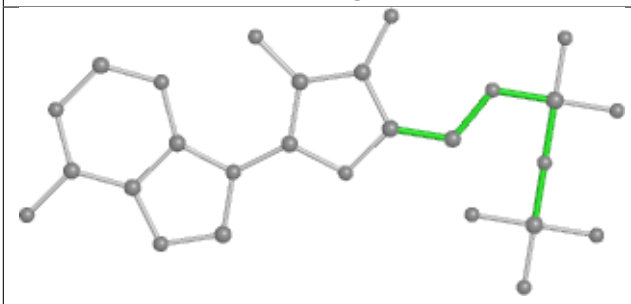
Ligand ADP D 902



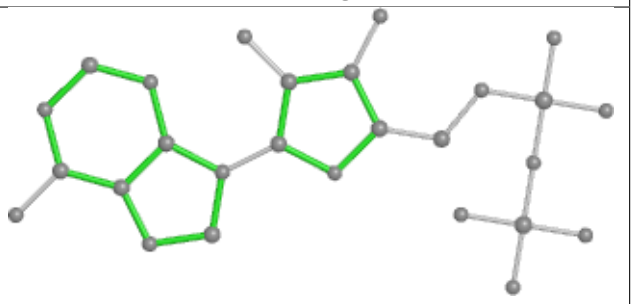
Bond lengths



Bond angles

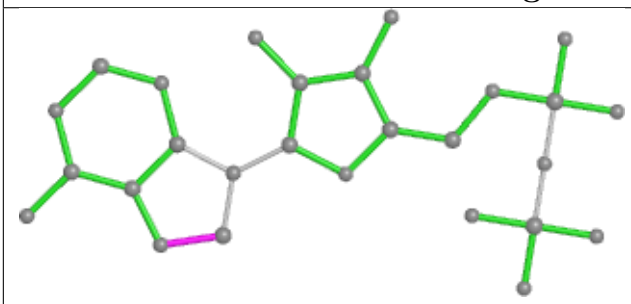


Torsions

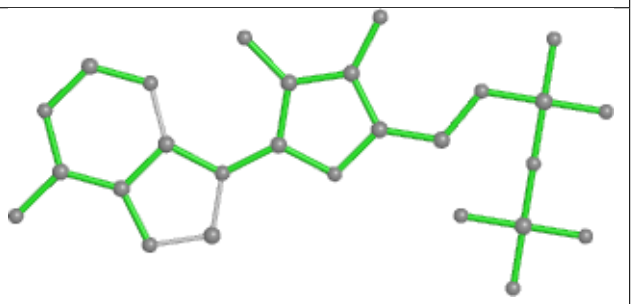


Rings

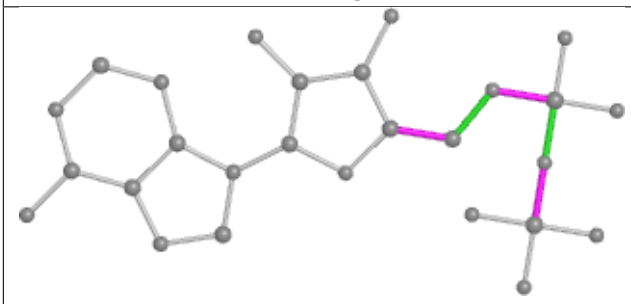
Ligand ADP E 901



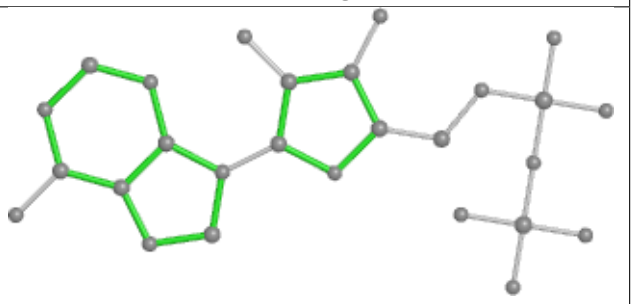
Bond lengths



Bond angles

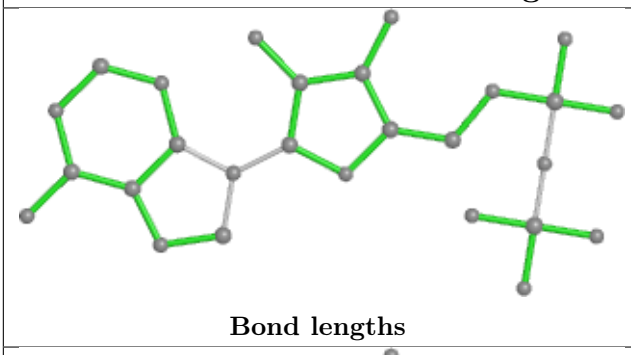


Torsions

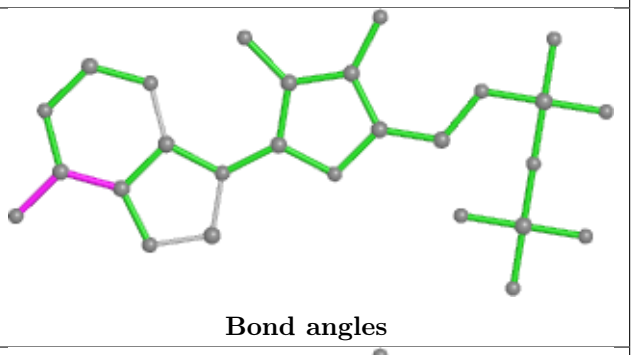


Rings

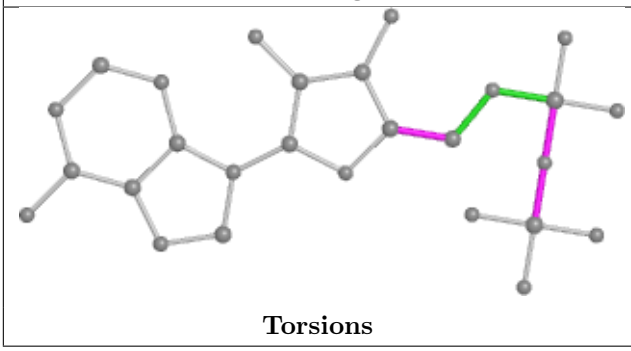
Ligand ADP B 901



