Full wwPDB X-ray Structure Validation Report (i)

Mar 4, 2024 – 03:35 AM EST

PDB ID	:	1PK8
Title	:	Crystal Structure of Rat Synapsin I C Domain Complexed to Ca.ATP
Authors	:	Brautigam, C.A.; Chelliah, Y.; Deisenhofer, J.
Deposited on	:	2003-06-05
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
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 (i)) were used in the production of this report:

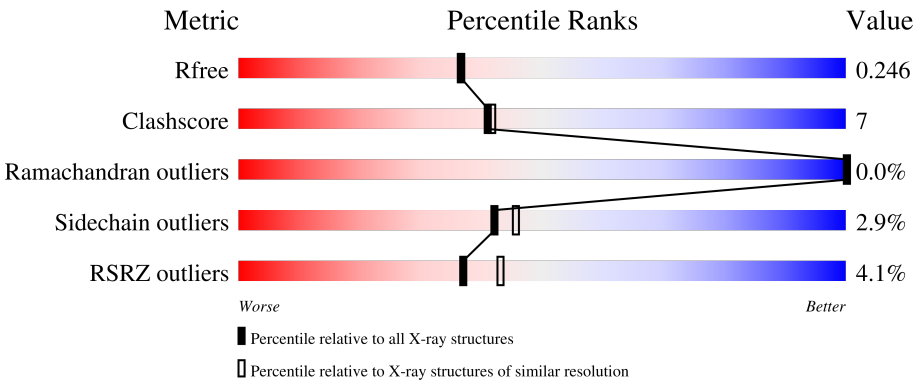
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	422	2%, 61%, 11%, 27%
1	B	422	%, 58%, 11%, 31%
1	C	422	4%, 54%, 12%, •, 32%
1	D	422	5%, 57%, 14%, 29%
1	E	422	2%, 55%, 12%, 32%

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Mol	Chain	Length	Quality of chain
1	F	422	4% 55% 12% 32%
1	G	422	4% 57% 12% 31%
1	H	422	% 54% 14% • 32%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19708 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 rat synapsin I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	306	2414	1535	417	448	14	25	0	0
1	B	292	2317	1476	397	430	14	8	0	0
1	C	285	2272	1451	389	419	13	18	0	0
1	D	300	2367	1506	406	441	14	7	0	0
1	E	286	2279	1455	390	421	13	40	0	0
1	F	286	2279	1455	390	421	13	24	0	0
1	G	293	2326	1482	399	431	14	5	0	0
1	H	286	2277	1454	390	420	13	25	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	cloning artifact	UNP P09951
A	1	SER	MET	cloning artifact	UNP P09951
B	0	GLY	-	cloning artifact	UNP P09951
B	1	SER	MET	cloning artifact	UNP P09951
C	0	GLY	-	cloning artifact	UNP P09951
C	1	SER	MET	cloning artifact	UNP P09951
D	0	GLY	-	cloning artifact	UNP P09951
D	1	SER	MET	cloning artifact	UNP P09951
E	0	GLY	-	cloning artifact	UNP P09951
E	1	SER	MET	cloning artifact	UNP P09951
F	0	GLY	-	cloning artifact	UNP P09951
F	1	SER	MET	cloning artifact	UNP P09951
G	0	GLY	-	cloning artifact	UNP P09951

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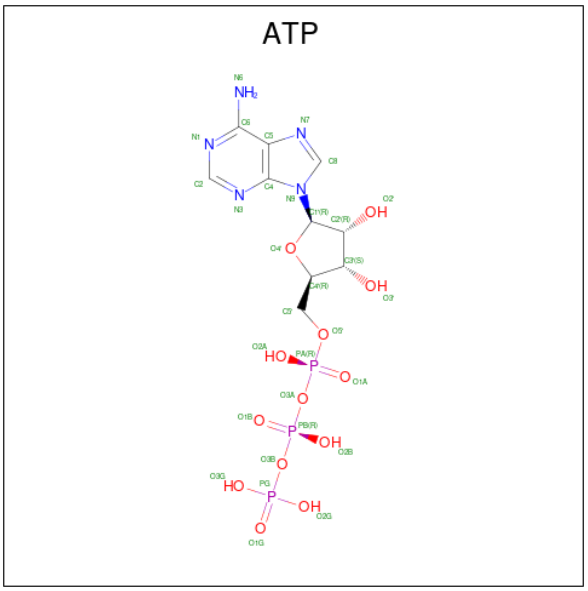
Chain	Residue	Modelled	Actual	Comment	Reference
G	1	SER	MET	cloning artifact	UNP P09951
H	0	GLY	-	cloning artifact	UNP P09951
H	1	SER	MET	cloning artifact	UNP P09951

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

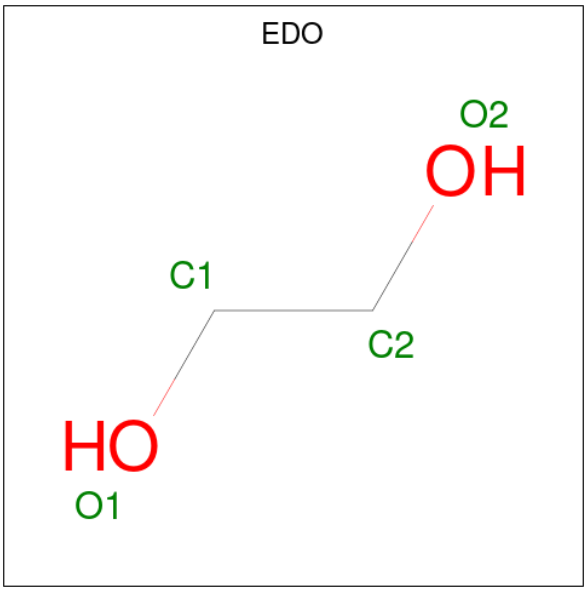
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0
2	G	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	62	20	10	26	6	0	1
3	B	1	62	20	10	26	6	0	1
3	C	1	62	20	10	26	6	0	1
3	D	1	62	20	10	26	6	0	1
3	E	1	62	20	10	26	6	0	1
3	F	1	62	20	10	26	6	0	1
3	G	1	62	20	10	26	6	0	1
3	H	1	62	20	10	26	6	0	1

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	2	2	0	0
4	B	1	4	2	2	0	0

- Molecule 5 is water.

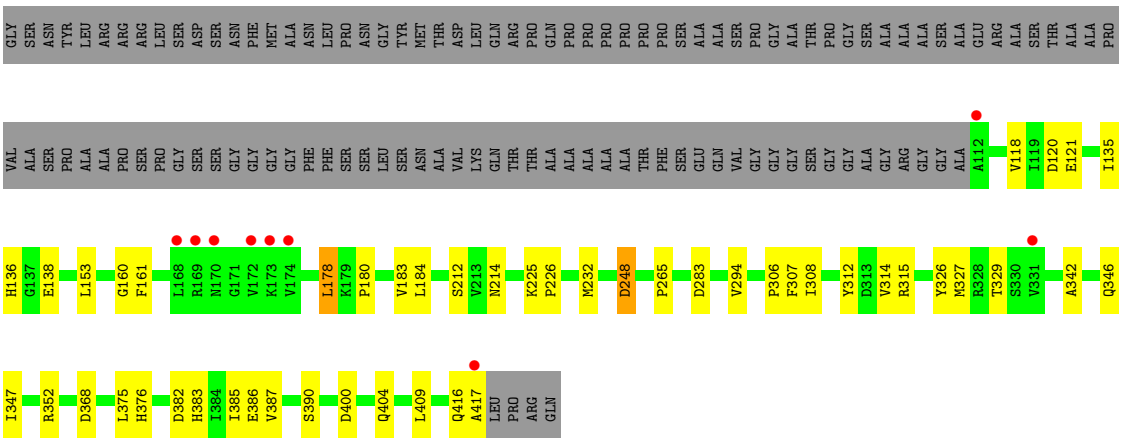
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	117	117	117	0	0
			Total	O		
5	B	127	127	127	0	0
			Total	O		
5	C	81	81	81	0	0
			Total	O		
5	D	77	77	77	0	0
			Total	O		
5	E	80	80	80	0	0
			Total	O		
5	F	39	39	39	0	0
			Total	O		
5	G	68	68	68	0	0
			Total	O		
5	H	76	76	76	0	0

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

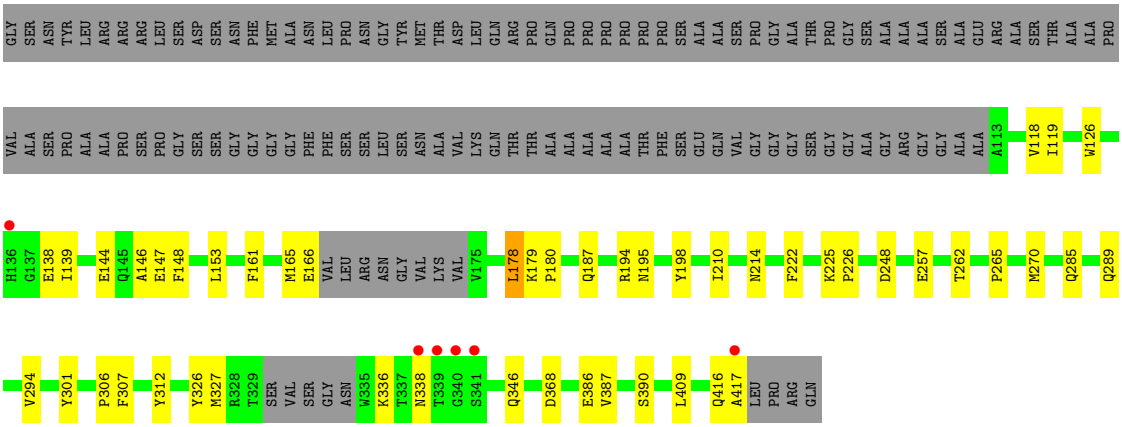
• Molecule 1: rat synapsin I

Chain A:



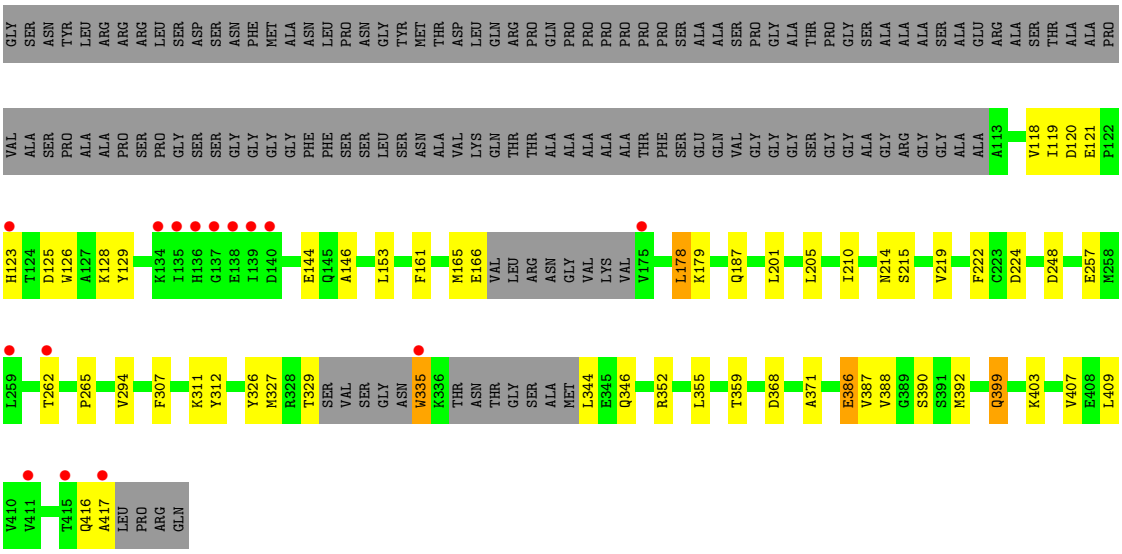
• Molecule 1: rat synapsin I

Chain B:



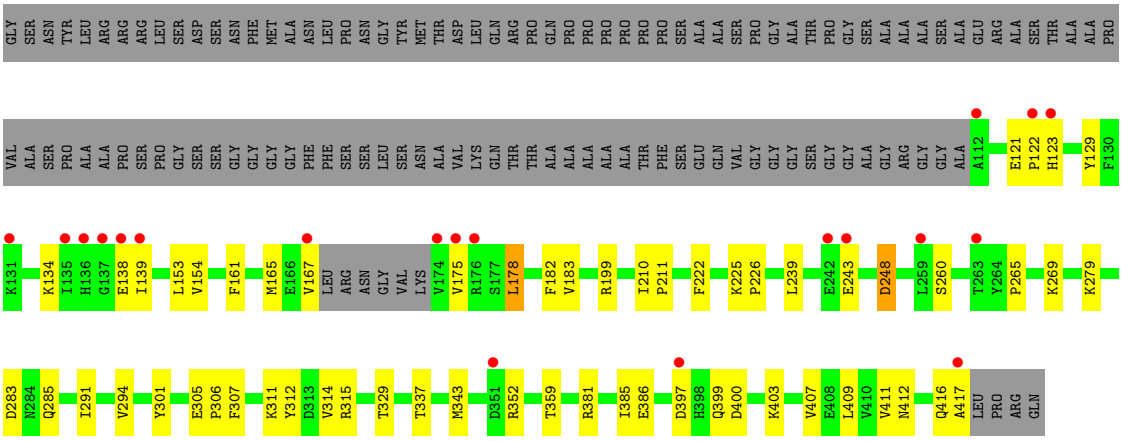
• Molecule 1: rat synapsin I

Chain C:



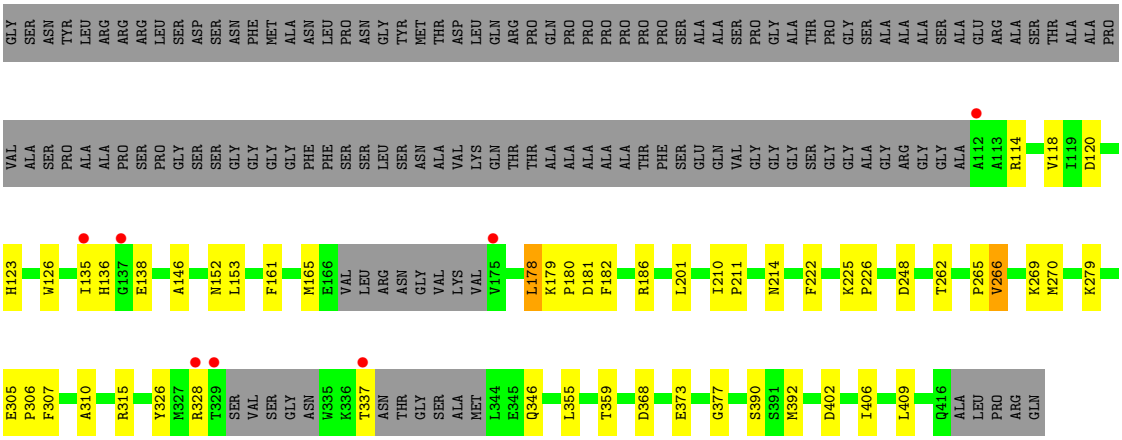
- Molecule 1: rat synapsin I

Chain D:



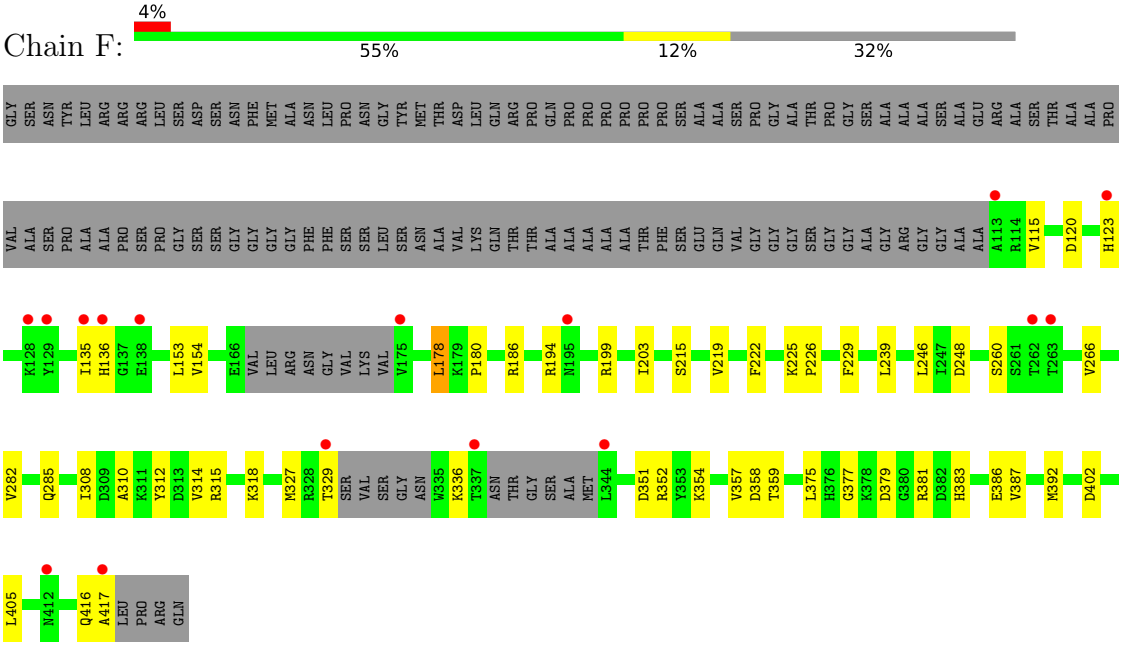
- Molecule 1: rat synapsin I

Chain E:



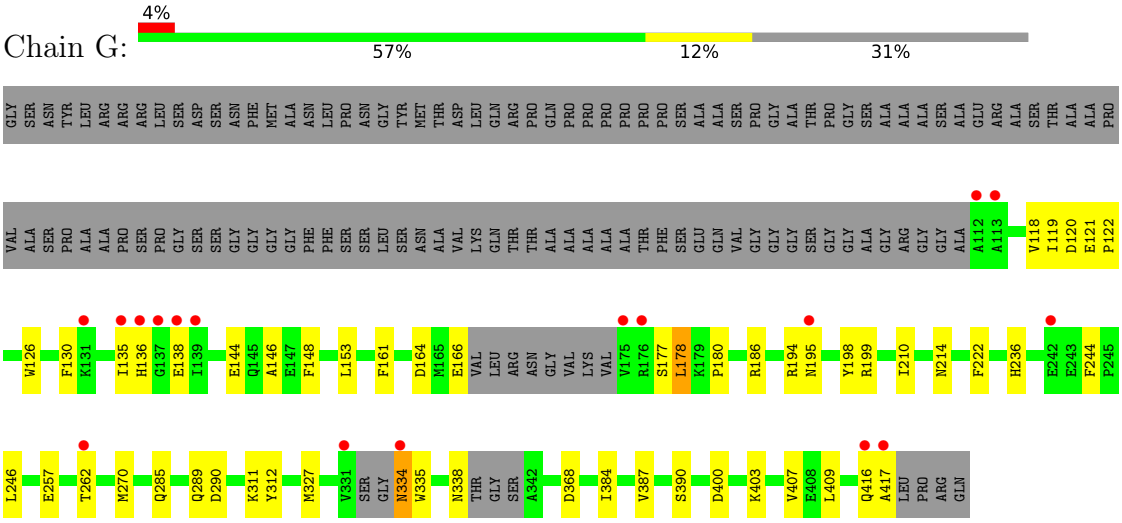
• Molecule 1: rat synapsin I

Chain F:



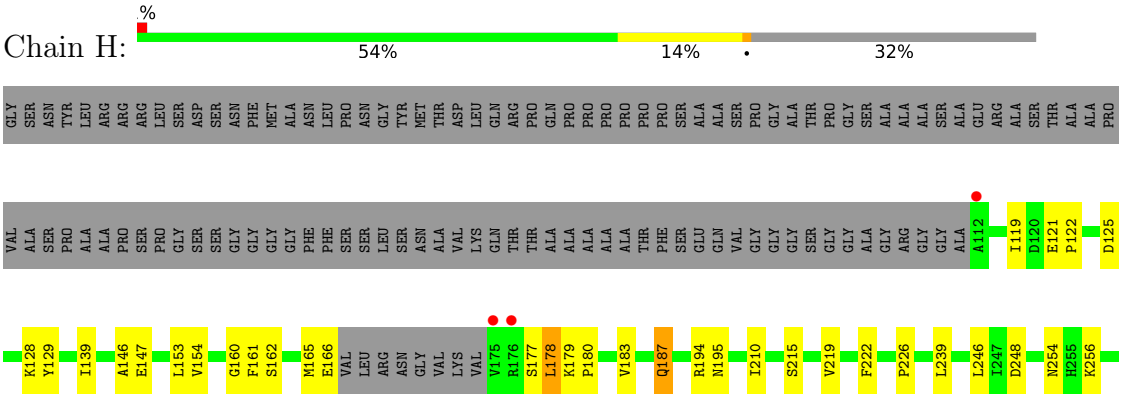
• Molecule 1: rat synapsin I

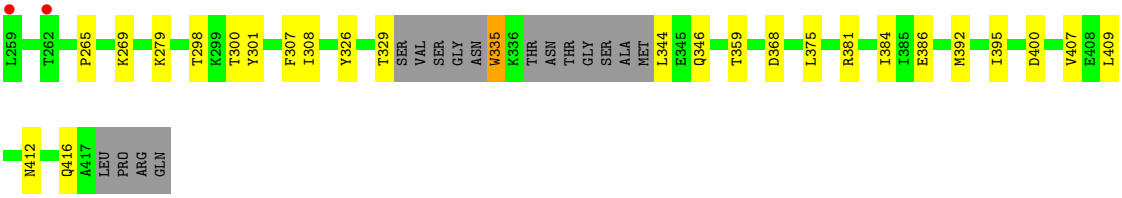
Chain G:



• Molecule 1: rat synapsin I

Chain H:




L259
T262
P265
K269
K279
T298
K299
T300
Y301
F307
I308
Y326
T329
SER
VAL
SER
GLY
ASN
W335
K336
THR
ASN
THR
GLY
SER
ALA
MET
L344
E345
Q346
T359
D368
L375
R381
I384
I385
E386
M392
I395
D400
V407
E408
L409
M412
Q416
A417
LEU
PRO
ARG
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	70.60Å 78.40Å 135.00Å 80.60° 76.90° 71.80°	Depositor
Resolution (Å)	20.00 – 2.10 37.16 – 2.09	Depositor EDS
% Data completeness (in resolution range)	91.9 (20.00-2.10) 91.5 (37.16-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.25 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.222 , 0.259 0.210 , 0.246	Depositor DCC
R_{free} test set	14970 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å^2)	27.7	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19708	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: CA, ATP, EDO

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	0.38	0/2466	0.62	0/3334
1	B	0.39	0/2367	0.64	0/3197
1	C	0.35	0/2321	0.62	0/3133
1	D	0.33	0/2418	0.61	0/3269
1	E	0.34	0/2328	0.60	0/3143
1	F	0.37	0/2328	0.61	0/3143
1	G	0.35	0/2375	0.62	0/3207
1	H	0.35	0/2326	0.60	0/3140
All	All	0.36	0/18929	0.62	0/25566

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 (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	2414	0	2397	36	0
1	B	2317	0	2289	33	0
1	C	2272	0	2246	34	0
1	D	2367	0	2341	39	0
1	E	2279	0	2253	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2279	0	2253	29	0
1	G	2326	0	2298	31	0
1	H	2277	0	2251	39	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	62	0	24	1	0
3	B	62	0	24	1	0
3	C	62	0	24	0	0
3	D	62	0	24	2	0
3	E	62	0	24	0	0
3	F	62	0	24	0	0
3	G	62	0	24	0	0
3	H	62	0	24	0	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
5	A	117	0	0	1	0
5	B	127	0	0	2	0
5	C	81	0	0	0	0
5	D	77	0	0	1	0
5	E	80	0	0	2	0
5	F	39	0	0	0	0
5	G	68	0	0	1	0
5	H	76	0	0	1	0
All	All	19708	0	18532	264	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 7.

All (264) 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:D:248:ASP:O	1:D:306:PRO:HD3	1.80	0.82
1:E:328:ARG:HD3	1:E:337:THR:HB	1.64	0.78
1:D:407:VAL:O	1:D:411:VAL:HG23	1.94	0.68
1:D:399:GLN:O	1:D:403:LYS:HG3	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:336:LYS:HE2	1:G:290:ASP:OD1	1.94	0.67
1:D:129:TYR:HB3	1:D:407:VAL:HG21	1.77	0.66
1:C:355:LEU:O	1:C:359:THR:HG23	1.96	0.66
1:E:328:ARG:HD3	1:E:337:THR:CB	2.27	0.64
1:G:403:LYS:O	1:G:407:VAL:HG23	1.98	0.63
1:C:165:MET:O	1:C:166:GLU:HB2	1.97	0.63
1:H:178:LEU:HD12	1:H:180:PRO:HG3	1.80	0.63
1:B:336:LYS:C	1:B:338:ASN:H	2.00	0.62
1:F:379:ASP:OD2	1:F:381:ARG:HD3	1.99	0.62
1:G:135:ILE:O	1:G:136:HIS:HB2	1.99	0.62
1:F:120:ASP:HB2	1:F:186:ARG:HB2	1.81	0.62
1:G:121:GLU:HB2	1:G:122:PRO:HD2	1.79	0.62
1:A:294:VAL:HG11	1:C:294:VAL:HG11	1.83	0.60
1:C:144:GLU:HG3	1:C:178:LEU:HD13	1.83	0.60
1:H:165:MET:O	1:H:166:GLU:HB2	2.01	0.60
1:C:257:GLU:HG3	1:D:153:LEU:O	2.03	0.59
1:D:161:PHE:CE2	1:D:210:ILE:HD11	2.37	0.59
1:F:115:VAL:HB	1:F:180:PRO:HA	1.84	0.59
1:H:161:PHE:CE2	1:H:210:ILE:HD11	2.38	0.59
1:F:178:LEU:HD12	1:F:180:PRO:HG3	1.85	0.59
1:G:130:PHE:CE1	1:G:407:VAL:HG13	2.38	0.59
1:A:416:GLN:O	1:A:417:ALA:HB2	2.02	0.58
1:H:269:LYS:HG2	1:H:279:LYS:HG3	1.85	0.58
1:B:144:GLU:HG3	1:B:178:LEU:HD13	1.86	0.58
1:E:355:LEU:O	1:E:359:THR:HG23	2.04	0.58
1:F:392:MET:HG3	1:F:392:MET:O	2.03	0.57
1:G:285:GLN:O	1:G:289:GLN:HG3	2.04	0.57
1:B:194:ARG:O	1:B:195:ASN:HB2	2.05	0.56
1:C:399:GLN:O	1:C:403:LYS:HG3	2.05	0.56
1:D:352:ARG:HG3	1:D:352:ARG:HH11	1.71	0.56
1:G:178:LEU:HD12	1:G:180:PRO:HG3	1.88	0.55
1:H:153:LEU:C	1:H:153:LEU:HD12	2.26	0.55
1:E:161:PHE:CE2	1:E:210:ILE:HD11	2.41	0.55
1:H:215:SER:O	1:H:219:VAL:HG23	2.07	0.55
1:D:139:ILE:HD12	1:D:139:ILE:N	2.22	0.55
1:H:226:PRO:HG2	1:H:301:TYR:CE1	2.42	0.55
1:H:368:ASP:HB3	1:H:409:LEU:HD21	1.88	0.55
1:G:148:PHE:HB3	1:G:198:TYR:CD1	2.42	0.54
1:G:130:PHE:CD1	1:G:407:VAL:HG13	2.43	0.54
1:D:121:GLU:HB2	1:D:122:PRO:HD2	1.89	0.54
1:G:257:GLU:HB3	1:H:154:VAL:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ILE:HD12	1:A:375:LEU:HD12	1.90	0.54
1:D:183:VAL:HG23	1:D:210:ILE:HG21	1.88	0.54
1:H:335:TRP:CE3	1:H:335:TRP:C	2.82	0.53
1:B:265:PRO:HG2	1:B:307:PHE:HB3	1.88	0.53
1:D:269:LYS:HG2	1:D:279:LYS:HG3	1.91	0.53
1:B:153:LEU:C	1:B:153:LEU:HD12	2.29	0.53
1:G:214:ASN:CG	1:G:390:SER:HB3	2.28	0.53
1:B:336:LYS:C	1:B:338:ASN:N	2.62	0.53
1:D:199:ARG:NH1	5:D:845:HOH:O	2.41	0.53
1:D:409:LEU:O	1:D:409:LEU:HD23	2.08	0.53
1:G:144:GLU:HG3	1:G:178:LEU:HD13	1.90	0.53
1:D:239:LEU:HD11	1:D:359:THR:HG21	1.91	0.53
1:H:139:ILE:N	1:H:139:ILE:HD12	2.24	0.53
1:A:312:TYR:CD1	1:A:327:MET:HG3	2.44	0.53
1:H:412:ASN:O	1:H:416:GLN:HG3	2.09	0.52
1:F:135:ILE:O	1:F:136:HIS:HB2	2.09	0.52
1:C:392:MET:O	1:C:392:MET:HG3	2.09	0.52
1:E:368:ASP:HB3	1:E:409:LEU:HD21	1.91	0.52
1:F:318:LYS:HB2	1:F:357:VAL:HG21	1.91	0.52
1:A:153:LEU:O	1:B:257:GLU:HG3	2.10	0.52
1:C:326:TYR:CE1	1:C:346:GLN:HB2	2.45	0.52
1:A:368:ASP:HB3	1:A:409:LEU:HD21	1.92	0.52
1:C:416:GLN:O	1:C:417:ALA:HB2	2.10	0.52
1:D:311:LYS:HE2	1:D:312:TYR:CE2	2.45	0.52
1:H:183:VAL:HG23	1:H:210:ILE:HG21	1.91	0.52
1:B:248:ASP:O	1:B:306:PRO:HD3	2.09	0.52
1:B:194:ARG:NH1	5:B:820:HOH:O	2.43	0.51
1:D:385:ILE:O	1:D:386:GLU:HB2	2.09	0.51
1:B:214:ASN:CG	1:B:390:SER:HB3	2.31	0.51
1:B:368:ASP:HB3	1:B:409:LEU:HD21	1.93	0.51
1:A:183:VAL:CG1	1:A:212:SER:HB2	2.41	0.51
1:C:125:ASP:OD2	1:C:128:LYS:HB2	2.11	0.51
1:G:153:LEU:HD12	1:G:153:LEU:C	2.31	0.51
1:B:416:GLN:O	1:B:417:ALA:HB2	2.12	0.50
1:A:327:MET:HE3	1:A:347:ILE:HG21	1.92	0.50
1:F:178:LEU:HD12	1:F:180:PRO:CG	2.41	0.50
1:H:335:TRP:C	1:H:335:TRP:HE3	2.14	0.50
1:G:119:ILE:HA	1:G:146:ALA:O	2.12	0.50
1:B:139:ILE:HD12	1:B:139:ILE:N	2.26	0.50
1:E:248:ASP:O	1:E:306:PRO:HD3	2.11	0.50
1:A:400:ASP:OD2	1:A:404:GLN:NE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ILE:HA	1:B:146:ALA:O	2.11	0.50
1:E:265:PRO:HG2	1:E:307:PHE:HB3	1.93	0.49
1:B:161:PHE:CE2	1:B:210:ILE:HD11	2.46	0.49
1:G:368:ASP:HB3	1:G:409:LEU:HD21	1.94	0.49
1:B:270:MET:HB3	5:B:848:HOH:O	2.12	0.49
1:D:305:GLU:HG3	3:D:803[B]:ATP:N6	2.27	0.49
1:E:135:ILE:O	1:E:136:HIS:HB2	2.13	0.49
1:D:260:SER:HB3	1:D:285:GLN:HE22	1.78	0.49
1:F:153:LEU:C	1:F:153:LEU:HD12	2.32	0.49
1:H:195:ASN:HA	5:H:836:HOH:O	2.12	0.49
1:E:182:PHE:CD2	1:E:211:PRO:HB2	2.47	0.49
1:E:315:ARG:HG3	1:E:373:GLU:HG2	1.95	0.49
1:B:139:ILE:HD12	1:B:139:ILE:H	1.77	0.49
1:B:294:VAL:HG11	1:D:294:VAL:HG11	1.95	0.49
1:C:119:ILE:HA	1:C:146:ALA:O	2.13	0.48
1:E:178:LEU:N	1:E:178:LEU:HD23	2.28	0.48
1:E:225:LYS:HB2	1:E:226:PRO:HD3	1.95	0.48
1:A:265:PRO:HG2	1:A:307:PHE:HB3	1.94	0.48
1:A:329:THR:O	1:A:342:ALA:HB1	2.14	0.48
1:A:386:GLU:HG2	1:A:387:VAL:N	2.28	0.48
1:C:352:ARG:HH11	1:C:352:ARG:HG3	1.77	0.48
1:H:254:ASN:OD1	1:H:256:LYS:HB2	2.14	0.48
1:H:392:MET:O	1:H:392:MET:HG3	2.14	0.48
1:B:178:LEU:N	1:B:178:LEU:HD23	2.29	0.48
1:D:225:LYS:HB2	1:D:226:PRO:HD3	1.94	0.48
1:D:305:GLU:HG3	3:D:803[B]:ATP:HN61	1.79	0.48
1:A:385:ILE:O	1:A:386:GLU:HB2	2.14	0.48
1:H:121:GLU:HB2	1:H:122:PRO:HD2	1.95	0.47
1:F:225:LYS:HB2	1:F:226:PRO:HD3	1.95	0.47
1:C:153:LEU:C	1:C:153:LEU:HD12	2.34	0.47
1:D:134:LYS:HE2	1:D:138:GLU:HA	1.96	0.47
1:G:118:VAL:HG11	1:G:126:TRP:CD1	2.50	0.47
1:H:125:ASP:O	1:H:128:LYS:HB3	2.15	0.47
1:F:416:GLN:O	1:F:417:ALA:HB2	2.13	0.47
1:A:178:LEU:HD12	1:A:180:PRO:HG3	1.97	0.47
1:F:153:LEU:HD12	1:F:154:VAL:N	2.30	0.47
1:A:376:HIS:ND1	1:A:382:ASP:OD1	2.45	0.47
1:H:147:GLU:HG2	1:H:187:GLN:HE22	1.80	0.47
1:C:118:VAL:HG11	1:C:126:TRP:CD1	2.50	0.47
1:F:308:ILE:HD12	1:F:375:LEU:HD12	1.97	0.46
1:A:214:ASN:CG	1:A:390:SER:HB3	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:409:LEU:HD23	1:D:409:LEU:C	2.36	0.46
1:F:266:VAL:HG12	1:F:282:VAL:HB	1.98	0.46
1:A:386:GLU:HG3	5:A:885:HOH:O	2.16	0.46
1:E:402:ASP:O	1:E:406:ILE:HG13	2.16	0.46
1:F:199:ARG:O	1:F:203:ILE:HG13	2.15	0.46
1:H:239:LEU:HD11	1:H:359:THR:HG21	1.97	0.46
1:H:265:PRO:HG2	1:H:307:PHE:HB3	1.96	0.46
1:G:246:LEU:HA	1:G:384:ILE:HB	1.97	0.46
1:B:161:PHE:CZ	1:B:179:LYS:HG2	2.50	0.46
1:C:371:ALA:HB3	1:C:388:VAL:CG2	2.46	0.46
1:A:265:PRO:HB3	1:A:283:ASP:HA	1.98	0.46
1:B:225:LYS:HE2	1:B:386:GLU:OE1	2.16	0.46
1:E:120:ASP:HB2	1:E:186:ARG:HB2	1.98	0.46
1:C:129:TYR:HB3	1:C:407:VAL:HG21	1.97	0.46
1:D:183:VAL:HG23	1:D:210:ILE:CG2	2.46	0.46
1:E:146:ALA:HB2	1:E:165:MET:SD	2.55	0.46
1:B:312:TYR:CD1	1:B:327:MET:HG3	2.50	0.46
1:D:265:PRO:HG2	1:D:307:PHE:HB3	1.98	0.46
1:G:257:GLU:OE1	1:H:154:VAL:HG23	2.16	0.46
1:D:182:PHE:CD2	1:D:211:PRO:HB2	2.50	0.45
1:G:195:ASN:N	1:G:195:ASN:HD22	2.14	0.45
1:G:416:GLN:O	1:G:417:ALA:HB2	2.15	0.45
1:H:125:ASP:OD2	1:H:128:LYS:HB2	2.15	0.45
1:B:338:ASN:HB2	3:B:801[B]:ATP:H4'	1.98	0.45
1:A:153:LEU:C	1:A:153:LEU:HD12	2.36	0.45
1:C:224:ASP:OD2	1:D:199:ARG:NH2	2.50	0.45
1:D:311:LYS:HE2	1:D:312:TYR:HE2	1.81	0.45
1:F:215:SER:O	1:F:219:VAL:HG23	2.17	0.45
1:A:135:ILE:O	1:A:136:HIS:HB2	2.17	0.45
1:B:161:PHE:CE1	1:B:179:LYS:HE2	2.52	0.45
1:E:248:ASP:O	1:E:306:PRO:CD	2.64	0.45
1:A:352:ARG:HG3	1:A:352:ARG:HH11	1.81	0.45
1:G:120:ASP:HB2	1:G:186:ARG:HB2	1.98	0.45
1:H:183:VAL:HG23	1:H:210:ILE:CG2	2.47	0.45
1:D:314:VAL:HG12	1:D:315:ARG:N	2.32	0.45
1:G:148:PHE:HB3	1:G:198:TYR:CG	2.52	0.45
1:H:308:ILE:HD12	1:H:375:LEU:HD12	1.99	0.45
1:F:402:ASP:HA	1:F:405:LEU:HD12	1.99	0.45
1:H:165:MET:O	1:H:166:GLU:CB	2.65	0.45
1:E:326:TYR:CE1	1:E:346:GLN:HB2	2.52	0.45
1:A:308:ILE:HD13	1:A:383:HIS:CG	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:239:LEU:HD11	1:F:359:THR:HG21	1.98	0.44
1:H:246:LEU:HA	1:H:384:ILE:HB	1.99	0.44
1:A:375:LEU:HD11	3:A:800[B]:ATP:C5	2.52	0.44
1:F:260:SER:HB3	1:F:285:GLN:OE1	2.17	0.44
1:G:199:ARG:HH11	1:G:199:ARG:HG2	1.81	0.44
1:H:298:THR:OG1	1:H:300:THR:HG22	2.16	0.44
1:B:118:VAL:HG11	1:B:126:TRP:CD1	2.52	0.44
1:H:119:ILE:HA	1:H:146:ALA:O	2.17	0.44
1:B:178:LEU:HD12	1:B:180:PRO:HG3	2.00	0.44
1:E:181:ASP:O	1:E:211:PRO:HD2	2.18	0.44
1:F:310:ALA:HA	1:F:377:GLY:HA2	1.99	0.44
1:C:161:PHE:O	1:C:179:LYS:HE2	2.18	0.44
1:E:269:LYS:HG2	1:E:279:LYS:CG	2.48	0.44
1:B:285:GLN:HG3	1:B:289:GLN:NE2	2.33	0.44
1:E:214:ASN:CG	1:E:390:SER:HB3	2.38	0.44
1:B:386:GLU:HG2	1:B:387:VAL:N	2.32	0.44
1:C:312:TYR:CD1	1:C:327:MET:HG3	2.53	0.44
1:H:129:TYR:HB3	1:H:407:VAL:HG21	1.99	0.44
1:C:201:LEU:O	1:C:205:LEU:HG	2.17	0.43
1:C:344:LEU:HD23	1:C:344:LEU:HA	1.73	0.43
1:D:265:PRO:HB3	1:D:283:ASP:HA	2.00	0.43
1:B:148:PHE:HB3	1:B:198:TYR:CD1	2.53	0.43
1:G:164:ASP:OD1	1:G:177:SER:HB3	2.18	0.43
1:F:194:ARG:HG2	1:F:194:ARG:HH11	1.83	0.43
1:G:270:MET:HB3	5:G:844:HOH:O	2.18	0.43
1:C:121:GLU:HB3	1:C:123:HIS:CD2	2.53	0.43
1:D:178:LEU:N	1:D:178:LEU:HD23	2.33	0.43
1:A:248:ASP:O	1:A:306:PRO:HD3	2.18	0.43
1:F:312:TYR:CD1	1:F:327:MET:HG3	2.54	0.43
1:D:165:MET:HG2	1:D:167:VAL:HG23	2.00	0.43
1:C:311:LYS:O	1:C:312:TYR:HB3	2.18	0.43
1:G:334:ASN:HB3	1:G:335:TRP:H	1.65	0.43
1:A:120:ASP:OD1	1:A:121:GLU:N	2.48	0.43
1:C:215:SER:O	1:C:219:VAL:HG23	2.18	0.43
1:A:160:GLY:O	1:A:161:PHE:HB3	2.19	0.42
1:A:416:GLN:O	1:A:417:ALA:CB	2.67	0.42
1:F:314:VAL:HG12	1:F:315:ARG:N	2.34	0.42
1:A:314:VAL:HG22	1:A:315:ARG:N	2.35	0.42
1:F:318:LYS:HB2	1:F:357:VAL:CG2	2.49	0.42
1:A:118:VAL:HG13	1:A:184:LEU:HD23	2.01	0.42
1:A:326:TYR:CE1	1:A:346:GLN:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:GLU:OE1	1:D:154:VAL:CG2	2.68	0.42
1:B:165:MET:O	1:B:166:GLU:HB2	2.18	0.42
1:C:161:PHE:CE2	1:C:210:ILE:HD11	2.53	0.42
1:E:161:PHE:CZ	1:E:179:LYS:HG2	2.54	0.42
1:E:310:ALA:HA	1:E:377:GLY:HA2	2.01	0.42
1:G:161:PHE:CE2	1:G:210:ILE:HD11	2.55	0.42
1:B:226:PRO:HG2	1:B:301:TYR:CE1	2.55	0.42
1:C:368:ASP:HB3	1:C:409:LEU:HD21	2.00	0.42
1:H:344:LEU:HD11	1:H:395:ILE:HB	2.00	0.42
1:D:381:ARG:HE	1:D:381:ARG:HB2	1.53	0.42
1:D:416:GLN:O	1:D:417:ALA:HB2	2.20	0.42
1:F:354:LYS:HG2	1:F:358:ASP:OD2	2.20	0.42
1:G:312:TYR:CD1	1:G:327:MET:HG3	2.55	0.42
1:A:248:ASP:O	1:A:306:PRO:CD	2.67	0.41
1:D:226:PRO:HG2	1:D:301:TYR:CE1	2.55	0.41
1:C:120:ASP:OD1	1:C:121:GLU:N	2.53	0.41
1:E:152:ASN:HA	1:E:201:LEU:HD21	2.02	0.41
1:G:236:HIS:HD2	1:G:244:PHE:O	2.03	0.41
1:A:232:MET:HE2	1:A:386:GLU:HA	2.01	0.41
1:G:257:GLU:HB3	1:H:154:VAL:CG2	2.50	0.41
1:A:386:GLU:CG	1:A:387:VAL:N	2.83	0.41
1:C:335:TRP:HE3	1:C:335:TRP:C	2.24	0.41
1:D:291:ILE:HD13	1:D:291:ILE:HA	1.91	0.41
1:C:214:ASN:CG	1:C:390:SER:HB3	2.41	0.41
1:E:182:PHE:CE2	1:E:211:PRO:HB2	2.56	0.41
1:E:210:ILE:HA	1:E:211:PRO:HD3	1.91	0.41
1:H:161:PHE:O	1:H:179:LYS:HE2	2.20	0.41
1:H:194:ARG:O	1:H:195:ASN:HB2	2.21	0.41
1:C:335:TRP:C	1:C:335:TRP:CE3	2.94	0.41
1:E:178:LEU:HD12	1:E:180:PRO:HG3	2.03	0.41
1:G:311:LYS:HE3	1:G:311:LYS:HB2	1.91	0.41
1:E:153:LEU:HD12	1:E:153:LEU:C	2.41	0.41
1:E:392:MET:O	1:E:392:MET:HG3	2.20	0.41
1:D:175:VAL:O	1:D:175:VAL:HG12	2.20	0.41
1:D:260:SER:CB	1:D:285:GLN:HE22	2.34	0.41
1:E:266:VAL:HG22	1:E:305:GLU:O	2.20	0.41
1:F:386:GLU:HG2	1:F:387:VAL:N	2.35	0.41
1:H:162:SER:OG	1:H:177:SER:HB2	2.20	0.41
1:H:326:TYR:CE1	1:H:346:GLN:HB2	2.56	0.41
1:F:229:PHE:CZ	1:F:246:LEU:HD11	2.56	0.41
1:F:308:ILE:HD13	1:F:383:HIS:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:160:GLY:O	1:H:161:PHE:HB3	2.19	0.41
1:A:232:MET:CE	1:A:386:GLU:HA	2.52	0.40
1:C:265:PRO:HG2	1:C:307:PHE:HB3	2.03	0.40
1:H:129:TYR:OH	1:H:400:ASP:OD1	2.30	0.40
1:A:183:VAL:HG12	1:A:212:SER:HB2	2.03	0.40
1:B:326:TYR:CE1	1:B:346:GLN:HB2	2.57	0.40
1:C:144:GLU:CG	1:C:178:LEU:HD13	2.50	0.40
1:E:118:VAL:HG11	1:E:126:TRP:CD1	2.56	0.40
1:E:270:MET:HB3	5:E:885:HOH:O	2.20	0.40
1:B:147:GLU:HG2	1:B:187:GLN:HE22	1.86	0.40
1:E:269:LYS:HG2	1:E:279:LYS:HG3	2.03	0.40
1:E:377:GLY:HA3	5:E:831:HOH:O	2.22	0.40
1:A:225:LYS:HB2	1:A:226:PRO:HD3	2.04	0.40
1:C:386:GLU:HG3	1:C:387:VAL:N	2.36	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 X-ray entries followed by that with respect to entries of similar resolution.

