Full wwPDB EM Validation Report (i)

May 18, 2024 – 04:35 PM EDT

PDB ID	:	7LMY
EMDB ID	:	EMD-23442
Title	:	Cryo-EM structure of human p97 in complex with NMS-873 in the presence of ATP, Npl4/Ufd1, and Ub6
Authors	:	Pan, M.; Yu, Y.; Liu, L.; Zhao, M.
Deposited on	:	2021-02-06
Resolution	:	2.40 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 (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:

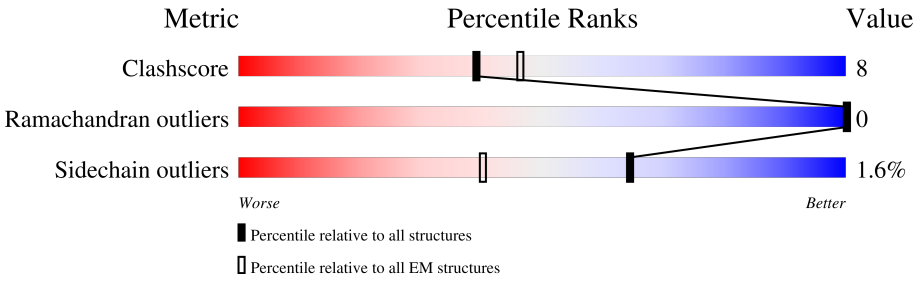
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.40 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	5% 74% 18% 8%
1	B	806	5% 74% 17% 8%
1	C	806	5% 75% 17% 8%
1	D	806	5% 74% 18% 8%
1	E	806	5% 74% 17% 8%
1	F	806	5% 74% 18% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 35646 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.

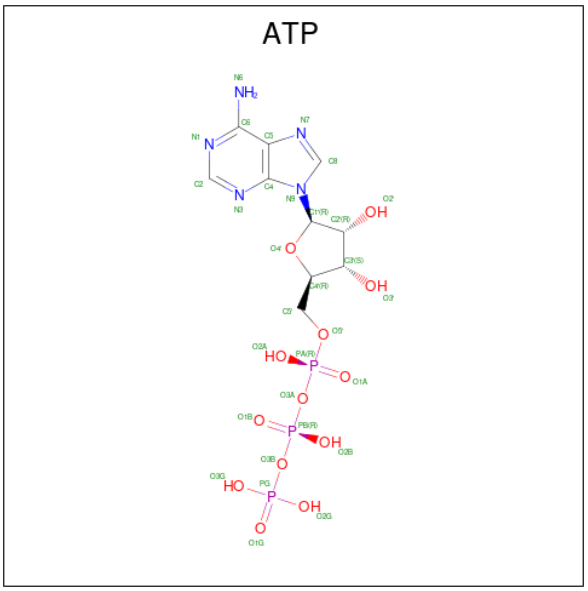
- Molecule 1 is a protein called Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	745	5841	3676	1036	1099	30	0	0
1	B	745	5841	3676	1036	1099	30	0	0
1	C	745	5841	3676	1036	1099	30	0	0
1	D	745	5841	3676	1036	1099	30	0	0
1	E	745	5841	3676	1036	1099	30	0	0
1	F	745	5841	3676	1036	1099	30	0	0

There are 12 discrepancies between the modelled and reference sequences:

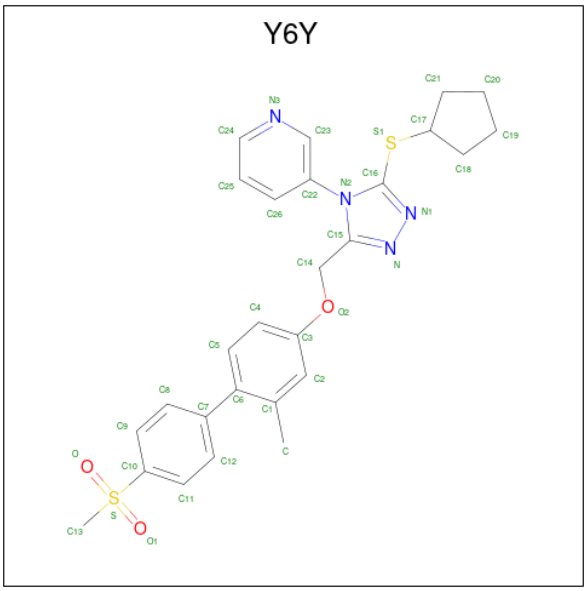
Chain	Residue	Modelled	Actual	Comment	Reference
A	232	GLU	ALA	engineered mutation	UNP P55072
A	578	GLN	GLU	engineered mutation	UNP P55072
B	232	GLU	ALA	engineered mutation	UNP P55072
B	578	GLN	GLU	engineered mutation	UNP P55072
C	232	GLU	ALA	engineered mutation	UNP P55072
C	578	GLN	GLU	engineered mutation	UNP P55072
D	232	GLU	ALA	engineered mutation	UNP P55072
D	578	GLN	GLU	engineered mutation	UNP P55072
E	232	GLU	ALA	engineered mutation	UNP P55072
E	578	GLN	GLU	engineered mutation	UNP P55072
F	232	GLU	ALA	engineered mutation	UNP P55072
F	578	GLN	GLU	engineered mutation	UNP P55072

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	31	10	5	13	3	0
			Total	C	N	O	P	
2	A	1	31	10	5	13	3	0
			Total	C	N	O	P	
2	B	1	31	10	5	13	3	0
			Total	C	N	O	P	
2	B	1	31	10	5	13	3	0
			Total	C	N	O	P	
2	C	1	31	10	5	13	3	0
			Total	C	N	O	P	
2	C	1	31	10	5	13	3	0
			Total	C	N	O	P	
2	D	1	31	10	5	13	3	0
			Total	C	N	O	P	
2	D	1	31	10	5	13	3	0
			Total	C	N	O	P	
2	E	1	31	10	5	13	3	0
			Total	C	N	O	P	
2	E	1	31	10	5	13	3	0
			Total	C	N	O	P	
2	F	1	31	10	5	13	3	0
			Total	C	N	O	P	
2	F	1	31	10	5	13	3	0

- Molecule 3 is 3-[3-cyclopentylsulfanyl-5-[[3-methyl-4-(4-methylsulfonylphenyl)phenoxy]methyl]-1,2,4-triazol-4-yl]pyridine (three-letter code: Y6Y) (formula: $C_{27}H_{28}N_4O_3S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
3	A	1	36	27	4	3	2	0
3	B	1	36	27	4	3	2	0
3	C	1	36	27	4	3	2	0
3	D	1	36	27	4	3	2	0
3	E	1	36	27	4	3	2	0
3	F	1	36	27	4	3	2	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

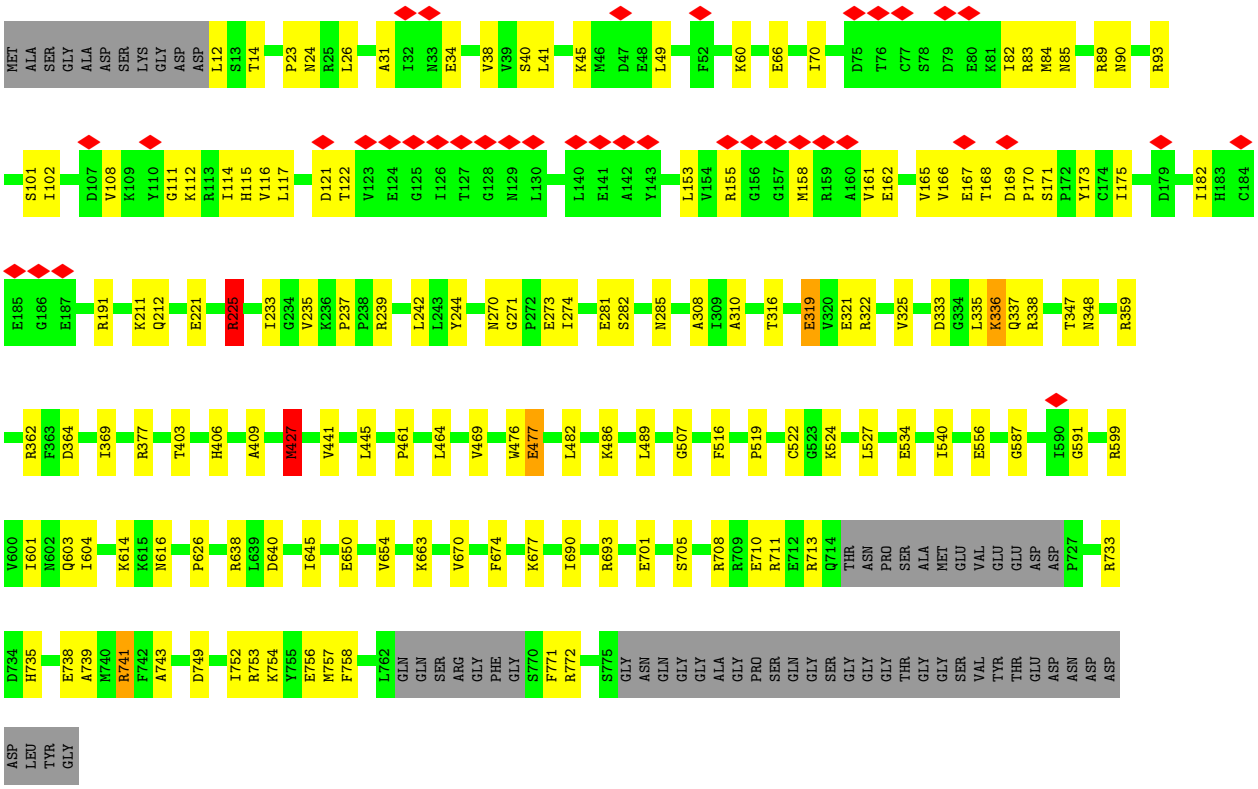
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	A	2	2	2	0
4	B	2	2	2	0
4	C	2	2	2	0
4	D	2	2	2	0
4	E	2	2	2	0
4	F	2	2	2	0

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.

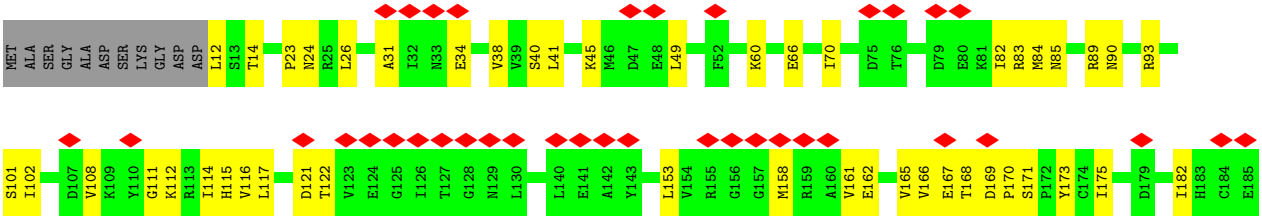
• Molecule 1: Transitional endoplasmic reticulum ATPase

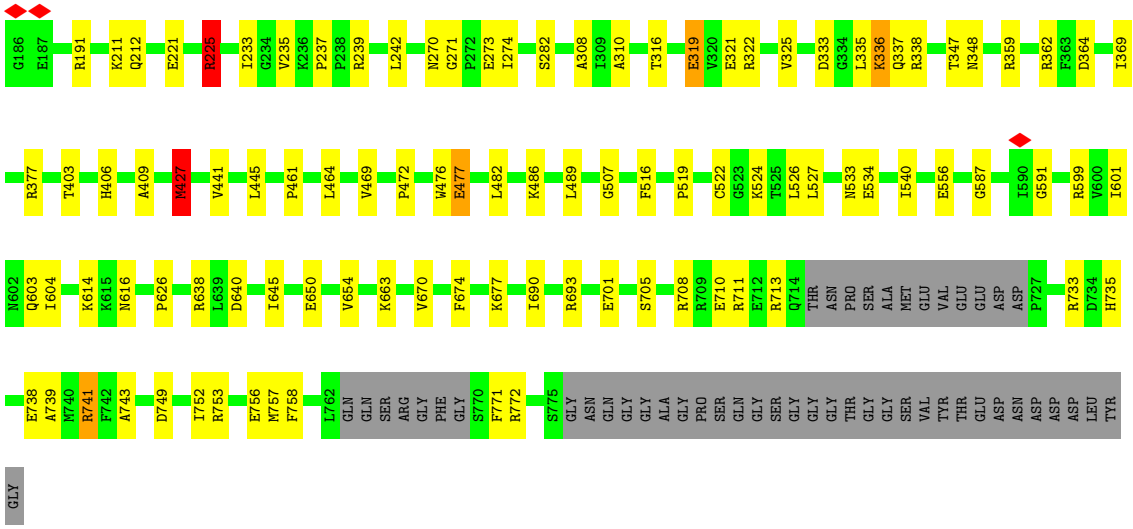
Chain A:



• Molecule 1: Transitional endoplasmic reticulum ATPase

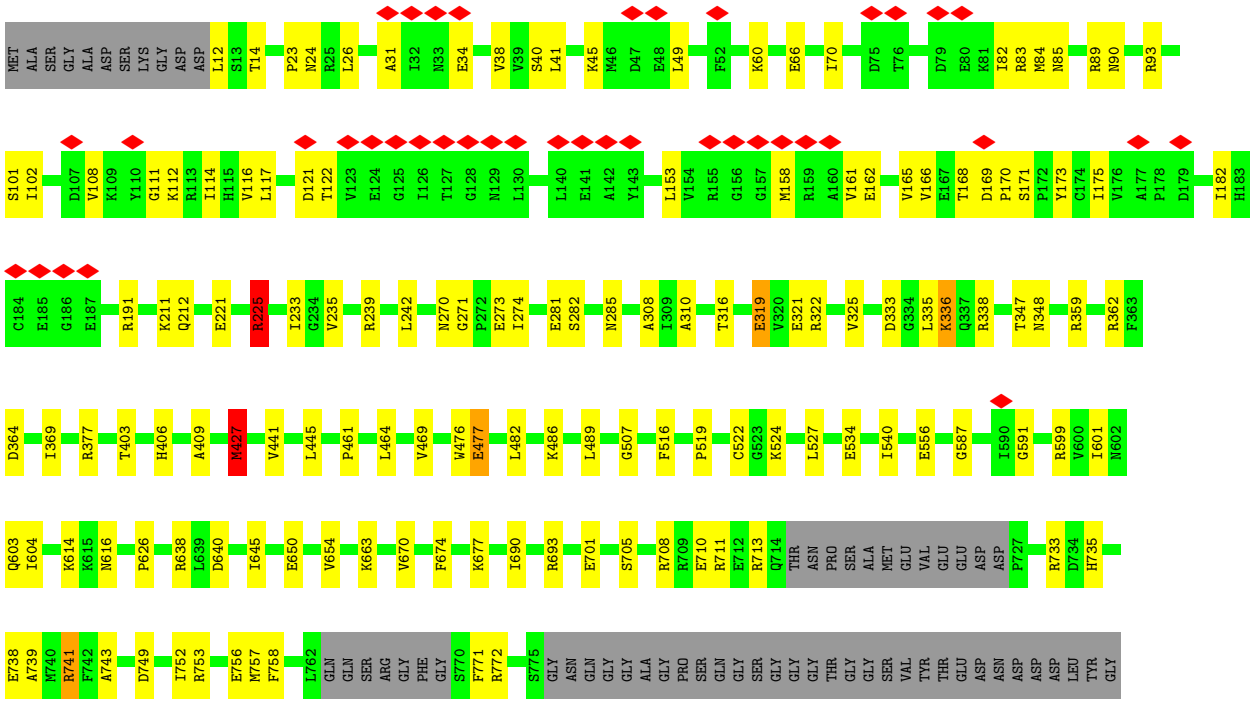
Chain B:





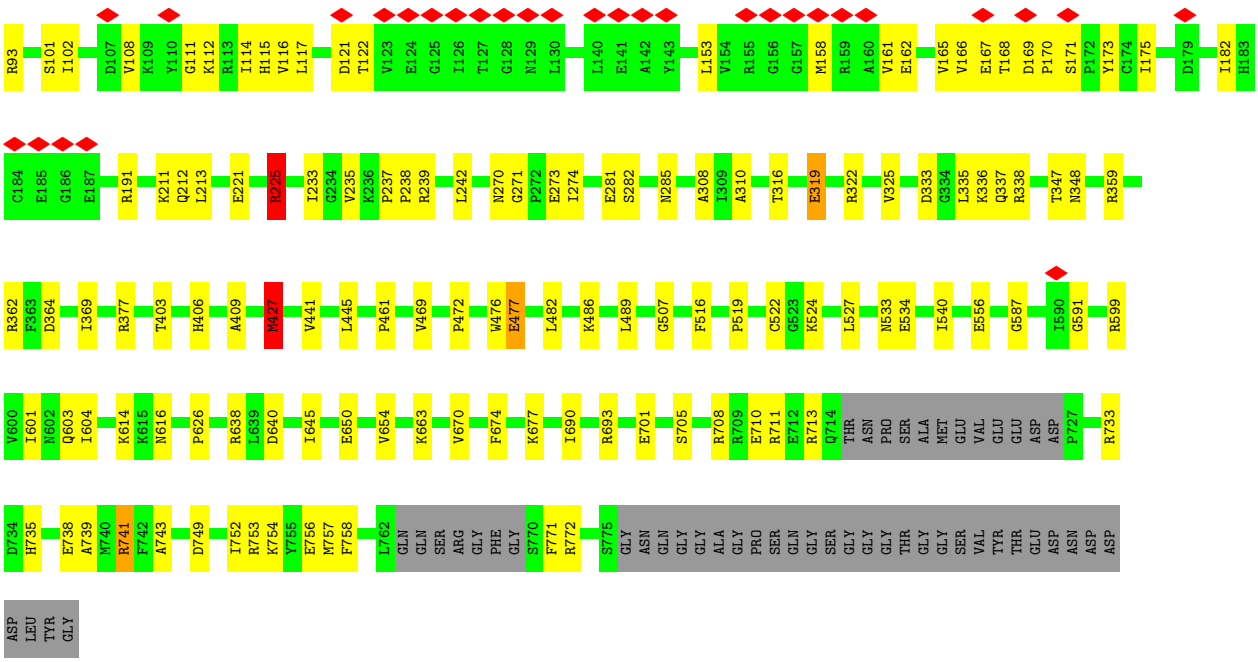
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain C:



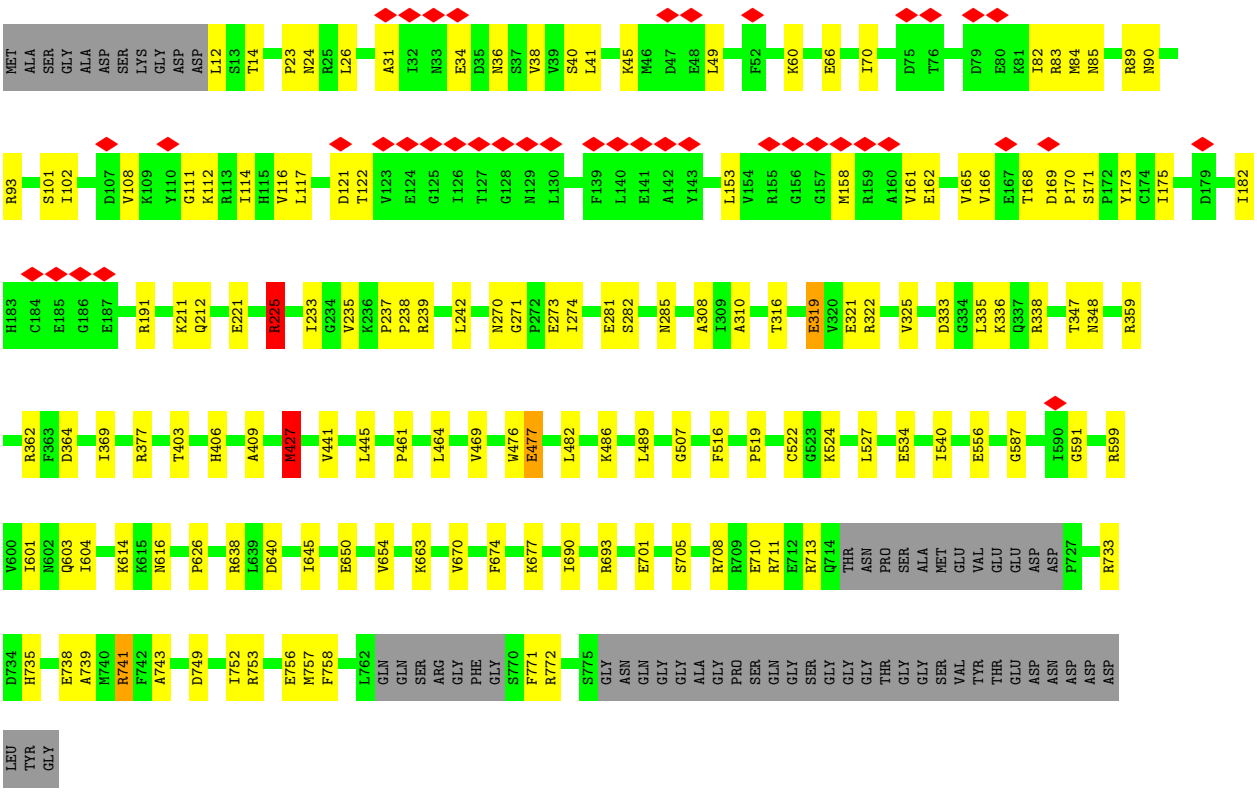
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain D:



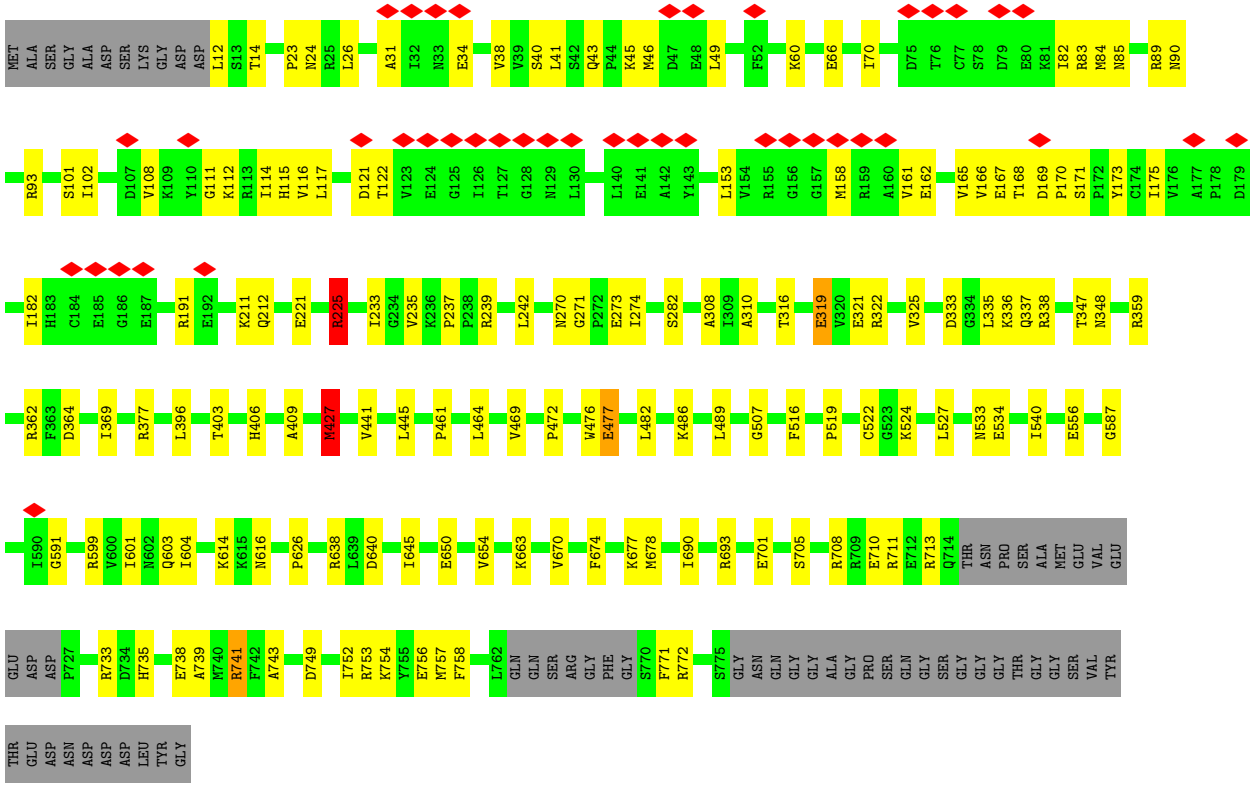
- Molecule 1: Transitional endoplasmic reticulum ATPase