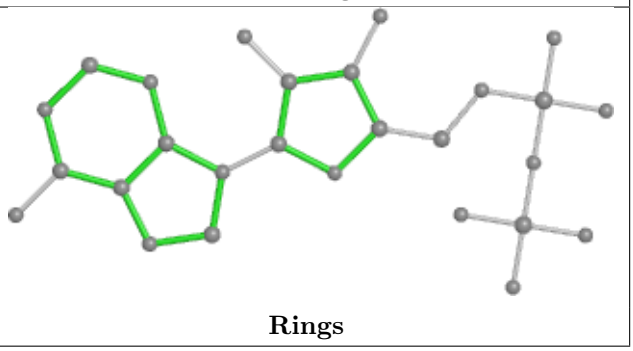
Bond lengths



Bond angles

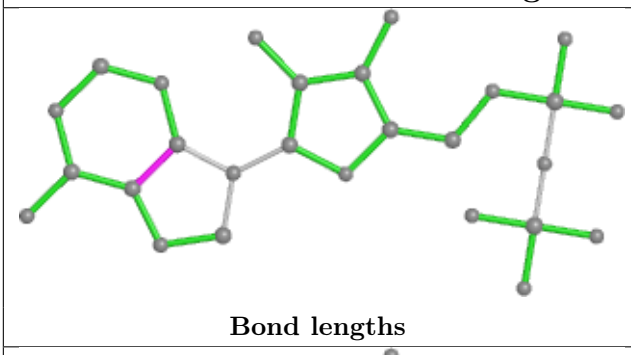


Torsions

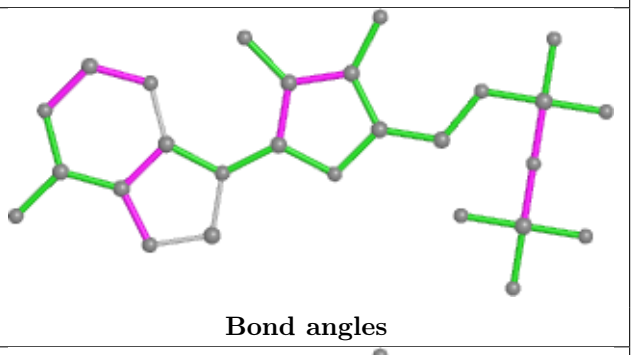


Rings

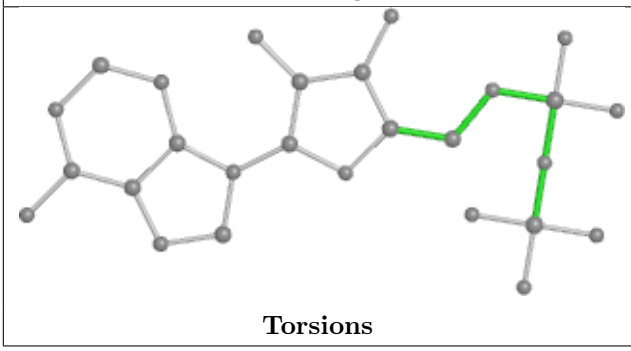
Ligand ADP E 902



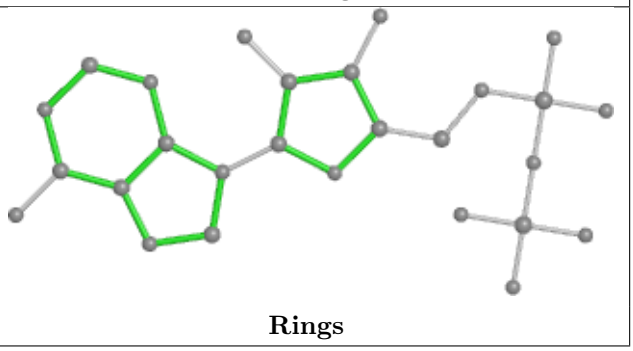
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

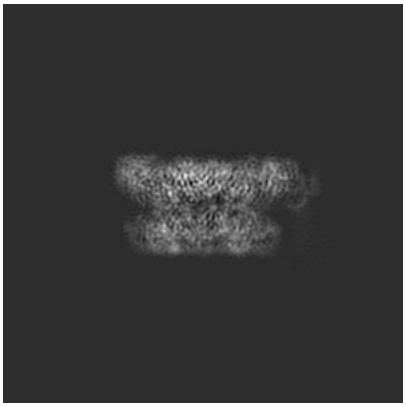
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-28983. These allow visual inspection of the internal detail of the map and identification of artifacts.