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	304/422 (72%)	297 (98%)	7 (2%)	0	100	100
1	B	286/422 (68%)	282 (99%)	4 (1%)	0	100	100
1	C	277/422 (66%)	272 (98%)	5 (2%)	0	100	100
1	D	296/422 (70%)	288 (97%)	7 (2%)	1 (0%)	41	41
1	E	278/422 (66%)	271 (98%)	7 (2%)	0	100	100
1	F	278/422 (66%)	270 (97%)	8 (3%)	0	100	100
1	G	285/422 (68%)	279 (98%)	6 (2%)	0	100	100
1	H	278/422 (66%)	271 (98%)	7 (2%)	0	100	100
All	All	2282/3376 (68%)	2230 (98%)	51 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	337	THR

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 X-ray entries followed by that with respect to entries of similar resolution.

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	263/340 (77%)	260 (99%)	3 (1%)	73	79
1	B	252/340 (74%)	248 (98%)	4 (2%)	62	69
1	C	247/340 (73%)	238 (96%)	9 (4%)	35	36
1	D	258/340 (76%)	248 (96%)	10 (4%)	32	33
1	E	248/340 (73%)	241 (97%)	7 (3%)	43	47
1	F	248/340 (73%)	241 (97%)	7 (3%)	43	47
1	G	253/340 (74%)	243 (96%)	10 (4%)	31	32
1	H	247/340 (73%)	239 (97%)	8 (3%)	39	41
All	All	2016/2720 (74%)	1958 (97%)	58 (3%)	42	46

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	GLU
1	A	178	LEU
1	A	248	ASP
1	B	138	GLU
1	B	178	LEU
1	B	222	PHE
1	B	262	THR
1	C	178	LEU
1	C	187	GLN
1	C	222	PHE
1	C	248	ASP
1	C	262	THR
1	C	329	THR

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Mol	Chain	Res	Type
1	C	335	TRP
1	C	386	GLU
1	C	399	GLN
1	D	123	HIS
1	D	178	LEU
1	D	222	PHE
1	D	243	GLU
1	D	248	ASP
1	D	329	THR
1	D	343	MET
1	D	397	ASP
1	D	400	ASP
1	D	412	ASN
1	E	114	ARG
1	E	123	HIS
1	E	138	GLU
1	E	178	LEU
1	E	222	PHE
1	E	262	THR
1	E	266	VAL
1	F	123	HIS
1	F	178	LEU
1	F	222	PHE
1	F	248	ASP
1	F	329	THR
1	F	351	ASP
1	F	352	ARG
1	G	138	GLU
1	G	166	GLU
1	G	178	LEU
1	G	194	ARG
1	G	222	PHE
1	G	262	THR
1	G	334	ASN
1	G	338	ASN
1	G	387	VAL
1	G	400	ASP
1	H	178	LEU
1	H	187	GLN
1	H	222	PHE
1	H	248	ASP
1	H	329	THR

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Mol	Chain	Res	Type
1	H	335	TRP
1	H	381	ARG
1	H	386	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	ASN
1	A	383	HIS
1	B	236	HIS
1	B	289	GLN
1	B	338	ASN
1	B	383	HIS
1	B	404	GLN
1	C	255	HIS
1	D	195	ASN
1	D	399	GLN
1	E	195	ASN
1	E	383	HIS
1	E	404	GLN
1	F	217	HIS
1	F	399	GLN
1	G	195	ASN
1	G	334	ASN
1	G	338	ASN
1	H	383	HIS

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 26 ligands modelled in this entry, 8 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	$\#\|Z\| > 2$
3	ATP	A	800[A]	2	26,33,33	0.78	0	31,52,52	0.98	2 (6%)
3	ATP	B	801[B]	2	26,33,33	0.79	0	31,52,52	0.99	4 (12%)
3	ATP	A	800[B]	2	26,33,33	0.84	0	31,52,52	0.98	2 (6%)
3	ATP	D	803[A]	2	26,33,33	0.77	0	31,52,52	0.98	3 (9%)
3	ATP	E	804[A]	2	26,33,33	0.83	0	31,52,52	1.01	4 (12%)
4	EDO	A	818	-	3,3,3	0.91	0	2,2,2	0.41	0
3	ATP	E	804[B]	2	26,33,33	0.80	0	31,52,52	0.97	3 (9%)
3	ATP	B	801[A]	2	26,33,33	0.79	0	31,52,52	0.98	3 (9%)
3	ATP	H	807[B]	2	26,33,33	0.80	0	31,52,52	0.97	4 (12%)
3	ATP	C	802[A]	2	26,33,33	0.77	0	31,52,52	1.00	4 (12%)
3	ATP	C	802[B]	2	26,33,33	0.80	0	31,52,52	0.98	4 (12%)
3	ATP	G	806[B]	2	26,33,33	0.80	0	31,52,52	0.99	3 (9%)
3	ATP	H	807[A]	2	26,33,33	0.78	0	31,52,52	0.98	4 (12%)
4	EDO	B	819	-	3,3,3	0.63	0	2,2,2	0.43	0
3	ATP	F	805[B]	2	26,33,33	0.82	0	31,52,52	0.99	4 (12%)
3	ATP	G	806[A]	2	26,33,33	0.81	0	31,52,52	0.97	3 (9%)
3	ATP	F	805[A]	2	26,33,33	0.80	0	31,52,52	0.97	3 (9%)
3	ATP	D	803[B]	2	26,33,33	0.80	0	31,52,52	0.98	3 (9%)

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	ATP	A	800[A]	2	-	0/18/38/38	0/3/3/3
3	ATP	B	801[B]	2	-	7/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	800[B]	2	-	6/18/38/38	0/3/3/3
3	ATP	D	803[A]	2	-	0/18/38/38	0/3/3/3
3	ATP	E	804[A]	2	-	0/18/38/38	0/3/3/3
4	EDO	A	818	-	-	0/1/1/1	-
3	ATP	E	804[B]	2	-	3/18/38/38	0/3/3/3
3	ATP	B	801[A]	2	-	0/18/38/38	0/3/3/3
3	ATP	H	807[B]	2	-	2/18/38/38	0/3/3/3
3	ATP	C	802[A]	2	-	2/18/38/38	0/3/3/3
3	ATP	C	802[B]	2	-	1/18/38/38	0/3/3/3
3	ATP	G	806[B]	2	-	5/18/38/38	0/3/3/3
3	ATP	H	807[A]	2	-	2/18/38/38	0/3/3/3
4	EDO	B	819	-	-	1/1/1/1	-
3	ATP	F	805[B]	2	-	3/18/38/38	0/3/3/3
3	ATP	G	806[A]	2	-	0/18/38/38	0/3/3/3
3	ATP	F	805[A]	2	-	0/18/38/38	0/3/3/3
3	ATP	D	803[B]	2	-	4/18/38/38	0/3/3/3

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	800[A]	ATP	C5-C6-N6	2.55	124.23	120.35
3	E	804[A]	ATP	O3G-PG-O2G	-2.35	98.66	107.64
3	A	800[B]	ATP	C5-C6-N6	2.32	123.88	120.35
3	D	803[A]	ATP	C5-C6-N6	2.31	123.86	120.35
3	E	804[B]	ATP	C5-C6-N6	2.27	123.81	120.35
3	A	800[B]	ATP	O3G-PG-O2G	-2.26	99.00	107.64
3	H	807[A]	ATP	C5-C6-N6	2.25	123.78	120.35
3	D	803[B]	ATP	C5-C6-N6	2.25	123.77	120.35
3	G	806[A]	ATP	C5-C6-N6	2.24	123.76	120.35
3	C	802[A]	ATP	O3G-PG-O2G	-2.24	99.06	107.64
3	H	807[B]	ATP	C5-C6-N6	2.24	123.75	120.35
3	C	802[B]	ATP	C5-C6-N6	2.23	123.74	120.35
3	E	804[A]	ATP	C5-C6-N6	2.23	123.74	120.35
3	F	805[B]	ATP	C5-C6-N6	2.23	123.74	120.35
3	G	806[B]	ATP	C5-C6-N6	2.23	123.74	120.35
3	C	802[A]	ATP	C5-C6-N6	2.21	123.72	120.35
3	E	804[A]	ATP	O2G-PG-O1G	2.20	119.29	110.68
3	B	801[B]	ATP	C5-C6-N6	2.19	123.69	120.35
3	H	807[A]	ATP	O3G-PG-O2G	-2.16	99.38	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	805[A]	ATP	C5-C6-N6	2.16	123.63	120.35
3	F	805[A]	ATP	O2G-PG-O1G	2.13	119.03	110.68
3	B	801[B]	ATP	O3G-PG-O2G	-2.13	99.51	107.64
3	C	802[A]	ATP	O2G-PG-O1G	2.10	118.92	110.68
3	C	802[B]	ATP	O3G-PG-O2G	-2.10	99.61	107.64
3	D	803[A]	ATP	O3G-PG-O1G	2.10	118.88	110.68
3	H	807[A]	ATP	O2G-PG-O1G	2.09	118.87	110.68
3	F	805[B]	ATP	O3G-PG-O1G	2.09	118.87	110.68
3	D	803[B]	ATP	O2G-PG-O1G	2.08	118.84	110.68
3	E	804[A]	ATP	O3G-PG-O1G	2.08	118.84	110.68
3	C	802[A]	ATP	O3G-PG-O1G	2.08	118.84	110.68
3	G	806[B]	ATP	O3G-PG-O1G	2.07	118.80	110.68
3	H	807[B]	ATP	O3G-PG-O2G	-2.07	99.73	107.64
3	B	801[B]	ATP	O2G-PG-O1G	2.06	118.76	110.68
3	E	804[B]	ATP	O3G-PG-O1G	2.06	118.76	110.68
3	C	802[B]	ATP	O3G-PG-O1G	2.06	118.75	110.68
3	D	803[A]	ATP	O2G-PG-O1G	2.06	118.75	110.68
3	F	805[B]	ATP	O3G-PG-O2G	-2.06	99.76	107.64
3	G	806[A]	ATP	O3G-PG-O2G	-2.06	99.77	107.64
3	D	803[B]	ATP	O3G-PG-O1G	2.06	118.73	110.68
3	H	807[B]	ATP	O3G-PG-O1G	2.06	118.73	110.68
3	F	805[A]	ATP	O3G-PG-O1G	2.06	118.73	110.68
3	B	801[A]	ATP	O2G-PG-O1G	2.05	118.73	110.68
3	F	805[B]	ATP	O2G-PG-O1G	2.05	118.71	110.68
3	B	801[A]	ATP	C5-C6-N6	2.05	123.47	120.35
3	B	801[B]	ATP	O3G-PG-O1G	2.05	118.70	110.68
3	C	802[B]	ATP	O2G-PG-O1G	2.05	118.69	110.68
3	G	806[A]	ATP	O3G-PG-O1G	2.04	118.67	110.68
3	A	800[A]	ATP	O2G-PG-O1G	2.04	118.65	110.68
3	H	807[A]	ATP	O3G-PG-O1G	2.03	118.63	110.68
3	G	806[B]	ATP	O3G-PG-O2G	-2.03	99.88	107.64
3	B	801[A]	ATP	O3G-PG-O1G	2.02	118.60	110.68
3	H	807[B]	ATP	O2G-PG-O1G	2.02	118.60	110.68
3	E	804[B]	ATP	O2G-PG-O1G	2.00	118.52	110.68

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	800[B]	ATP	PB-O3B-PG-O3G
3	B	801[B]	ATP	PB-O3B-PG-O3G
3	C	802[A]	ATP	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
3	E	804[B]	ATP	PB-O3B-PG-O3G
3	F	805[B]	ATP	PB-O3B-PG-O3G
3	G	806[B]	ATP	PB-O3B-PG-O3G
3	H	807[A]	ATP	PB-O3B-PG-O2G
3	H	807[B]	ATP	PB-O3B-PG-O3G
3	A	800[B]	ATP	PB-O3B-PG-O1G
3	C	802[A]	ATP	PB-O3B-PG-O1G
3	F	805[B]	ATP	PB-O3B-PG-O1G
3	G	806[B]	ATP	PA-O3A-PB-O1B
3	A	800[B]	ATP	O4'-C4'-C5'-O5'
4	B	819	EDO	O1-C1-C2-O2
3	D	803[B]	ATP	PA-O3A-PB-O2B
3	G	806[B]	ATP	PA-O3A-PB-O2B
3	D	803[B]	ATP	C4'-C5'-O5'-PA
3	H	807[A]	ATP	PB-O3B-PG-O1G
3	G	806[B]	ATP	C4'-C5'-O5'-PA
3	B	801[B]	ATP	PA-O3A-PB-O1B
3	B	801[B]	ATP	PA-O3A-PB-O2B
3	F	805[B]	ATP	PA-O3A-PB-O2B
3	B	801[B]	ATP	C4'-C5'-O5'-PA
3	A	800[B]	ATP	C3'-C4'-C5'-O5'
3	B	801[B]	ATP	PB-O3B-PG-O1G
3	E	804[B]	ATP	PB-O3B-PG-O1G
3	H	807[B]	ATP	PB-O3B-PG-O1G
3	B	801[B]	ATP	PB-O3B-PG-O2G
3	C	802[B]	ATP	PB-O3B-PG-O2G
3	E	804[B]	ATP	PB-O3B-PG-O2G
3	B	801[B]	ATP	C5'-O5'-PA-O3A
3	D	803[B]	ATP	C5'-O5'-PA-O3A
3	G	806[B]	ATP	C5'-O5'-PA-O3A
3	A	800[B]	ATP	PA-O3A-PB-O2B
3	D	803[B]	ATP	PA-O3A-PB-O1B
3	A	800[B]	ATP	C4'-C5'-O5'-PA