Chain E:



- Molecule 1: Transitional endoplasmic reticulum ATPase

Chain F:


MET ALA SER GLY ALA ASP SER LYS GLY ASP ASP L12 S13 T14 P23 N24 R25 L26 A31 I32 N33 E34 V38 V39 S40 L41 S42 Q43 P44 K45 M46 D47 E48 L49 F52 K60 E66 I70 D75 T76 C77 S78 D79 E80 K81 I82 R83 M84 N85 R89 N90
R93 S101 I102 D107 V108 K109 Y110 G111 K112 R113 I114 H115 V116 L117 D121 T122 V123 E124 G125 I126 T127 G128 N129 L130 L140 E141 A142 Y143 L153 V154 R155 G156 G157 M158 R159 A160 V161 E162 V165 V166 E167 T168 D169 P170 S171 P172 Y173 C174 I175 V176 A177 P178 D179
I182 H183 C184 E185 G186 E187 R191 E192 K211 Q212 E221 R225 I233 G234 V235 K236 P237 P238 R239 L242 N270 G271 P272 E273 I274 S282 A308 I309 A310 T316 E319 V320 E321 R322 V325 D333 G334 L335 K336 Q337 R338 T347 N348 R359
R362 F363 D364 I369 R377 L396 T403 H406 A409 M427 V441 L445 P461 L464 V469 P472 W476 E477 L482 K486 L489 G507 F516 P519 C522 G523 K524 L527 N533 E534 I540 E556 G587
I590 G591 R599 V600 I601 N602 Q603 I604 K614 K615 N616 P626 R638 L639 D640 I645 E650 V654 K663 V670 F674 K677 M678 I690 R693 E701 S705 R708 R709 E710 R711 E712 R713 Q714 THR ASN PRO SER ALA MET GLU VAL GLU
GLU ASP ASP P727 R733 D734 H735 E738 A739 M740 R741 F742 A743 D749 I752 R753 K754 Y755 E756 M757 F758 L762 GLN GLN SER ARG GLY PHE GLY S770 F771 R772 S775 GLY ASN GLN GLY GLY ALA GLY PRO SER GLN GLY SER GLY GLY GLY THR GLY GLY SER VAL TYR
THR GLU ASP ASN ASP ASP ASP LEU TYR GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	372419	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.109	Depositor
Minimum map value	-0.028	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	340.15997, 340.15997, 340.15997	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.063, 1.063, 1.063	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, Y6Y, ATP

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	0.26	0/5936	0.54	4/8011 (0.0%)
1	B	0.26	0/5936	0.54	4/8011 (0.0%)
1	C	0.26	0/5936	0.54	4/8011 (0.0%)
1	D	0.26	0/5936	0.54	4/8011 (0.0%)
1	E	0.26	0/5936	0.54	4/8011 (0.0%)
1	F	0.26	0/5936	0.54	4/8011 (0.0%)
All	All	0.26	0/35616	0.54	24/48066 (0.0%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	225	ARG	CB-CG-CD	5.64	126.26	111.60
1	E	427	MET	CB-CG-SD	5.63	129.30	112.40
1	B	225	ARG	CB-CG-CD	5.63	126.24	111.60
1	D	427	MET	CB-CG-SD	5.63	129.29	112.40
1	D	225	ARG	CB-CG-CD	5.62	126.22	111.60
1	E	225	ARG	CB-CG-CD	5.62	126.22	111.60
1	F	225	ARG	CB-CG-CD	5.62	126.22	111.60
1	C	427	MET	CB-CG-SD	5.62	129.26	112.40
1	F	427	MET	CB-CG-SD	5.62	129.26	112.40
1	A	225	ARG	CB-CG-CD	5.62	126.20	111.60
1	A	427	MET	CB-CG-SD	5.61	129.24	112.40
1	B	427	MET	CB-CG-SD	5.60	129.20	112.40
1	C	319	GLU	CA-CB-CG	5.60	125.72	113.40
1	E	319	GLU	CA-CB-CG	5.59	125.70	113.40
1	B	319	GLU	CA-CB-CG	5.59	125.69	113.40
1	A	319	GLU	CA-CB-CG	5.57	125.66	113.40
1	D	319	GLU	CA-CB-CG	5.57	125.66	113.40
1	F	319	GLU	CA-CB-CG	5.56	125.64	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	427	MET	CG-SD-CE	5.46	108.94	100.20
1	A	427	MET	CG-SD-CE	5.46	108.94	100.20
1	C	427	MET	CG-SD-CE	5.43	108.90	100.20
1	F	427	MET	CG-SD-CE	5.42	108.88	100.20
1	D	427	MET	CG-SD-CE	5.42	108.87	100.20
1	E	427	MET	CG-SD-CE	5.41	108.86	100.20

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	5841	0	5922	96	0
1	B	5841	0	5922	93	0
1	C	5841	0	5922	90	0
1	D	5841	0	5922	93	0
1	E	5841	0	5922	91	0
1	F	5841	0	5922	94	0
2	A	62	0	24	3	0
2	B	62	0	24	4	0
2	C	62	0	24	3	0
2	D	62	0	24	3	0
2	E	62	0	24	3	0
2	F	62	0	24	3	0
3	A	36	0	0	0	0
3	B	36	0	0	0	0
3	C	36	0	0	0	0
3	D	36	0	0	0	0
3	E	36	0	0	0	0
3	F	36	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	2	0	0	0	0
All	All	35646	0	35676	556	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 8.

