



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:51 AM UTC

PDB ID : 1PK8 / pdb_00001pk8
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

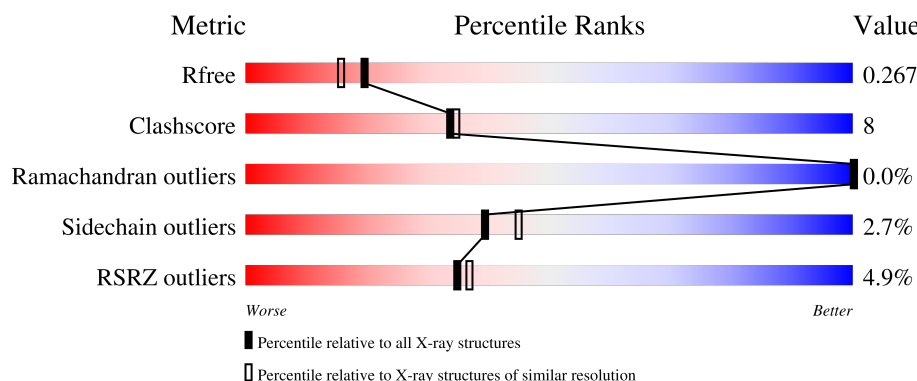
1 Overall quality at a glance

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.



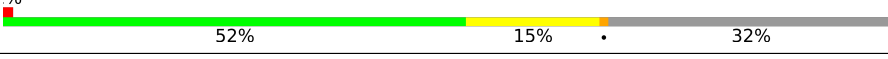
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 $\leq 5\%$. 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	
1	B	422	
1	C	422	
1	D	422	
1	E	422	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	422	 8% 53% 14% 25%
1	G	422	 4% 55% 13% 31%
1	H	422	 % 52% 15% 32%

2 Entry composition

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

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

Continued on next page...

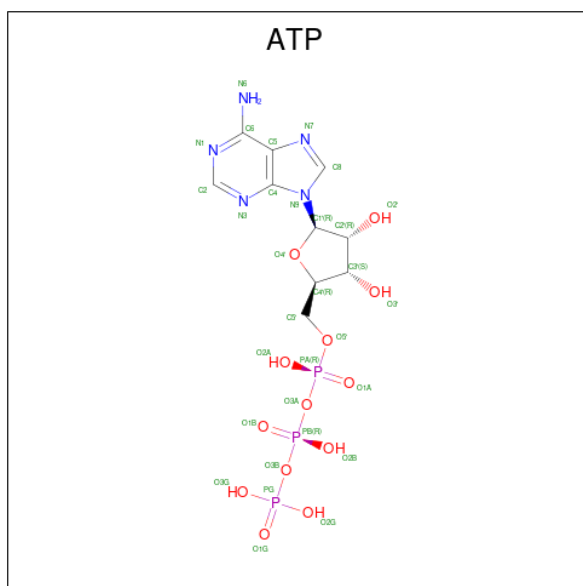
Continued from previous page...

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 (CCD ID: CA) (formula: Ca).

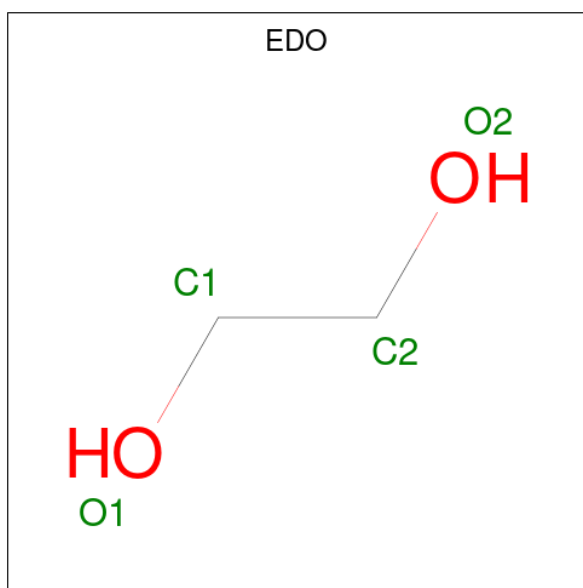
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0
2	G	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