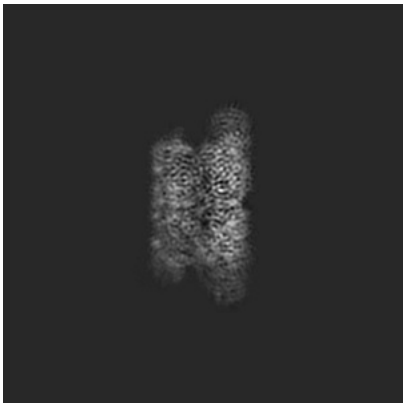
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

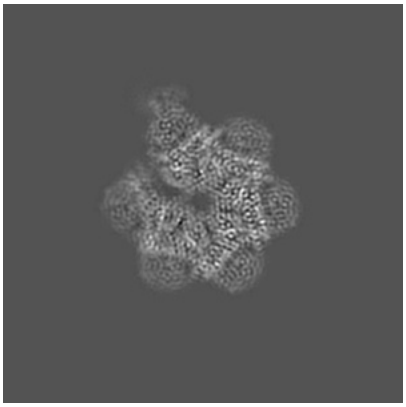
6.1.1 Primary map



X



Y



Z

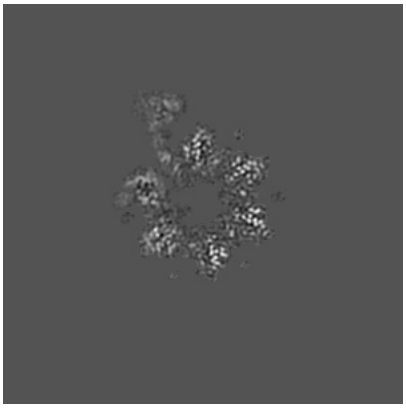
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 200

Y Index: 200



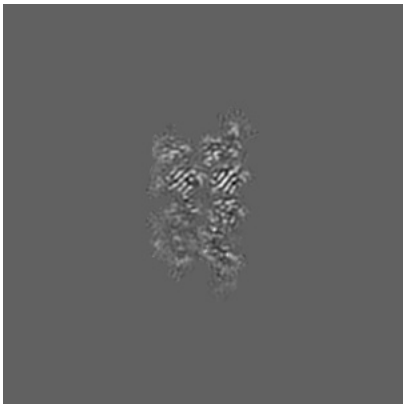
Z Index: 200

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

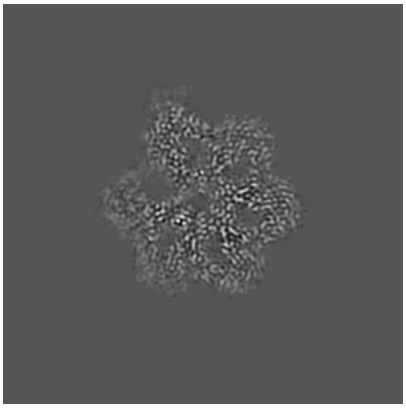
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 225