All (556) 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:701:GLU:OE1	1:C:735:HIS:NE2	2.10	0.85
1:E:701:GLU:OE1	1:E:735:HIS:NE2	2.10	0.85
1:D:556:GLU:OE2	1:D:599:ARG:NH1	2.10	0.85
1:A:556:GLU:OE2	1:A:599:ARG:NH1	2.10	0.84
1:E:556:GLU:OE2	1:E:599:ARG:NH1	2.10	0.84
1:F:556:GLU:OE2	1:F:599:ARG:NH1	2.10	0.84
1:C:556:GLU:OE2	1:C:599:ARG:NH1	2.10	0.84
1:F:701:GLU:OE1	1:F:735:HIS:NE2	2.10	0.84
1:B:556:GLU:OE2	1:B:599:ARG:NH1	2.10	0.83
1:D:701:GLU:OE1	1:D:735:HIS:NE2	2.10	0.83
1:A:476:TRP:NE1	1:A:534:GLU:OE1	2.12	0.83
1:B:476:TRP:NE1	1:B:534:GLU:OE1	2.12	0.83
1:B:701:GLU:OE1	1:B:735:HIS:NE2	2.10	0.83
1:A:701:GLU:OE1	1:A:735:HIS:NE2	2.10	0.82
1:C:476:TRP:NE1	1:C:534:GLU:OE1	2.12	0.81
1:F:476:TRP:NE1	1:F:534:GLU:OE1	2.12	0.81
1:E:476:TRP:NE1	1:E:534:GLU:OE1	2.11	0.81
1:D:476:TRP:NE1	1:D:534:GLU:OE1	2.12	0.81
1:E:507:GLY:O	1:F:663:LYS:NZ	2.14	0.80
1:B:507:GLY:O	1:C:663:LYS:NZ	2.17	0.76
1:C:771:PHE:O	1:C:772:ARG:NH1	2.21	0.74
1:A:663:LYS:NZ	1:F:507:GLY:O	2.20	0.74
1:D:771:PHE:O	1:D:772:ARG:NH1	2.21	0.74
1:D:507:GLY:O	1:E:663:LYS:NZ	2.19	0.74
1:E:771:PHE:O	1:E:772:ARG:NH1	2.20	0.74
1:B:771:PHE:O	1:B:772:ARG:NH1	2.21	0.74
1:C:507:GLY:O	1:D:663:LYS:NZ	2.19	0.74
1:F:771:PHE:O	1:F:772:ARG:NH1	2.21	0.74
1:A:771:PHE:O	1:A:772:ARG:NH1	2.21	0.73
1:E:239:ARG:NH1	1:E:335:LEU:O	2.24	0.71
1:D:239:ARG:NH1	1:D:335:LEU:O	2.24	0.71
1:F:239:ARG:NH1	1:F:335:LEU:O	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ARG:NH1	1:C:335:LEU:O	2.24	0.70
1:B:239:ARG:NH1	1:B:335:LEU:O	2.24	0.70
1:B:710:GLU:OE2	1:B:713:ARG:NH2	2.20	0.70
1:A:239:ARG:NH1	1:A:335:LEU:O	2.24	0.70
1:A:710:GLU:OE2	1:A:713:ARG:NH2	2.20	0.68
1:F:710:GLU:OE2	1:F:713:ARG:NH2	2.20	0.68
1:E:710:GLU:OE2	1:E:713:ARG:NH2	2.20	0.67
1:D:710:GLU:OE2	1:D:713:ARG:NH2	2.20	0.67
1:C:710:GLU:OE2	1:C:713:ARG:NH2	2.20	0.66
1:A:12:LEU:HD23	1:A:14:THR:H	1.62	0.65
1:C:12:LEU:HD23	1:C:14:THR:H	1.62	0.64
1:B:270:ASN:HB2	1:B:273:GLU:HB2	1.80	0.64
1:C:270:ASN:HB2	1:C:273:GLU:HB2	1.80	0.64
1:D:12:LEU:HD23	1:D:14:THR:H	1.62	0.64
1:E:12:LEU:HD23	1:E:14:THR:H	1.62	0.64
1:A:270:ASN:HB2	1:A:273:GLU:HB2	1.80	0.64
1:E:90:ASN:O	1:E:93:ARG:NH1	2.31	0.64
1:D:90:ASN:O	1:D:93:ARG:NH1	2.31	0.64
1:F:90:ASN:O	1:F:93:ARG:NH1	2.31	0.64
1:B:12:LEU:HD23	1:B:14:THR:H	1.62	0.63
1:D:270:ASN:HB2	1:D:273:GLU:HB2	1.80	0.63
1:A:90:ASN:O	1:A:93:ARG:NH1	2.31	0.63
1:E:270:ASN:HB2	1:E:273:GLU:HB2	1.80	0.63
1:F:12:LEU:HD23	1:F:14:THR:H	1.62	0.63
1:F:270:ASN:HB2	1:F:273:GLU:HB2	1.80	0.63
1:C:90:ASN:O	1:C:93:ARG:NH1	2.31	0.63
1:A:507:GLY:O	1:B:663:LYS:NZ	2.30	0.62
1:B:90:ASN:O	1:B:93:ARG:NH1	2.31	0.62
1:D:674:PHE:HA	1:D:677:LYS:HG2	1.83	0.61
1:C:674:PHE:HA	1:C:677:LYS:HG2	1.83	0.61
1:A:674:PHE:HA	1:A:677:LYS:HG2	1.83	0.60
1:D:406:HIS:CE1	1:D:461:PRO:HG3	2.37	0.60
1:A:38:VAL:HG12	1:A:70:ILE:HB	1.84	0.60
1:B:38:VAL:HG12	1:B:70:ILE:HB	1.84	0.60
1:E:406:HIS:CE1	1:E:461:PRO:HG3	2.37	0.60
1:E:674:PHE:HA	1:E:677:LYS:HG2	1.83	0.60
1:F:406:HIS:CE1	1:F:461:PRO:HG3	2.37	0.60
1:A:406:HIS:CE1	1:A:461:PRO:HG3	2.37	0.60
1:B:674:PHE:HA	1:B:677:LYS:HG2	1.83	0.59
1:C:406:HIS:CE1	1:C:461:PRO:HG3	2.37	0.59
1:F:38:VAL:HG12	1:F:70:ILE:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:HIS:CE1	1:B:461:PRO:HG3	2.37	0.59
1:E:38:VAL:HG12	1:E:70:ILE:HB	1.84	0.59
1:F:674:PHE:HA	1:F:677:LYS:HG2	1.83	0.59
1:C:38:VAL:HG12	1:C:70:ILE:HB	1.84	0.59
1:D:38:VAL:HG12	1:D:70:ILE:HB	1.84	0.58
1:C:111:GLY:HA2	1:C:170:PRO:HD2	1.85	0.58
1:D:111:GLY:HA2	1:D:170:PRO:HD2	1.85	0.58
1:E:111:GLY:HA2	1:E:170:PRO:HD2	1.85	0.58
1:B:111:GLY:HA2	1:B:170:PRO:HD2	1.85	0.57
1:A:111:GLY:HA2	1:A:170:PRO:HD2	1.85	0.57
1:B:556:GLU:OE1	1:B:556:GLU:N	2.30	0.57
1:F:111:GLY:HA2	1:F:170:PRO:HD2	1.85	0.57
1:F:31:ALA:HB1	1:F:34:GLU:HB2	1.87	0.57
1:E:556:GLU:HB3	1:E:603:GLN:HG3	1.86	0.57
1:E:482:LEU:HD13	1:E:527:LEU:HD11	1.87	0.57
1:B:482:LEU:HD13	1:B:527:LEU:HD11	1.87	0.57
1:D:482:LEU:HD13	1:D:527:LEU:HD11	1.87	0.57
1:F:482:LEU:HD13	1:F:527:LEU:HD11	1.87	0.57
1:B:556:GLU:HB3	1:B:603:GLN:HG3	1.86	0.56
1:C:482:LEU:HD13	1:C:527:LEU:HD11	1.87	0.56
1:C:556:GLU:HB3	1:C:603:GLN:HG3	1.86	0.56
1:A:31:ALA:HB1	1:A:34:GLU:HB2	1.87	0.56
1:A:482:LEU:HD13	1:A:527:LEU:HD11	1.87	0.56
1:D:556:GLU:HB3	1:D:603:GLN:HG3	1.86	0.56
1:E:31:ALA:HB1	1:E:34:GLU:HB2	1.87	0.56
1:F:556:GLU:HB3	1:F:603:GLN:HG3	1.86	0.56
1:A:225:ARG:HE	1:A:225:ARG:HA	1.70	0.56
1:A:556:GLU:HB3	1:A:603:GLN:HG3	1.86	0.56
1:D:316:THR:O	1:D:322:ARG:NH2	2.39	0.56
1:F:556:GLU:OE1	1:F:556:GLU:N	2.30	0.56
1:B:225:ARG:HE	1:B:225:ARG:HA	1.70	0.56
1:B:31:ALA:HB1	1:B:34:GLU:HB2	1.87	0.55
1:C:225:ARG:HE	1:C:225:ARG:HA	1.70	0.55
1:C:316:THR:O	1:C:322:ARG:NH2	2.39	0.55
1:E:316:THR:O	1:E:322:ARG:NH2	2.39	0.55
1:B:316:THR:O	1:B:322:ARG:NH2	2.39	0.55
1:F:225:ARG:HE	1:F:225:ARG:HA	1.70	0.55
1:D:31:ALA:HB1	1:D:34:GLU:HB2	1.87	0.55
1:D:225:ARG:HE	1:D:225:ARG:HA	1.70	0.55
1:E:587:GLY:HA3	1:E:591:GLY:HA3	1.89	0.55
1:A:316:THR:O	1:A:322:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:ALA:HB1	1:C:34:GLU:HB2	1.87	0.55
1:F:587:GLY:HA3	1:F:591:GLY:HA3	1.89	0.55
1:C:587:GLY:HA3	1:C:591:GLY:HA3	1.89	0.55
1:D:112:LYS:N	1:D:169:ASP:O	2.37	0.55
1:F:316:THR:O	1:F:322:ARG:NH2	2.39	0.55
1:B:587:GLY:HA3	1:B:591:GLY:HA3	1.89	0.55
1:D:587:GLY:HA3	1:D:591:GLY:HA3	1.89	0.55
1:A:587:GLY:HA3	1:A:591:GLY:HA3	1.89	0.55
1:E:112:LYS:N	1:E:169:ASP:O	2.37	0.55
1:E:225:ARG:HE	1:E:225:ARG:HA	1.70	0.55
1:A:348:ASN:HD21	1:F:359:ARG:NH1	2.05	0.54
1:D:270:ASN:O	1:D:273:GLU:HB3	2.08	0.54
1:F:112:LYS:N	1:F:169:ASP:O	2.37	0.54
1:E:270:ASN:O	1:E:273:GLU:HB3	2.08	0.54
1:F:477:GLU:N	1:F:477:GLU:OE1	2.41	0.54
1:D:477:GLU:N	1:D:477:GLU:OE1	2.41	0.54
1:E:477:GLU:N	1:E:477:GLU:OE1	2.41	0.54
1:C:270:ASN:O	1:C:273:GLU:HB3	2.08	0.54
1:C:752:ILE:O	1:C:756:GLU:HG2	2.08	0.54
1:D:117:LEU:HD12	1:D:166:VAL:HG11	1.90	0.54
1:B:112:LYS:N	1:B:169:ASP:O	2.37	0.54
1:C:477:GLU:OE1	1:C:477:GLU:N	2.41	0.54
1:D:752:ILE:O	1:D:756:GLU:HG2	2.08	0.54
1:E:117:LEU:HD12	1:E:166:VAL:HG11	1.90	0.54
1:F:270:ASN:O	1:F:273:GLU:HB3	2.08	0.54
1:A:752:ILE:O	1:A:756:GLU:HG2	2.08	0.54
1:B:752:ILE:O	1:B:756:GLU:HG2	2.08	0.54
1:F:117:LEU:HD12	1:F:166:VAL:HG11	1.90	0.54
1:A:477:GLU:OE1	1:A:477:GLU:N	2.41	0.54
1:E:752:ILE:O	1:E:756:GLU:HG2	2.08	0.54
1:A:112:LYS:N	1:A:169:ASP:O	2.37	0.53
1:B:270:ASN:O	1:B:273:GLU:HB3	2.08	0.53
1:C:117:LEU:HD12	1:C:166:VAL:HG11	1.90	0.53
1:A:117:LEU:HD12	1:A:166:VAL:HG11	1.90	0.53
1:B:122:THR:HB	1:B:161:VAL:HA	1.91	0.53
1:C:122:THR:HB	1:C:161:VAL:HA	1.91	0.53
1:A:270:ASN:O	1:A:273:GLU:HB3	2.08	0.53
1:F:752:ILE:O	1:F:756:GLU:HG2	2.08	0.53
1:B:117:LEU:HD12	1:B:166:VAL:HG11	1.90	0.53
1:A:122:THR:HB	1:A:161:VAL:HA	1.91	0.53
1:B:477:GLU:N	1:B:477:GLU:OE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:THR:HB	1:D:161:VAL:HA	1.91	0.53
1:F:556:GLU:OE2	1:F:599:ARG:HD3	2.10	0.52
1:A:556:GLU:OE2	1:A:599:ARG:HD3	2.10	0.52
1:B:556:GLU:OE2	1:B:599:ARG:HD3	2.10	0.52
1:E:556:GLU:OE1	1:E:556:GLU:N	2.30	0.52
1:F:122:THR:HB	1:F:161:VAL:HA	1.91	0.52
1:C:556:GLU:OE2	1:C:599:ARG:HD3	2.10	0.51
1:E:122:THR:HB	1:E:161:VAL:HA	1.91	0.51
1:E:556:GLU:OE2	1:E:599:ARG:HD3	2.10	0.51
1:D:359:ARG:NH1	1:E:348:ASN:HD21	2.08	0.51
1:D:556:GLU:OE2	1:D:599:ARG:HD3	2.10	0.51
1:C:556:GLU:OE1	1:C:556:GLU:N	2.30	0.51
1:E:40:SER:HB2	1:E:83:ARG:HB2	1.93	0.51
1:D:556:GLU:OE1	1:D:556:GLU:N	2.30	0.51
1:E:524:LYS:HG2	1:E:645:ILE:HG13	1.93	0.51
1:D:441:VAL:O	1:D:445:LEU:HG	2.11	0.51
1:F:40:SER:HB2	1:F:83:ARG:HB2	1.93	0.51
1:D:524:LYS:HG2	1:D:645:ILE:HG13	1.93	0.50
1:A:23:PRO:HB2	1:A:49:LEU:HD21	1.93	0.50
1:A:441:VAL:O	1:A:445:LEU:HG	2.11	0.50
1:C:441:VAL:O	1:C:445:LEU:HG	2.11	0.50
1:D:40:SER:HB2	1:D:83:ARG:HB2	1.93	0.50
1:F:524:LYS:HG2	1:F:645:ILE:HG13	1.93	0.50
1:F:556:GLU:HB3	1:F:603:GLN:CG	2.42	0.50
1:E:23:PRO:HB2	1:E:49:LEU:HD21	1.93	0.50
1:E:441:VAL:O	1:E:445:LEU:HG	2.11	0.50
1:A:556:GLU:HB3	1:A:603:GLN:CG	2.42	0.50
1:B:23:PRO:HB2	1:B:49:LEU:HD21	1.93	0.50
1:B:40:SER:HB2	1:B:83:ARG:HB2	1.93	0.50
1:A:556:GLU:OE1	1:A:556:GLU:N	2.30	0.50
1:B:556:GLU:HB3	1:B:603:GLN:CG	2.42	0.50
1:B:441:VAL:O	1:B:445:LEU:HG	2.11	0.50
1:C:556:GLU:HB3	1:C:603:GLN:CG	2.42	0.50
1:D:23:PRO:HB2	1:D:49:LEU:HD21	1.93	0.50
1:F:441:VAL:O	1:F:445:LEU:HG	2.11	0.50
1:D:556:GLU:HB3	1:D:603:GLN:CG	2.42	0.49
1:E:556:GLU:HB3	1:E:603:GLN:CG	2.42	0.49
1:F:556:GLU:HG3	1:F:599:ARG:HB2	1.94	0.49
1:C:40:SER:HB2	1:C:83:ARG:HB2	1.93	0.49
1:A:40:SER:HB2	1:A:83:ARG:HB2	1.93	0.49
1:A:524:LYS:HG2	1:A:645:ILE:HG13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:524:LYS:HG2	1:C:645:ILE:HG13	1.93	0.49
1:F:23:PRO:HB2	1:F:49:LEU:HD21	1.93	0.49
1:C:556:GLU:HG3	1:C:599:ARG:HB2	1.94	0.49
1:E:556:GLU:HG3	1:E:599:ARG:HB2	1.94	0.49
1:A:556:GLU:HG3	1:A:599:ARG:HB2	1.94	0.49
1:B:524:LYS:HG2	1:B:645:ILE:HG13	1.93	0.49
1:B:556:GLU:HG3	1:B:599:ARG:HB2	1.94	0.49
1:C:23:PRO:HB2	1:C:49:LEU:HD21	1.93	0.49
1:B:121:ASP:OD1	1:B:122:THR:N	2.47	0.48
1:B:626:PRO:HB2	1:B:758:PHE:CZ	2.49	0.48
1:A:121:ASP:OD1	1:A:122:THR:N	2.47	0.48
1:F:333:ASP:OD2	1:F:362:ARG:NH2	2.44	0.48
1:A:626:PRO:HB2	1:A:758:PHE:CZ	2.49	0.48
1:C:626:PRO:HB2	1:C:758:PHE:CZ	2.48	0.48
1:E:362:ARG:O	1:E:364:ASP:N	2.47	0.48
1:F:362:ARG:O	1:F:364:ASP:N	2.47	0.48
1:F:626:PRO:HB2	1:F:758:PHE:CZ	2.48	0.48
1:C:212:GLN:HG2	1:C:369:ILE:HD13	1.96	0.48
1:D:556:GLU:HG3	1:D:599:ARG:HB2	1.94	0.48
1:E:626:PRO:HB2	1:E:758:PHE:CZ	2.49	0.48
1:D:362:ARG:O	1:D:364:ASP:N	2.47	0.48
1:F:121:ASP:OD1	1:F:122:THR:N	2.47	0.48
1:B:212:GLN:HG2	1:B:369:ILE:HD13	1.96	0.48
1:C:112:LYS:N	1:C:169:ASP:O	2.37	0.48
1:A:362:ARG:O	1:A:364:ASP:N	2.47	0.47
1:B:333:ASP:OD2	1:B:362:ARG:NH2	2.44	0.47
1:C:519:PRO:HG2	1:C:522:CYS:SG	2.54	0.47
1:F:519:PRO:HG2	1:F:522:CYS:SG	2.54	0.47
1:A:601:ILE:HD13	1:A:604:ILE:HD12	1.96	0.47
1:C:121:ASP:OD1	1:C:122:THR:N	2.47	0.47
1:D:626:PRO:HB2	1:D:758:PHE:CZ	2.49	0.47
1:E:121:ASP:OD1	1:E:122:THR:N	2.46	0.47
1:C:359:ARG:NH1	1:D:348:ASN:HD21	2.12	0.47
1:C:362:ARG:O	1:C:364:ASP:N	2.47	0.47
1:D:66:GLU:OE1	1:D:173:TYR:OH	2.33	0.47
1:D:519:PRO:HG2	1:D:522:CYS:SG	2.54	0.47
1:A:212:GLN:HG2	1:A:369:ILE:HD13	1.96	0.47
1:A:333:ASP:OD2	1:A:362:ARG:NH2	2.44	0.47
1:A:519:PRO:HG2	1:A:522:CYS:SG	2.54	0.47
1:C:310:ALA:HA	1:C:325:VAL:HG22	1.96	0.47
1:F:212:GLN:HG2	1:F:369:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LYS:HD3	1:A:45:LYS:HA	1.73	0.47
1:B:362:ARG:O	1:B:364:ASP:N	2.47	0.47
1:D:242:LEU:HD11	1:D:347:THR:HG22	1.97	0.47
1:E:26:LEU:HD13	1:E:82:ILE:HB	1.97	0.47
1:E:242:LEU:HD11	1:E:347:THR:HG22	1.97	0.47
1:A:310:ALA:HA	1:A:325:VAL:HG22	1.96	0.47
1:B:66:GLU:OE1	1:B:173:TYR:OH	2.33	0.47
1:C:601:ILE:HD13	1:C:604:ILE:HD12	1.96	0.47
1:D:310:ALA:HA	1:D:325:VAL:HG22	1.96	0.47
1:F:66:GLU:OE1	1:F:173:TYR:OH	2.33	0.47
1:A:66:GLU:OE1	1:A:173:TYR:OH	2.33	0.47
1:B:519:PRO:HG2	1:B:522:CYS:SG	2.54	0.47
1:D:26:LEU:HD13	1:D:82:ILE:HB	1.97	0.47
1:D:212:GLN:HG2	1:D:369:ILE:HD13	1.96	0.47
1:D:601:ILE:HD13	1:D:604:ILE:HD12	1.96	0.47
1:E:114:ILE:HD11	1:E:182:ILE:HG12	1.96	0.47
1:E:212:GLN:HG2	1:E:369:ILE:HD13	1.96	0.47
1:E:333:ASP:OD2	1:E:362:ARG:NH2	2.45	0.47
1:E:519:PRO:HG2	1:E:522:CYS:SG	2.54	0.47
1:F:310:ALA:HA	1:F:325:VAL:HG22	1.96	0.47
1:C:26:LEU:HD13	1:C:82:ILE:HB	1.97	0.47
1:C:242:LEU:HD11	1:C:347:THR:HG22	1.97	0.47
1:C:556:GLU:H	1:C:556:GLU:CD	2.17	0.47
1:D:121:ASP:OD1	1:D:122:THR:N	2.46	0.47
1:F:114:ILE:HD11	1:F:182:ILE:HG12	1.96	0.47
1:A:489:LEU:HD11	1:A:516:PHE:CZ	2.50	0.47
1:B:601:ILE:HD13	1:B:604:ILE:HD12	1.96	0.47
1:C:114:ILE:HD11	1:C:182:ILE:HG12	1.96	0.47
1:D:556:GLU:H	1:D:556:GLU:CD	2.17	0.47
1:F:26:LEU:HD13	1:F:82:ILE:HB	1.97	0.47
1:B:489:LEU:HD11	1:B:516:PHE:CZ	2.50	0.47
1:F:601:ILE:HD13	1:F:604:ILE:HD12	1.96	0.47
1:B:26:LEU:HD13	1:B:82:ILE:HB	1.97	0.46
1:D:638:ARG:O	1:D:640:ASP:N	2.49	0.46
1:E:60:LYS:HG2	1:E:66:GLU:HG2	1.97	0.46
1:E:638:ARG:O	1:E:640:ASP:N	2.49	0.46
1:F:60:LYS:HG2	1:F:66:GLU:HG2	1.98	0.46
1:B:114:ILE:HD11	1:B:182:ILE:HG12	1.96	0.46
1:D:60:LYS:HG2	1:D:66:GLU:HG2	1.98	0.46
1:F:242:LEU:HD11	1:F:347:THR:HG22	1.97	0.46
1:F:489:LEU:HD11	1:F:516:PHE:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ILE:HD11	1:A:182:ILE:HG12	1.96	0.46
1:A:359:ARG:NH1	1:B:348:ASN:HD21	2.13	0.46
1:C:638:ARG:O	1:C:640:ASP:N	2.49	0.46
1:F:638:ARG:O	1:F:640:ASP:N	2.48	0.46
1:A:26:LEU:HD13	1:A:82:ILE:HB	1.97	0.46
1:B:84:MET:O	1:B:89:ARG:NH1	2.49	0.46
1:B:310:ALA:HA	1:B:325:VAL:HG22	1.96	0.46
1:C:489:LEU:HD11	1:C:516:PHE:CZ	2.50	0.46
1:E:66:GLU:OE1	1:E:173:TYR:OH	2.33	0.46
1:E:489:LEU:HD11	1:E:516:PHE:CZ	2.50	0.46
1:A:84:MET:O	1:A:89:ARG:NH1	2.49	0.46
1:C:66:GLU:OE1	1:C:173:TYR:OH	2.33	0.46
1:E:310:ALA:HA	1:E:325:VAL:HG22	1.96	0.46
1:E:359:ARG:NH1	1:F:348:ASN:HD21	2.13	0.46
1:E:409:ALA:HB2	2:E:901:ATP:H5'2	1.98	0.46
1:A:242:LEU:HD11	1:A:347:THR:HG22	1.97	0.46
1:E:601:ILE:HD13	1:E:604:ILE:HD12	1.96	0.46
1:B:556:GLU:H	1:B:556:GLU:CD	2.17	0.46
1:C:84:MET:O	1:C:89:ARG:NH1	2.49	0.46
1:C:333:ASP:OD2	1:C:362:ARG:NH2	2.44	0.46
1:D:489:LEU:HD11	1:D:516:PHE:CZ	2.50	0.46
1:A:377:ARG:HD3	1:A:403:THR:OG1	2.16	0.46
1:A:409:ALA:HB2	2:A:901:ATP:H5'2	1.98	0.46
1:B:638:ARG:O	1:B:640:ASP:N	2.48	0.46
1:D:114:ILE:HD11	1:D:182:ILE:HG12	1.96	0.46
1:E:84:MET:O	1:E:89:ARG:NH1	2.49	0.46
1:F:377:ARG:HD3	1:F:403:THR:OG1	2.16	0.46
1:B:237:PRO:O	1:B:337:GLN:NE2	2.37	0.45
1:B:377:ARG:HD3	1:B:403:THR:OG1	2.16	0.45
1:B:409:ALA:HB2	2:B:901:ATP:H5'2	1.98	0.45
1:C:336:LYS:HE2	1:C:336:LYS:HB2	1.39	0.45
1:D:84:MET:O	1:D:89:ARG:NH1	2.49	0.45
1:D:333:ASP:OD2	1:D:362:ARG:NH2	2.44	0.45
1:B:242:LEU:HD11	1:B:347:THR:HG22	1.97	0.45
1:C:60:LYS:HG2	1:C:66:GLU:HG2	1.97	0.45
1:E:556:GLU:H	1:E:556:GLU:CD	2.17	0.45
1:B:359:ARG:NH1	1:C:348:ASN:HD21	2.14	0.45
1:F:84:MET:O	1:F:89:ARG:NH1	2.49	0.45
1:A:60:LYS:HG2	1:A:66:GLU:HG2	1.98	0.45
1:A:638:ARG:O	1:A:640:ASP:N	2.48	0.45
1:C:85:ASN:O	1:C:89:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:ILE:HG23	1:C:235:VAL:HG22	1.99	0.45
1:F:85:ASN:O	1:F:89:ARG:HG3	2.17	0.45
1:A:233:ILE:HG23	1:A:235:VAL:HG22	1.99	0.45
1:C:409:ALA:HB2	2:C:901:ATP:H5'2	1.98	0.45
1:A:754:LYS:HE3	1:A:754:LYS:HB3	1.86	0.45
1:B:60:LYS:HG2	1:B:66:GLU:HG2	1.98	0.45
1:B:233:ILE:HG23	1:B:235:VAL:HG22	1.99	0.45
1:D:24:ASN:ND2	1:D:102:ILE:O	2.50	0.45
1:A:24:ASN:ND2	1:A:102:ILE:O	2.50	0.45
1:C:377:ARG:HD3	1:C:403:THR:OG1	2.17	0.45
1:A:85:ASN:O	1:A:89:ARG:HG3	2.17	0.45
1:B:24:ASN:ND2	1:B:102:ILE:O	2.50	0.45
1:B:85:ASN:O	1:B:89:ARG:HG3	2.17	0.45
1:D:85:ASN:O	1:D:89:ARG:HG3	2.17	0.45
1:D:377:ARG:HD3	1:D:403:THR:OG1	2.16	0.45
1:D:409:ALA:HB2	2:D:901:ATP:H5'2	1.97	0.45
1:B:705:SER:OG	1:B:708:ARG:NH2	2.50	0.44
1:C:705:SER:OG	1:C:708:ARG:NH2	2.50	0.44
1:E:24:ASN:ND2	1:E:102:ILE:O	2.50	0.44
1:F:754:LYS:HE3	1:F:754:LYS:HB3	1.85	0.44
1:D:233:ILE:HG23	1:D:235:VAL:HG22	1.99	0.44
1:E:168:THR:O	1:E:171:SER:OG	2.35	0.44
1:E:85:ASN:O	1:E:89:ARG:HG3	2.17	0.44
1:C:168:THR:O	1:C:171:SER:OG	2.35	0.44
1:F:24:ASN:ND2	1:F:102:ILE:O	2.50	0.44
2:A:901:ATP:H5'1	2:A:901:ATP:H8	1.83	0.44
1:C:24:ASN:ND2	1:C:102:ILE:O	2.50	0.44
1:E:377:ARG:HD3	1:E:403:THR:OG1	2.17	0.44
1:F:409:ALA:HB2	2:F:901:ATP:H5'2	1.98	0.44
1:F:705:SER:OG	1:F:708:ARG:NH2	2.50	0.44
1:A:168:THR:O	1:A:171:SER:OG	2.35	0.44
1:A:705:SER:OG	1:A:708:ARG:NH2	2.50	0.44
1:D:705:SER:OG	1:D:708:ARG:NH2	2.50	0.44
1:E:427:MET:HA	1:E:427:MET:CE	2.48	0.44
1:F:45:LYS:HA	1:F:45:LYS:HD3	1.73	0.44
1:A:427:MET:HA	1:A:427:MET:CE	2.48	0.44
1:A:556:GLU:H	1:A:556:GLU:CD	2.17	0.44
1:B:225:ARG:HA	1:B:225:ARG:NE	2.33	0.44
1:F:233:ILE:HG23	1:F:235:VAL:HG22	1.99	0.44
1:F:237:PRO:O	1:F:337:GLN:NE2	2.37	0.44
1:A:336:LYS:HE2	1:A:336:LYS:HB2	1.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:705:SER:OG	1:E:708:ARG:NH2	2.50	0.44
2:B:901:ATP:H5'1	2:B:901:ATP:H8	1.83	0.43
1:C:753:ARG:O	1:C:757:MET:SD	2.76	0.43
2:C:901:ATP:H5'1	2:C:901:ATP:H8	1.83	0.43
1:F:427:MET:HA	1:F:427:MET:CE	2.48	0.43
1:F:738:GLU:O	1:F:741:ARG:HB2	2.18	0.43
2:F:901:ATP:H5'1	2:F:901:ATP:C8	2.53	0.43
1:A:237:PRO:O	1:A:337:GLN:NE2	2.37	0.43
1:A:738:GLU:O	1:A:741:ARG:HB2	2.18	0.43
1:A:753:ARG:O	1:A:757:MET:SD	2.76	0.43
1:B:274:ILE:HG23	1:B:282:SER:HB3	2.00	0.43
1:B:753:ARG:O	1:B:757:MET:SD	2.76	0.43
1:D:753:ARG:O	1:D:757:MET:SD	2.76	0.43
2:D:901:ATP:H5'1	2:D:901:ATP:H8	1.83	0.43
1:E:753:ARG:O	1:E:757:MET:SD	2.76	0.43
1:F:168:THR:O	1:F:171:SER:OG	2.35	0.43
1:F:271:GLY:HA3	1:F:308:ALA:HB3	2.00	0.43
1:F:749:ASP:HA	1:F:752:ILE:HD12	2.01	0.43
2:F:901:ATP:H5'1	2:F:901:ATP:H8	1.83	0.43
1:A:749:ASP:HA	1:A:752:ILE:HD12	2.00	0.43
1:B:271:GLY:HA3	1:B:308:ALA:HB3	2.00	0.43
1:C:271:GLY:HA3	1:C:308:ALA:HB3	2.00	0.43
1:C:274:ILE:HG23	1:C:282:SER:HB3	2.00	0.43
1:D:271:GLY:HA3	1:D:308:ALA:HB3	2.00	0.43
1:E:233:ILE:HG23	1:E:235:VAL:HG22	1.99	0.43
1:E:749:ASP:HA	1:E:752:ILE:HD12	2.01	0.43
1:A:221:GLU:HG3	1:A:225:ARG:HG2	2.00	0.43
1:B:168:THR:O	1:B:171:SER:OG	2.35	0.43
1:B:472:PRO:O	1:B:533:ASN:ND2	2.37	0.43
2:E:901:ATP:C8	2:E:901:ATP:H5'1	2.53	0.43
2:E:901:ATP:H5'1	2:E:901:ATP:H8	1.83	0.43
1:B:221:GLU:HG3	1:B:225:ARG:HG2	2.00	0.43
1:F:753:ARG:O	1:F:757:MET:SD	2.76	0.43
1:B:427:MET:CE	1:B:427:MET:HA	2.48	0.43
1:C:225:ARG:HA	1:C:225:ARG:NE	2.33	0.43
1:D:221:GLU:HG3	1:D:225:ARG:HG2	2.00	0.43
1:D:225:ARG:HA	1:D:225:ARG:NE	2.33	0.43
1:B:116:VAL:HG12	1:B:165:VAL:HA	2.01	0.43
1:D:108:VAL:HG12	1:D:175:ILE:HG12	2.01	0.43
1:D:650:GLU:O	1:D:654:VAL:HG23	2.19	0.43
2:D:901:ATP:H5'1	2:D:901:ATP:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:VAL:HG12	1:C:175:ILE:HG12	2.01	0.43
1:D:738:GLU:O	1:D:741:ARG:HB2	2.18	0.43
1:E:274:ILE:HG23	1:E:282:SER:HB3	2.00	0.43
1:F:556:GLU:H	1:F:556:GLU:CD	2.17	0.43
1:B:108:VAL:HG12	1:B:175:ILE:HG12	2.01	0.43
1:B:153:LEU:HD13	1:B:162:GLU:HG3	2.01	0.43
1:C:221:GLU:HG3	1:C:225:ARG:HG2	2.00	0.43
1:D:749:ASP:HA	1:D:752:ILE:HD12	2.01	0.43
1:E:45:LYS:HA	1:E:45:LYS:HD3	1.73	0.43
1:B:45:LYS:HA	1:B:45:LYS:HD3	1.73	0.43
2:B:901:ATP:H5'1	2:B:901:ATP:C8	2.54	0.43
1:C:650:GLU:O	1:C:654:VAL:HG23	2.19	0.43
2:C:901:ATP:H5'1	2:C:901:ATP:C8	2.54	0.43
1:D:121:ASP:OD2	1:D:191:ARG:HD2	2.19	0.43
1:D:472:PRO:O	1:D:533:ASN:ND2	2.37	0.43
1:F:650:GLU:O	1:F:654:VAL:HG23	2.19	0.43
1:B:122:THR:HG21	1:B:162:GLU:HB2	2.02	0.42
1:C:116:VAL:HG12	1:C:165:VAL:HA	2.01	0.42
1:D:274:ILE:HG23	1:D:282:SER:HB3	2.00	0.42
1:E:108:VAL:HG12	1:E:175:ILE:HG12	2.01	0.42
1:E:221:GLU:HG3	1:E:225:ARG:HG2	2.00	0.42
1:F:614:LYS:HE3	1:F:616:ASN:OD1	2.20	0.42
1:A:122:THR:HG21	1:A:162:GLU:HB2	2.01	0.42
1:B:336:LYS:HB2	1:B:336:LYS:HE2	1.39	0.42
1:B:614:LYS:HE3	1:B:616:ASN:OD1	2.19	0.42
1:B:738:GLU:O	1:B:741:ARG:HB2	2.18	0.42
1:C:153:LEU:HD13	1:C:162:GLU:HG3	2.01	0.42
1:D:153:LEU:HD13	1:D:162:GLU:HG3	2.01	0.42
1:E:153:LEU:HD13	1:E:162:GLU:HG3	2.01	0.42
1:B:650:GLU:O	1:B:654:VAL:HG23	2.19	0.42
1:C:121:ASP:OD2	1:C:191:ARG:HD2	2.19	0.42
1:C:749:ASP:HA	1:C:752:ILE:HD12	2.01	0.42
1:D:168:THR:O	1:D:171:SER:OG	2.35	0.42
1:E:121:ASP:OD2	1:E:191:ARG:HD2	2.19	0.42
1:E:271:GLY:HA3	1:E:308:ALA:HB3	2.00	0.42
1:E:738:GLU:O	1:E:741:ARG:HB2	2.18	0.42
1:A:153:LEU:HD13	1:A:162:GLU:HG3	2.01	0.42
1:C:427:MET:HA	1:C:427:MET:CE	2.48	0.42
1:C:738:GLU:O	1:C:741:ARG:HB2	2.18	0.42
1:D:427:MET:HA	1:D:427:MET:CE	2.48	0.42
1:E:225:ARG:HA	1:E:225:ARG:NE	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:614:LYS:HE3	1:E:616:ASN:OD1	2.20	0.42
1:E:650:GLU:O	1:E:654:VAL:HG23	2.19	0.42
1:F:116:VAL:HG12	1:F:165:VAL:HA	2.01	0.42
1:F:122:THR:HG21	1:F:162:GLU:HB2	2.01	0.42
1:A:108:VAL:HG12	1:A:175:ILE:HG12	2.01	0.42
1:A:476:TRP:CZ3	1:A:486:LYS:HG2	2.55	0.42
1:A:650:GLU:O	1:A:654:VAL:HG23	2.19	0.42
2:A:901:ATP:H5'1	2:A:901:ATP:C8	2.53	0.42
1:B:121:ASP:OD2	1:B:191:ARG:HD2	2.19	0.42
1:C:41:LEU:HD23	1:C:45:LYS:HG3	2.02	0.42
1:F:108:VAL:HG12	1:F:175:ILE:HG12	2.01	0.42
1:F:225:ARG:HA	1:F:225:ARG:NE	2.33	0.42
1:F:274:ILE:HG23	1:F:282:SER:HB3	2.00	0.42
1:A:271:GLY:HA3	1:A:308:ALA:HB3	2.00	0.42
1:A:614:LYS:HE3	1:A:616:ASN:OD1	2.19	0.42
1:B:749:ASP:HA	1:B:752:ILE:HD12	2.01	0.42
1:D:116:VAL:HG12	1:D:165:VAL:HA	2.01	0.42
1:E:116:VAL:HG12	1:E:165:VAL:HA	2.01	0.42
1:F:153:LEU:HD13	1:F:162:GLU:HG3	2.01	0.42
1:F:221:GLU:HG3	1:F:225:ARG:HG2	2.00	0.42
1:D:614:LYS:HE3	1:D:616:ASN:OD1	2.20	0.42
1:E:41:LEU:HD23	1:E:45:LYS:HG3	2.02	0.42
1:B:476:TRP:CZ3	1:B:486:LYS:HG2	2.55	0.42
1:C:614:LYS:HE3	1:C:616:ASN:OD1	2.19	0.42
1:D:41:LEU:HD23	1:D:45:LYS:HG3	2.02	0.42
1:E:122:THR:HG21	1:E:162:GLU:HB2	2.02	0.42
1:B:41:LEU:HD23	1:B:45:LYS:HG3	2.02	0.42
1:C:122:THR:HG21	1:C:162:GLU:HB2	2.02	0.42
1:F:41:LEU:HD23	1:F:45:LYS:HG3	2.02	0.42
1:F:476:TRP:CZ3	1:F:486:LYS:HG2	2.55	0.42
1:A:41:LEU:HD23	1:A:45:LYS:HG3	2.02	0.41
1:A:461:PRO:HB2	1:A:464:LEU:HG	2.02	0.41
1:D:213:LEU:HD23	1:D:213:LEU:HA	1.91	0.41
1:E:670:VAL:HG22	1:E:733:ARG:HG2	2.03	0.41
1:F:121:ASP:OD2	1:F:191:ARG:HD2	2.19	0.41
1:F:396:LEU:HD23	1:F:396:LEU:HA	1.92	0.41
1:A:34:GLU:HG3	1:A:38:VAL:HG23	2.03	0.41
1:A:274:ILE:HG23	1:A:282:SER:HB3	2.01	0.41
1:C:670:VAL:HG22	1:C:733:ARG:HG2	2.02	0.41
1:E:476:TRP:CZ3	1:E:486:LYS:HG2	2.55	0.41
1:F:34:GLU:HG3	1:F:38:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LYS:HB2	1:A:101:SER:OG	2.20	0.41
1:A:116:VAL:HG12	1:A:165:VAL:HA	2.01	0.41
1:A:670:VAL:HG22	1:A:733:ARG:HG2	2.02	0.41
1:A:690:ILE:HG12	1:A:743:ALA:HB2	2.03	0.41
1:B:670:VAL:HG22	1:B:733:ARG:HG2	2.03	0.41
1:C:476:TRP:CZ3	1:C:486:LYS:HG2	2.55	0.41
1:C:677:LYS:HE2	1:C:677:LYS:HB2	1.96	0.41
1:D:122:THR:HG21	1:D:162:GLU:HB2	2.01	0.41
1:F:60:LYS:HB2	1:F:101:SER:OG	2.20	0.41
1:F:461:PRO:HB2	1:F:464:LEU:HG	2.02	0.41
1:B:34:GLU:HG3	1:B:38:VAL:HG23	2.03	0.41
1:B:690:ILE:HG12	1:B:743:ALA:HB2	2.03	0.41
1:D:237:PRO:O	1:D:337:GLN:NE2	2.37	0.41
1:F:670:VAL:HG22	1:F:733:ARG:HG2	2.03	0.41
1:A:115:HIS:HB3	1:A:167:GLU:HB3	2.02	0.41
1:E:34:GLU:HG3	1:E:38:VAL:HG23	2.03	0.41
1:E:237:PRO:HA	1:E:238:PRO:HD2	1.97	0.41
1:A:121:ASP:OD2	1:A:191:ARG:HD2	2.19	0.41
1:E:60:LYS:HB2	1:E:101:SER:OG	2.20	0.41
1:A:693:ARG:HD2	1:A:739:ALA:HA	2.03	0.41
1:B:60:LYS:HB2	1:B:101:SER:OG	2.20	0.41
1:B:461:PRO:HB2	1:B:464:LEU:HG	2.02	0.41
1:B:489:LEU:HD11	1:B:516:PHE:HZ	1.86	0.41
1:B:693:ARG:HD2	1:B:739:ALA:HA	2.03	0.41
1:D:670:VAL:HG22	1:D:733:ARG:HG2	2.02	0.41
1:D:754:LYS:HE3	1:D:754:LYS:HB3	1.85	0.41
1:F:472:PRO:O	1:F:533:ASN:ND2	2.37	0.41
1:C:693:ARG:HD2	1:C:739:ALA:HA	2.03	0.41
1:D:693:ARG:HD2	1:D:739:ALA:HA	2.03	0.41
1:F:115:HIS:HB3	1:F:167:GLU:HB3	2.02	0.41
1:F:693:ARG:HD2	1:F:739:ALA:HA	2.03	0.41
1:A:225:ARG:HA	1:A:225:ARG:NE	2.33	0.41
1:B:526:LEU:HD11	2:B:902:ATP:H2'	2.03	0.41
1:C:489:LEU:HD11	1:C:516:PHE:HZ	1.86	0.41
1:C:690:ILE:HG12	1:C:743:ALA:HB2	2.03	0.41
1:D:34:GLU:HG3	1:D:38:VAL:HG23	2.03	0.41
1:D:237:PRO:HA	1:D:238:PRO:HD2	1.97	0.41
1:D:270:ASN:HB2	1:D:273:GLU:CB	2.51	0.41
1:D:281:GLU:HG2	1:D:285:ASN:ND2	2.36	0.41
1:D:476:TRP:CZ3	1:D:486:LYS:HG2	2.55	0.41
1:E:461:PRO:HB2	1:E:464:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:690:ILE:HG12	1:E:743:ALA:HB2	2.03	0.41
1:E:693:ARG:HD2	1:E:739:ALA:HA	2.03	0.41
1:F:321:GLU:O	1:F:325:VAL:HG23	2.21	0.41
1:B:115:HIS:HB3	1:B:167:GLU:HB3	2.02	0.41
1:C:60:LYS:HB2	1:C:101:SER:OG	2.20	0.41
1:D:36:ASN:HA	1:D:85:ASN:HD21	1.86	0.41
1:D:115:HIS:HB3	1:D:167:GLU:HB3	2.02	0.41
1:C:321:GLU:O	1:C:325:VAL:HG23	2.21	0.40
1:C:469:VAL:HG22	1:C:540:ILE:HG12	2.04	0.40
1:E:469:VAL:HG22	1:E:540:ILE:HG12	2.03	0.40
1:A:155:ARG:HA	1:A:155:ARG:HD3	1.94	0.40
1:A:489:LEU:HD11	1:A:516:PHE:HZ	1.86	0.40
1:B:469:VAL:HG22	1:B:540:ILE:HG12	2.03	0.40
1:C:34:GLU:HG3	1:C:38:VAL:HG23	2.03	0.40
1:D:60:LYS:HB2	1:D:101:SER:OG	2.20	0.40
1:D:469:VAL:HG22	1:D:540:ILE:HG12	2.04	0.40
1:D:690:ILE:HG12	1:D:743:ALA:HB2	2.03	0.40
1:E:281:GLU:HG2	1:E:285:ASN:ND2	2.36	0.40
1:E:321:GLU:O	1:E:325:VAL:HG23	2.21	0.40
1:A:321:GLU:O	1:A:325:VAL:HG23	2.21	0.40
1:A:281:GLU:HG2	1:A:285:ASN:ND2	2.36	0.40
1:F:469:VAL:HG22	1:F:540:ILE:HG12	2.04	0.40
1:A:244:TYR:HA	1:A:347:THR:O	2.22	0.40
1:A:274:ILE:O	1:A:282:SER:OG	2.32	0.40
1:A:469:VAL:HG22	1:A:540:ILE:HG12	2.03	0.40
1:B:321:GLU:O	1:B:325:VAL:HG23	2.21	0.40
1:C:281:GLU:HG2	1:C:285:ASN:ND2	2.36	0.40
1:C:461:PRO:HB2	1:C:464:LEU:HG	2.02	0.40
1:E:36:ASN:HA	1:E:85:ASN:HD21	1.86	0.40
1:E:771:PHE:HE1	1:F:678:MET:HG3	1.86	0.40
1:F:43:GLN:HA	1:F:46:MET:HE2	2.03	0.40
1:F:690:ILE:HG12	1:F:743:ALA:HB2	2.03	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	739/806 (92%)	719 (97%)	20 (3%)	0	100	100
1	B	739/806 (92%)	719 (97%)	20 (3%)	0	100	100
1	C	739/806 (92%)	719 (97%)	20 (3%)	0	100	100
1	D	739/806 (92%)	719 (97%)	20 (3%)	0	100	100
1	E	739/806 (92%)	719 (97%)	20 (3%)	0	100	100
1	F	739/806 (92%)	719 (97%)	20 (3%)	0	100	100
All	All	4434/4836 (92%)	4314 (97%)	120 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	634/679 (93%)	624 (98%)	10 (2%)	62	79
1	B	634/679 (93%)	624 (98%)	10 (2%)	62	79
1	C	634/679 (93%)	624 (98%)	10 (2%)	62	79
1	D	634/679 (93%)	624 (98%)	10 (2%)	62	79
1	E	634/679 (93%)	624 (98%)	10 (2%)	62	79
1	F	634/679 (93%)	624 (98%)	10 (2%)	62	79
All	All	3804/4074 (93%)	3744 (98%)	60 (2%)	64	79