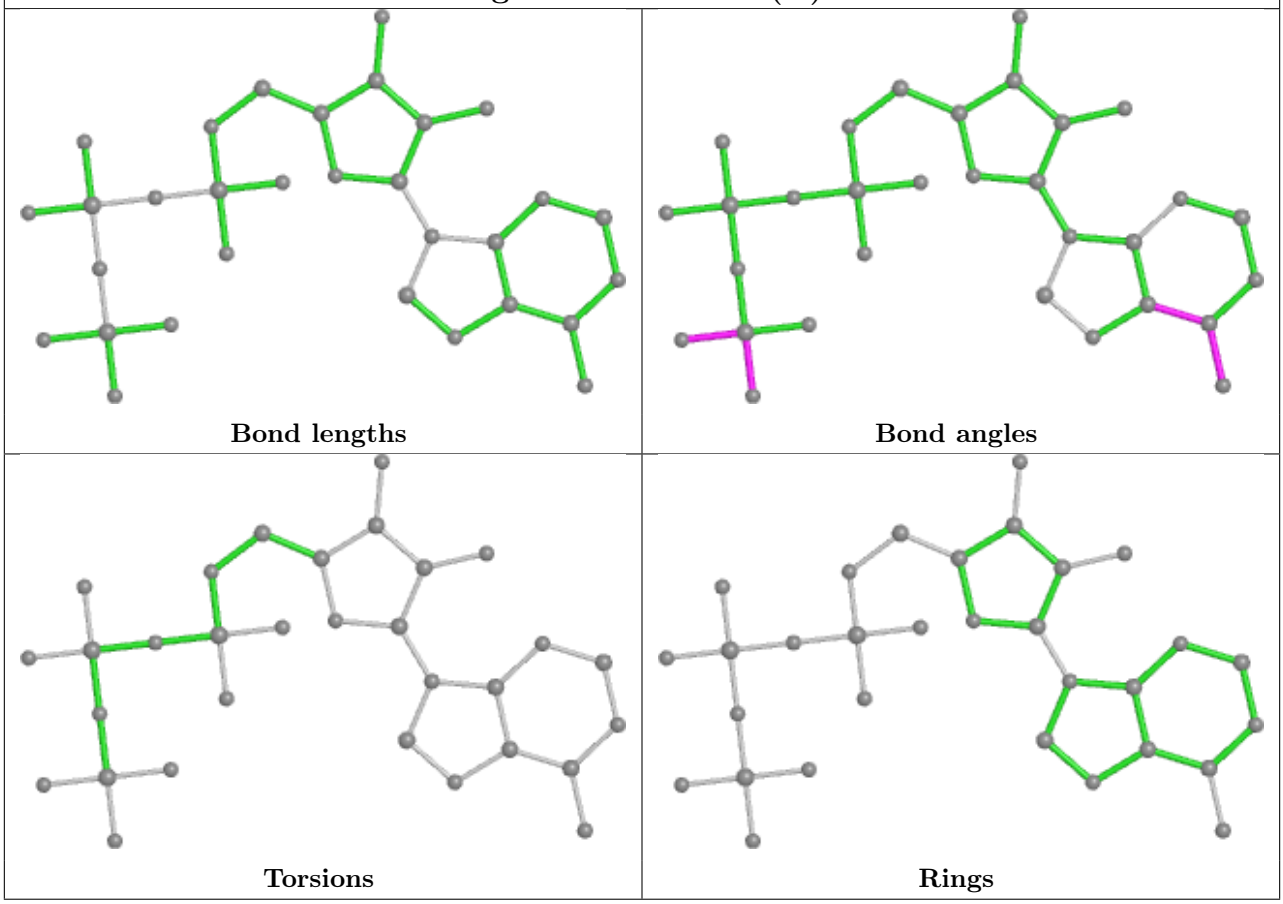
There are no ring outliers.

3 monomers are involved in 4 short contacts:

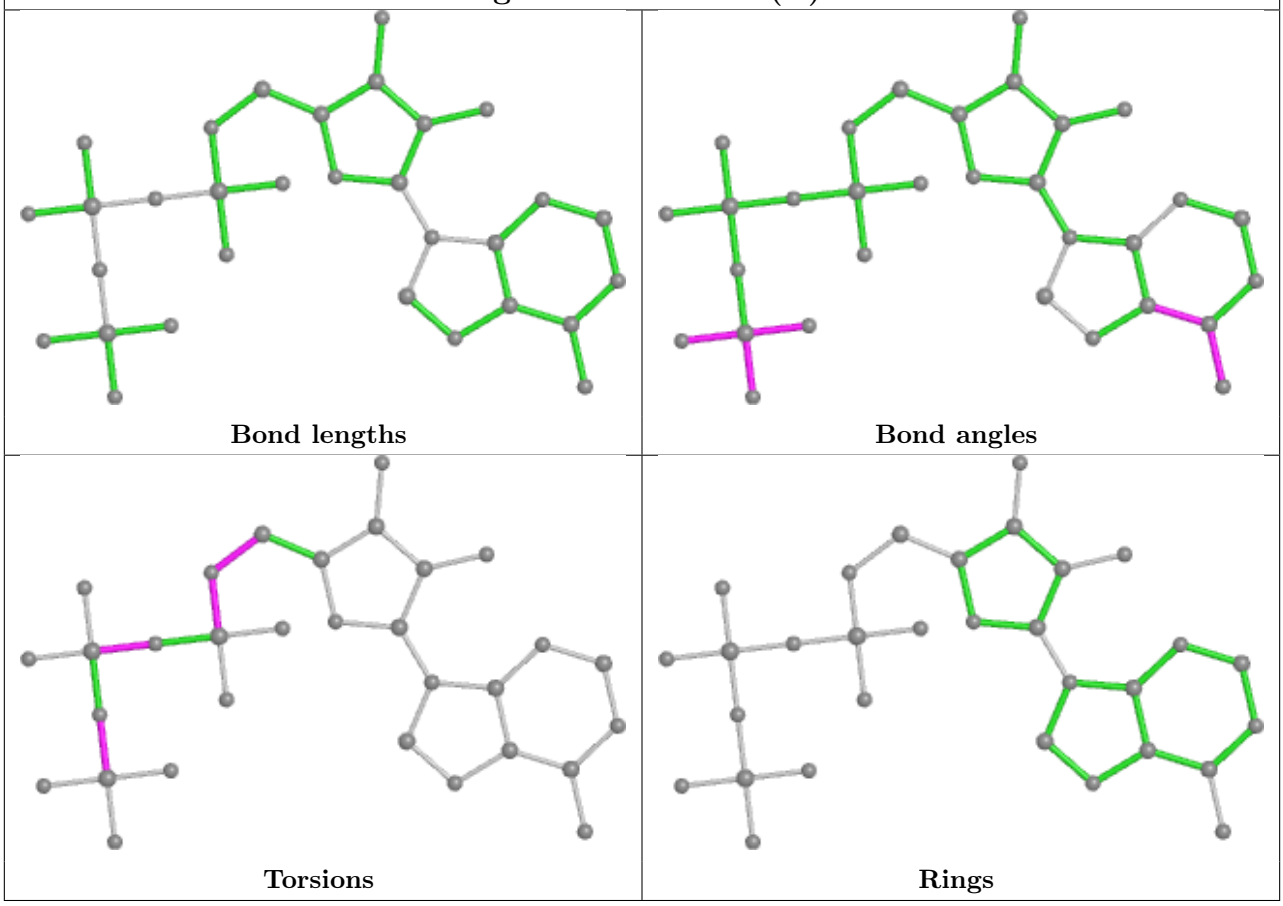
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	801[B]	ATP	1	0
3	A	800[B]	ATP	1	0
3	D	803[B]	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

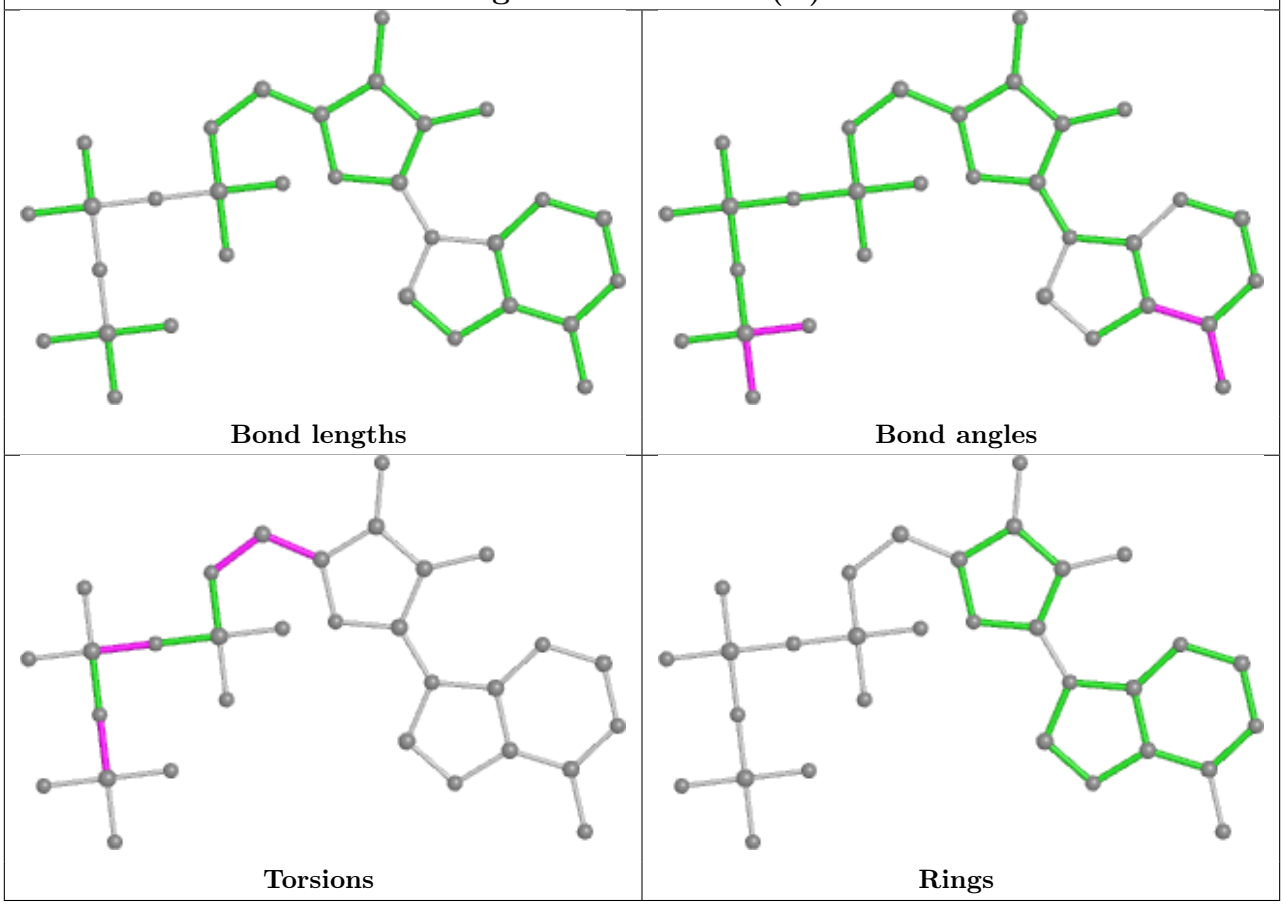
Ligand ATP A 800 (A)



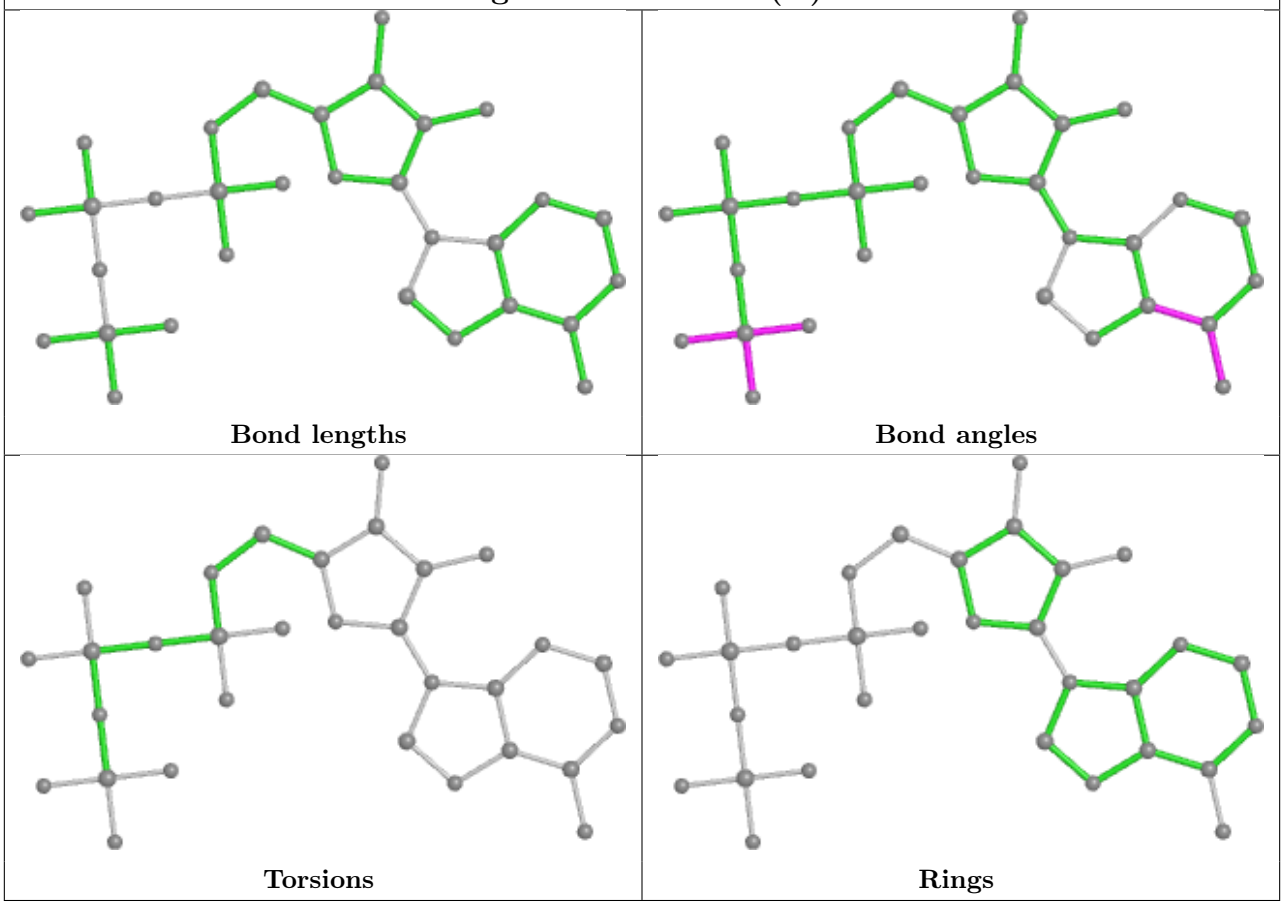
Ligand ATP B 801 (B)



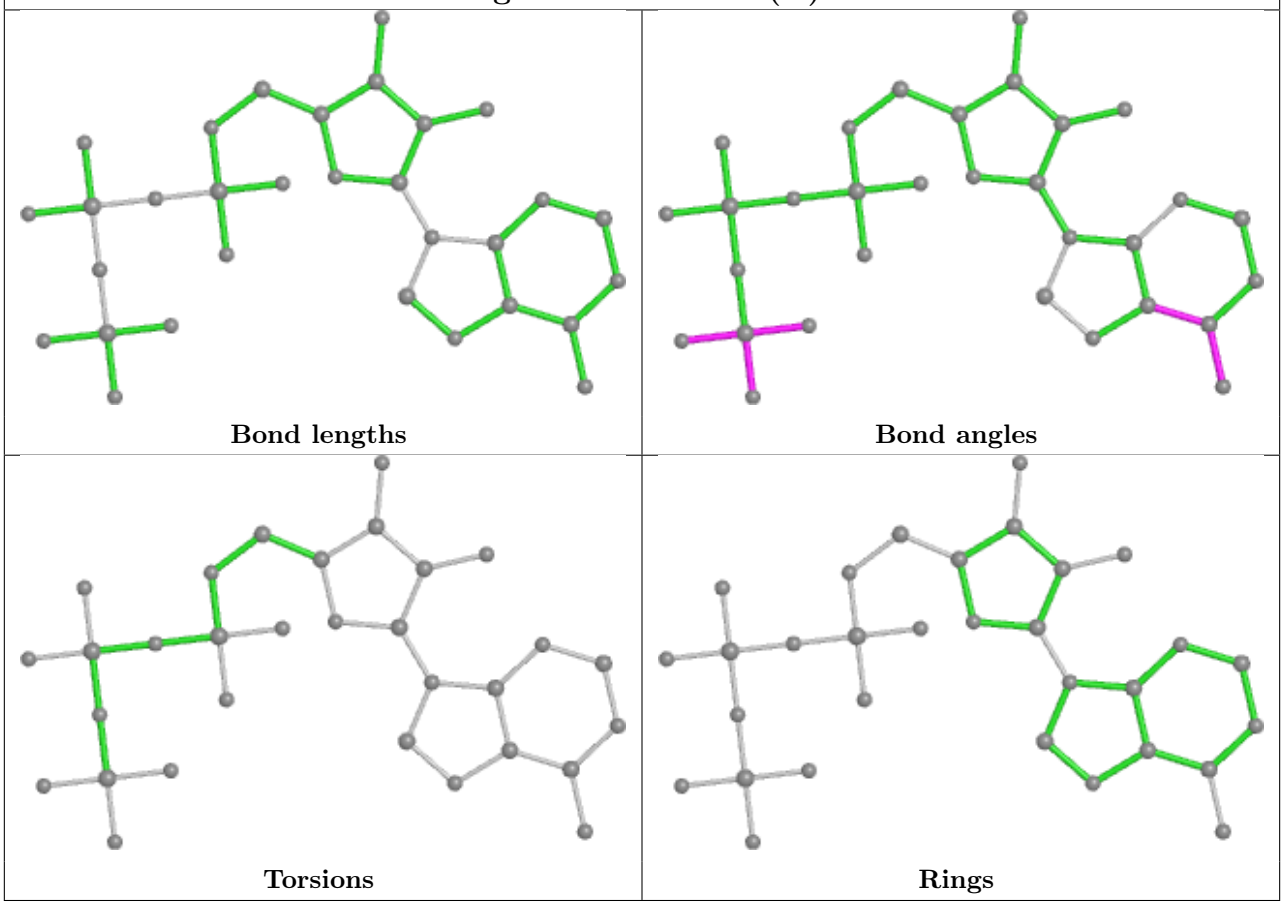
Ligand ATP A 800 (B)