Y Index: 172

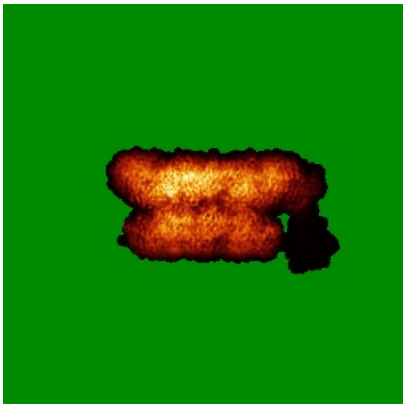


Z Index: 226

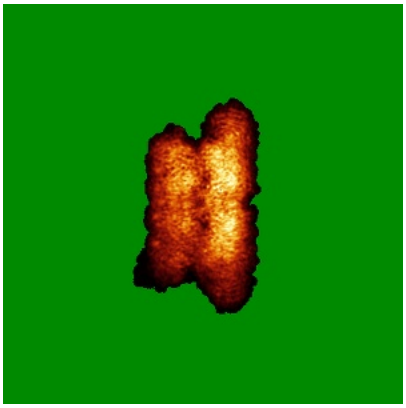
The images above show the largest variance slices of the map in three orthogonal directions.

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

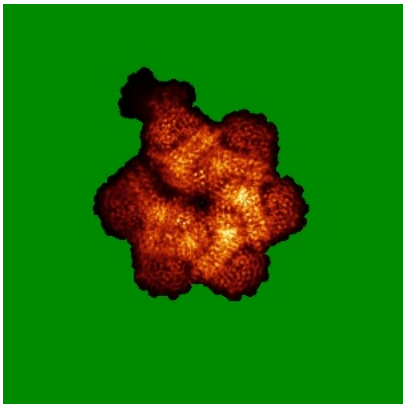
6.4.1 Primary map



X



Y



Z

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 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

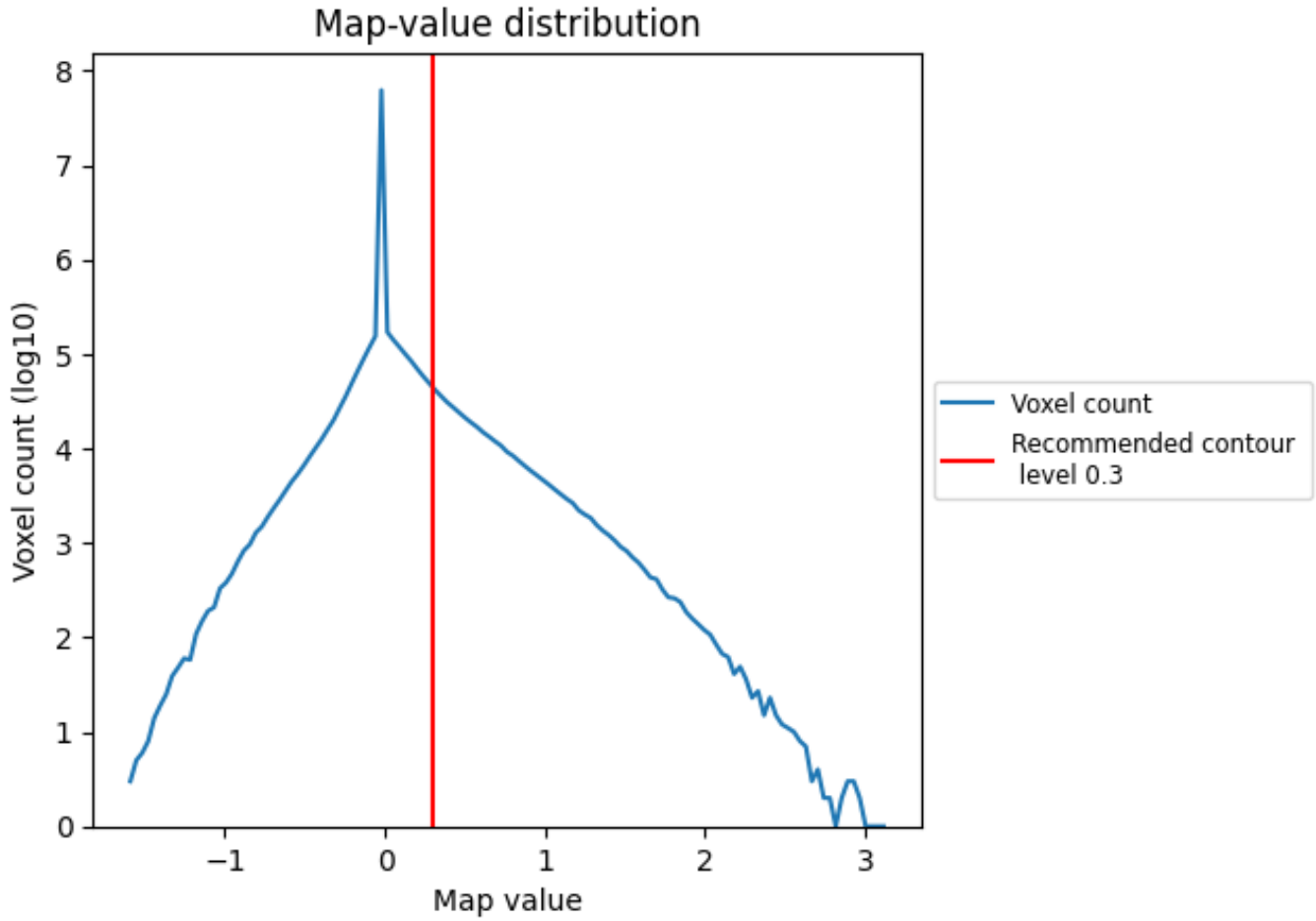
6.6 Mask visualisation (i)