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	MET
1	A	211	LYS
1	A	225	ARG

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Mol	Chain	Res	Type
1	A	319	GLU
1	A	336	LYS
1	A	338	ARG
1	A	427	MET
1	A	477	GLU
1	A	711	ARG
1	A	741	ARG
1	B	158	MET
1	B	211	LYS
1	B	225	ARG
1	B	319	GLU
1	B	336	LYS
1	B	338	ARG
1	B	427	MET
1	B	477	GLU
1	B	711	ARG
1	B	741	ARG
1	C	158	MET
1	C	211	LYS
1	C	225	ARG
1	C	319	GLU
1	C	336	LYS
1	C	338	ARG
1	C	427	MET
1	C	477	GLU
1	C	711	ARG
1	C	741	ARG
1	D	158	MET
1	D	211	LYS
1	D	225	ARG
1	D	319	GLU
1	D	336	LYS
1	D	338	ARG
1	D	427	MET
1	D	477	GLU
1	D	711	ARG
1	D	741	ARG
1	E	158	MET
1	E	211	LYS
1	E	225	ARG
1	E	319	GLU
1	E	336	LYS

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Mol	Chain	Res	Type
1	E	338	ARG
1	E	427	MET
1	E	477	GLU
1	E	711	ARG
1	E	741	ARG
1	F	158	MET
1	F	211	LYS
1	F	225	ARG
1	F	319	GLU
1	F	336	LYS
1	F	338	ARG
1	F	427	MET
1	F	477	GLU
1	F	711	ARG
1	F	741	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	ASN
1	E	348	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)

Of 30 ligands modelled in this entry, 12 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ATP	E	901	4	26,33,33	0.64	0	31,52,52	0.77	2 (6%)
2	ATP	F	901	4	26,33,33	0.63	0	31,52,52	0.77	2 (6%)
3	Y6Y	B	903	-	37,40,40	3.19	6 (16%)	41,57,57	1.52	6 (14%)
2	ATP	C	901	4	26,33,33	0.64	0	31,52,52	0.77	2 (6%)
2	ATP	C	902	4	26,33,33	0.61	0	31,52,52	0.75	2 (6%)
2	ATP	F	902	4	26,33,33	0.61	0	31,52,52	0.75	2 (6%)
2	ATP	D	901	4	26,33,33	0.65	0	31,52,52	0.77	2 (6%)
2	ATP	E	902	4	26,33,33	0.62	0	31,52,52	0.75	2 (6%)
2	ATP	A	902	4	26,33,33	0.61	0	31,52,52	0.75	2 (6%)
2	ATP	B	902	4	26,33,33	0.62	0	31,52,52	0.74	2 (6%)
3	Y6Y	D	903	-	37,40,40	3.18	6 (16%)	41,57,57	1.52	6 (14%)
3	Y6Y	C	903	-	37,40,40	3.18	6 (16%)	41,57,57	1.52	6 (14%)
3	Y6Y	E	903	-	37,40,40	3.18	6 (16%)	41,57,57	1.52	6 (14%)
2	ATP	D	902	4	26,33,33	0.61	0	31,52,52	0.75	2 (6%)
2	ATP	B	901	4	26,33,33	0.64	0	31,52,52	0.78	2 (6%)
3	Y6Y	A	903	-	37,40,40	3.19	6 (16%)	41,57,57	1.52	6 (14%)
3	Y6Y	F	903	-	37,40,40	3.18	6 (16%)	41,57,57	1.52	6 (14%)
2	ATP	A	901	4	26,33,33	0.64	0	31,52,52	0.77	2 (6%)

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
2	ATP	E	901	4	-	5/18/38/38	0/3/3/3
2	ATP	F	901	4	-	5/18/38/38	0/3/3/3
3	Y6Y	B	903	-	-	4/19/30/30	0/5/5/5
2	ATP	C	901	4	-	5/18/38/38	0/3/3/3
2	ATP	C	902	4	-	6/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	F	902	4	-	6/18/38/38	0/3/3/3
2	ATP	D	901	4	-	5/18/38/38	0/3/3/3
2	ATP	E	902	4	-	6/18/38/38	0/3/3/3
2	ATP	A	902	4	-	6/18/38/38	0/3/3/3
2	ATP	B	902	4	-	6/18/38/38	0/3/3/3
3	Y6Y	D	903	-	-	4/19/30/30	0/5/5/5
3	Y6Y	C	903	-	-	4/19/30/30	0/5/5/5
3	Y6Y	E	903	-	-	4/19/30/30	0/5/5/5
2	ATP	D	902	4	-	6/18/38/38	0/3/3/3
2	ATP	B	901	4	-	5/18/38/38	0/3/3/3
3	Y6Y	A	903	-	-	4/19/30/30	0/5/5/5
3	Y6Y	F	903	-	-	4/19/30/30	0/5/5/5
2	ATP	A	901	4	-	4/18/38/38	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	903	Y6Y	C10-S	-16.10	1.59	1.77
3	B	903	Y6Y	C10-S	-16.08	1.59	1.77
3	F	903	Y6Y	C10-S	-16.03	1.59	1.77
3	D	903	Y6Y	C10-S	-16.01	1.59	1.77
3	E	903	Y6Y	C10-S	-15.99	1.59	1.77
3	C	903	Y6Y	C10-S	-15.98	1.59	1.77
3	B	903	Y6Y	C22-N2	-8.74	1.34	1.46
3	E	903	Y6Y	C22-N2	-8.68	1.34	1.46
3	D	903	Y6Y	C22-N2	-8.68	1.34	1.46
3	A	903	Y6Y	C22-N2	-8.67	1.34	1.46
3	C	903	Y6Y	C22-N2	-8.67	1.34	1.46
3	F	903	Y6Y	C22-N2	-8.63	1.34	1.46
3	A	903	Y6Y	C6-C1	4.75	1.49	1.40
3	D	903	Y6Y	C6-C1	4.75	1.49	1.40
3	E	903	Y6Y	C6-C1	4.74	1.49	1.40
3	F	903	Y6Y	C6-C1	4.74	1.49	1.40
3	C	903	Y6Y	C6-C1	4.73	1.49	1.40
3	B	903	Y6Y	C6-C1	4.72	1.49	1.40
3	D	903	Y6Y	N-N1	2.27	1.42	1.37
3	F	903	Y6Y	N-N1	2.26	1.42	1.37
3	E	903	Y6Y	N-N1	2.24	1.42	1.37
3	A	903	Y6Y	N-N1	2.23	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	903	Y6Y	N-N1	2.22	1.42	1.37
3	C	903	Y6Y	N-N1	2.21	1.41	1.37
3	D	903	Y6Y	C13-S	-2.18	1.66	1.75
3	E	903	Y6Y	C13-S	-2.17	1.66	1.75
3	F	903	Y6Y	C13-S	-2.17	1.66	1.75
3	C	903	Y6Y	C13-S	-2.16	1.66	1.75
3	A	903	Y6Y	C13-S	-2.16	1.66	1.75
3	B	903	Y6Y	C13-S	-2.14	1.66	1.75
3	A	903	Y6Y	C15-N2	-2.13	1.33	1.37
3	F	903	Y6Y	C15-N2	-2.12	1.33	1.37
3	D	903	Y6Y	C15-N2	-2.08	1.34	1.37
3	E	903	Y6Y	C15-N2	-2.08	1.34	1.37
3	C	903	Y6Y	C15-N2	-2.06	1.34	1.37
3	B	903	Y6Y	C15-N2	-2.04	1.34	1.37

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	903	Y6Y	O1-S-O	-5.12	109.10	117.92
3	F	903	Y6Y	O1-S-O	-5.12	109.10	117.92
3	D	903	Y6Y	O1-S-O	-5.12	109.10	117.92
3	A	903	Y6Y	O1-S-O	-5.11	109.11	117.92
3	B	903	Y6Y	O1-S-O	-5.10	109.13	117.92
3	C	903	Y6Y	O1-S-O	-5.10	109.14	117.92
3	F	903	Y6Y	C13-S-C10	4.20	109.55	104.58
3	D	903	Y6Y	C13-S-C10	4.19	109.53	104.58
3	B	903	Y6Y	C13-S-C10	4.19	109.53	104.58
3	E	903	Y6Y	C13-S-C10	4.19	109.53	104.58
3	A	903	Y6Y	C13-S-C10	4.17	109.51	104.58
3	C	903	Y6Y	C13-S-C10	4.17	109.50	104.58
3	E	903	Y6Y	C26-C22-N2	2.97	123.35	119.19
3	B	903	Y6Y	C26-C22-N2	2.97	123.34	119.19
3	A	903	Y6Y	C26-C22-N2	2.96	123.34	119.19
3	D	903	Y6Y	C26-C22-N2	2.96	123.33	119.19
3	C	903	Y6Y	C26-C22-N2	2.95	123.31	119.19
3	F	903	Y6Y	C26-C22-N2	2.93	123.30	119.19
3	B	903	Y6Y	C25-C26-C22	2.69	122.12	118.63
3	C	903	Y6Y	C25-C26-C22	2.68	122.11	118.63
3	E	903	Y6Y	C25-C26-C22	2.68	122.11	118.63
3	F	903	Y6Y	C25-C26-C22	2.67	122.09	118.63
3	A	903	Y6Y	C25-C26-C22	2.66	122.09	118.63
3	D	903	Y6Y	C25-C26-C22	2.65	122.07	118.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	903	Y6Y	C24-N3-C23	2.63	121.40	116.85
3	E	903	Y6Y	C24-N3-C23	2.62	121.39	116.85
3	F	903	Y6Y	C24-N3-C23	2.62	121.38	116.85
3	A	903	Y6Y	C24-N3-C23	2.62	121.38	116.85
3	B	903	Y6Y	C24-N3-C23	2.62	121.38	116.85
3	D	903	Y6Y	C24-N3-C23	2.61	121.36	116.85
2	F	902	ATP	C5-C6-N6	2.32	123.88	120.35
2	D	902	ATP	C5-C6-N6	2.32	123.88	120.35
2	B	901	ATP	C5-C6-N6	2.32	123.87	120.35
2	C	901	ATP	C5-C6-N6	2.31	123.86	120.35
2	C	902	ATP	C5-C6-N6	2.31	123.86	120.35
2	A	902	ATP	C5-C6-N6	2.30	123.84	120.35
2	E	902	ATP	C5-C6-N6	2.30	123.84	120.35
2	B	902	ATP	C5-C6-N6	2.29	123.84	120.35
2	E	901	ATP	C5-C6-N6	2.28	123.82	120.35
2	A	901	ATP	C5-C6-N6	2.28	123.82	120.35
2	D	901	ATP	C5-C6-N6	2.26	123.79	120.35
2	F	901	ATP	C5-C6-N6	2.26	123.78	120.35
3	B	903	Y6Y	C23-C22-N2	2.23	122.35	119.26
3	F	903	Y6Y	C23-C22-N2	2.23	122.35	119.26
3	A	903	Y6Y	C23-C22-N2	2.22	122.33	119.26
3	C	903	Y6Y	C23-C22-N2	2.21	122.32	119.26
3	E	903	Y6Y	C23-C22-N2	2.20	122.31	119.26
3	D	903	Y6Y	C23-C22-N2	2.19	122.30	119.26
2	A	901	ATP	PB-O3B-PG	2.10	140.04	132.83
2	C	901	ATP	PB-O3B-PG	2.10	140.04	132.83
2	F	901	ATP	PB-O3B-PG	2.09	140.01	132.83
2	D	901	ATP	PB-O3B-PG	2.09	139.99	132.83
2	E	901	ATP	PB-O3B-PG	2.08	139.97	132.83
2	B	901	ATP	PB-O3B-PG	2.08	139.97	132.83
2	D	902	ATP	PB-O3B-PG	2.06	139.89	132.83
2	A	902	ATP	PB-O3B-PG	2.06	139.88	132.83
2	F	902	ATP	PB-O3B-PG	2.06	139.88	132.83
2	B	902	ATP	PB-O3B-PG	2.05	139.88	132.83
2	C	902	ATP	PB-O3B-PG	2.05	139.85	132.83
2	E	902	ATP	PB-O3B-PG	2.05	139.84	132.83

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	ATP	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
2	A	902	ATP	PB-O3B-PG-O2G
2	B	901	ATP	PB-O3B-PG-O2G
2	B	902	ATP	PB-O3B-PG-O2G
2	C	901	ATP	PB-O3B-PG-O2G
2	C	902	ATP	PB-O3B-PG-O2G
2	D	901	ATP	PB-O3B-PG-O2G
2	D	902	ATP	PB-O3B-PG-O2G
2	E	901	ATP	PB-O3B-PG-O2G
2	E	902	ATP	PB-O3B-PG-O2G
2	F	901	ATP	PB-O3B-PG-O2G
2	F	902	ATP	PB-O3B-PG-O2G
3	A	903	Y6Y	C11-C10-S-O1
3	B	903	Y6Y	C11-C10-S-O1
3	C	903	Y6Y	C11-C10-S-O1
3	D	903	Y6Y	C11-C10-S-O1
3	E	903	Y6Y	C11-C10-S-O1
3	F	903	Y6Y	C11-C10-S-O1
3	A	903	Y6Y	C9-C10-S-O1
3	B	903	Y6Y	C9-C10-S-O1
3	C	903	Y6Y	C9-C10-S-O1
3	D	903	Y6Y	C9-C10-S-O1
3	E	903	Y6Y	C9-C10-S-O1
3	F	903	Y6Y	C9-C10-S-O1
3	A	903	Y6Y	C9-C10-S-C13
3	A	903	Y6Y	C11-C10-S-C13
3	B	903	Y6Y	C9-C10-S-C13
3	B	903	Y6Y	C11-C10-S-C13
3	C	903	Y6Y	C9-C10-S-C13
3	C	903	Y6Y	C11-C10-S-C13
3	D	903	Y6Y	C9-C10-S-C13
3	D	903	Y6Y	C11-C10-S-C13
3	E	903	Y6Y	C9-C10-S-C13
3	E	903	Y6Y	C11-C10-S-C13
3	F	903	Y6Y	C9-C10-S-C13
3	F	903	Y6Y	C11-C10-S-C13
2	A	901	ATP	PB-O3B-PG-O1G
2	B	901	ATP	PB-O3B-PG-O1G
2	C	901	ATP	PB-O3B-PG-O1G
2	D	901	ATP	PB-O3B-PG-O1G
2	E	901	ATP	PB-O3B-PG-O1G
2	F	901	ATP	PB-O3B-PG-O1G
2	A	902	ATP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
2	B	902	ATP	C5'-O5'-PA-O3A
2	C	902	ATP	C5'-O5'-PA-O3A
2	D	902	ATP	C5'-O5'-PA-O3A
2	E	902	ATP	C5'-O5'-PA-O3A
2	F	902	ATP	C5'-O5'-PA-O3A
2	A	901	ATP	O4'-C4'-C5'-O5'
2	B	901	ATP	O4'-C4'-C5'-O5'
2	C	901	ATP	O4'-C4'-C5'-O5'
2	D	901	ATP	O4'-C4'-C5'-O5'
2	E	901	ATP	O4'-C4'-C5'-O5'
2	F	901	ATP	O4'-C4'-C5'-O5'
2	A	901	ATP	PA-O3A-PB-O1B
2	B	901	ATP	PA-O3A-PB-O1B
2	C	901	ATP	PA-O3A-PB-O1B
2	D	901	ATP	PA-O3A-PB-O1B
2	E	901	ATP	PA-O3A-PB-O1B
2	F	901	ATP	PA-O3A-PB-O1B
2	A	902	ATP	PB-O3B-PG-O1G
2	B	902	ATP	PB-O3B-PG-O1G
2	C	902	ATP	PB-O3B-PG-O1G
2	D	902	ATP	PB-O3B-PG-O1G
2	E	902	ATP	PB-O3B-PG-O1G
2	F	902	ATP	PB-O3B-PG-O1G
2	A	902	ATP	PB-O3B-PG-O3G
2	B	902	ATP	PB-O3B-PG-O3G
2	C	902	ATP	PB-O3B-PG-O3G
2	D	902	ATP	PB-O3B-PG-O3G
2	E	902	ATP	PB-O3B-PG-O3G
2	F	902	ATP	PB-O3B-PG-O3G
2	A	902	ATP	PA-O3A-PB-O1B
2	A	902	ATP	PA-O3A-PB-O2B
2	B	901	ATP	PA-O3A-PB-O2B
2	B	902	ATP	PA-O3A-PB-O1B
2	B	902	ATP	PA-O3A-PB-O2B
2	C	901	ATP	PA-O3A-PB-O2B
2	C	902	ATP	PA-O3A-PB-O1B
2	C	902	ATP	PA-O3A-PB-O2B
2	D	901	ATP	PA-O3A-PB-O2B
2	D	902	ATP	PA-O3A-PB-O1B
2	D	902	ATP	PA-O3A-PB-O2B
2	E	901	ATP	PA-O3A-PB-O2B
2	E	902	ATP	PA-O3A-PB-O1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	902	ATP	PA-O3A-PB-O2B
2	F	901	ATP	PA-O3A-PB-O2B
2	F	902	ATP	PA-O3A-PB-O1B
2	F	902	ATP	PA-O3A-PB-O2B

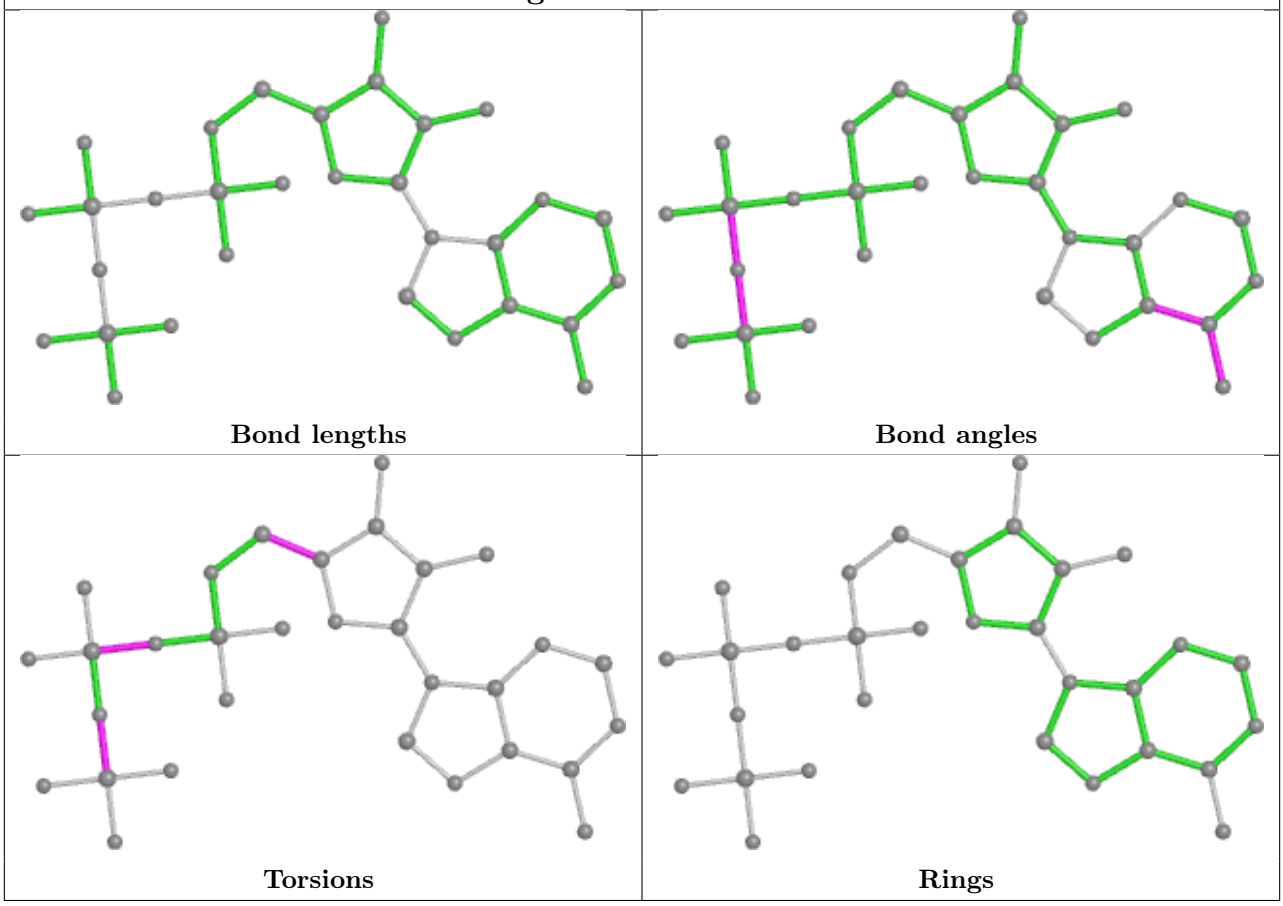
There are no ring outliers.