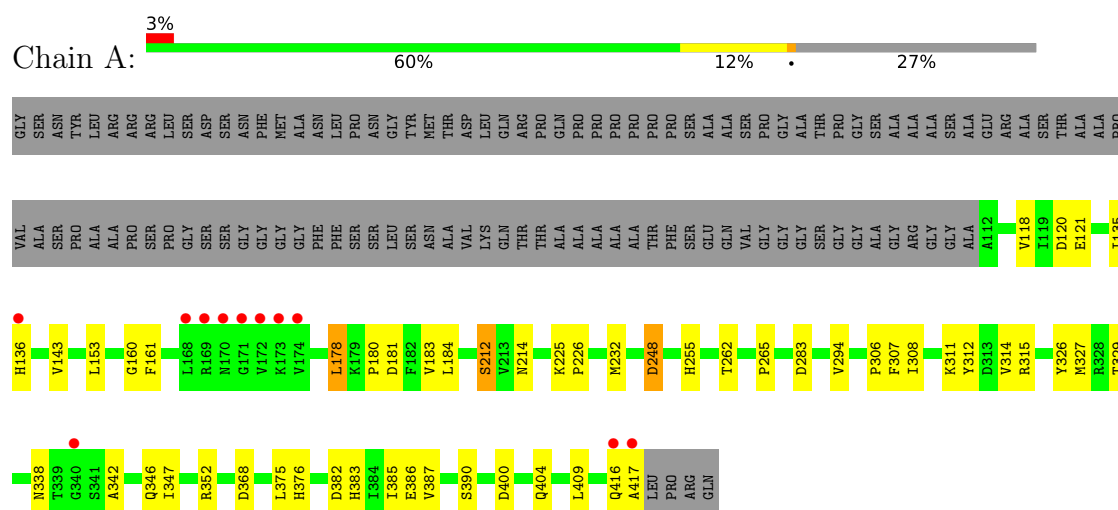
- Molecule 5 is water.

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

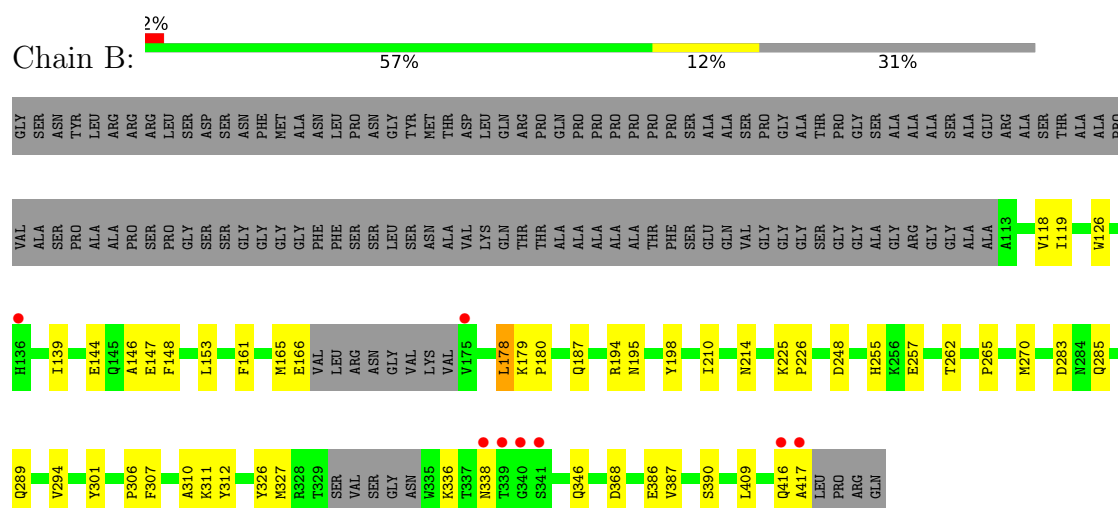
3 Residue-property plots

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.