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

7 Map analysis

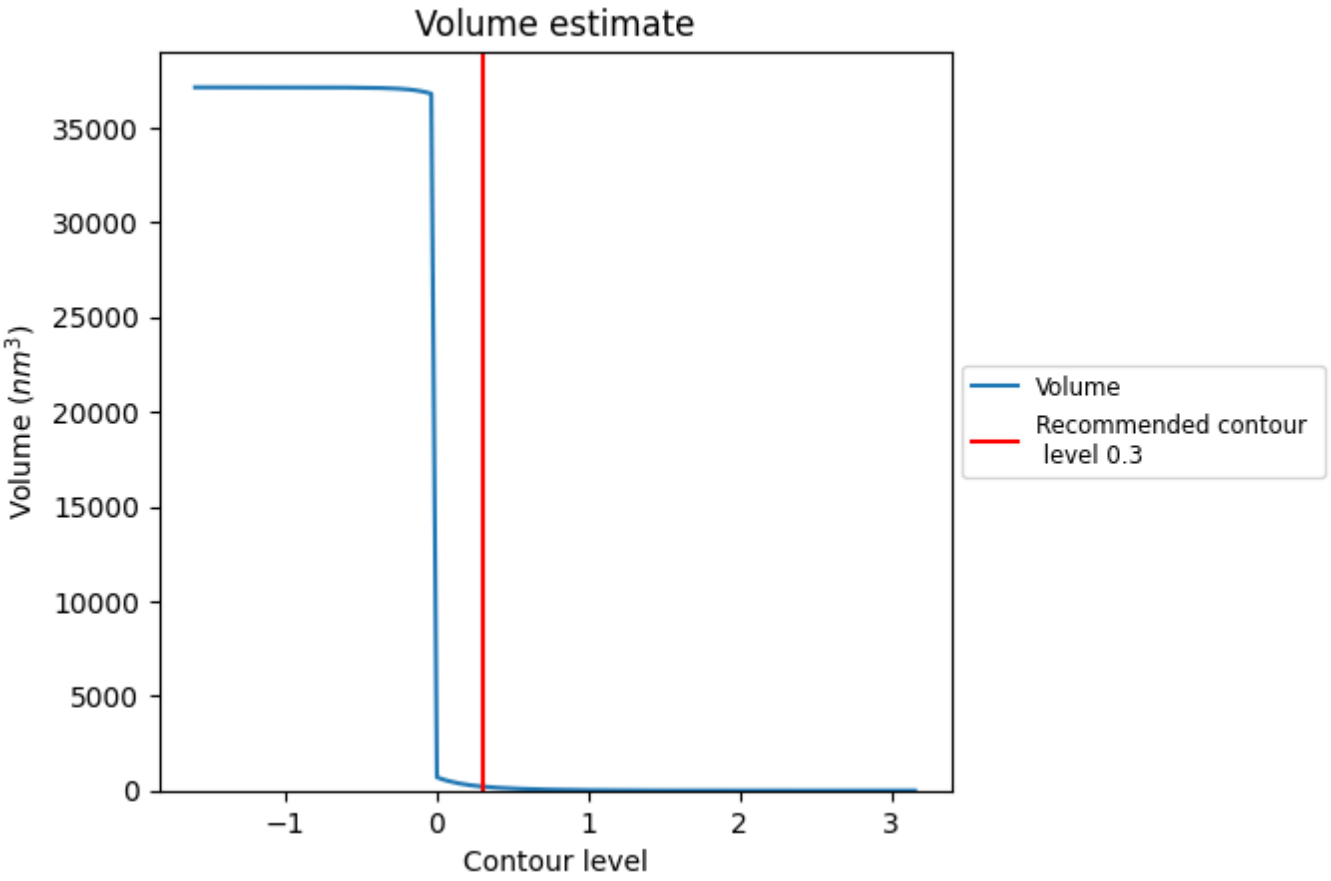
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