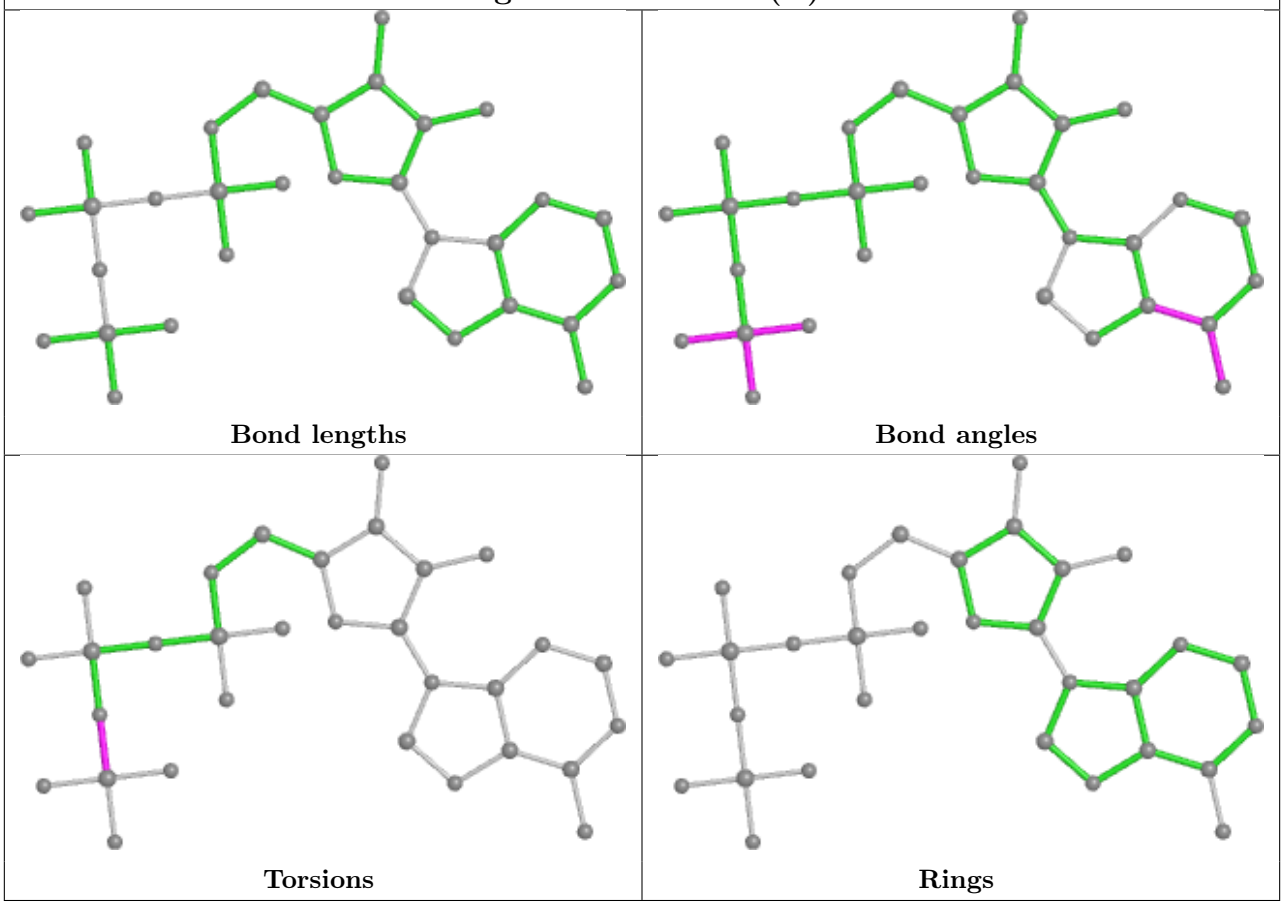
Ligand ATP D 803 (A)



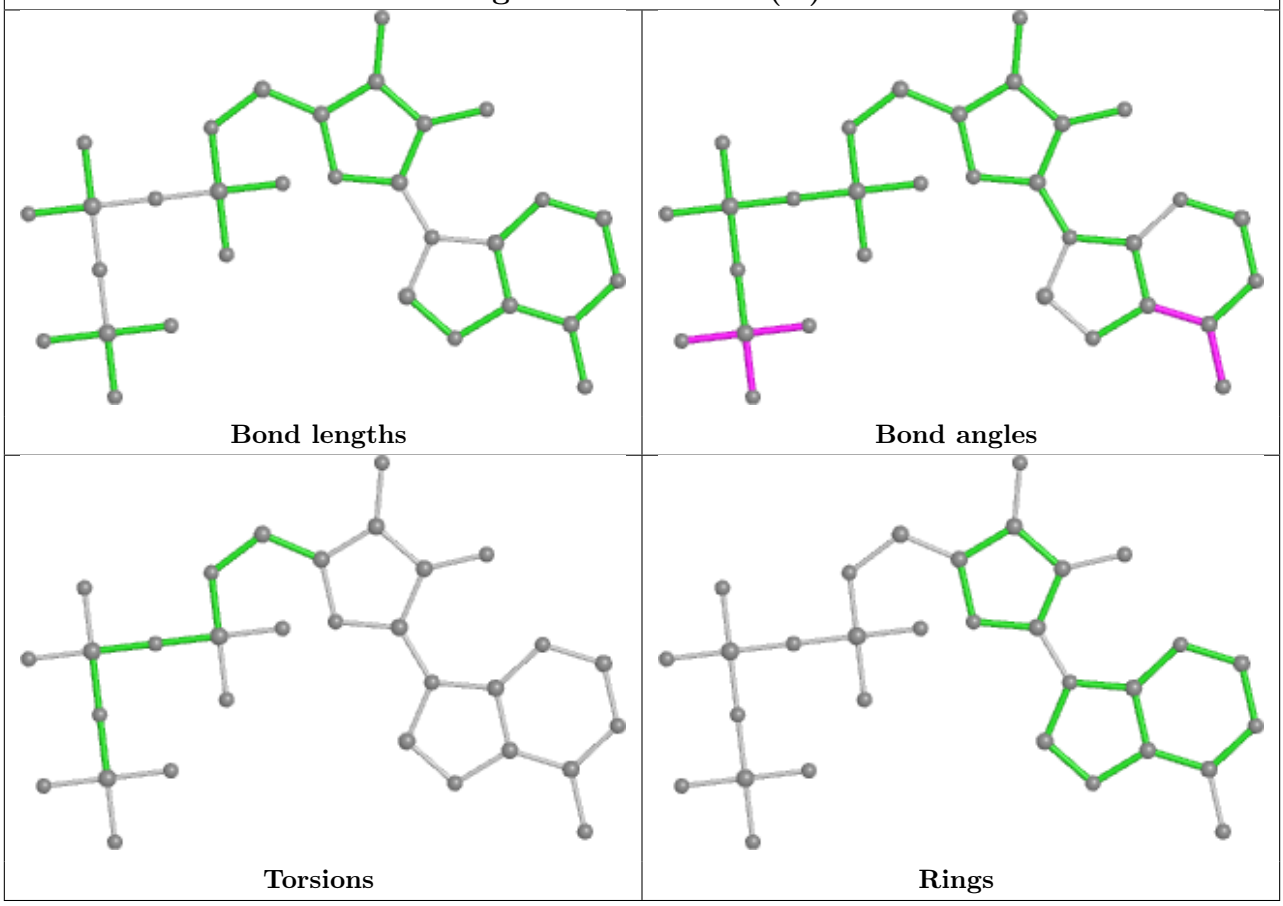
Ligand ATP E 804 (A)



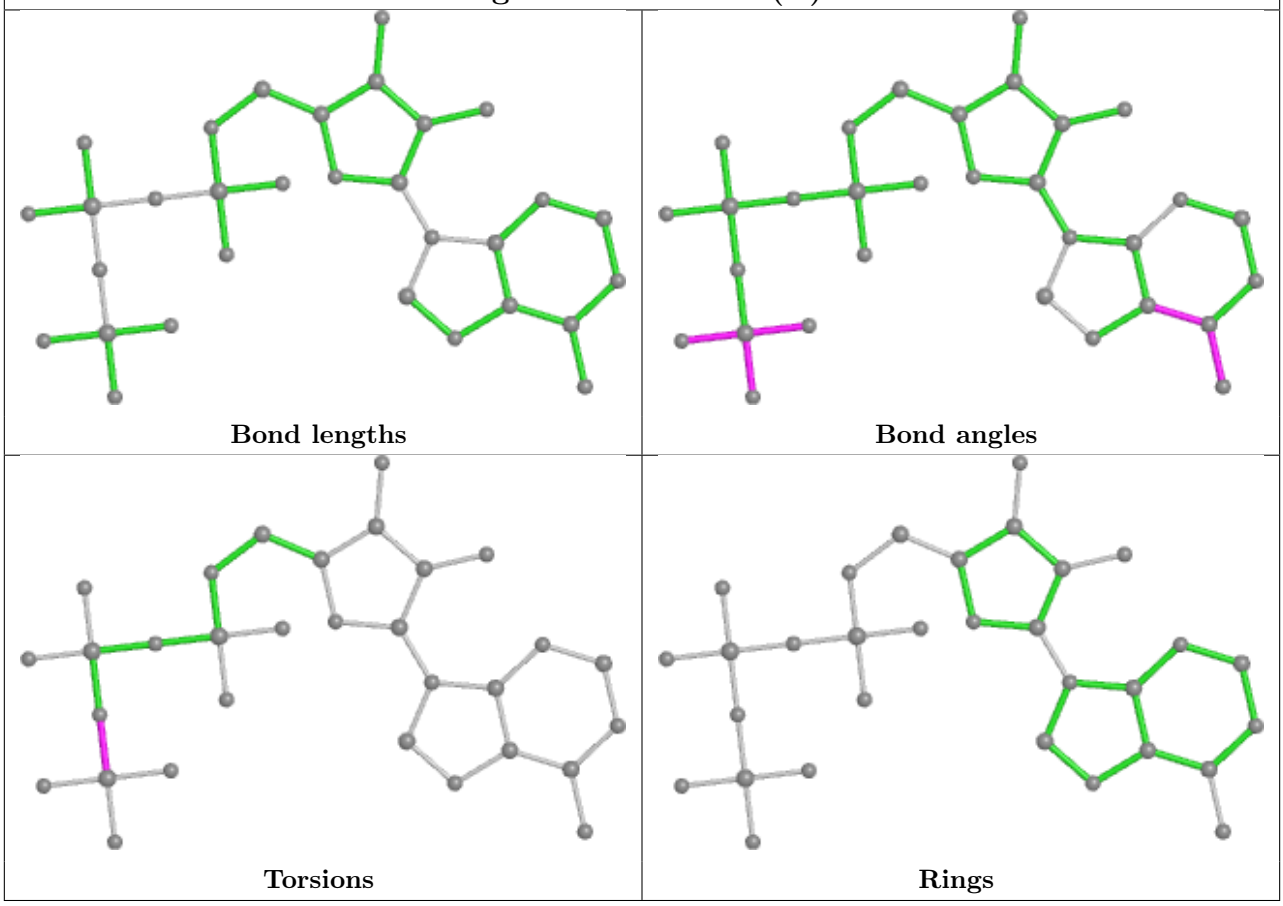
Ligand ATP E 804 (B)



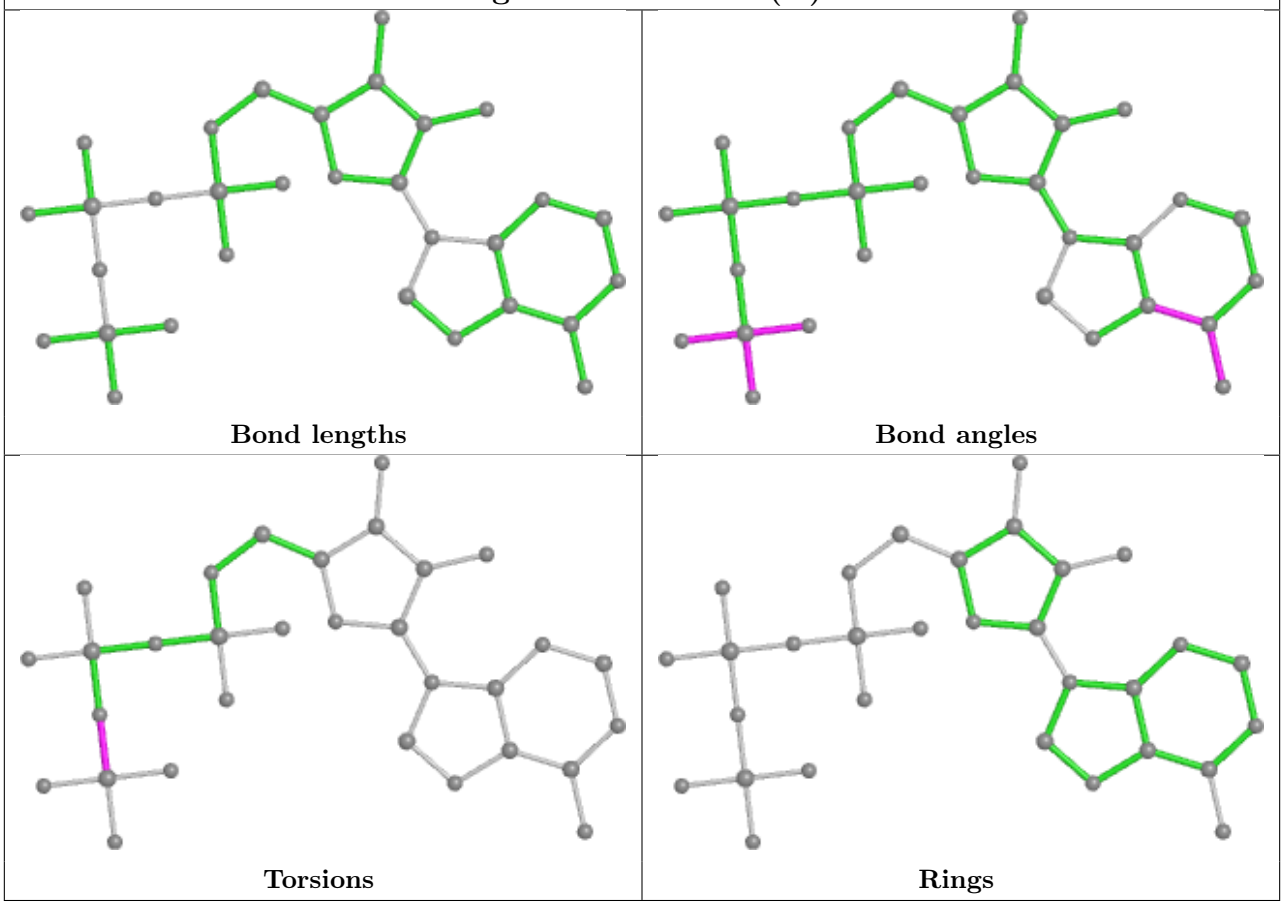
Ligand ATP B 801 (A)



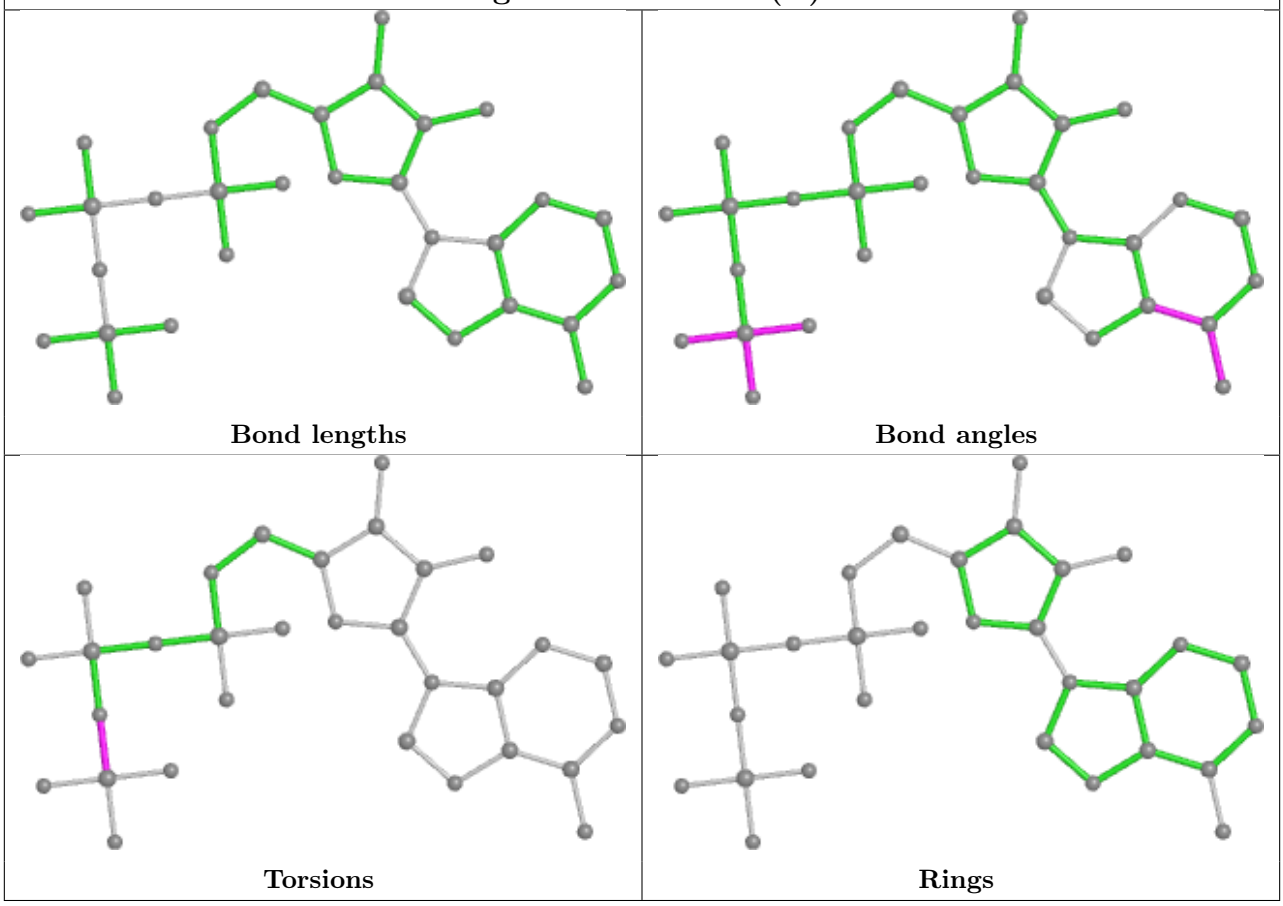
Ligand ATP H 807 (B)