7 monomers are involved in 19 short contacts:

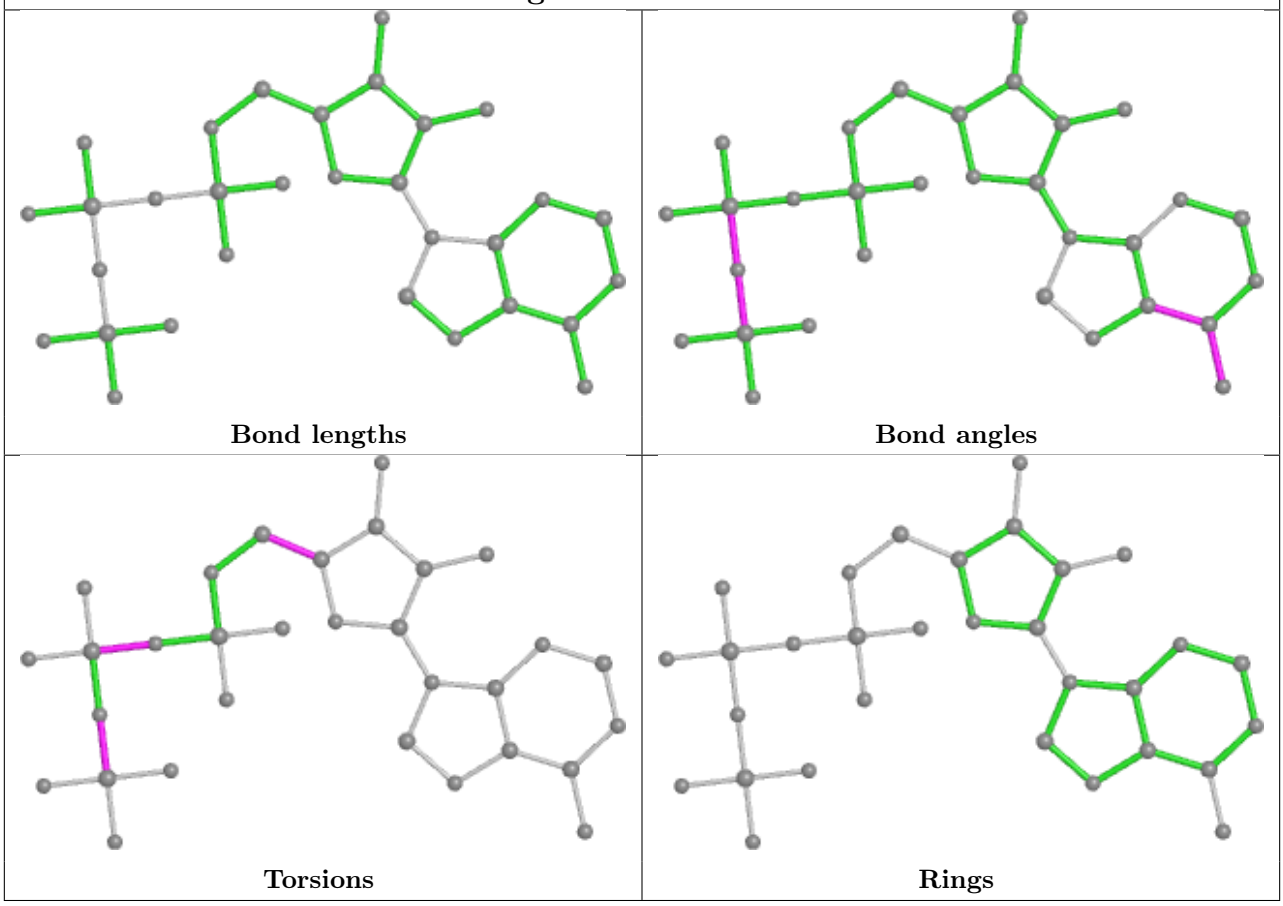
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	901	ATP	3	0
2	F	901	ATP	3	0
2	C	901	ATP	3	0
2	D	901	ATP	3	0
2	B	902	ATP	1	0
2	B	901	ATP	3	0
2	A	901	ATP	3	0