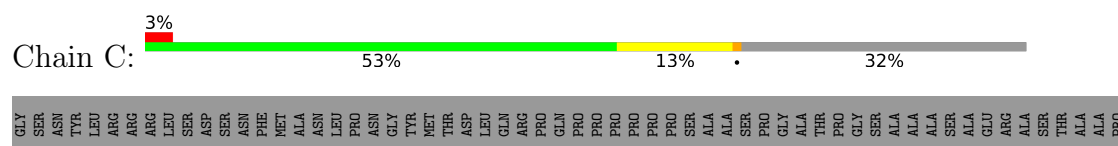
- Molecule 1: rat synapsin I

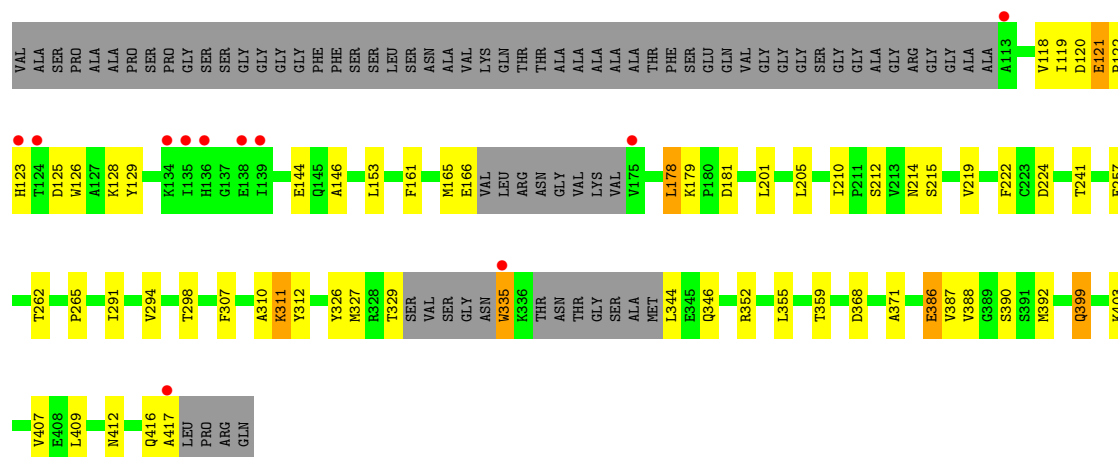


- Molecule 1: rat synapsin I

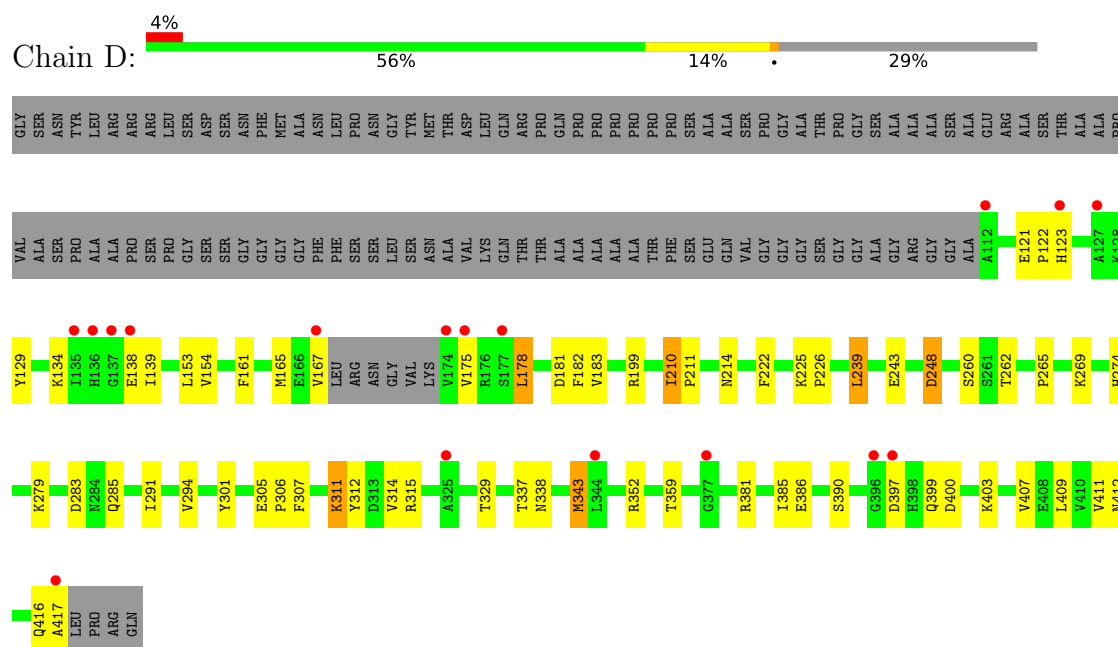


- Molecule 1: rat synapsin I

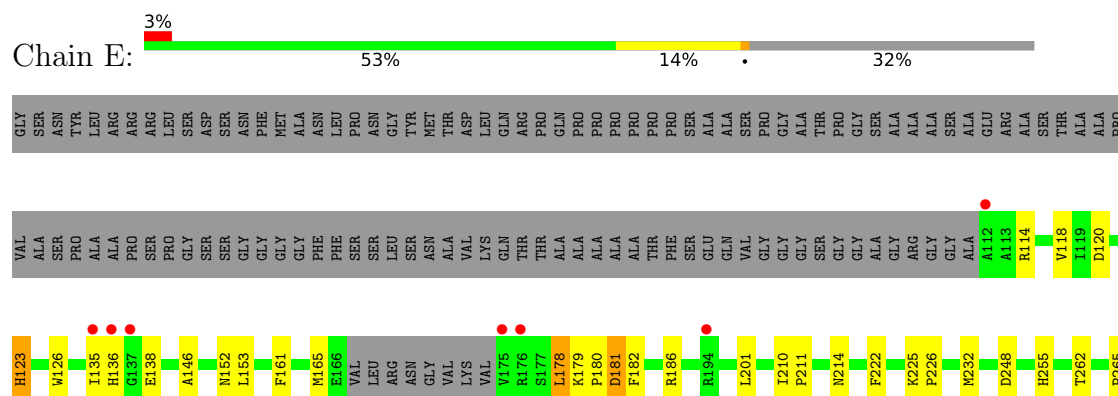


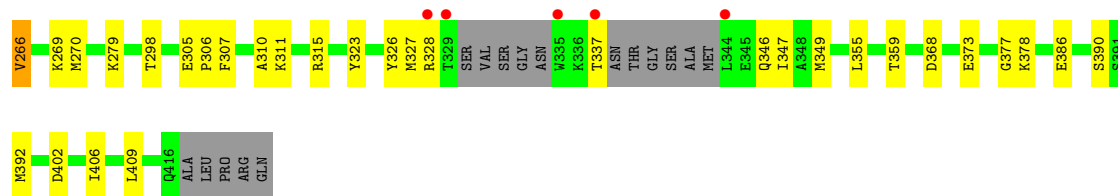


- Molecule 1: rat synapsin I

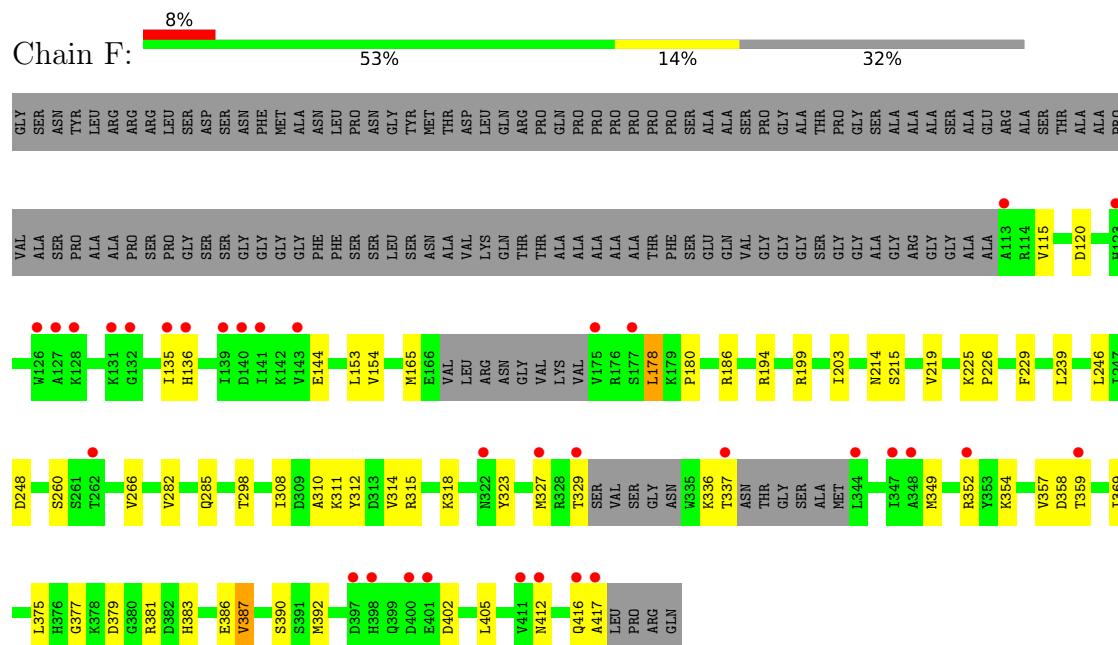


- Molecule 1: rat synapsin I

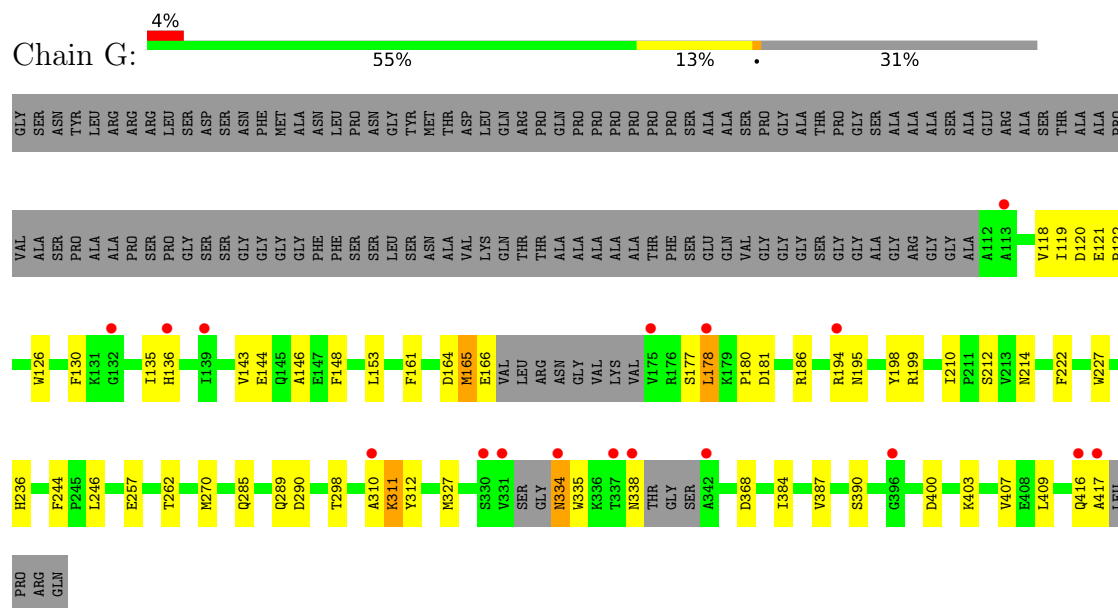




- Molecule 1: rat synapsin I

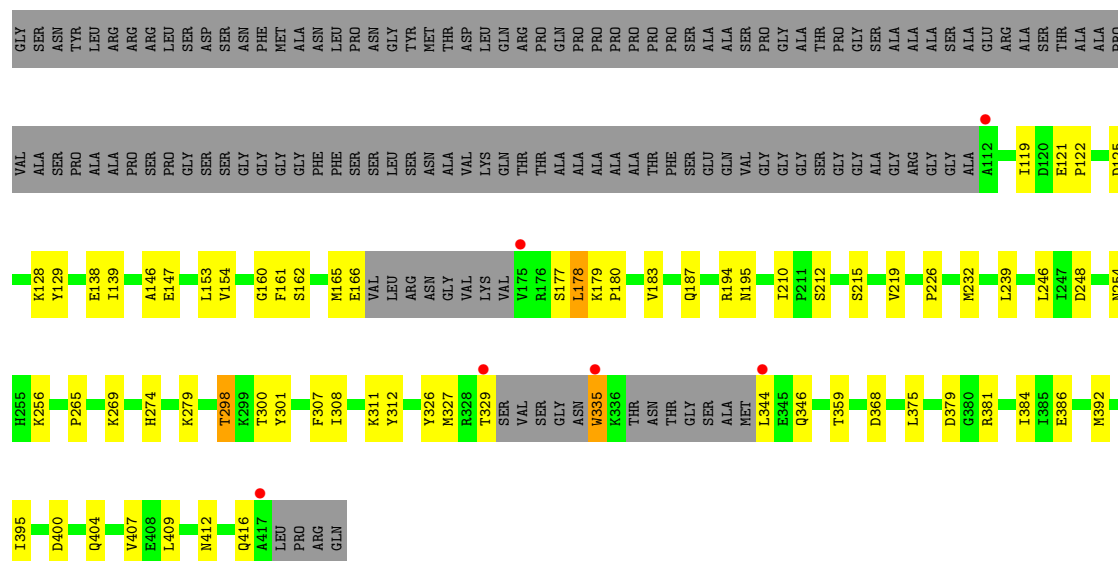


- Molecule 1: rat synapsin I



- Molecule 1: rat synapsin I





4 Data and refinement statistics

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 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.9 (20.00-2.10) 91.8 (20.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.222 , 0.259 0.232 , 0.267	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)	0.36 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.43	0/2466	0.92	6/3334 (0.2%)
1	B	0.45	0/2367	0.94	4/3197 (0.1%)
1	C	0.40	0/2321	0.93	9/3133 (0.3%)
1	D	0.37	0/2418	0.91	6/3269 (0.2%)
1	E	0.38	0/2328	0.90	5/3143 (0.2%)
1	F	0.41	1/2328 (0.0%)	0.90	2/3143 (0.1%)
1	G	0.40	0/2375	0.94	8/3207 (0.2%)
1	H	0.39	0/2326	0.89	4/3140 (0.1%)
All	All	0.40	1/18929 (0.0%)	0.92	44/25566 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	337	THR	CA-C	5.57	1.64	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	311	LYS	N-CA-C	-7.54	103.14	111.36
1	C	311	LYS	N-CA-C	-7.50	103.93	113.23
1	D	181	ASP	N-CA-C	-7.11	104.63	113.38
1	D	311	LYS	N-CA-C	-6.95	103.47	112.23
1	A	311	LYS	N-CA-C	-6.91	103.80	111.82
1	F	311	LYS	N-CA-C	-6.88	103.86	111.36
1	E	311	LYS	N-CA-C	-6.61	104.24	112.90
1	G	310	ALA	N-CA-C	6.54	120.16	109.76
1	H	311	LYS	N-CA-C	-6.25	104.00	111.69
1	C	212	SER	N-CA-C	6.24	117.71	108.60
1	C	121	GLU	CA-C-N	6.23	125.92	119.56
1	C	121	GLU	C-N-CA	6.23	125.92	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	298	THR	N-CA-C	-6.15	105.26	112.89