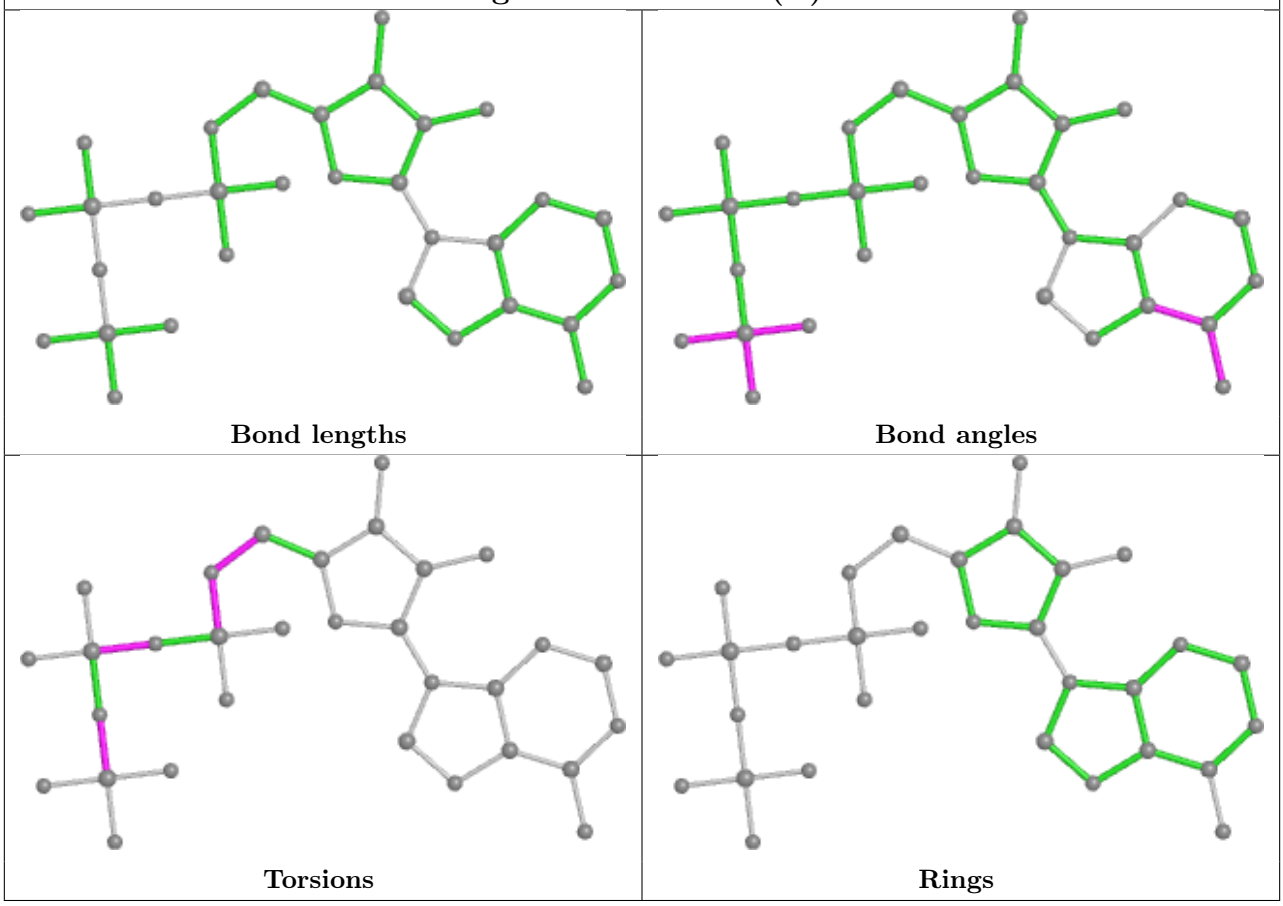
Ligand ATP C 802 (A)



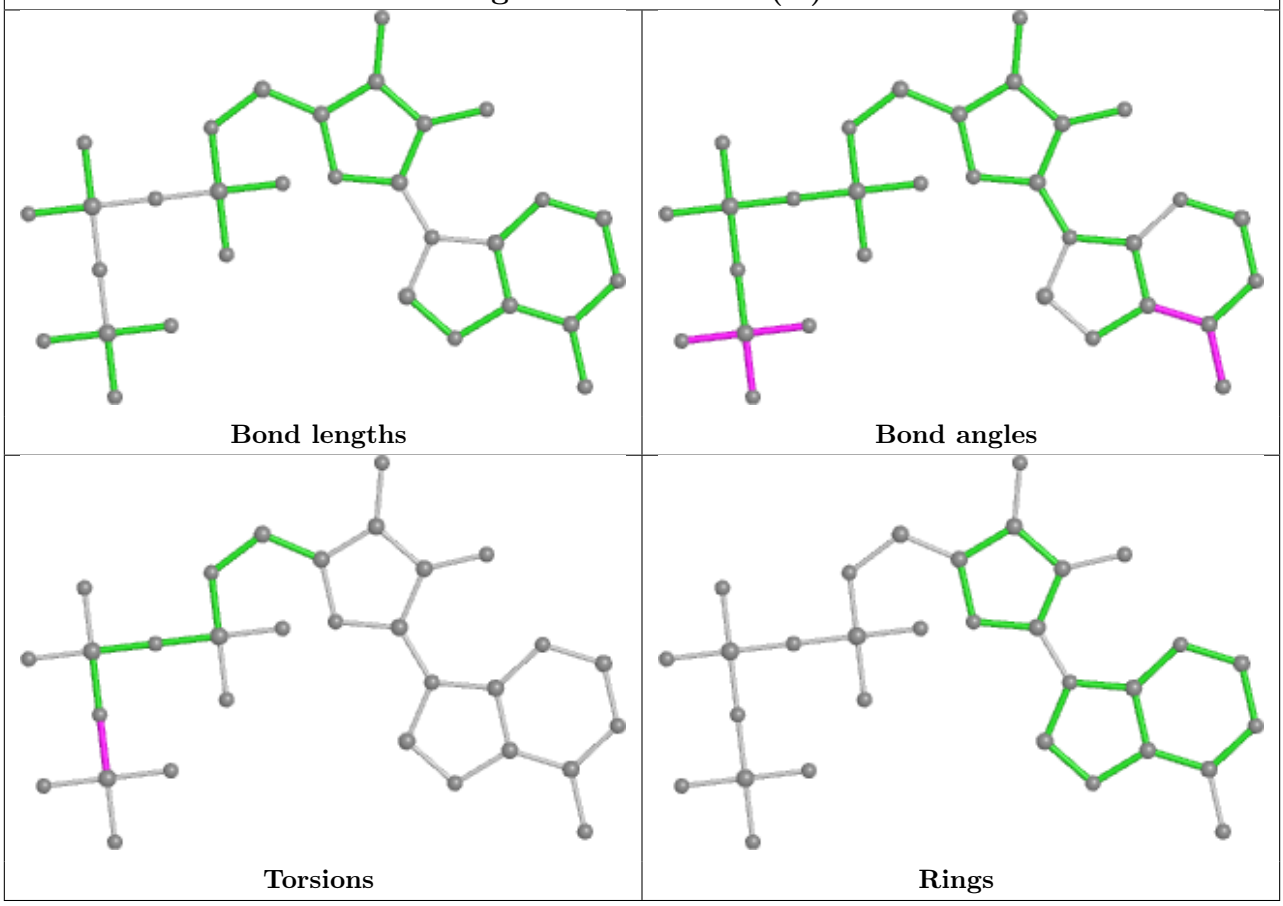
Ligand ATP C 802 (B)



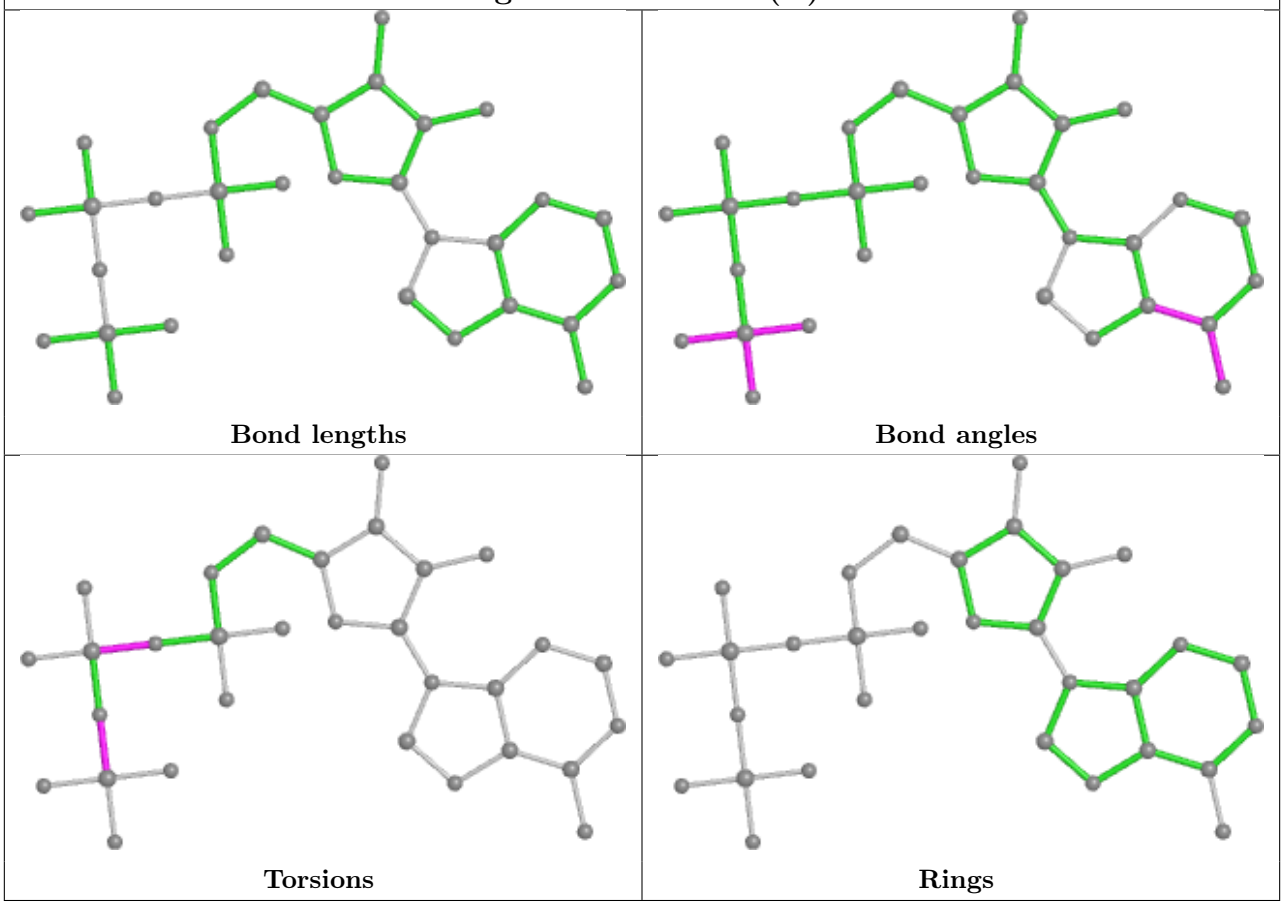
Ligand ATP G 806 (B)



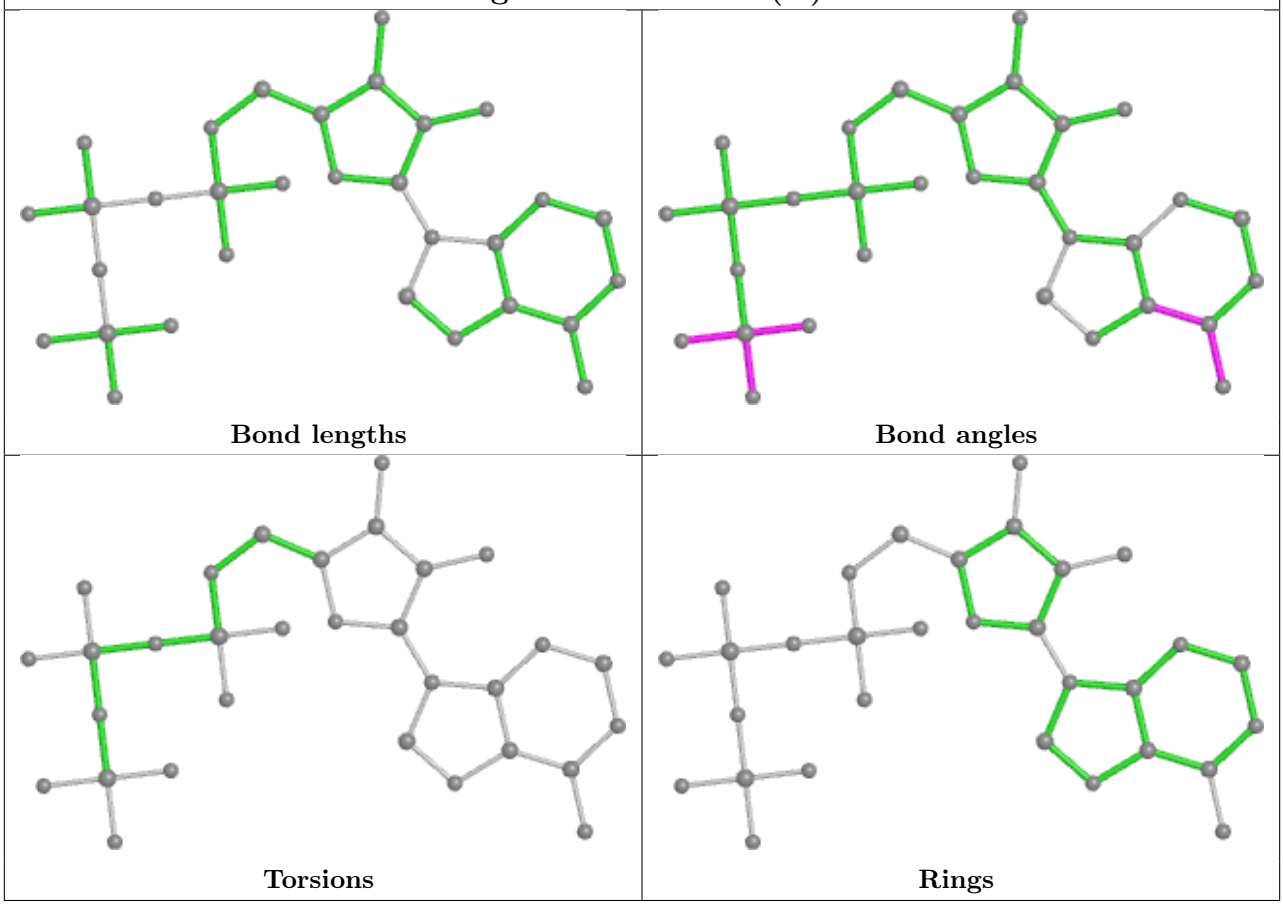
Ligand ATP H 807 (A)



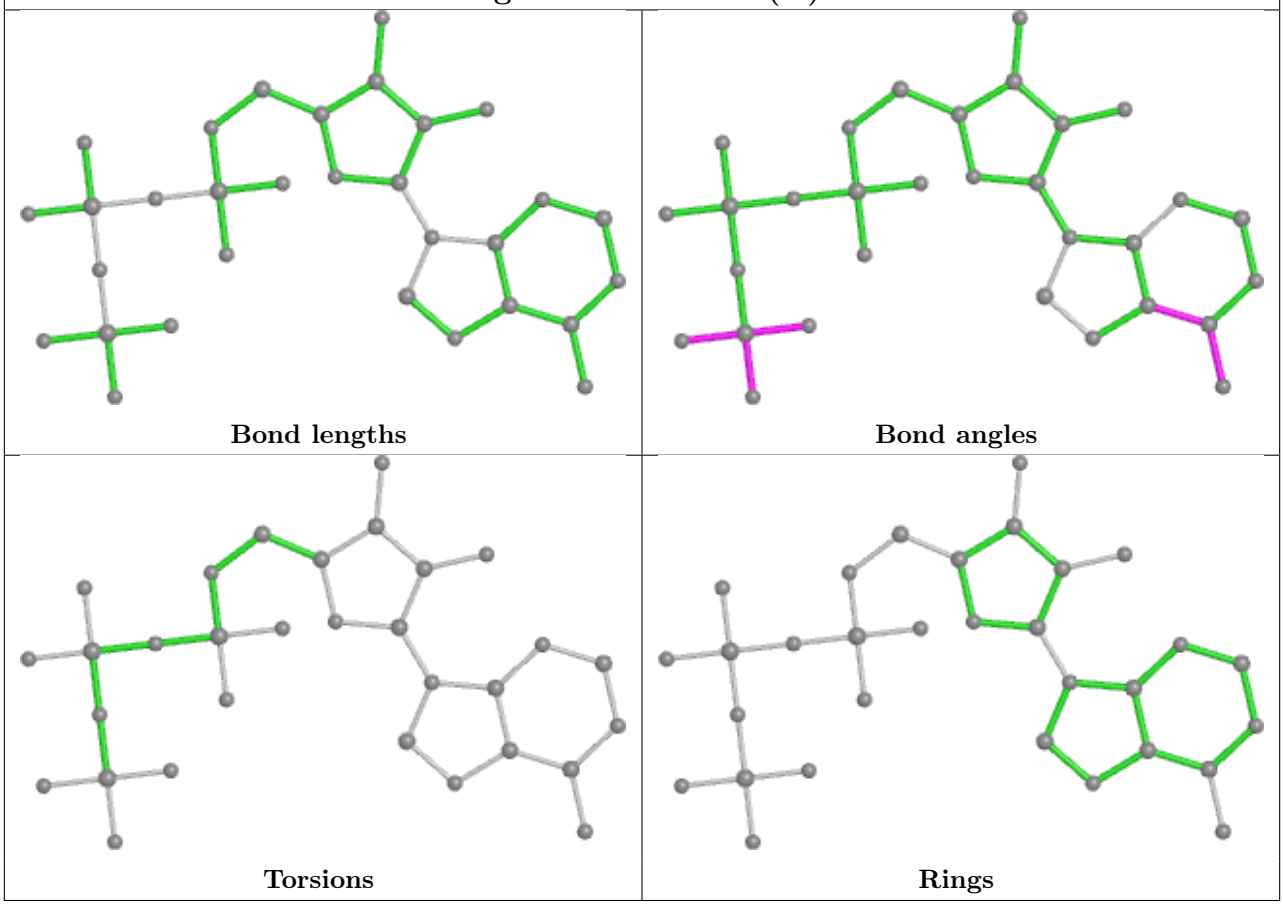
Ligand ATP F 805 (B)