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

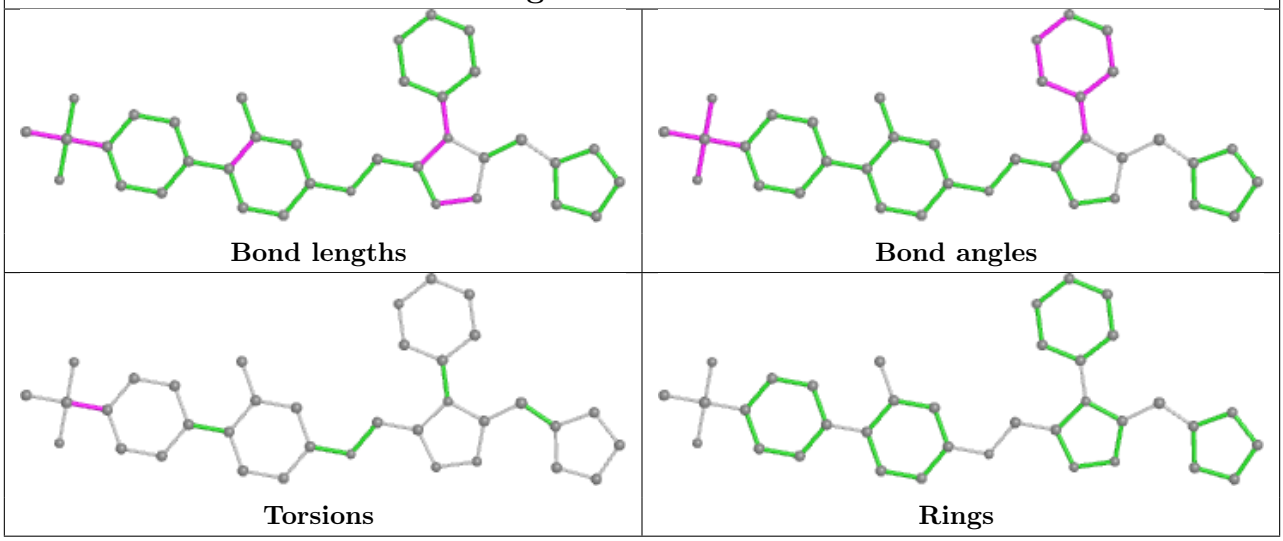
Ligand ATP E 901



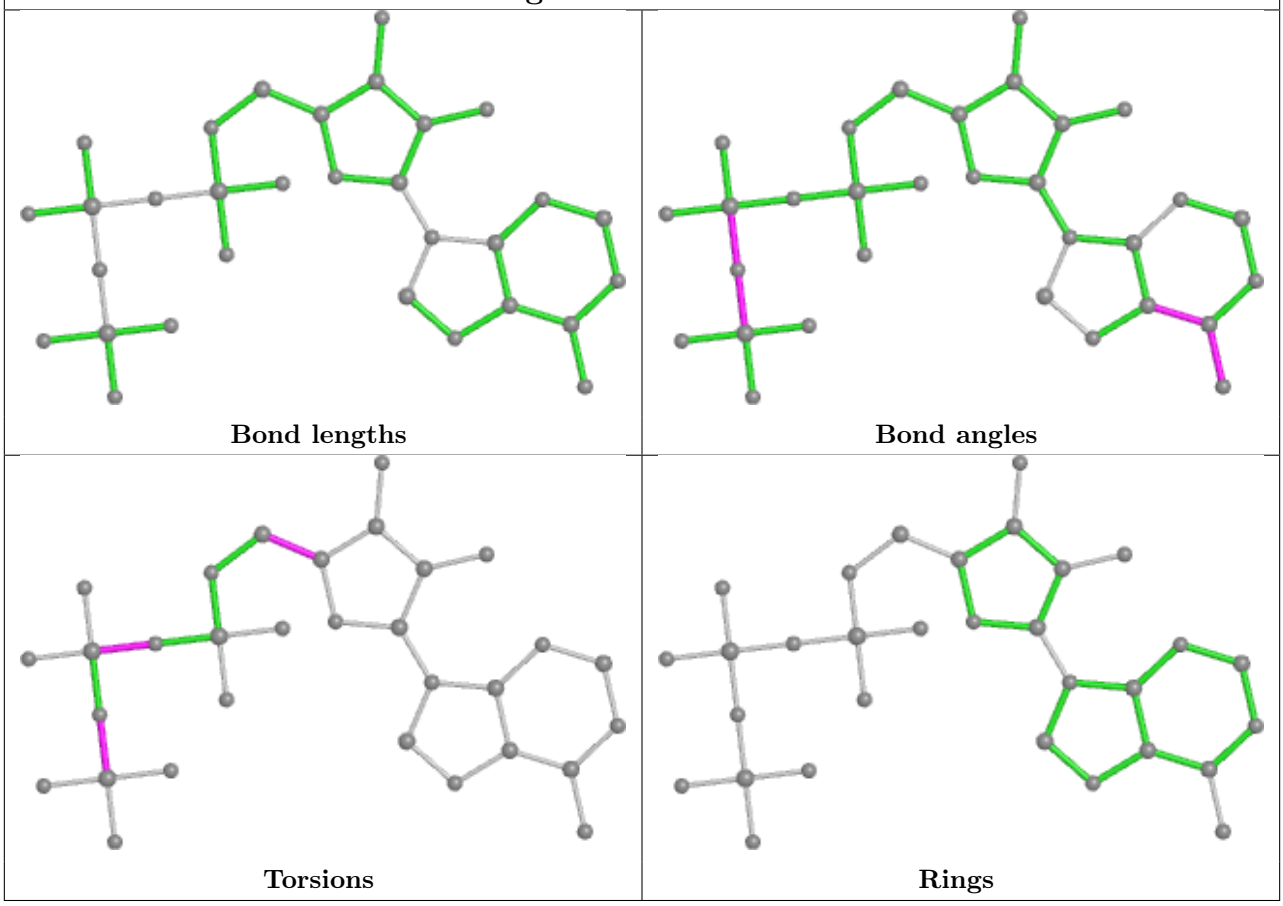
Ligand ATP F 901



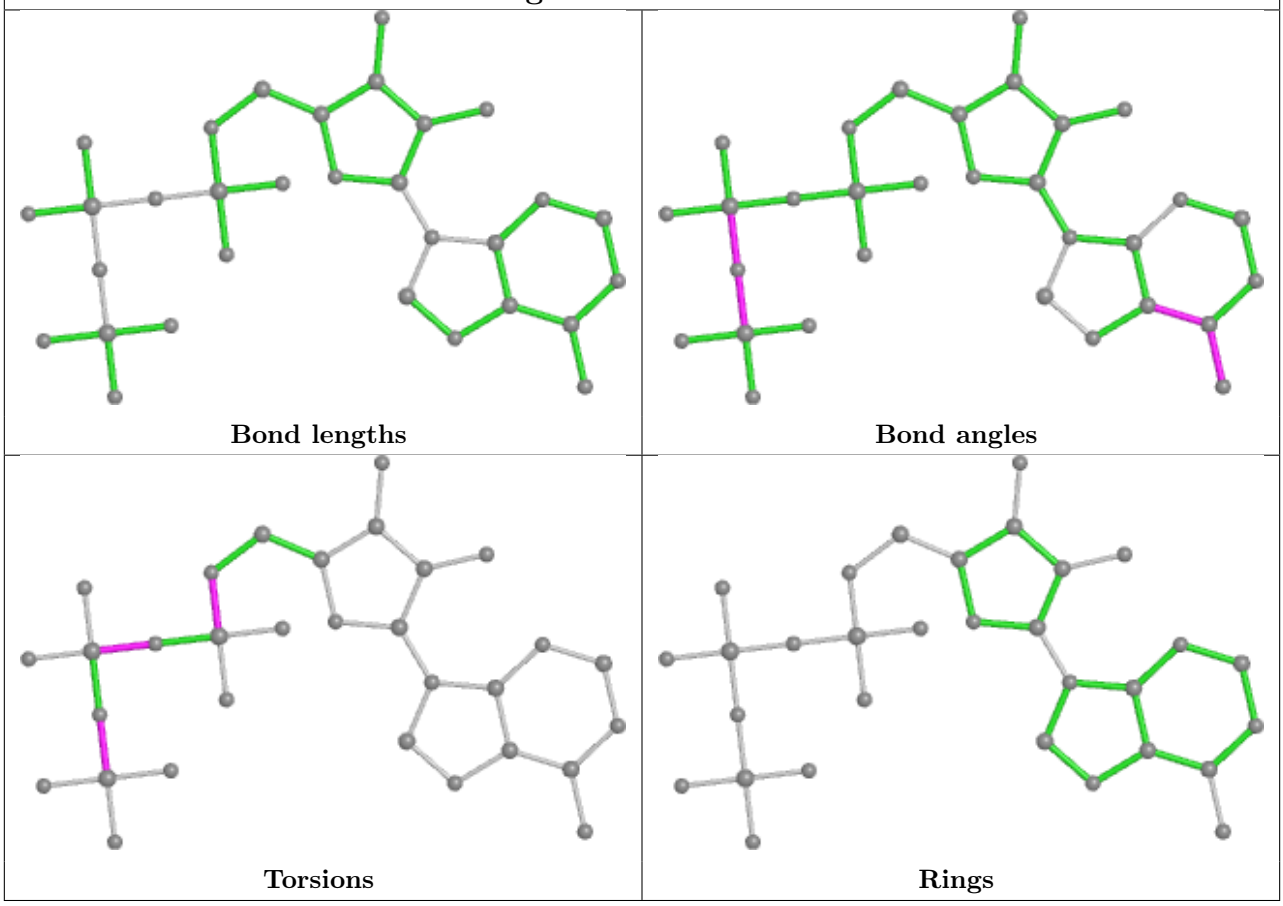
Ligand Y6Y B 903



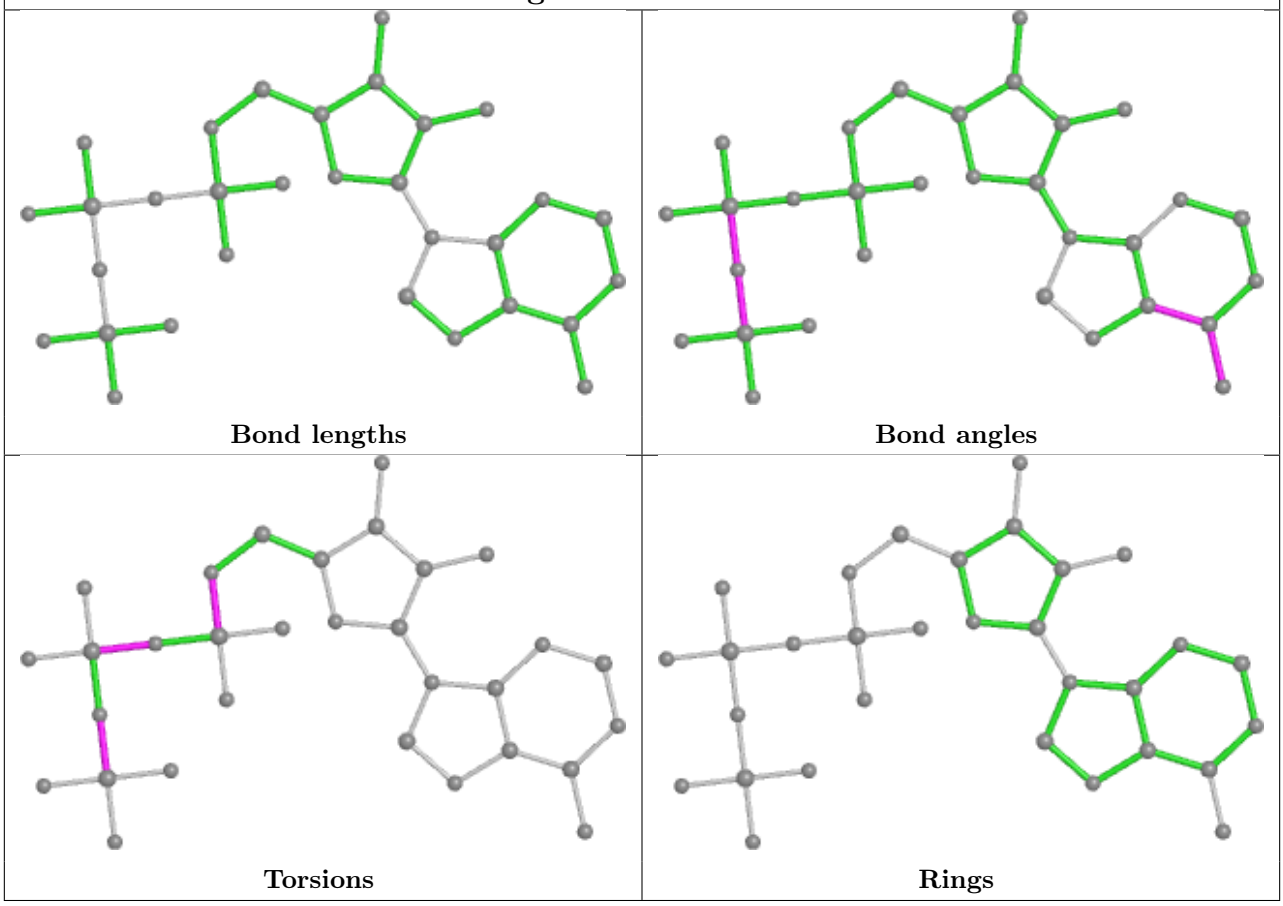
Ligand ATP C 901



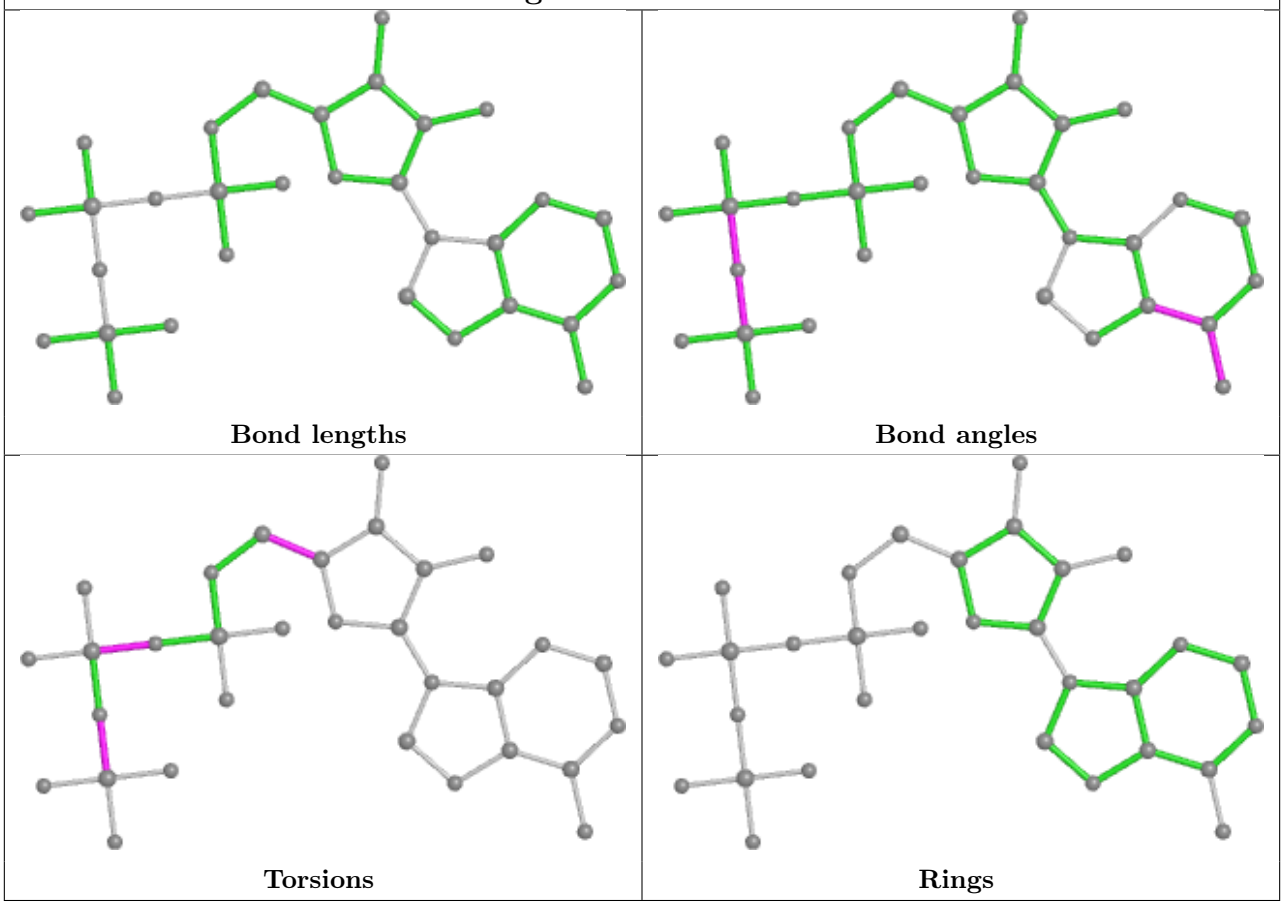
Ligand ATP C 902



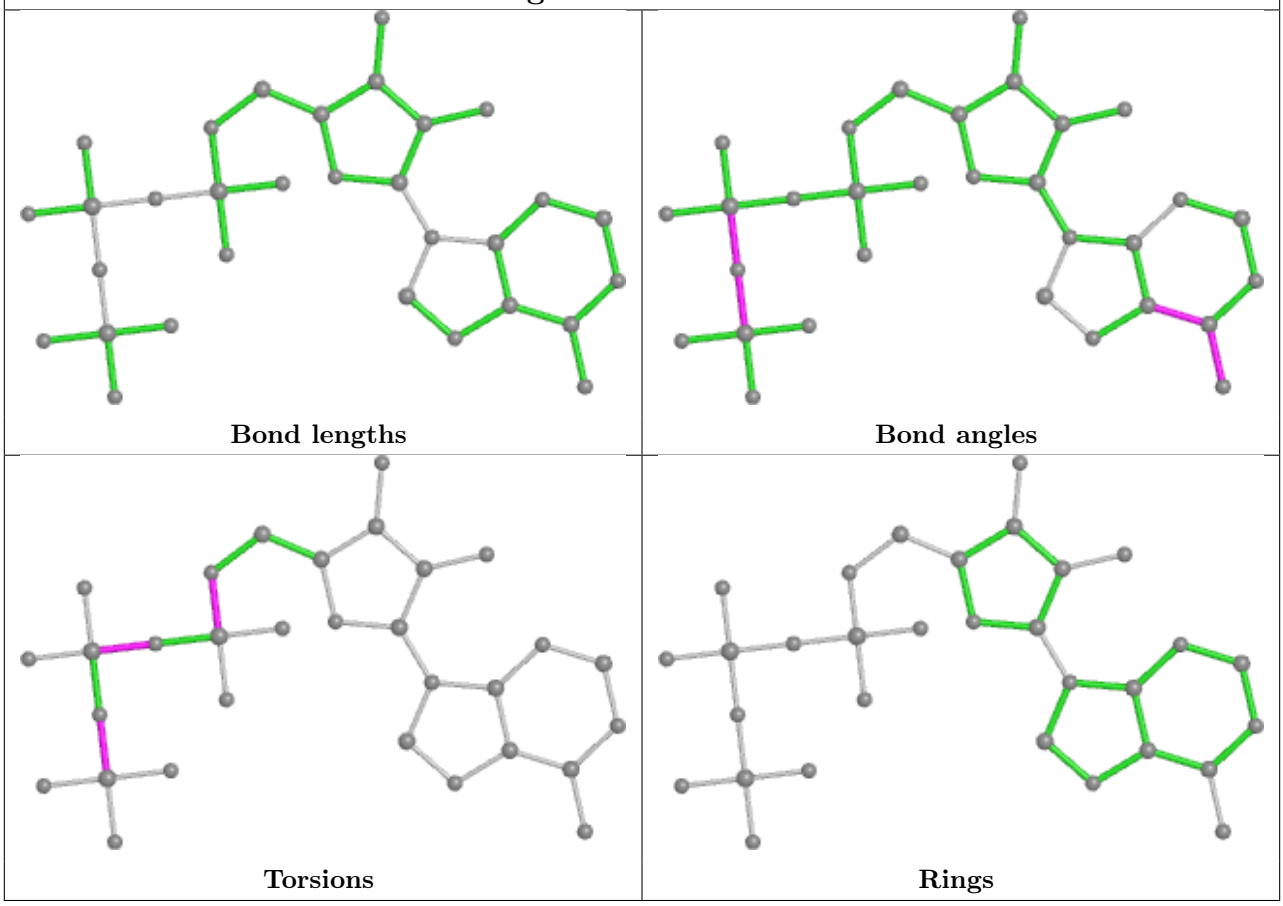
Ligand ATP F 902



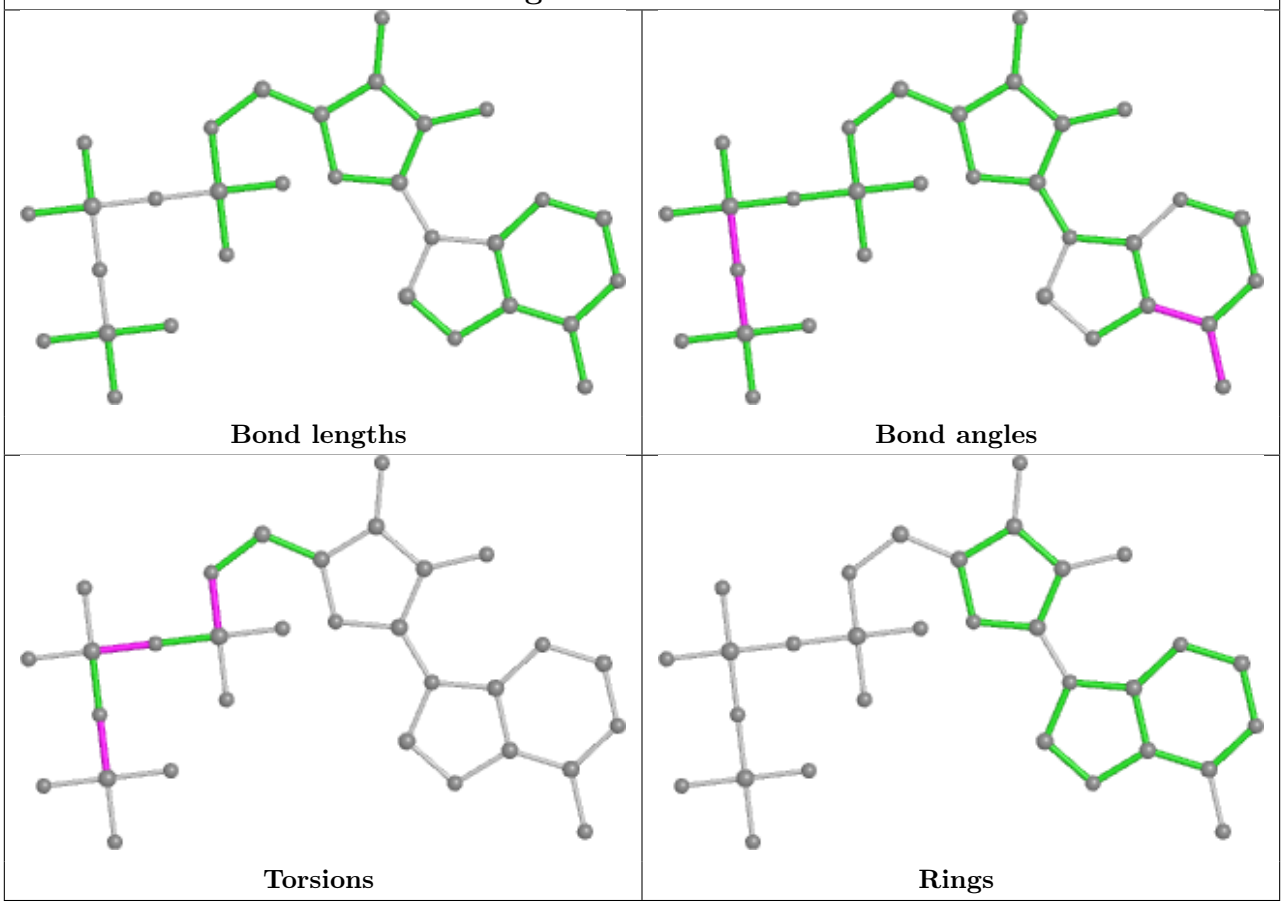
Ligand ATP D 901



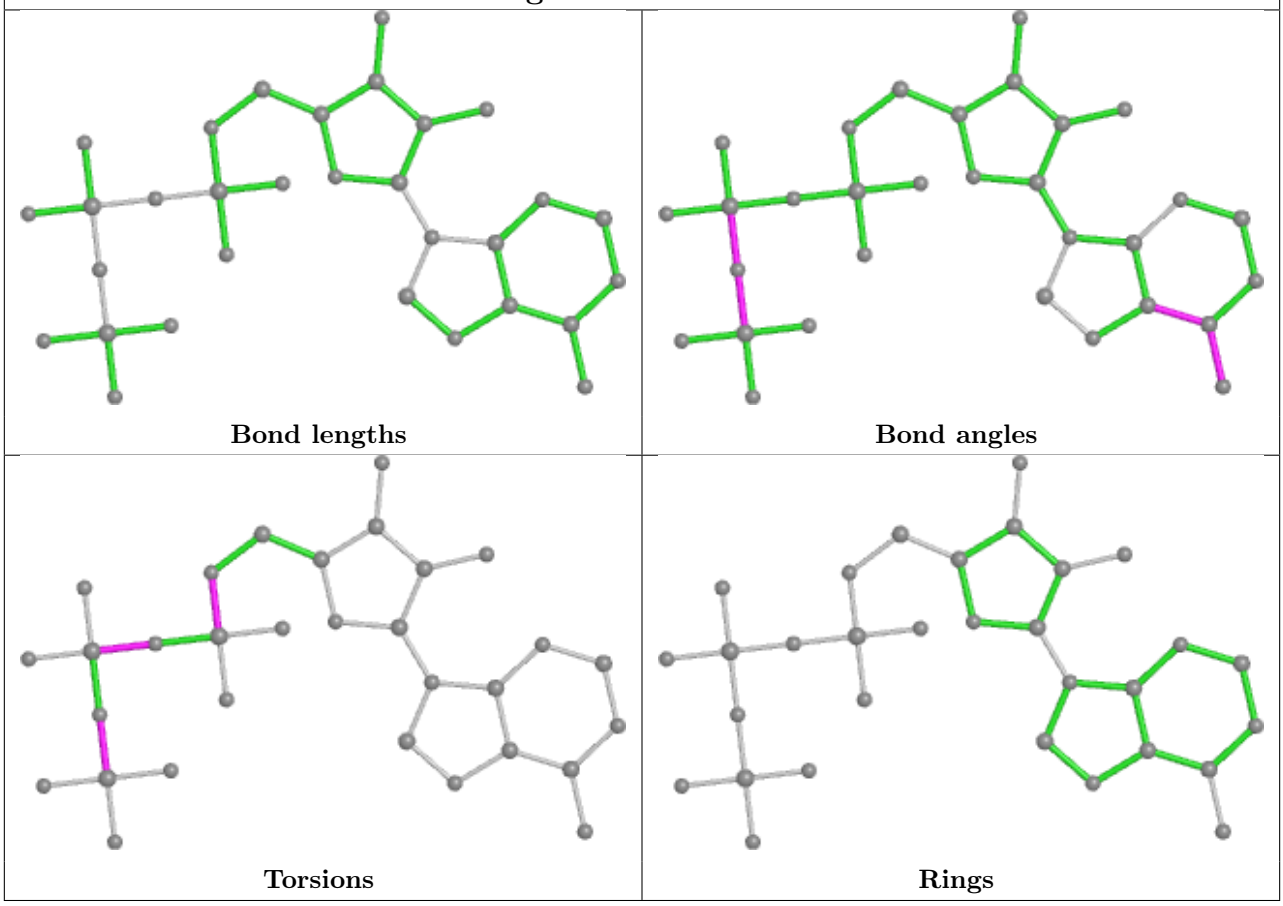
Ligand ATP E 902



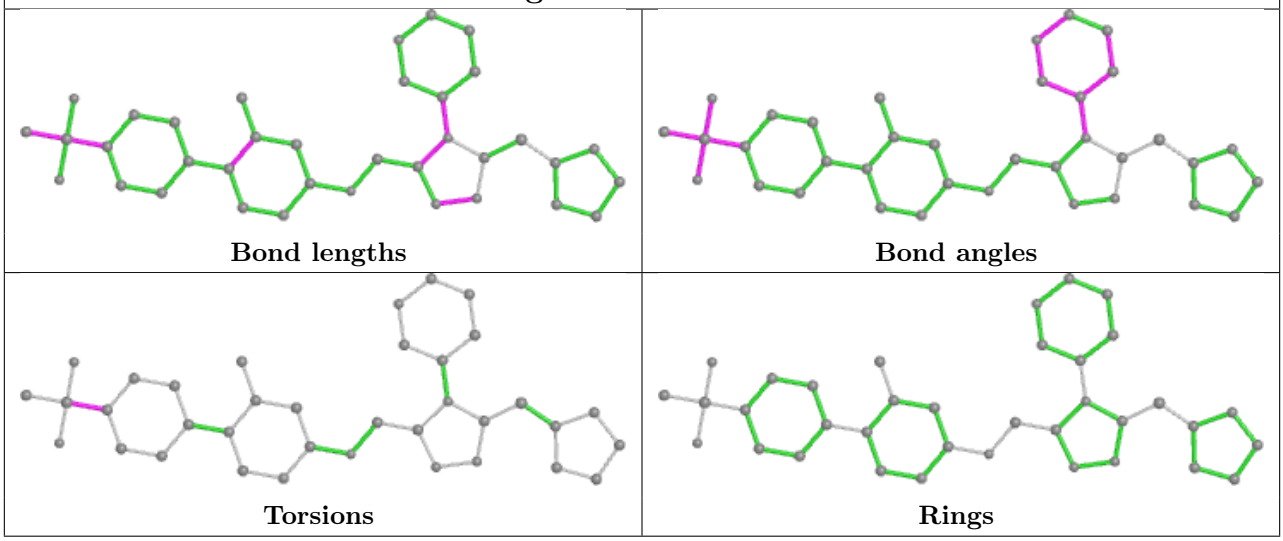
Ligand ATP A 902

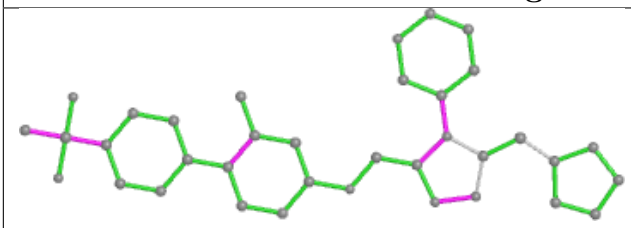
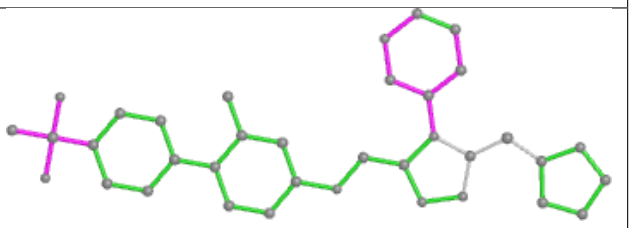
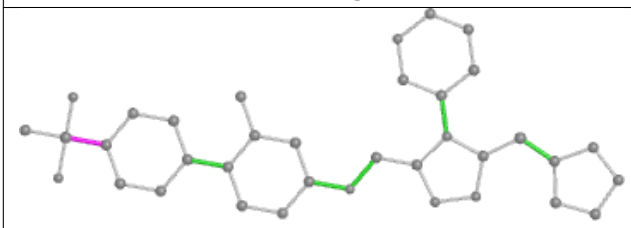
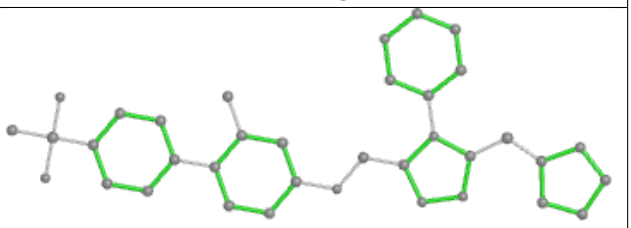


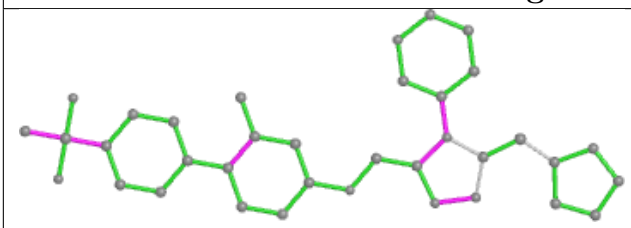
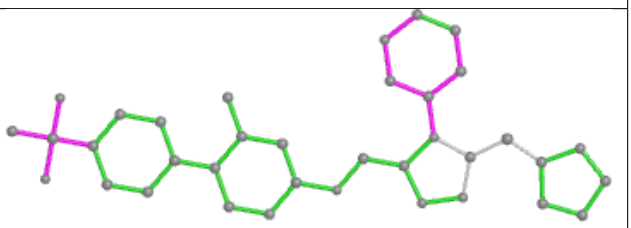
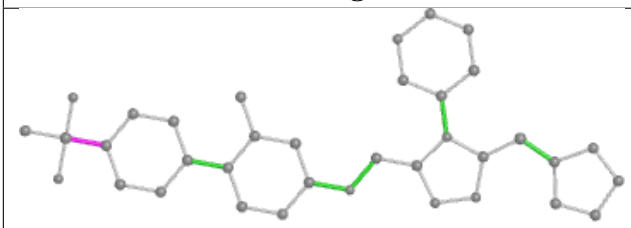
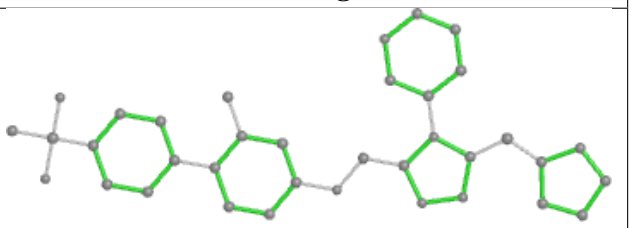
Ligand ATP B 902



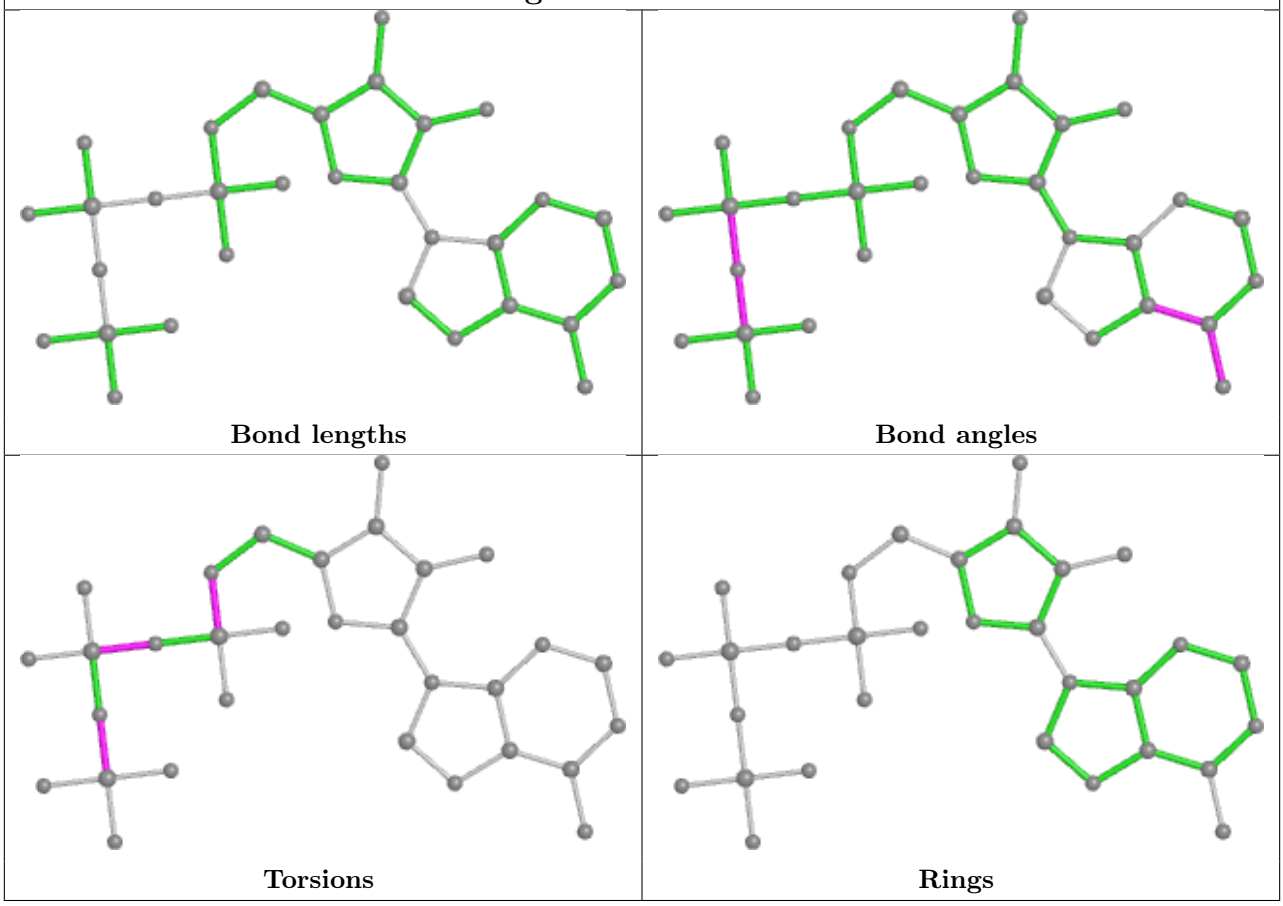
Ligand Y6Y D 903



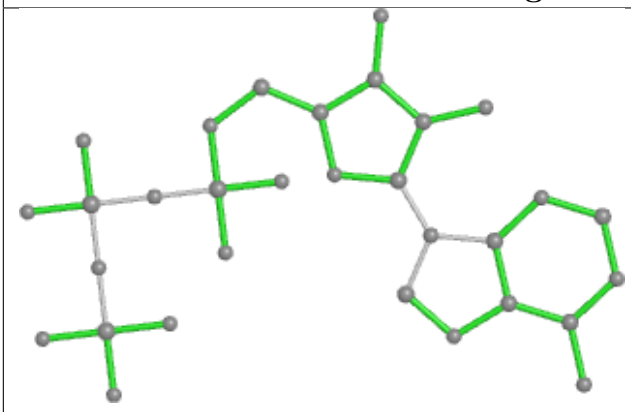
Ligand Y6Y C 903	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand Y6Y E 903	
 Bond lengths	 Bond angles
 Torsions	 Rings