1	D	239	LEU	N-CA-C	6.11	119.93	112.23
1	G	143	VAL	N-CA-C	6.01	116.52	107.80
1	B	310	ALA	N-CA-C	5.98	119.27	109.76
1	C	181	ASP	N-CA-C	-5.96	105.83	113.23
1	C	241	THR	N-CA-C	5.91	117.72	111.28
1	E	181	ASP	N-CA-C	-5.89	106.26	113.50
1	E	298	THR	N-CA-C	-5.81	105.69	112.89
1	B	311	LYS	N-CA-C	-5.79	105.05	111.36
1	B	255	HIS	N-CA-C	5.61	118.16	111.71
1	G	181	ASP	N-CA-C	-5.58	106.51	113.38
1	F	298	THR	N-CA-C	-5.49	106.43	113.01
1	C	298	THR	N-CA-C	-5.46	106.12	112.89
1	G	165	MET	N-CA-C	5.41	117.72	108.90
1	H	212	SER	N-CA-C	5.41	117.07	108.79
1	A	143	VAL	N-CA-C	5.39	116.07	108.36
1	D	274	HIS	N-CA-C	5.38	116.82	109.18
1	G	212	SER	N-CA-C	5.38	116.97	108.96
1	A	181	ASP	N-CA-C	-5.37	106.89	113.50
1	A	338	ASN	N-CA-C	-5.30	106.49	113.17
1	H	298	THR	N-CA-C	-5.30	106.32	112.89
1	B	283	ASP	N-CA-C	5.28	119.78	113.23
1	C	122	PRO	N-CA-C	5.24	120.65	113.84
1	D	338	ASN	N-CA-C	-5.19	105.63	112.94
1	G	227	TRP	N-CA-C	-5.18	105.71	111.36
1	E	123	HIS	N-CA-C	5.17	118.69	112.38
1	C	310	ALA	N-CA-C	5.08	118.49	109.96
1	E	255	HIS	N-CA-C	5.03	118.19	111.75
1	H	274	HIS	N-CA-C	5.03	117.50	109.81
1	A	255	HIS	N-CA-C	5.03	117.65	111.82
1	D	210	ILE	N-CA-C	5.03	112.84	107.76
1	A	212	SER	N-CA-C	5.01	116.42	108.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2414	0	2397	36	0
1	B	2317	0	2289	35	0
1	C	2272	0	2246	37	0
1	D	2367	0	2341	42	0
1	E	2279	0	2253	37	0
1	F	2279	0	2253	35	0
1	G	2326	0	2298	32	0
1	H	2277	0	2251	42	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	285	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 (285) 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:E:327:MET:HE3	1:E:347:ILE:HG21	1.66	0.78
1:D:343:MET:HE2	1:E:378:LYS:HE2	1.70	0.74
1:D:407:VAL:O	1:D:411:VAL:HG23	1.94	0.68
1:A:327:MET:HE3	1:A:347:ILE:HG21	1.74	0.68
1:D:399:GLN:O	1:D:403:LYS:HG3	1.93	0.67
1:E:232:MET:HE1	1:E:386:GLU:HA	1.76	0.67
1:F:336:LYS:HE2	1:G:290:ASP:OD1	1.94	0.67
1:B:336:LYS:C	1:B:338:ASN:H	2.00	0.67
1:H:232:MET:HE1	1:H:386:GLU:HA	1.77	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:F:144:GLU:HG3	1:F:165:MET:HE1	1.80	0.64