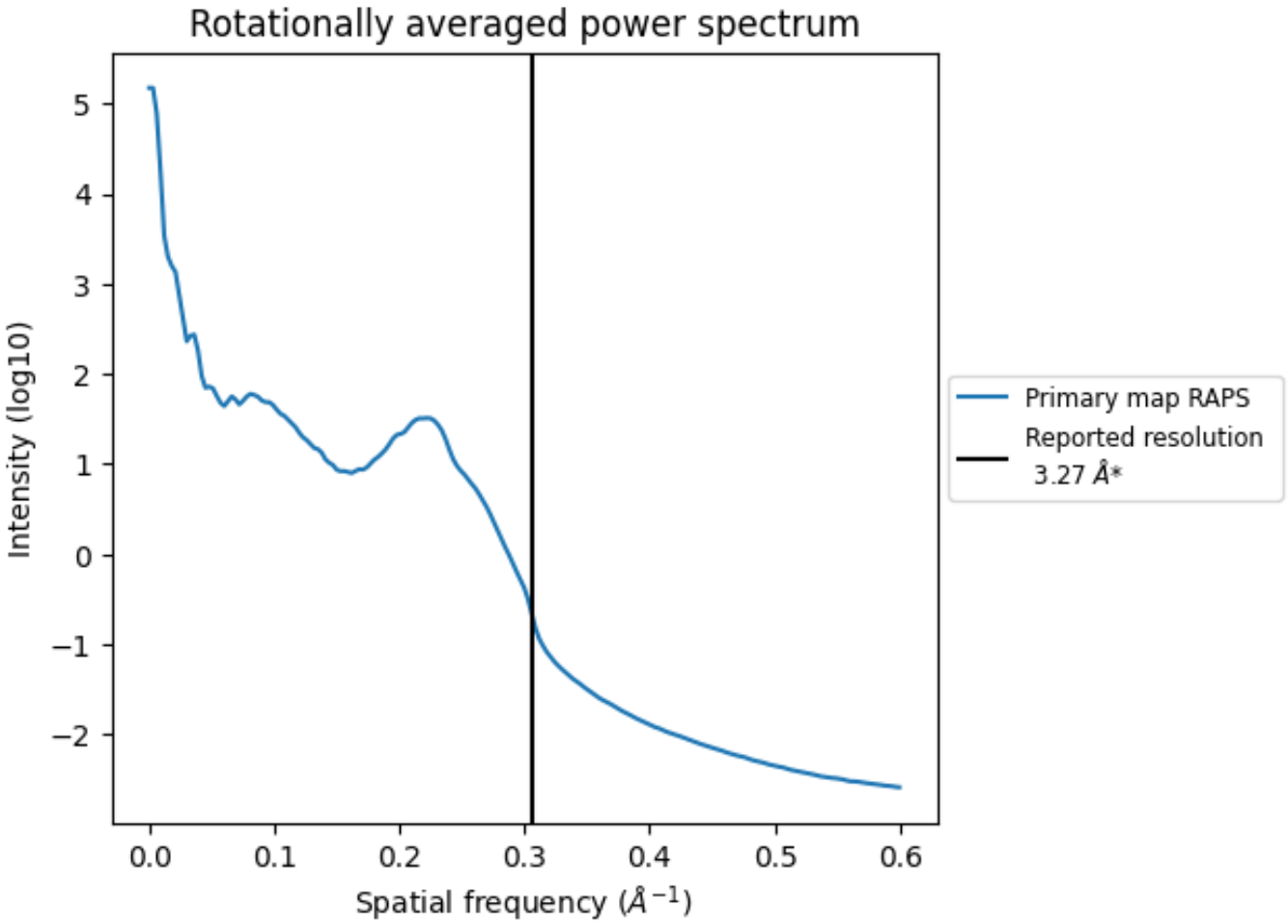
7.2 Volume estimate



The volume at the recommended contour level is 213 nm^3; this corresponds to an approximate mass of 193 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 0.306 Å^{-1}