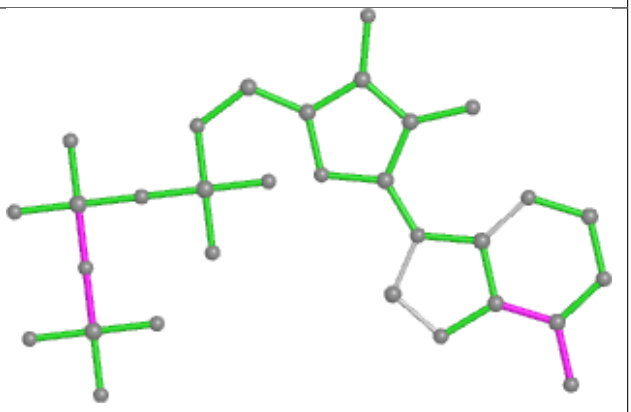
Ligand ATP D 902



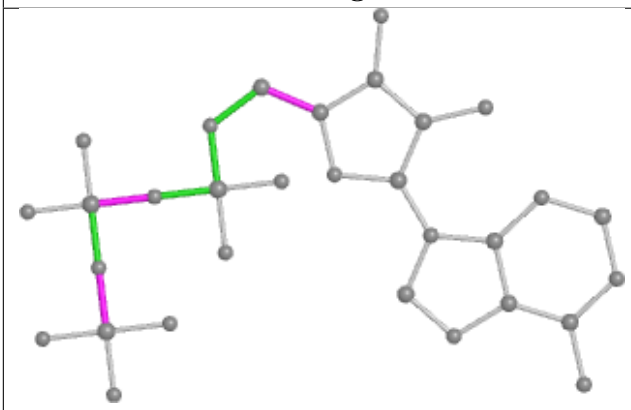
Ligand ATP B 901



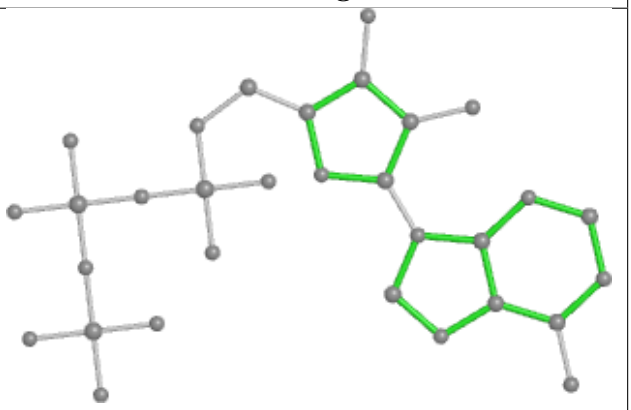
Bond lengths



Bond angles

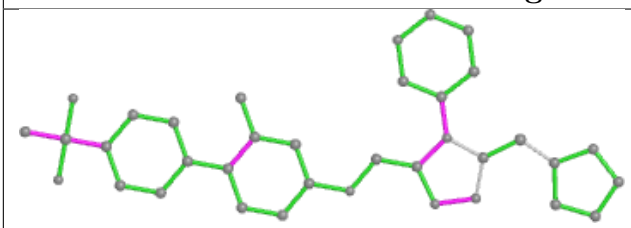


Torsions

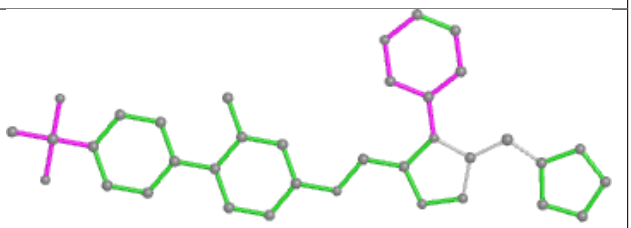


Rings

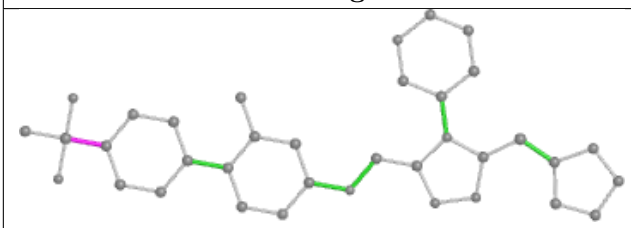
Ligand Y6Y A 903



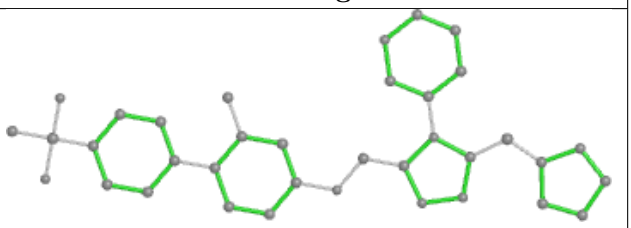
Bond lengths



Bond angles

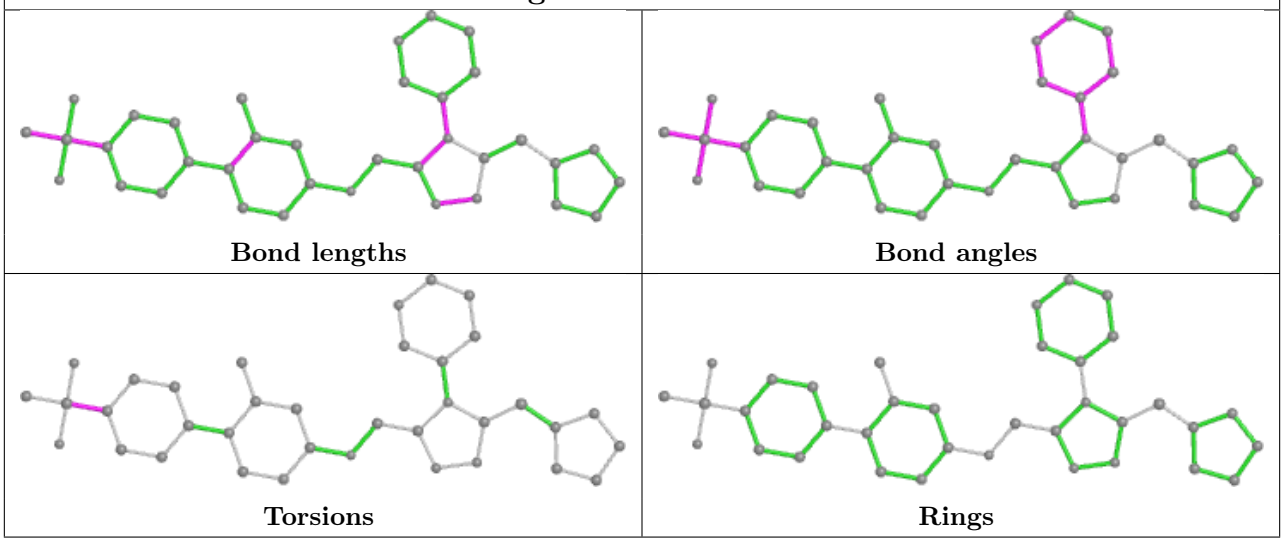


Torsions

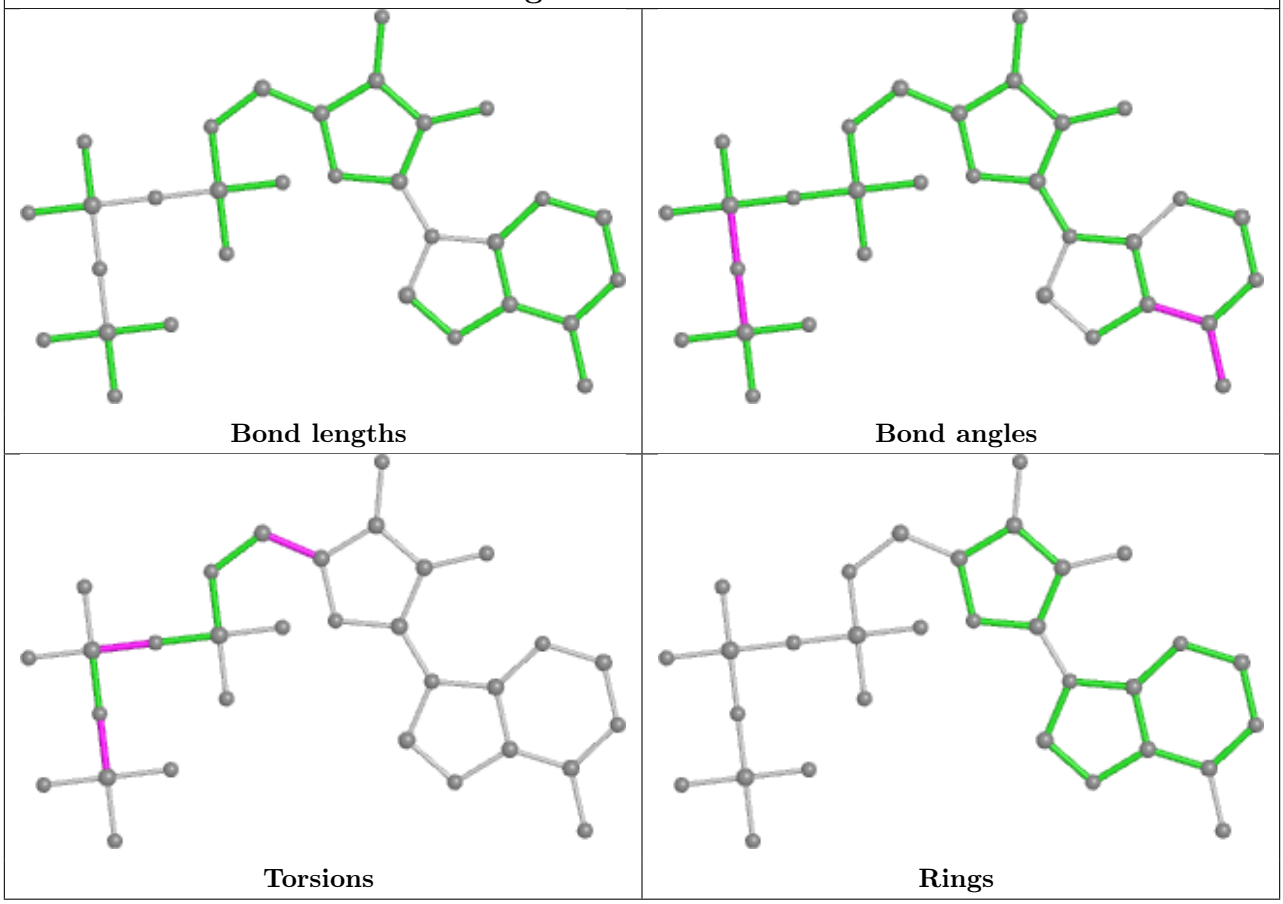


Rings

Ligand Y6Y F 903



Ligand ATP A 901



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.

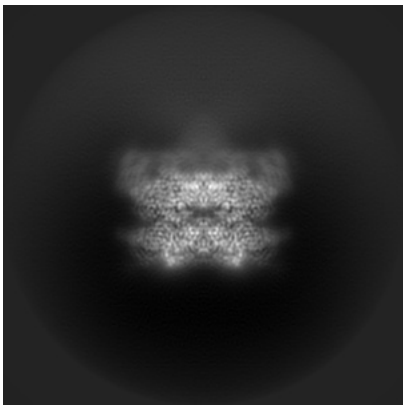
6 Map visualisation (i)

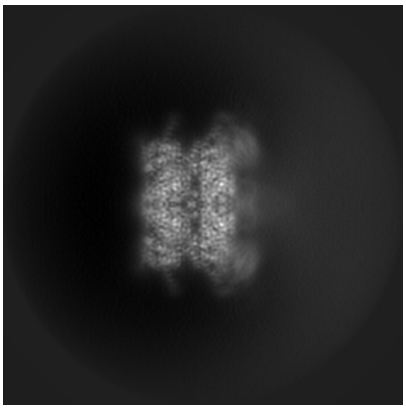
This section contains visualisations of the EMDB entry EMD-23442. These allow visual inspection of the internal detail of the map and identification of artifacts.

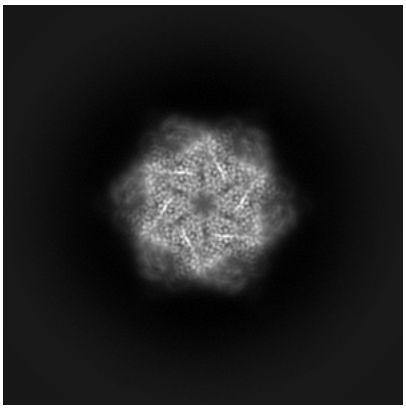
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

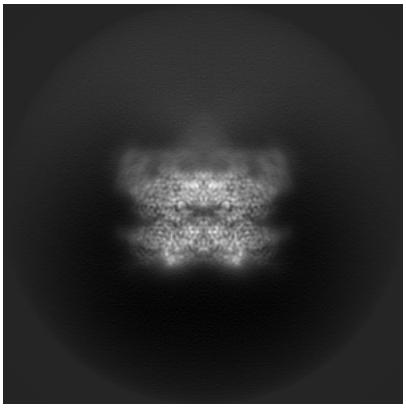
6.1.1 Primary map

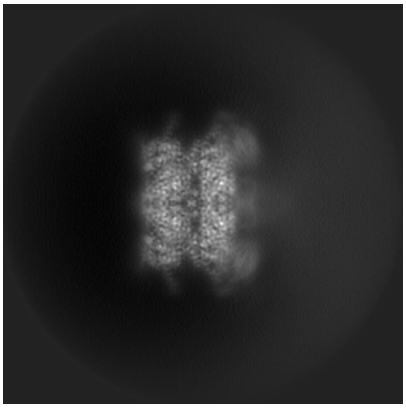

X

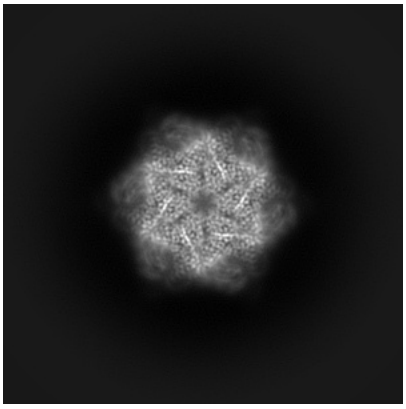

Y


Z

6.1.2 Raw map


X

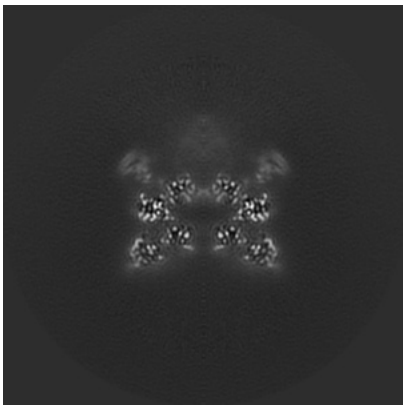

Y

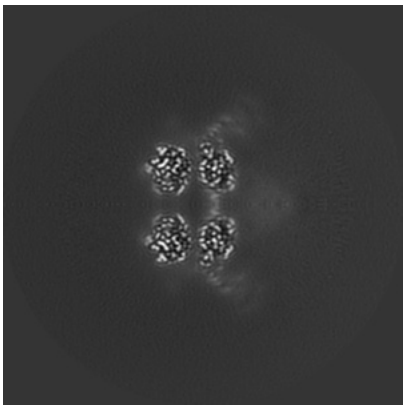

Z

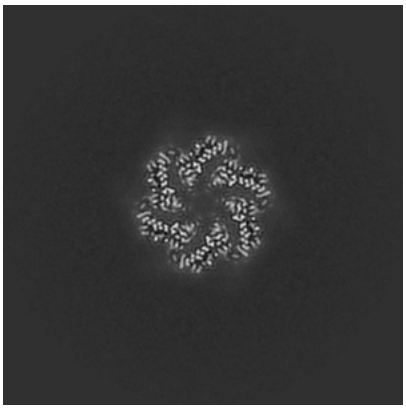
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

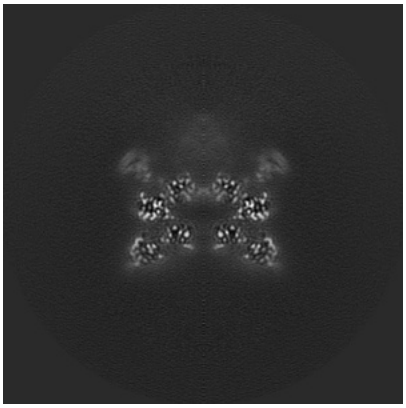
6.2.1 Primary map

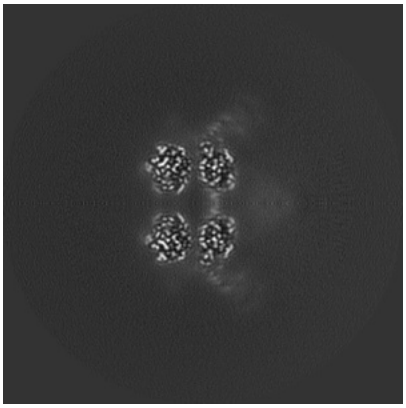

X Index: 160

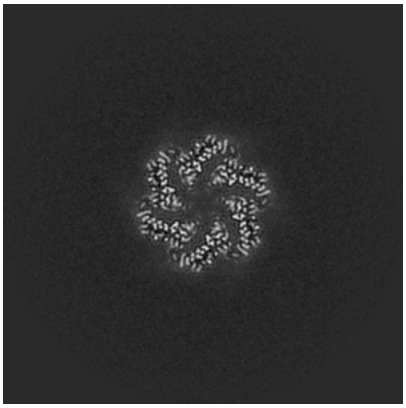

Y Index: 160


Z Index: 160

6.2.2 Raw map


X Index: 160

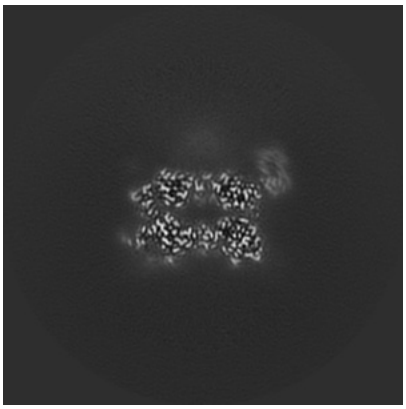

Y Index: 160

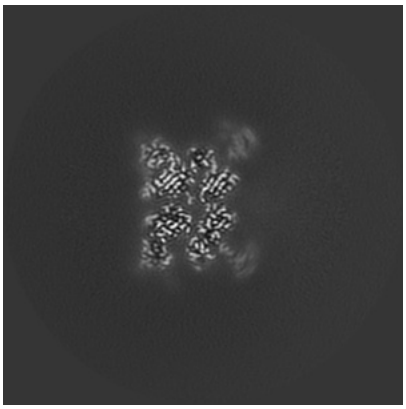

Z Index: 160

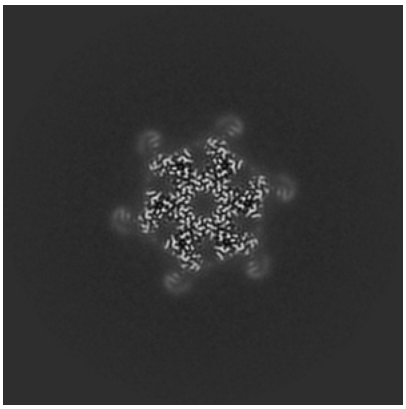
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

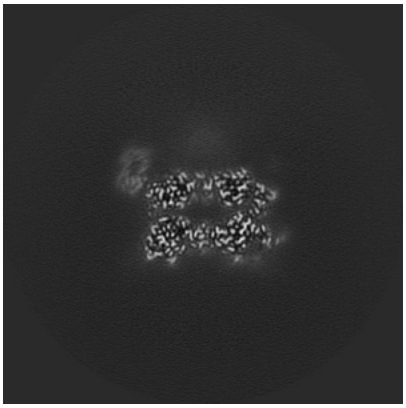
6.3.1 Primary map

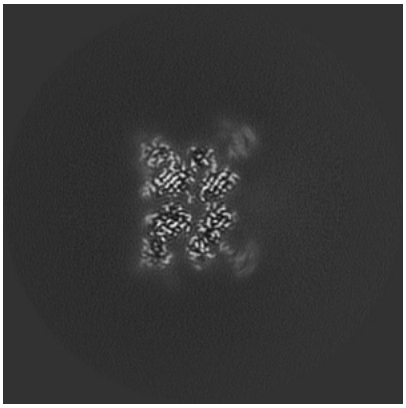

X Index: 148

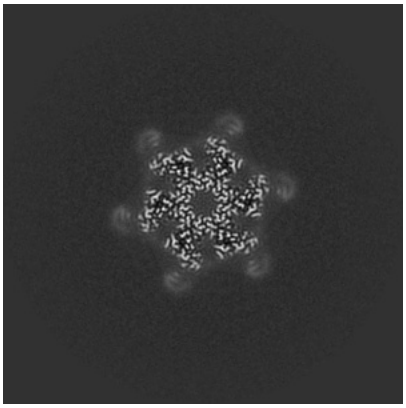

Y Index: 134


Z Index: 137

6.3.2 Raw map


X Index: 172

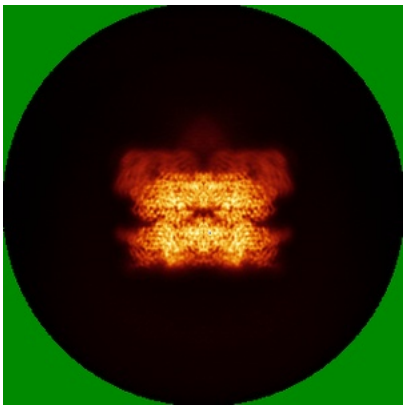

Y Index: 134

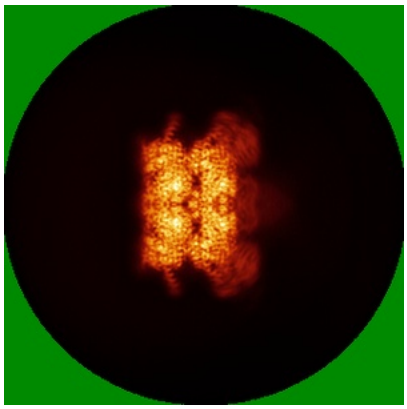

Z Index: 137

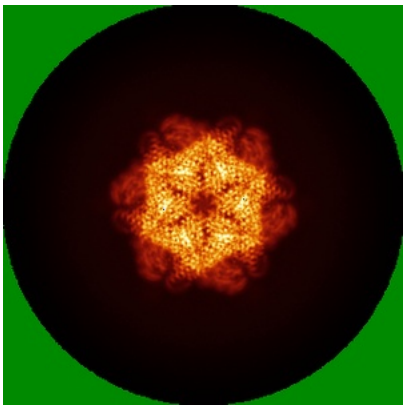
The images above show the largest variance slices of the map in three orthogonal directions.

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

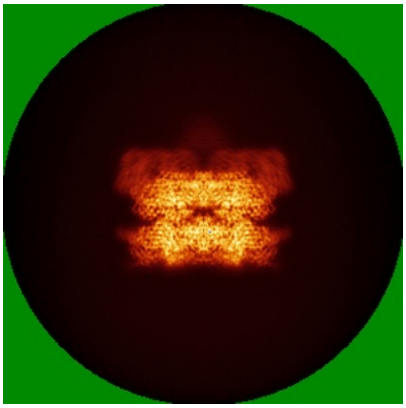
6.4.1 Primary map

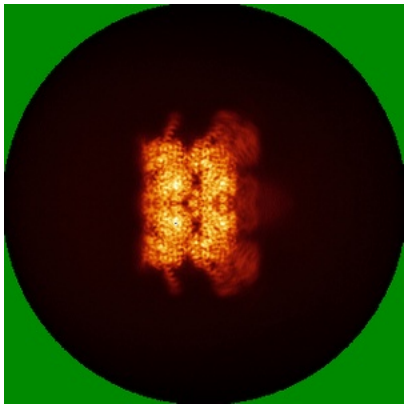

X

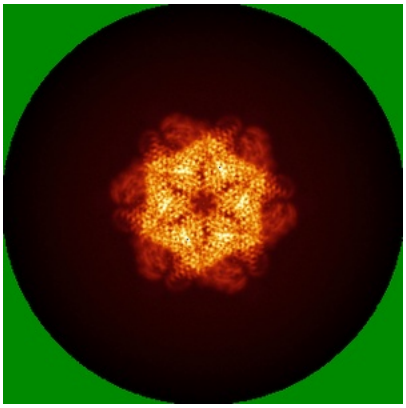

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

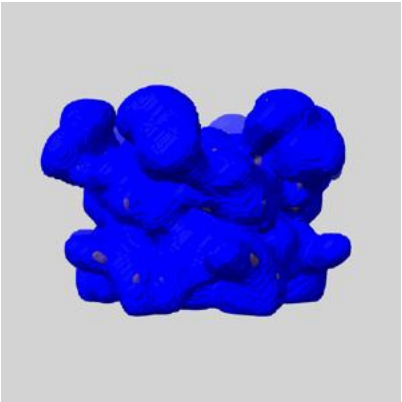
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

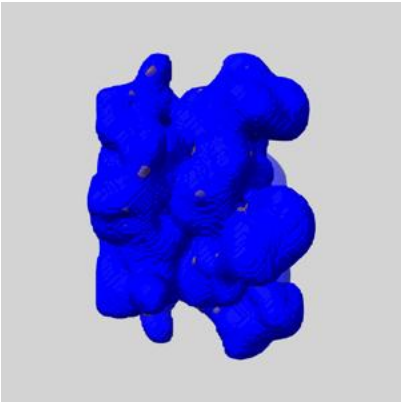
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

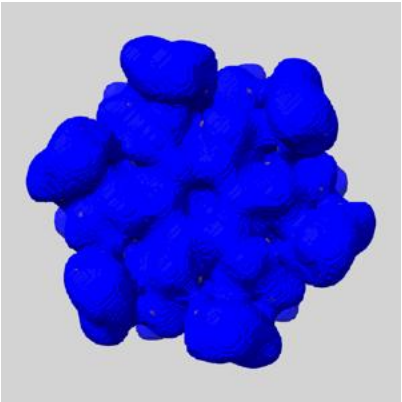
6.6.1 emd_23442_msk_1.map (i)