1:E:328:ARG:HD3	1:E:337:THR:CB	2.27	0.64
1:C:312:TYR:CZ	1:C:327:MET:HE2	2.33	0.63
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: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:H:153:LEU:C	1:H:153:LEU:HD12	2.26	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:E:323:TYR:HB3	1:E:349:MET:HE2	1.84	0.59
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:H:335:TRP:CE3	1:H:335:TRP:C	2.82	0.58
1:G:165:MET:HE3	1:G:178:LEU:HD21	1.85	0.58
1:E:355:LEU:O	1:E:359:THR:HG23	2.04	0.58
1:G:214:ASN:CG	1:G:390:SER:HB3	2.28	0.58
1:B:153:LEU:C	1:B:153:LEU:HD12	2.29	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:LYS:C	1:B:338:ASN:N	2.62	0.57
1:G:285:GLN:O	1:G:289:GLN:HG3	2.04	0.57
1:F:323:TYR:HB3	1:F:349:MET:HE2	1.85	0.57
1:F:392:MET:HG3	1:F:392:MET:O	2.03	0.57
1:F:369:ILE:CG2	1:F:392:MET:HE2	2.35	0.56
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:B:214:ASN:CG	1:B:390:SER:HB3	2.31	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:E:161:PHE:CE2	1:E:210:ILE:HD11	2.41	0.55
1:G:153:LEU:HD12	1:G:153:LEU:C	2.31	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:335:TRP:C	1:H:335:TRP:HE3	2.14	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
1:A:308:ILE:HD12	1:A:375:LEU:HD12	1.90	0.54
1:F:153:LEU:C	1:F:153:LEU:HD12	2.32	0.54
1:D:183:VAL:HG23	1:D:210:ILE:HG21	1.88	0.54
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:C:153:LEU:C	1:C:153:LEU:HD12	2.34	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:F:369:ILE:HG23	1:F:392:MET:HE2	1.91	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:B:312:TYR:CE2	1:B:327:MET:HE2	2.44	0.52
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:A:232:MET:HE1	1:A:386:GLU:HA	1.90	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:214:ASN:CG	1:A:390:SER:HB3	2.35	0.51
1:D:409:LEU:HD23	1:D:409:LEU:C	2.36	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:B:416:GLN:O	1:B:417:ALA:HB2	2.12	0.50