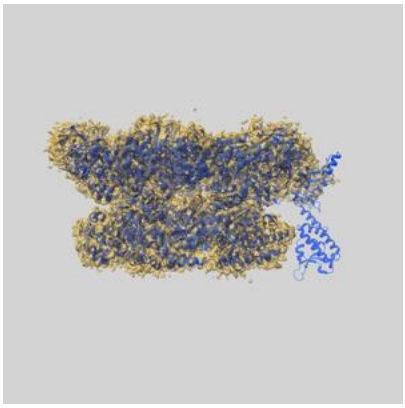
8 Fourier-Shell correlation (i)

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

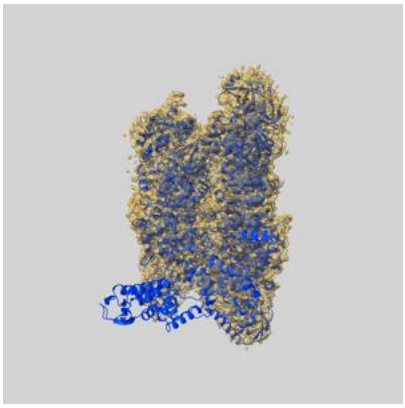
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-28983 and PDB model 8FCM. Per-residue inclusion information can be found in section 3 on page 5.

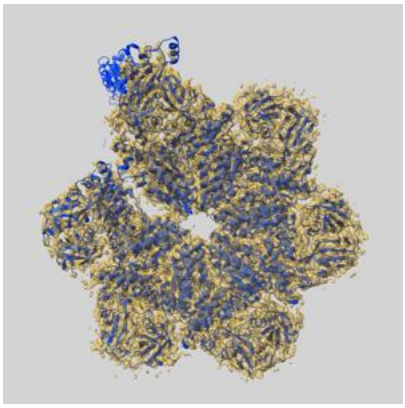
9.1 Map-model overlay



X



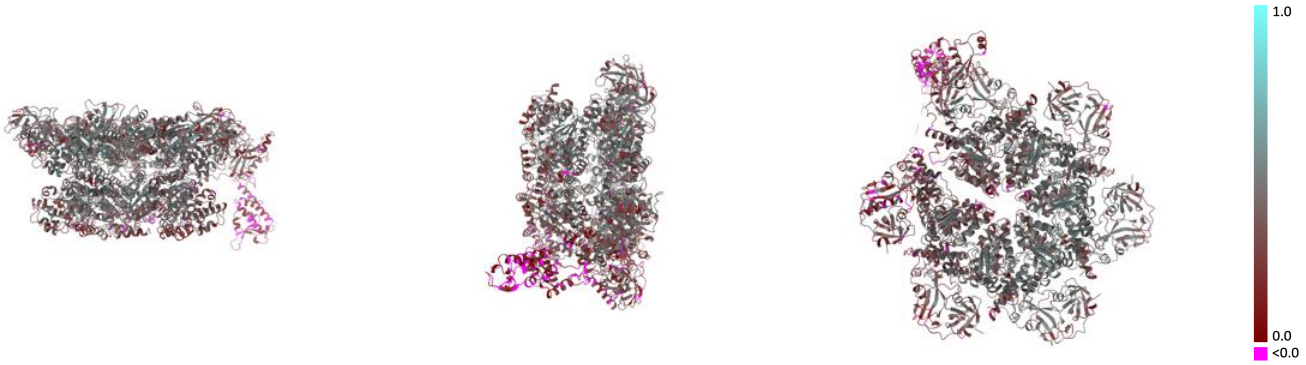
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

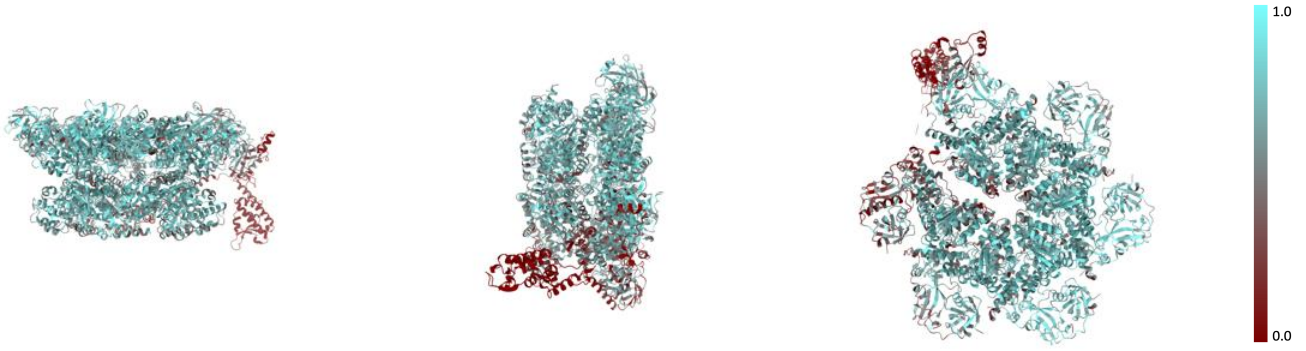
9.2 Q-score mapped to coordinate model



X Y Z

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.