X



Y

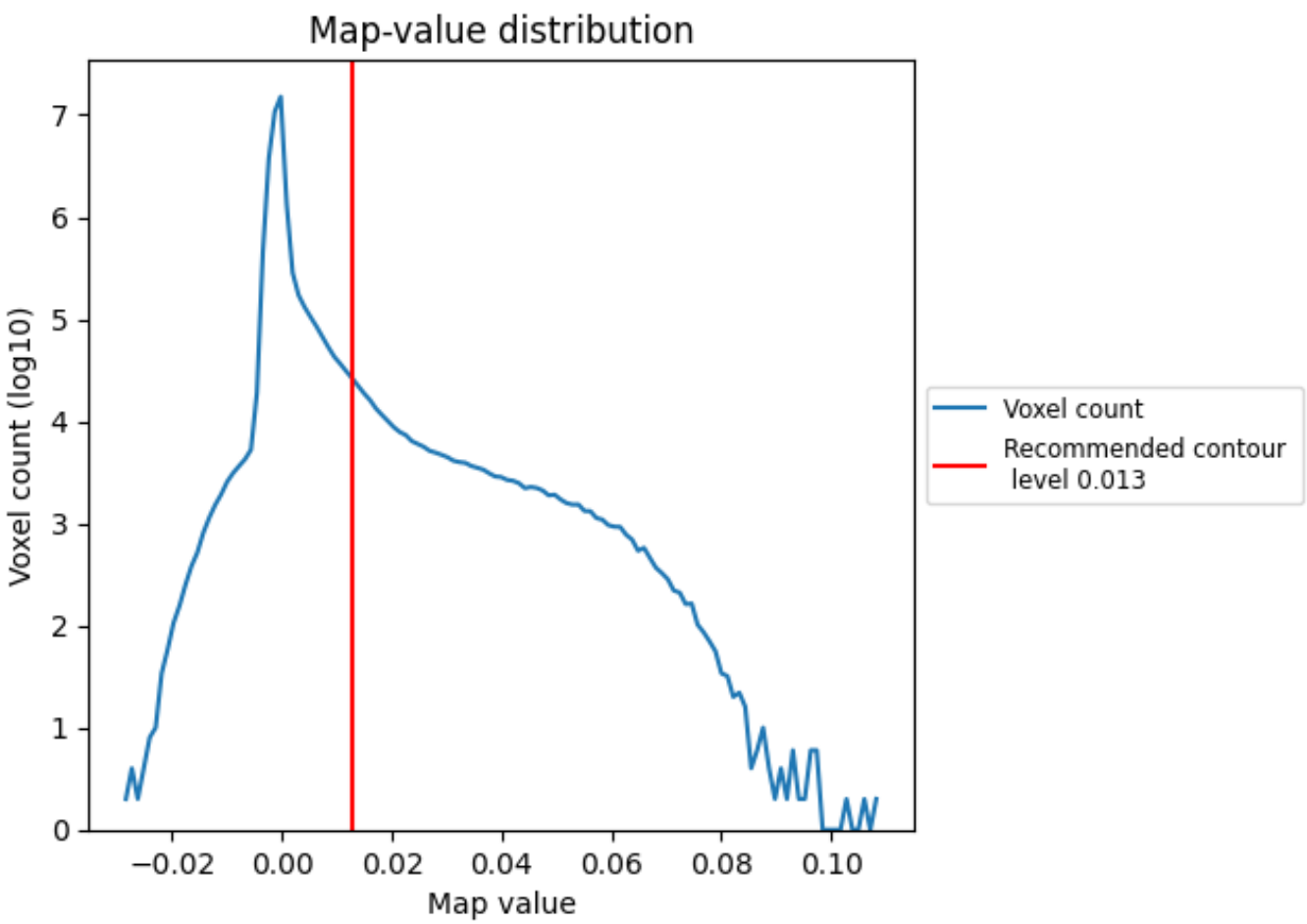


Z

7 Map analysis (i)

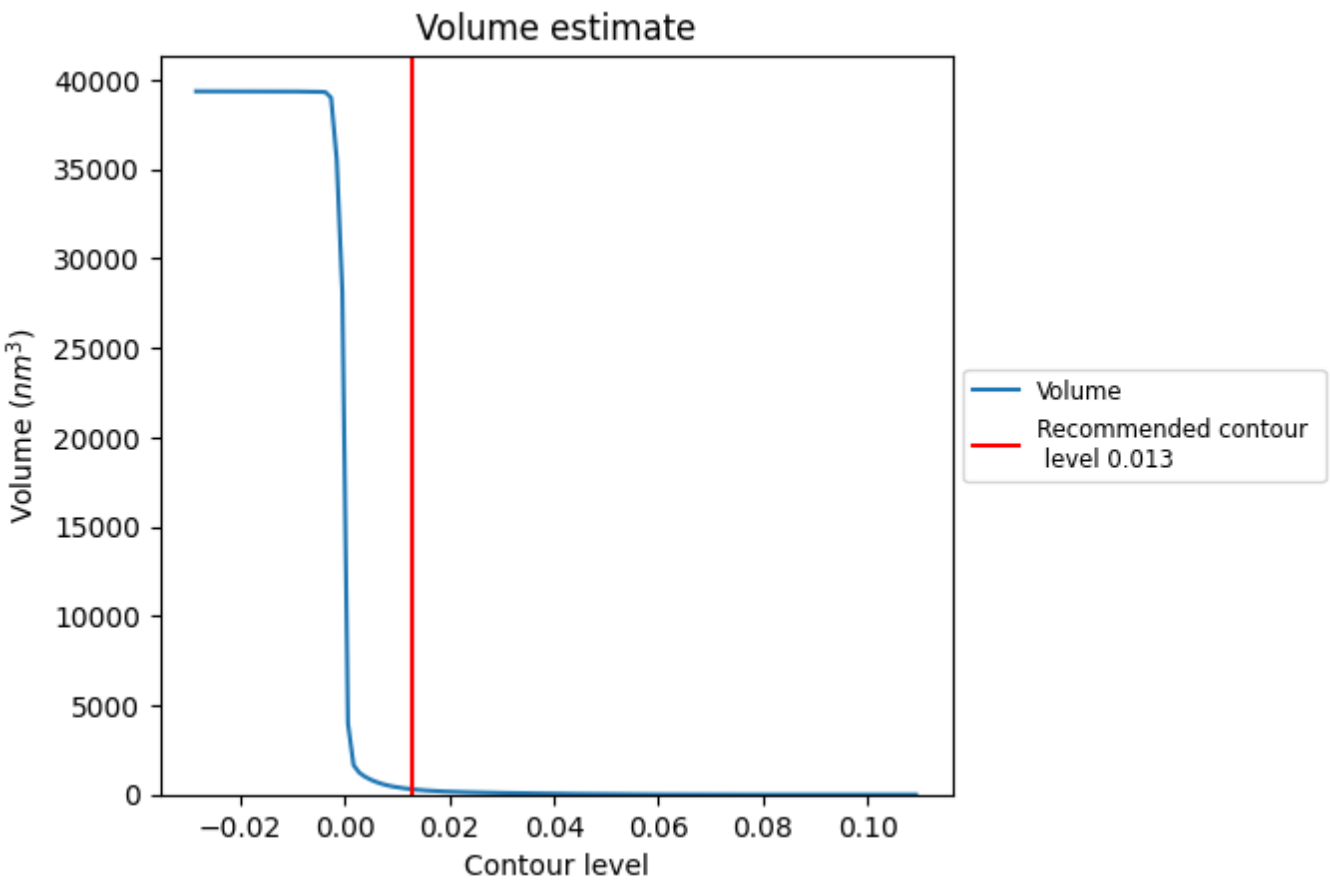
This section contains the results of statistical analysis of the map.

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.

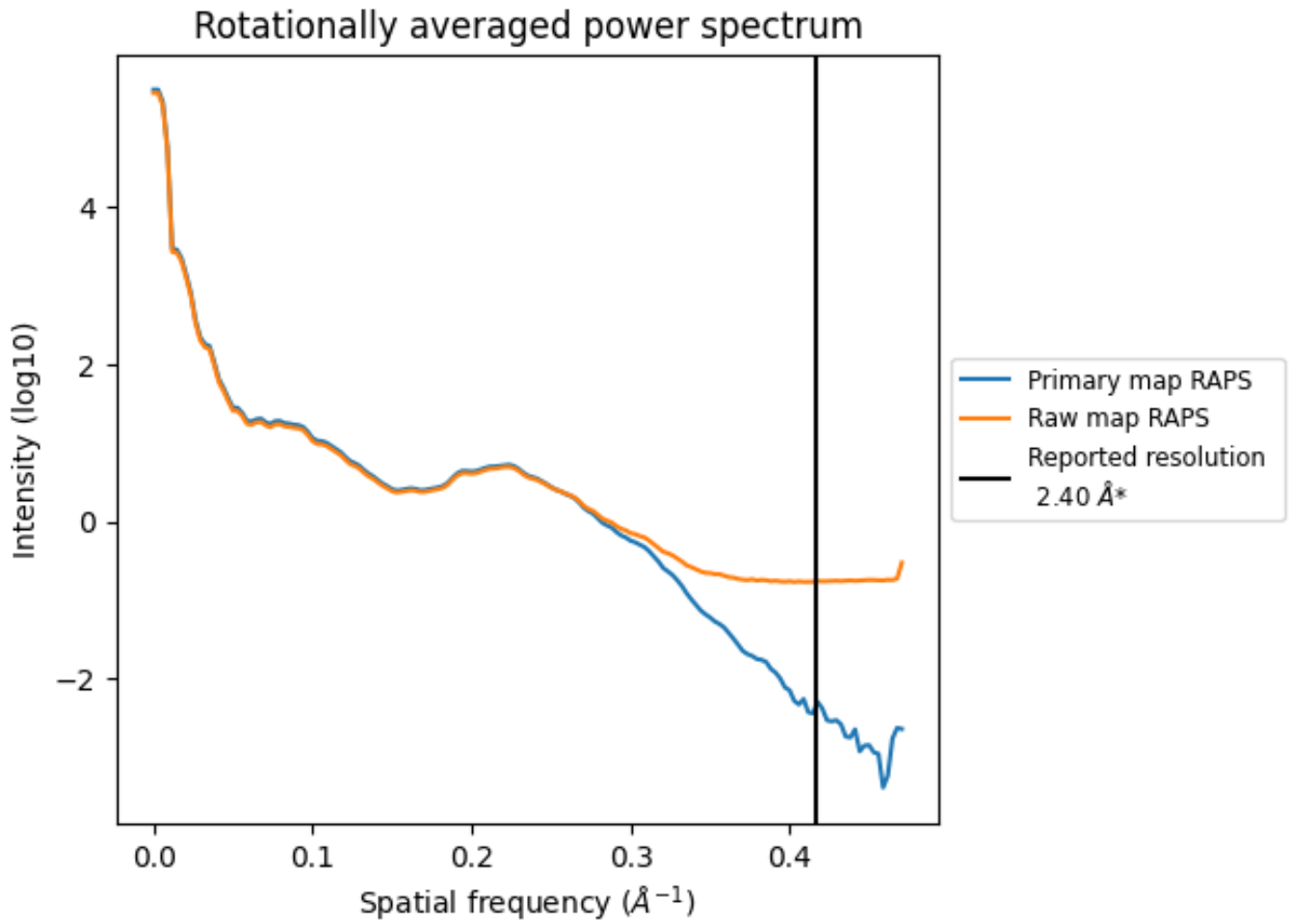
7.2 Volume estimate (i)



The volume at the recommended contour level is 296 nm^3; this corresponds to an approximate mass of 267 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)

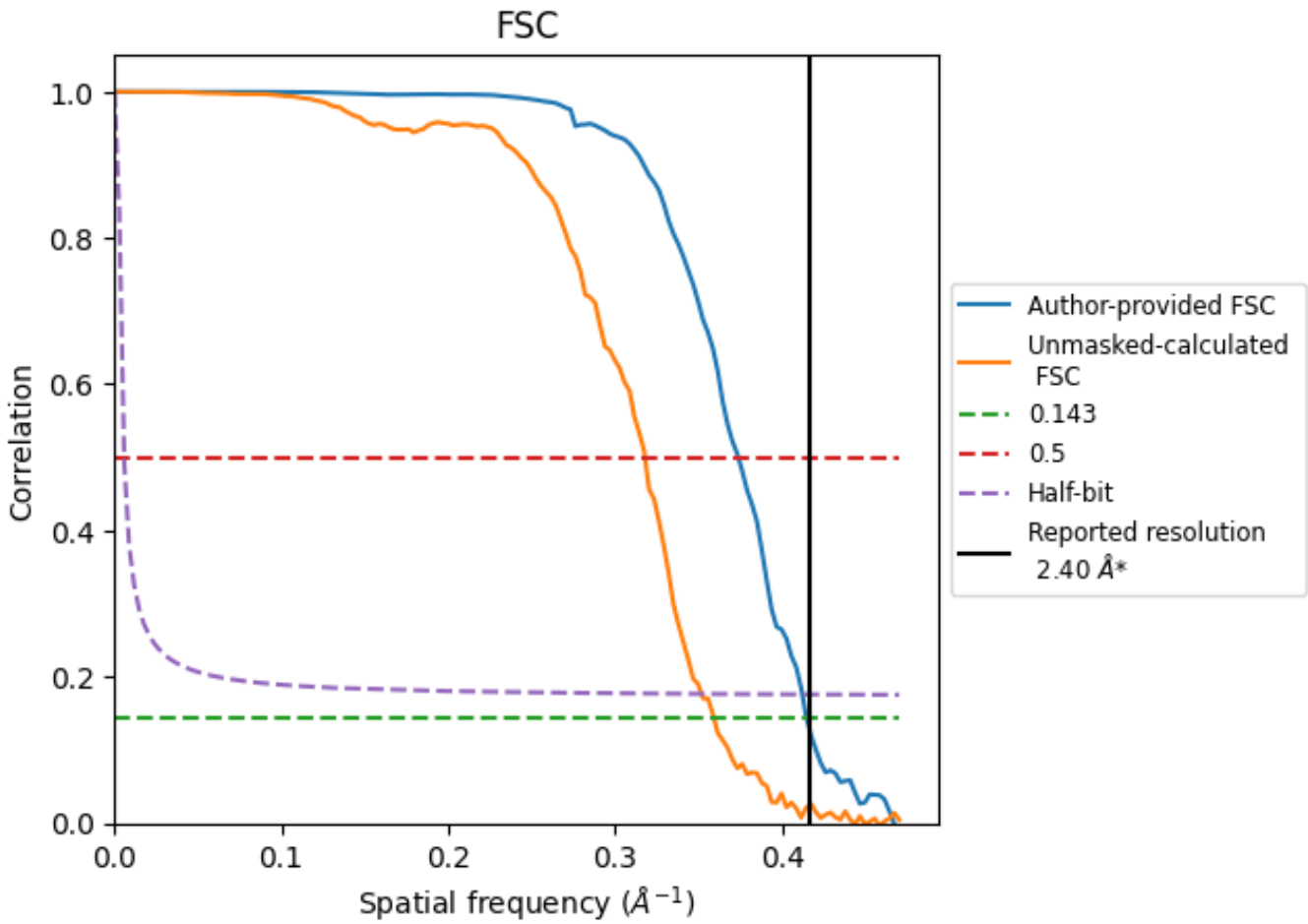


*Reported resolution corresponds to spatial frequency of 0.417 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.417 Å^{-1}

8.2 Resolution estimates (i)

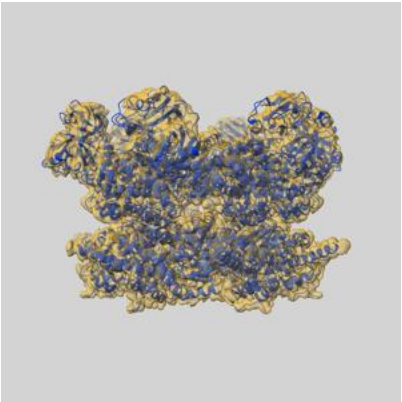
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.41	2.67	2.43
Unmasked-calculated*	2.78	3.14	2.84

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.78 differs from the reported value 2.4 by more than 10 %

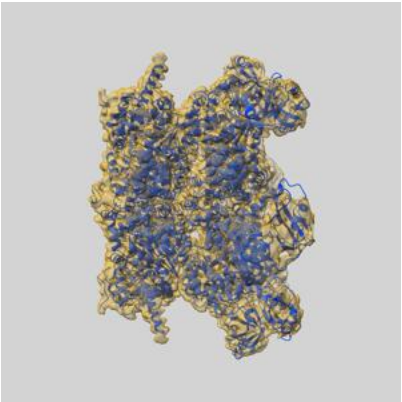
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-23442 and PDB model 7LMY. Per-residue inclusion information can be found in section 3 on page 6.

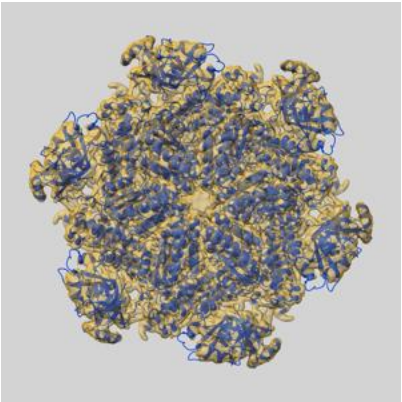
9.1 Map-model overlay (i)



X



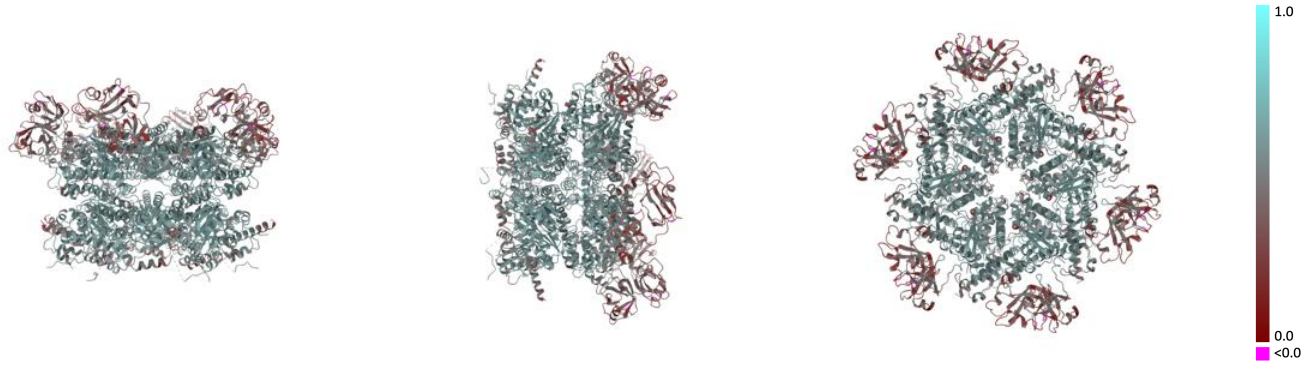
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013 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.

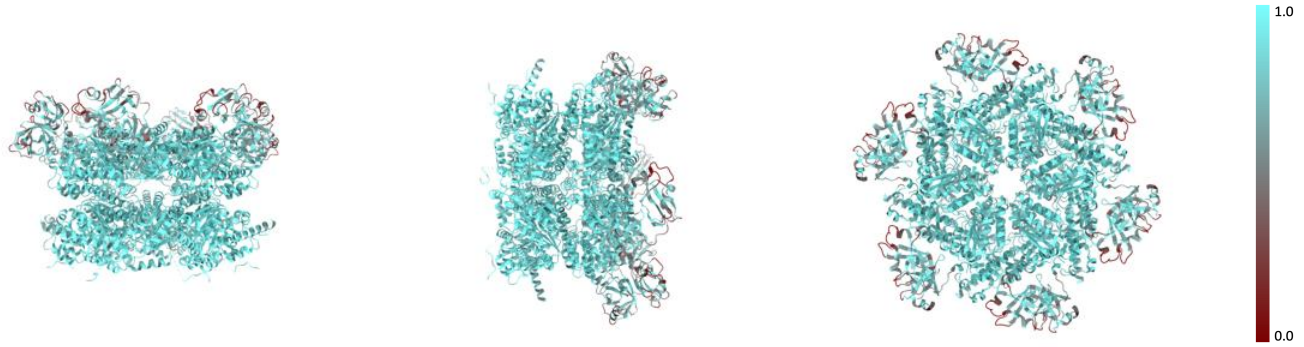
9.2 Q-score mapped to coordinate model (i)



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.

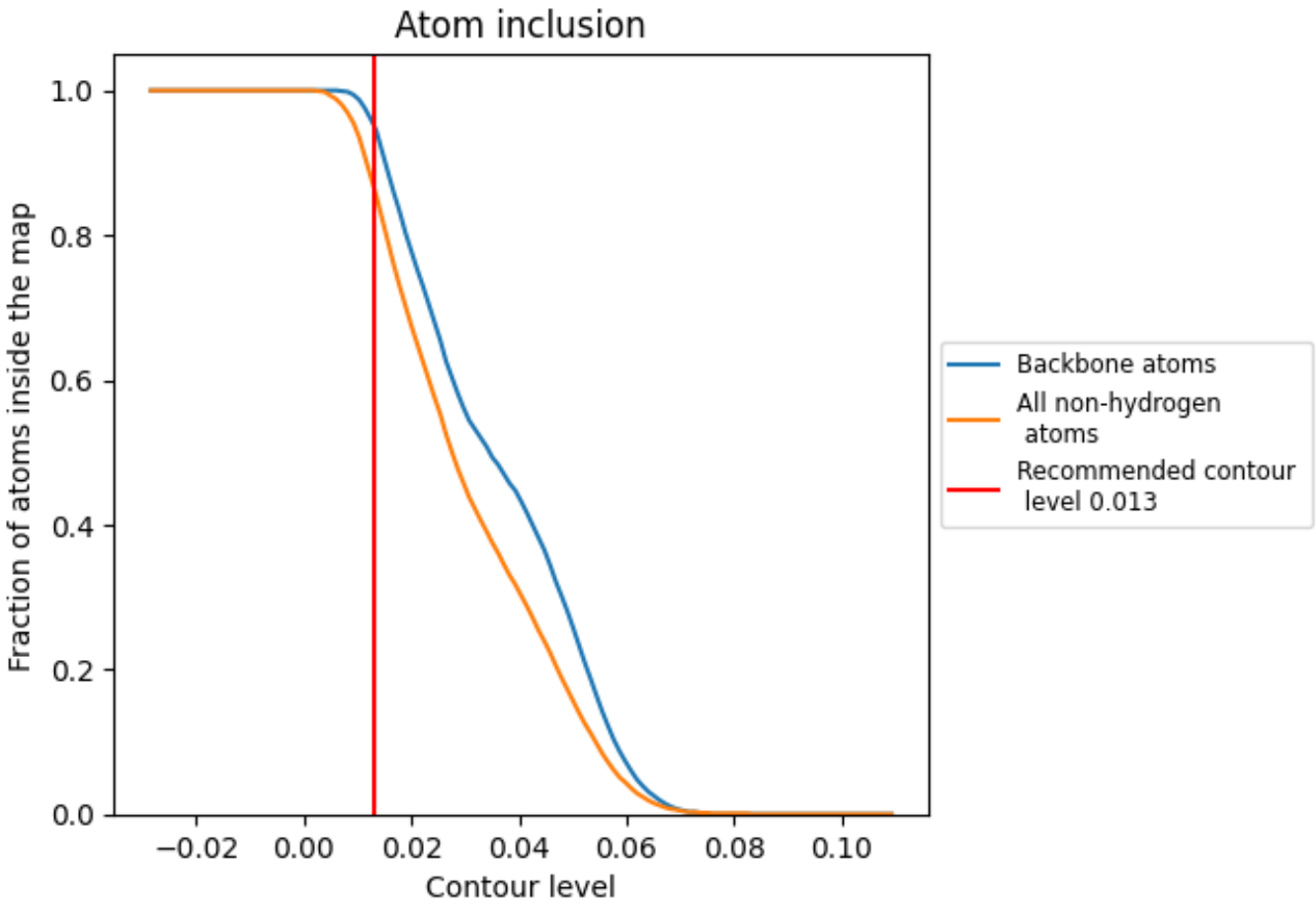
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.013).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 87% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8680	0.5120
A	0.8670	0.5120
B	0.8690	0.5120
C	0.8680	0.5130
D	0.8680	0.5130
E	0.8700	0.5130
F	0.8680	0.5120