1:F:178:LEU:HD12	1:F:180:PRO:CG	2.41	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:A:153:LEU:C	1:A:153:LEU:HD12	2.36	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
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: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:C:312:TYR:CE1	1:C:327:MET:HE2	2.48	0.49
1:B:294:VAL:HG11	1:D:294:VAL:HG11	1.95	0.49
1:E:214:ASN:CG	1:E:390:SER:HB3	2.38	0.48
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:F:323:TYR:CB	1:F:349:MET:HE2	2.45	0.46
1:A:385:ILE:O	1:A:386:GLU:HB2	2.14	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:335:TRP:HE3	1:C:335:TRP:C	2.24	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:C:214:ASN:CG	1:C:390:SER:HB3	2.41	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:C:335:TRP:C	1:C:335:TRP:CE3	2.94	0.46
1:D:265:PRO:HG2	1:D:307:PHE:HB3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:LEU:HD12	1:E:153:LEU:C	2.41	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: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: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
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:H:379:ASP:C	1:H:379:ASP:OD1	2.60	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:H:312:TYR:CZ	1:H:327:MET:HE2	2.53	0.44
1:A:135:ILE:O	1:A:136:HIS:HB2	2.17	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:214:ASN:CG	1:D:390:SER:HB3	2.42	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:153:LEU:C	1:D:153:LEU:HD12	2.44	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:C:165:MET:HE3	1:C:178:LEU:HD21	2.01	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:291:ILE:HD13	1:D:291:ILE:HA	1.91	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: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:B:312:TYR:CZ	1:B:327:MET:HE2	2.55	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
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:F:214:ASN:CG	1:F:390:SER:HB3	2.46	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