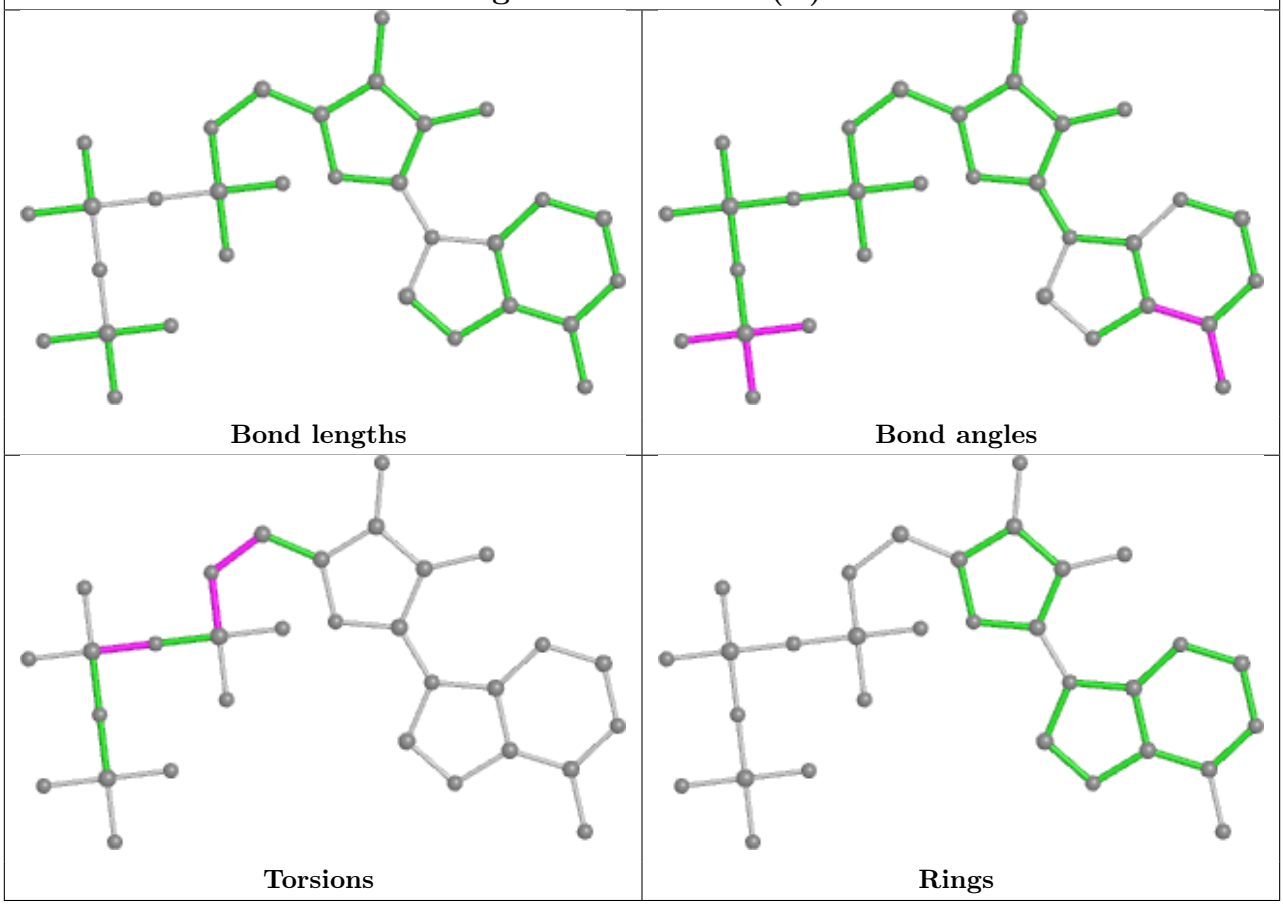
Ligand ATP G 806 (A)



Ligand ATP F 805 (A)



Ligand ATP D 803 (B)



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 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	306/422 (72%)	0.16	9 (2%)	51	57	11, 24, 47, 69	6 (1%)
1	B	292/422 (69%)	0.03	6 (2%)	63	68	12, 22, 43, 60	2 (0%)
1	C	285/422 (67%)	0.29	15 (5%)	26	32	17, 31, 56, 82	5 (1%)
1	D	300/422 (71%)	0.53	20 (6%)	17	22	19, 35, 59, 72	2 (0%)
1	E	286/422 (67%)	0.22	7 (2%)	59	64	20, 33, 56, 72	10 (3%)
1	F	286/422 (67%)	0.48	16 (5%)	24	29	19, 38, 66, 83	7 (2%)
1	G	293/422 (69%)	0.31	17 (5%)	23	28	15, 33, 58, 73	1 (0%)
1	H	286/422 (67%)	0.16	5 (1%)	70	74	15, 30, 50, 61	6 (2%)
All	All	2334/3376 (69%)	0.27	95 (4%)	37	43	11, 31, 58, 83	39 (1%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	174	VAL	7.3
1	A	168	LEU	7.0
1	D	167	VAL	6.6
1	A	172	VAL	6.3
1	C	139	ILE	5.9
1	C	137	GLY	5.3
1	F	123	HIS	5.2
1	D	138	GLU	4.9
1	F	136	HIS	4.7
1	C	138	GLU	4.7
1	D	175	VAL	4.4
1	G	136	HIS	4.3
1	C	136	HIS	4.3
1	G	138	GLU	4.0
1	D	135	ILE	4.0
1	G	137	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	135	ILE	4.0
1	F	337	THR	3.9
1	A	170	ASN	3.9
1	G	262	THR	3.9
1	D	417	ALA	3.8
1	F	329	THR	3.7
1	B	338	ASN	3.7
1	E	135	ILE	3.6
1	B	340	GLY	3.5
1	F	417	ALA	3.5
1	A	173	LYS	3.4
1	D	136	HIS	3.3
1	B	341	SER	3.3
1	A	169	ARG	3.2
1	F	262	THR	3.2
1	C	123	HIS	3.2
1	G	112	ALA	3.2
1	H	175	VAL	3.1
1	C	134	LYS	3.1
1	C	140	ASP	3.1
1	G	176	ARG	3.0
1	A	417	ALA	3.0
1	G	139	ILE	3.0
1	D	139	ILE	2.9
1	E	112	ALA	2.9
1	G	175	VAL	2.9
1	G	417	ALA	2.9
1	D	243	GLU	2.9
1	G	135	ILE	2.8
1	D	351	ASP	2.8
1	E	328	ARG	2.8
1	D	397	ASP	2.8
1	C	417	ALA	2.7
1	C	175	VAL	2.7
1	E	329	THR	2.7
1	C	259	LEU	2.7
1	E	337	THR	2.6
1	A	331	VAL	2.6
1	D	112	ALA	2.6
1	D	137	GLY	2.6
1	G	331	VAL	2.6
1	B	339	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	131	LYS	2.5
1	C	415	THR	2.5
1	D	122	PRO	2.5
1	C	335	TRP	2.5
1	H	262	THR	2.5
1	D	263	THR	2.5
1	A	174	VAL	2.4
1	G	195	ASN	2.4
1	G	242	GLU	2.4
1	F	412	ASN	2.4
1	D	123	HIS	2.4
1	B	136	HIS	2.4
1	C	262	THR	2.4
1	B	417	ALA	2.3
1	G	113	ALA	2.3
1	D	131	LYS	2.3
1	D	176	ARG	2.3
1	G	416	GLN	2.3
1	F	128	LYS	2.3
1	A	112	ALA	2.3
1	C	411	VAL	2.3
1	F	113	ALA	2.3
1	F	175	VAL	2.3
1	H	112	ALA	2.2
1	D	259	LEU	2.2
1	H	176	ARG	2.2
1	F	195	ASN	2.2
1	F	263	THR	2.2
1	F	135	ILE	2.1
1	D	242	GLU	2.1
1	G	334	ASN	2.1
1	E	137	GLY	2.1
1	F	344	LEU	2.1
1	F	138	GLU	2.0
1	E	175	VAL	2.0
1	F	129	TYR	2.0
1	H	259	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

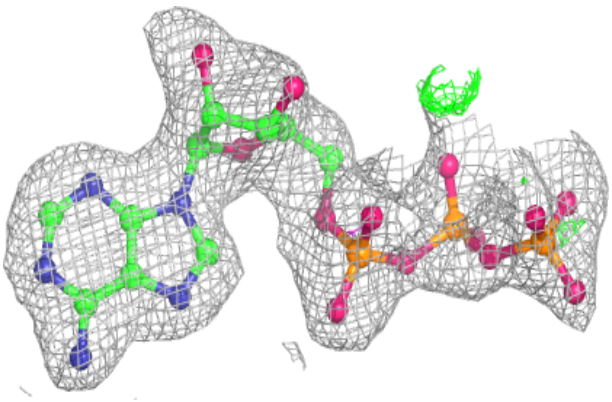
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

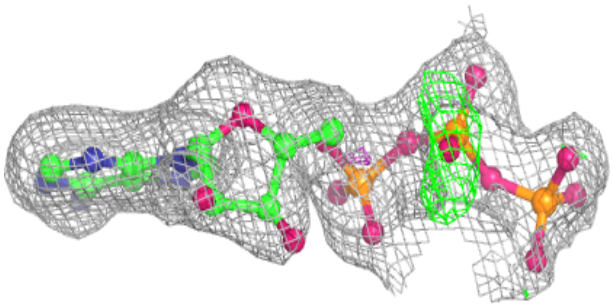
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	818	4/4	0.79	0.18	20,22,26,26	0
2	CA	E	817	1/1	0.83	0.12	56,56,56,56	0
2	CA	F	817	1/1	0.84	0.15	48,48,48,48	0
3	ATP	C	802[B]	31/31	0.92	0.15	30,33,36,37	31
3	ATP	C	802[A]	31/31	0.92	0.15	21,27,36,37	31
3	ATP	E	804[A]	31/31	0.94	0.15	28,32,37,39	31
3	ATP	E	804[B]	31/31	0.94	0.15	33,35,38,40	31
3	ATP	F	805[A]	31/31	0.94	0.14	26,35,39,41	31
3	ATP	F	805[B]	31/31	0.94	0.14	33,35,37,37	31
3	ATP	H	807[A]	31/31	0.94	0.14	28,33,43,43	31
3	ATP	H	807[B]	31/31	0.94	0.14	28,31,34,36	31
2	CA	D	817	1/1	0.94	0.11	39,39,39,39	0
3	ATP	D	803[B]	31/31	0.95	0.16	27,29,33,33	31
2	CA	G	817	1/1	0.95	0.10	39,39,39,39	0
2	CA	H	817	1/1	0.95	0.10	38,38,38,38	0
3	ATP	D	803[A]	31/31	0.95	0.16	23,27,30,31	31
4	EDO	B	819	4/4	0.95	0.13	26,28,30,32	0
3	ATP	B	801[A]	31/31	0.96	0.13	15,20,23,23	31
3	ATP	B	801[B]	31/31	0.96	0.13	28,31,32,32	31
3	ATP	G	806[A]	31/31	0.96	0.12	23,26,30,31	31
3	ATP	G	806[B]	31/31	0.96	0.12	24,26,28,28	31
3	ATP	A	800[A]	31/31	0.97	0.15	11,19,21,22	31
3	ATP	A	800[B]	31/31	0.97	0.15	21,30,33,33	31
2	CA	C	817	1/1	0.98	0.09	44,44,44,44	0
2	CA	A	817	1/1	0.98	0.14	29,29,29,29	0
2	CA	B	817	1/1	0.98	0.11	28,28,28,28	0

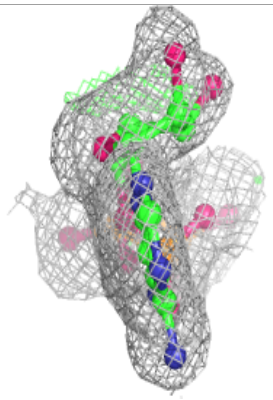
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATP C 802 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

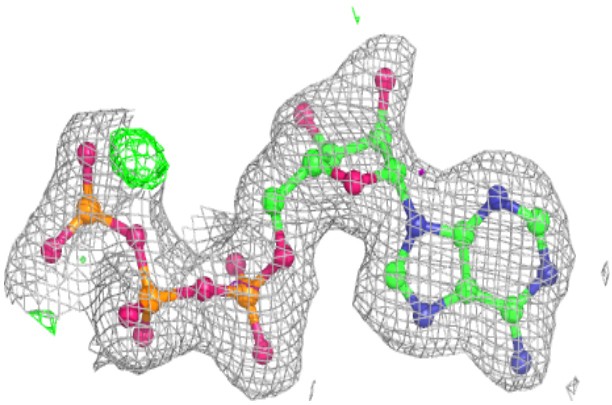


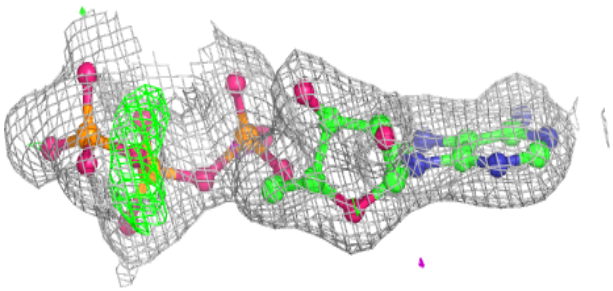


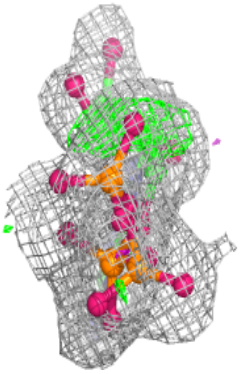


Electron density around ATP C 802 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

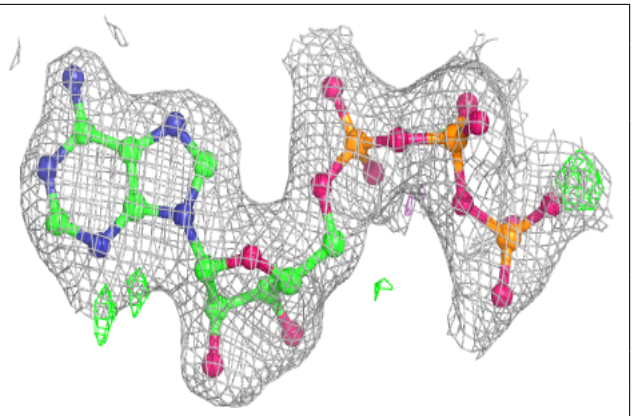


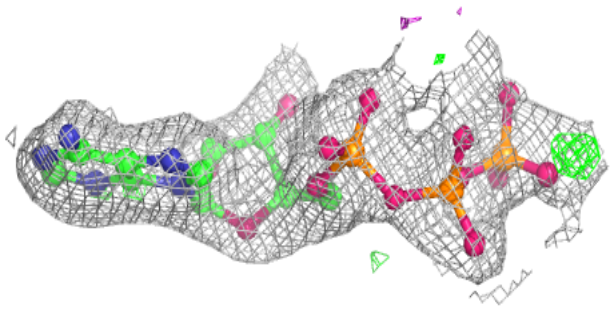


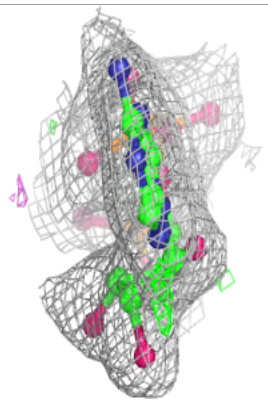


Electron density around ATP E 804 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

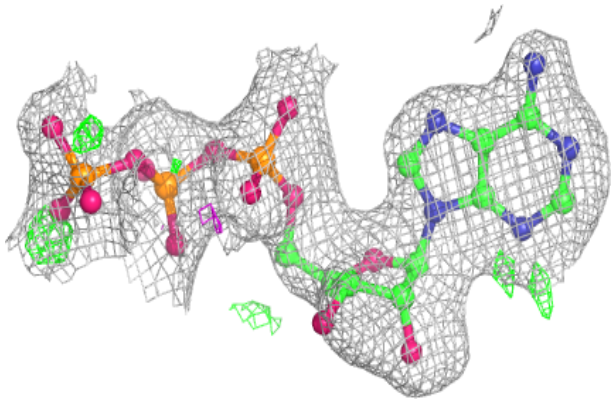


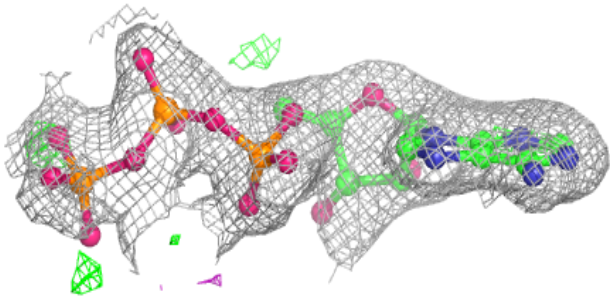


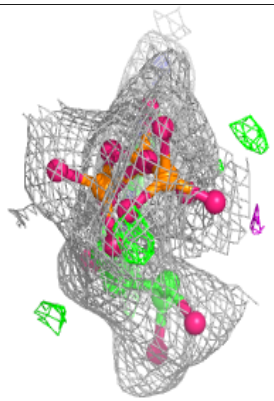


Electron density around ATP E 804 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

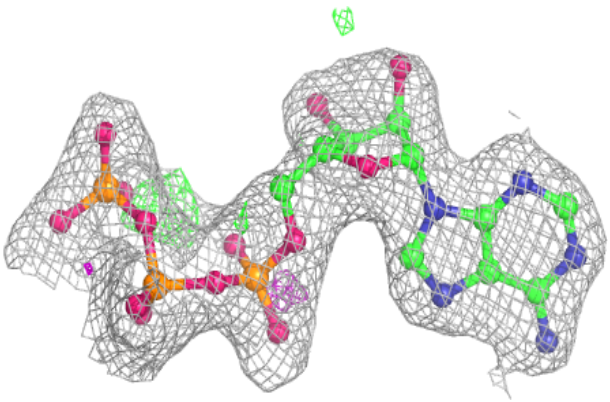


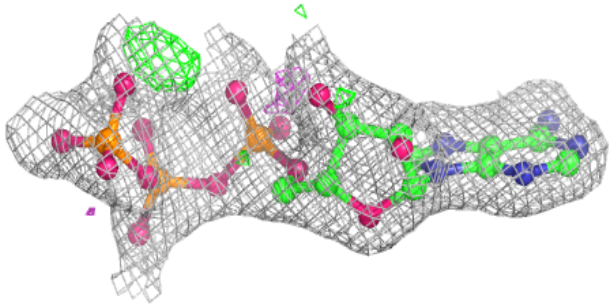


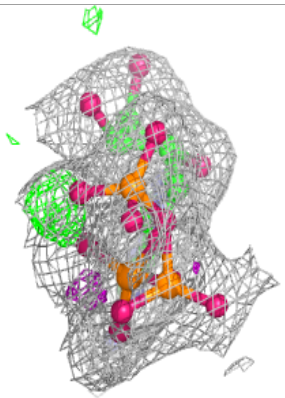


Electron density around ATP F 805 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

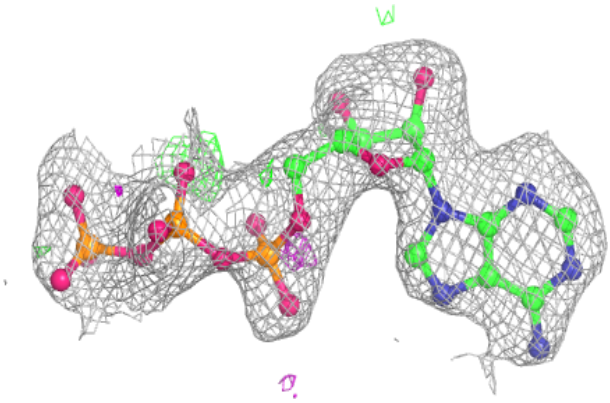


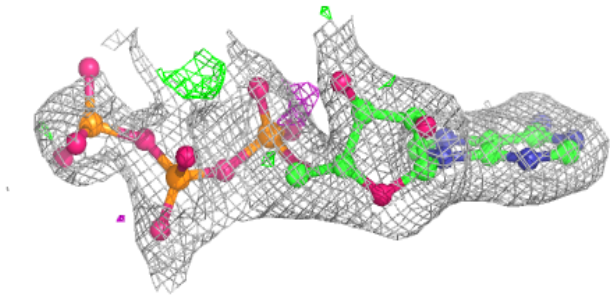


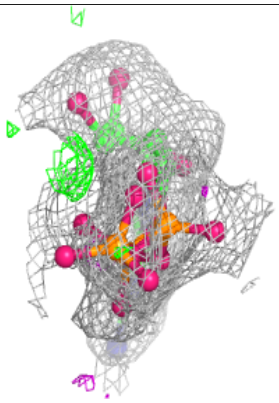


Electron density around ATP F 805 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