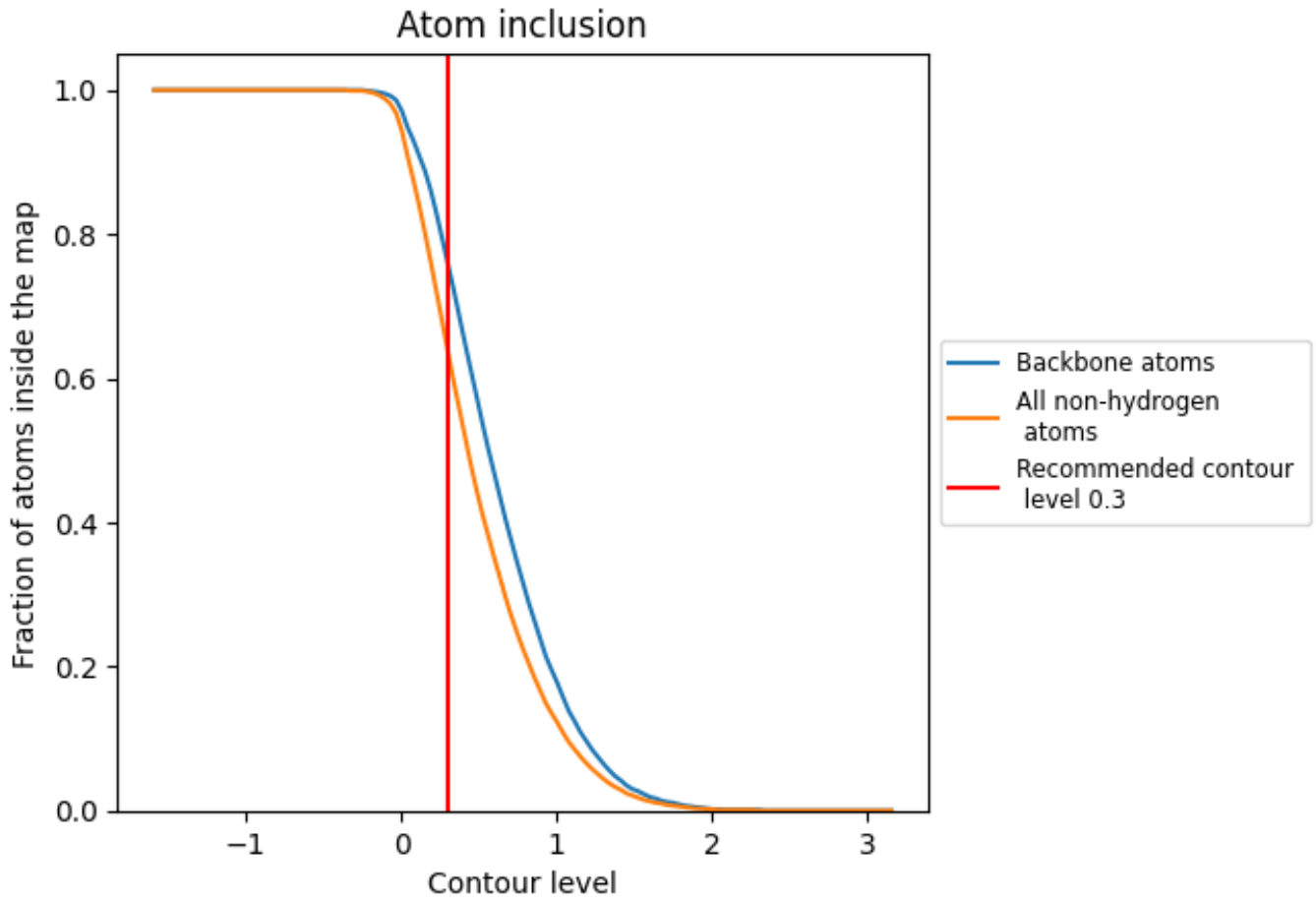
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 64% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6350	0.3640
A	0.5250	0.3030
B	0.6480	0.3580
C	0.7370	0.4260
D	0.7520	0.4340
E	0.6890	0.3920
F	0.6810	0.3740
G	0.1720	0.1560