5.3.1 Protein backbone

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%)	36	36
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

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%)	65	74
1	B	252/340 (74%)	250 (99%)	2 (1%)	73	81
1	C	247/340 (73%)	238 (96%)	9 (4%)	31	34
1	D	258/340 (76%)	247 (96%)	11 (4%)	26	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	248/340 (73%)	241 (97%)	7 (3%)	38	43
1	F	248/340 (73%)	242 (98%)	6 (2%)	43	49
1	G	253/340 (74%)	244 (96%)	9 (4%)	31	34
1	H	247/340 (73%)	240 (97%)	7 (3%)	38	43
All	All	2016/2720 (74%)	1962 (97%)	54 (3%)	39	45

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	LEU
1	A	248	ASP
1	A	262	THR
1	B	178	LEU
1	B	262	THR
1	C	178	LEU
1	C	222	PHE
1	C	262	THR
1	C	291	ILE
1	C	329	THR
1	C	335	TRP
1	C	386	GLU
1	C	399	GLN
1	C	412	ASN
1	D	123	HIS
1	D	178	LEU
1	D	222	PHE
1	D	243	GLU
1	D	248	ASP
1	D	262	THR
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	178	LEU
1	F	248	ASP
1	F	329	THR
1	F	352	ARG
1	F	387	VAL
1	F	412	ASN
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	138	GLU
1	H	178	LEU
1	H	248	ASP
1	H	329	THR
1	H	335	TRP
1	H	381	ARG
1	H	404	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	ASN
1	A	249	GLN
1	A	255	HIS
1	A	404	GLN
1	B	236	HIS
1	B	249	GLN
1	B	255	HIS
1	B	289	GLN
1	B	338	ASN
1	B	383	HIS
1	B	404	GLN
1	C	236	HIS
1	C	249	GLN
1	C	255	HIS
1	C	346	GLN
1	C	404	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	195	ASN
1	D	255	HIS
1	E	195	ASN
1	E	289	GLN
1	E	383	HIS
1	F	217	HIS
1	F	249	GLN
1	F	255	HIS
1	F	399	GLN
1	G	195	ASN
1	G	249	GLN
1	G	285	GLN
1	G	334	ASN
1	G	338	ASN
1	G	398	HIS
1	H	249	GLN
1	H	289	GLN
1	H	346	GLN
1	H	383	HIS
1	H	398	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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[B]	2	32,33,33	0.67	0	48,52,52	0.76	1 (2%)
3	ATP	B	801[B]	2	32,33,33	0.60	0	48,52,52	0.77	3 (6%)
3	ATP	A	800[A]	2	32,33,33	0.61	0	48,52,52	0.69	1 (2%)
3	ATP	E	804[B]	2	32,33,33	0.60	0	48,52,52	0.75	2 (4%)
3	ATP	H	807[B]	2	32,33,33	0.63	0	48,52,52	0.76	2 (4%)
3	ATP	F	805[A]	2	32,33,33	0.57	0	48,52,52	0.71	2 (4%)
3	ATP	F	805[B]	2	32,33,33	0.61	0	48,52,52	0.78	3 (6%)
3	ATP	G	806[A]	2	32,33,33	0.60	0	48,52,52	0.72	2 (4%)
3	ATP	G	806[B]	2	32,33,33	0.59	0	48,52,52	0.77	2 (4%)
3	ATP	D	803[A]	2	32,33,33	0.57	0	48,52,52	0.71	3 (6%)
4	EDO	B	819	-	3,3,3	0.63	0	2,2,2	0.40	0
3	ATP	D	803[B]	2	32,33,33	0.59	0	48,52,52	0.78	3 (6%)
3	ATP	C	802[A]	2	32,33,33	0.60	0	48,52,52	0.75	3 (6%)
3	ATP	C	802[B]	2	32,33,33	0.60	0	48,52,52	0.79	3 (6%)
3	ATP	E	804[A]	2	32,33,33	0.62	0	48,52,52	0.76	3 (6%)
3	ATP	H	807[A]	2	32,33,33	0.59	0	48,52,52	0.73	3 (6%)
4	EDO	A	818	-	3,3,3	0.91	0	2,2,2	0.37	0
3	ATP	B	801[A]	2	32,33,33	0.60	0	48,52,52	0.74	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	800[B]	2	-	6/22/38/38	0/3/3/3
3	ATP	B	801[B]	2	-	6/22/38/38	0/3/3/3
3	ATP	A	800[A]	2	-	1/22/38/38	0/3/3/3
3	ATP	E	804[B]	2	-	3/22/38/38	0/3/3/3
3	ATP	H	807[B]	2	-	2/22/38/38	0/3/3/3
3	ATP	F	805[A]	2	-	0/22/38/38	0/3/3/3
3	ATP	F	805[B]	2	-	3/22/38/38	0/3/3/3
3	ATP	G	806[A]	2	-	0/22/38/38	0/3/3/3
3	ATP	G	806[B]	2	-	4/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	D	803[A]	2	-	0/22/38/38	0/3/3/3
4	EDO	B	819	-	-	1/1/1/1	-
3	ATP	D	803[B]	2	-	3/22/38/38	0/3/3/3
3	ATP	C	802[A]	2	-	2/22/38/38	0/3/3/3
3	ATP	C	802[B]	2	-	1/22/38/38	0/3/3/3
3	ATP	E	804[A]	2	-	0/22/38/38	0/3/3/3
3	ATP	H	807[A]	2	-	2/22/38/38	0/3/3/3
4	EDO	A	818	-	-	0/1/1/1	-
3	ATP	B	801[A]	2	-	0/22/38/38	0/3/3/3