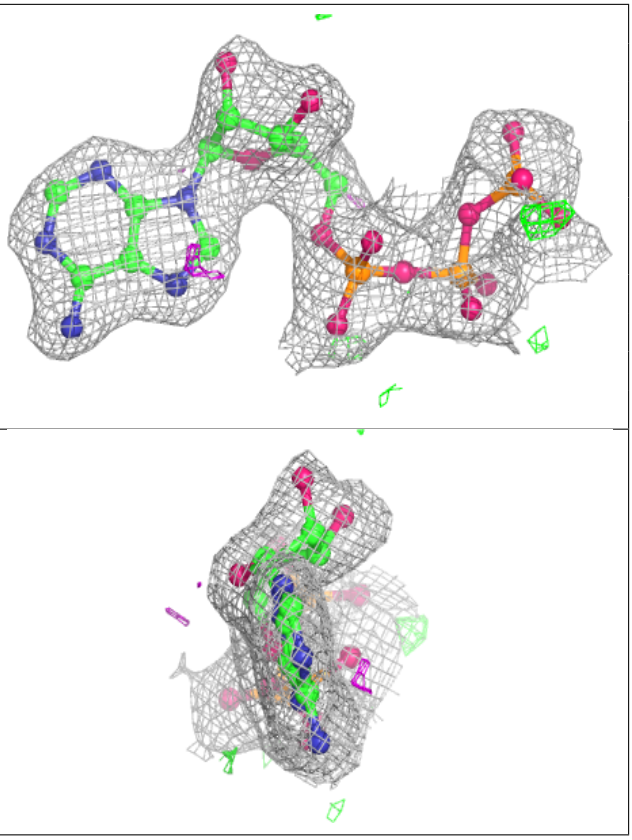


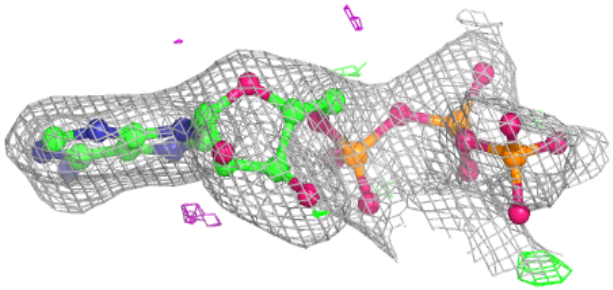




Electron density around ATP H 807 (A):

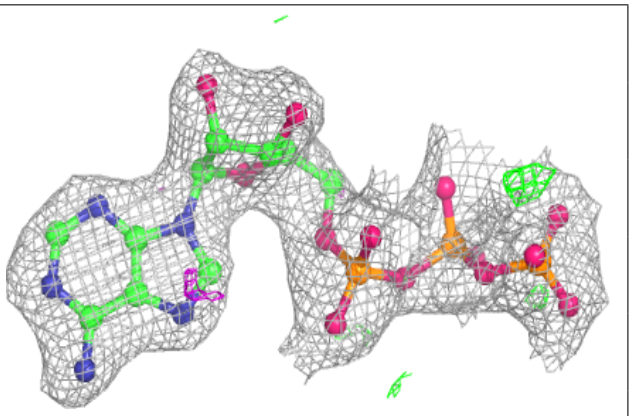
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

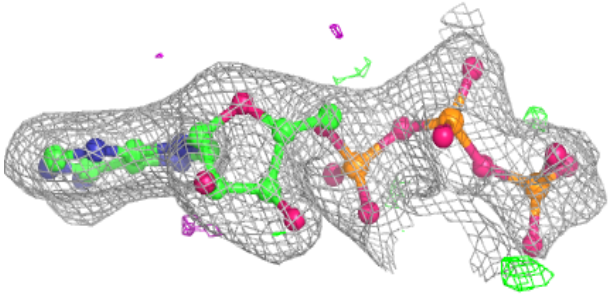


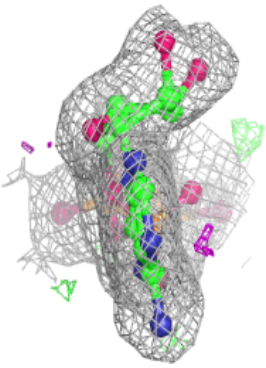


Electron density around ATP H 807 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

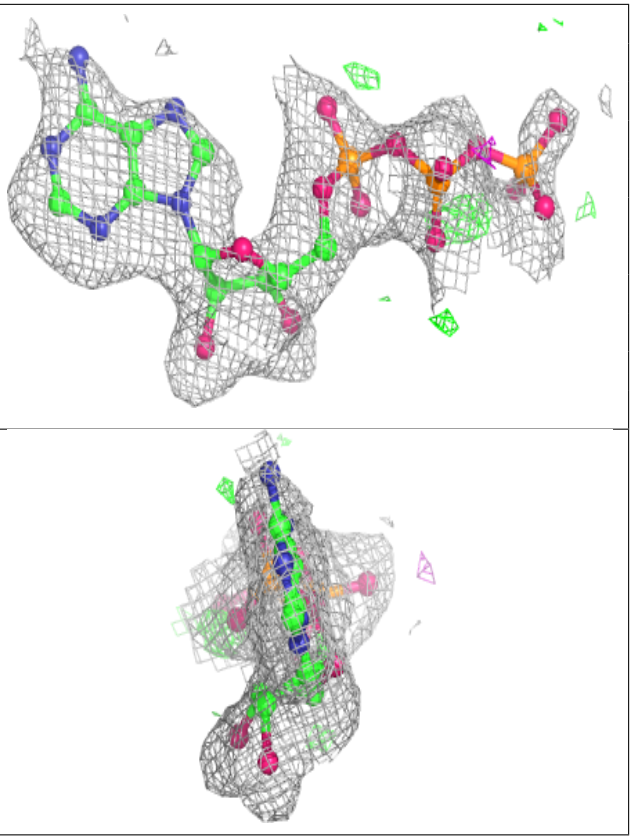


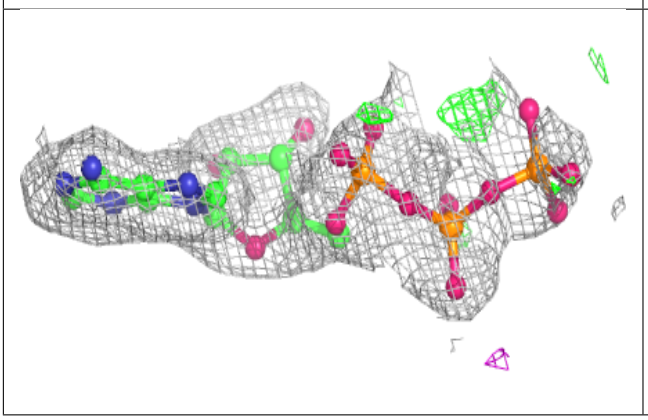




Electron density around ATP D 803 (B):

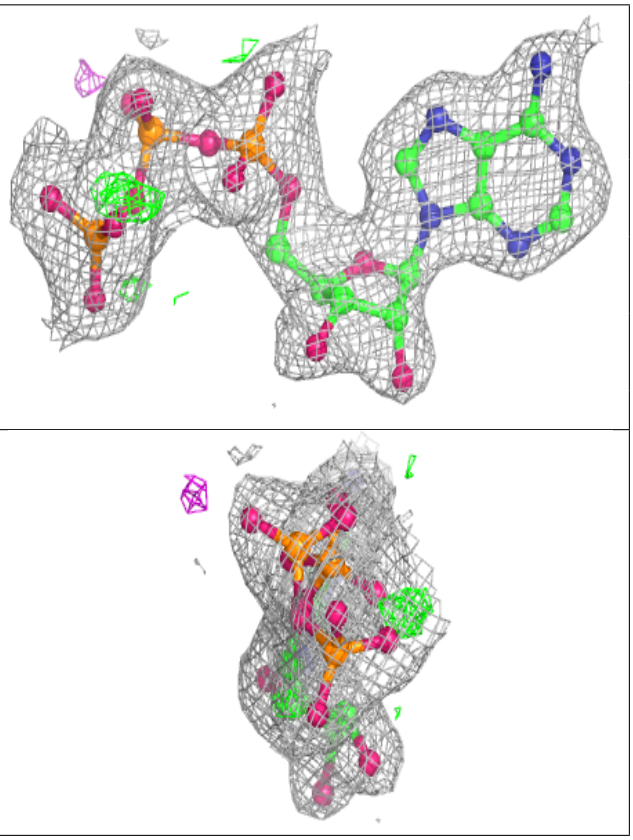
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

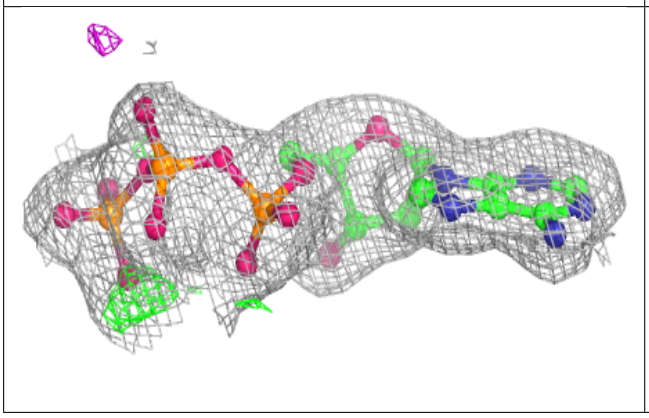




Electron density around ATP D 803 (A):

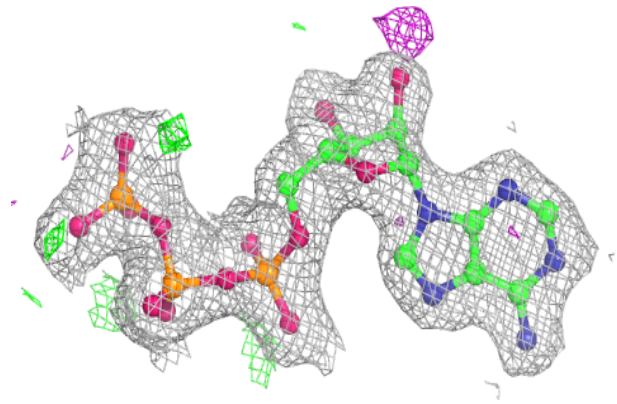
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

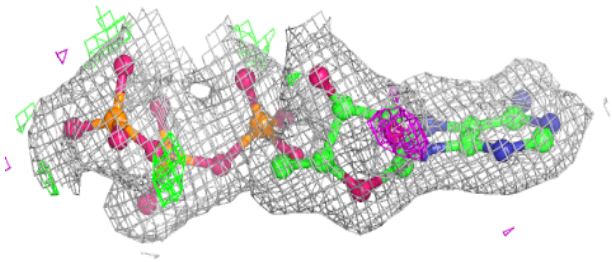


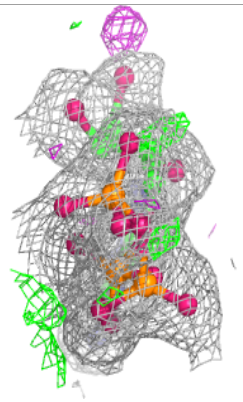


Electron density around ATP B 801 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

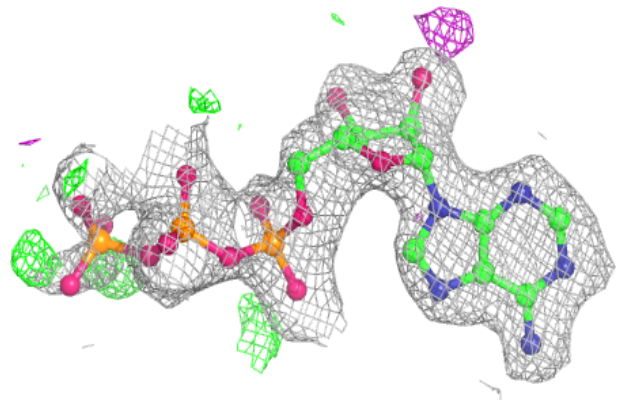


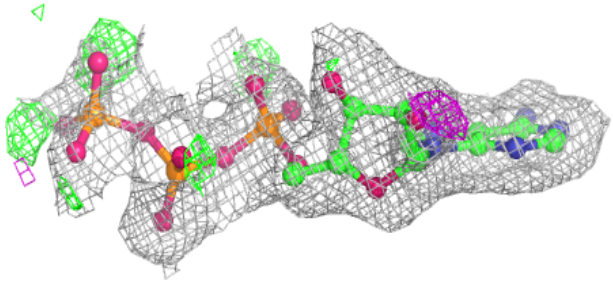


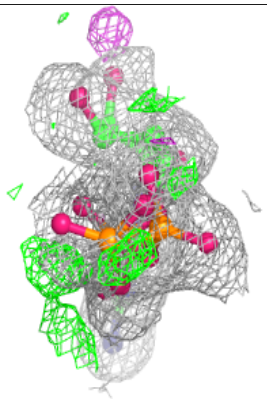


Electron density around ATP B 801 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

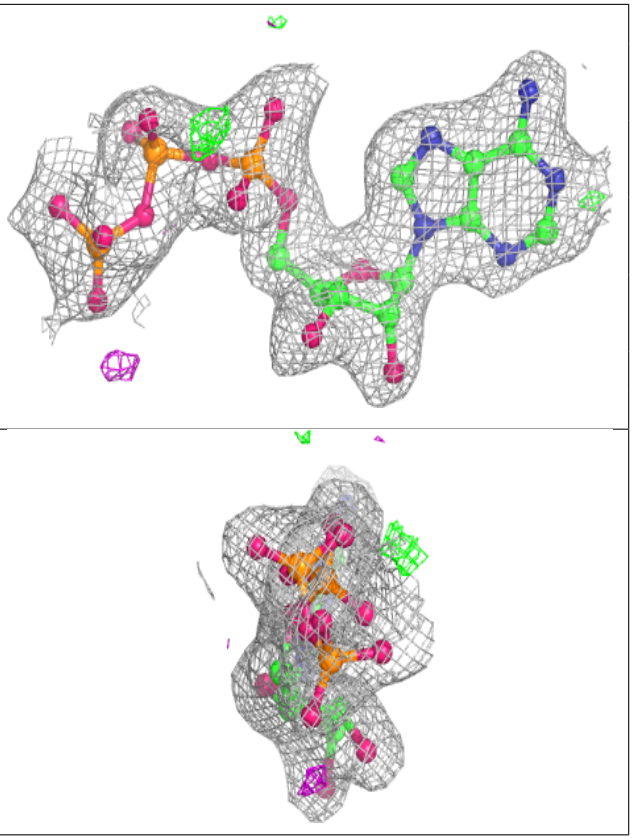






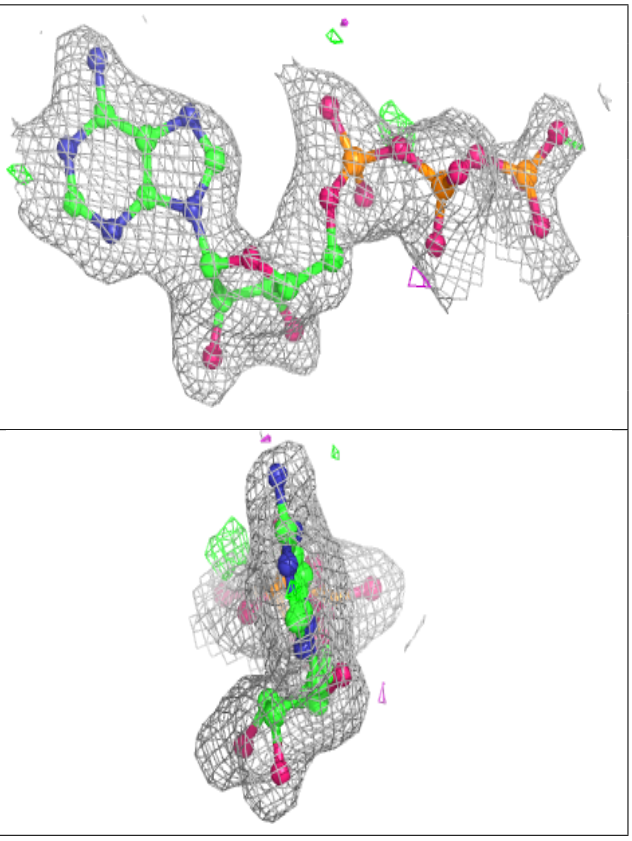
Electron density around ATP G 806 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



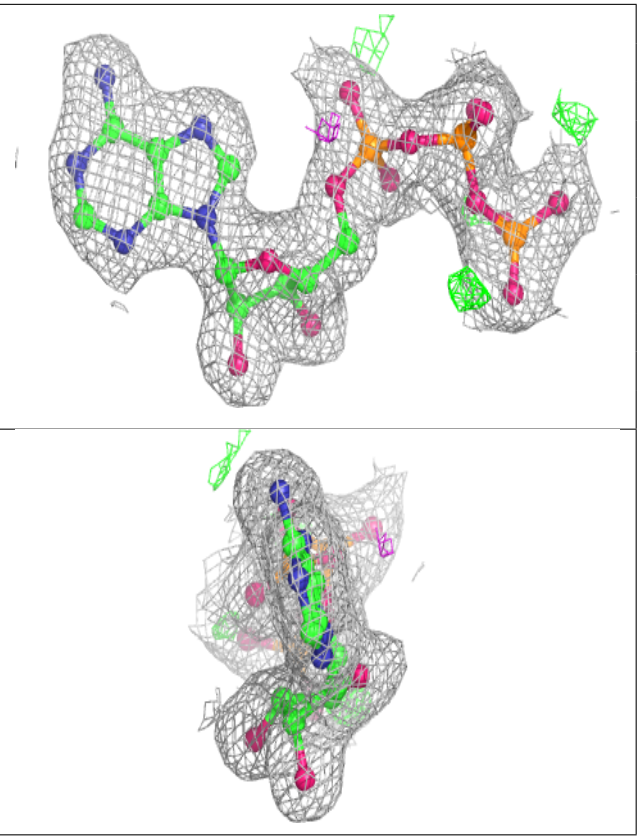
Electron density around ATP G 806 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



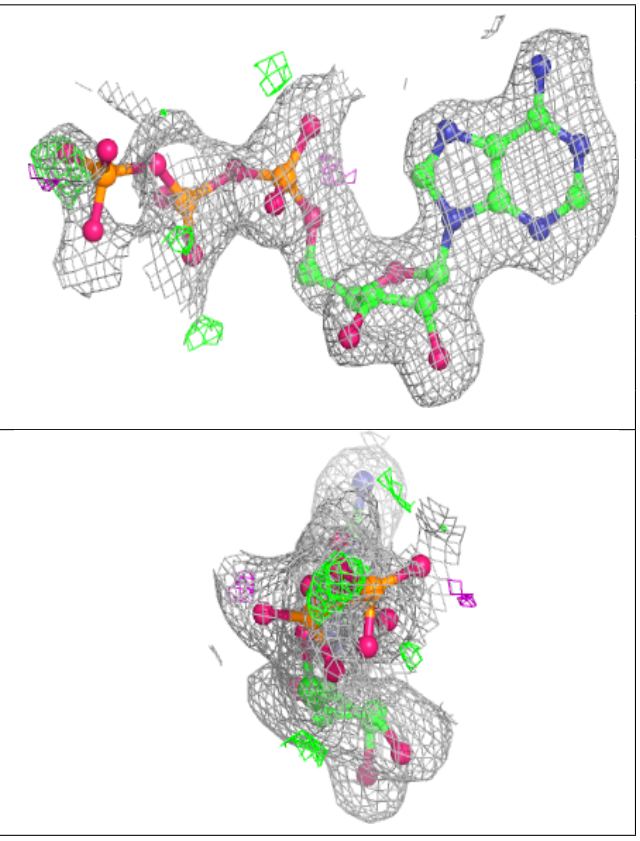
Electron density around ATP A 800 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ATP A 800 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.