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	804[A]	ATP	O3G-PG-O2G	-2.44	98.66	107.80
3	A	800[B]	ATP	O3G-PG-O2G	-2.35	99.00	107.80
3	C	802[A]	ATP	O3G-PG-O2G	-2.33	99.06	107.80
3	H	807[A]	ATP	O3G-PG-O2G	-2.25	99.38	107.80
3	B	801[B]	ATP	O3G-PG-O2G	-2.21	99.51	107.80
3	C	802[B]	ATP	O3G-PG-O2G	-2.19	99.61	107.80
3	E	804[A]	ATP	O2G-PG-O1G	2.17	119.29	110.83
3	H	807[B]	ATP	O3G-PG-O2G	-2.15	99.73	107.80
3	F	805[B]	ATP	O3G-PG-O2G	-2.14	99.76	107.80
3	G	806[A]	ATP	O3G-PG-O2G	-2.14	99.77	107.80
3	G	806[B]	ATP	O3G-PG-O2G	-2.11	99.88	107.80
3	F	805[A]	ATP	O2G-PG-O1G	2.10	119.03	110.83
3	D	803[A]	ATP	O3G-PG-O2G	-2.08	99.99	107.80
3	C	802[A]	ATP	O2G-PG-O1G	2.08	118.92	110.83
3	D	803[A]	ATP	O3G-PG-O1G	2.07	118.88	110.83
3	D	803[B]	ATP	O3G-PG-O2G	-2.06	100.07	107.80
3	H	807[A]	ATP	O2G-PG-O1G	2.06	118.87	110.83
3	F	805[B]	ATP	O3G-PG-O1G	2.06	118.87	110.83
3	E	804[B]	ATP	O3G-PG-O2G	-2.06	100.08	107.80
3	D	803[B]	ATP	O2G-PG-O1G	2.06	118.84	110.83
3	E	804[A]	ATP	O3G-PG-O1G	2.06	118.84	110.83
3	C	802[A]	ATP	O3G-PG-O1G	2.05	118.84	110.83
3	G	806[B]	ATP	O3G-PG-O1G	2.04	118.80	110.83
3	B	801[B]	ATP	O2G-PG-O1G	2.03	118.76	110.83
3	E	804[B]	ATP	O3G-PG-O1G	2.03	118.76	110.83
3	C	802[B]	ATP	O3G-PG-O1G	2.03	118.75	110.83
3	D	803[A]	ATP	O2G-PG-O1G	2.03	118.75	110.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	803[B]	ATP	O3G-PG-O1G	2.03	118.73	110.83
3	H	807[B]	ATP	O3G-PG-O1G	2.03	118.73	110.83
3	F	805[A]	ATP	O3G-PG-O1G	2.03	118.73	110.83
3	B	801[A]	ATP	O2G-PG-O1G	2.03	118.73	110.83
3	F	805[B]	ATP	O2G-PG-O1G	2.02	118.71	110.83
3	B	801[B]	ATP	O3G-PG-O1G	2.02	118.70	110.83
3	C	802[B]	ATP	O2G-PG-O1G	2.02	118.69	110.83
3	G	806[A]	ATP	O3G-PG-O1G	2.01	118.67	110.83
3	A	800[A]	ATP	O2G-PG-O1G	2.01	118.65	110.83
3	H	807[A]	ATP	O3G-PG-O1G	2.00	118.63	110.83

There are no chirality outliers.

All (34) 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
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'
3	D	803[B]	ATP	PA-O3A-PB-O2B
3	G	806[B]	ATP	PA-O3A-PB-O2B
3	H	807[A]	ATP	PB-O3B-PG-O1G
4	B	819	EDO	O1-C1-C2-O2
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	D	803[B]	ATP	C4'-C5'-O5'-PA
3	G	806[B]	ATP	C4'-C5'-O5'-PA
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

Continued on next page...

Continued from previous page...

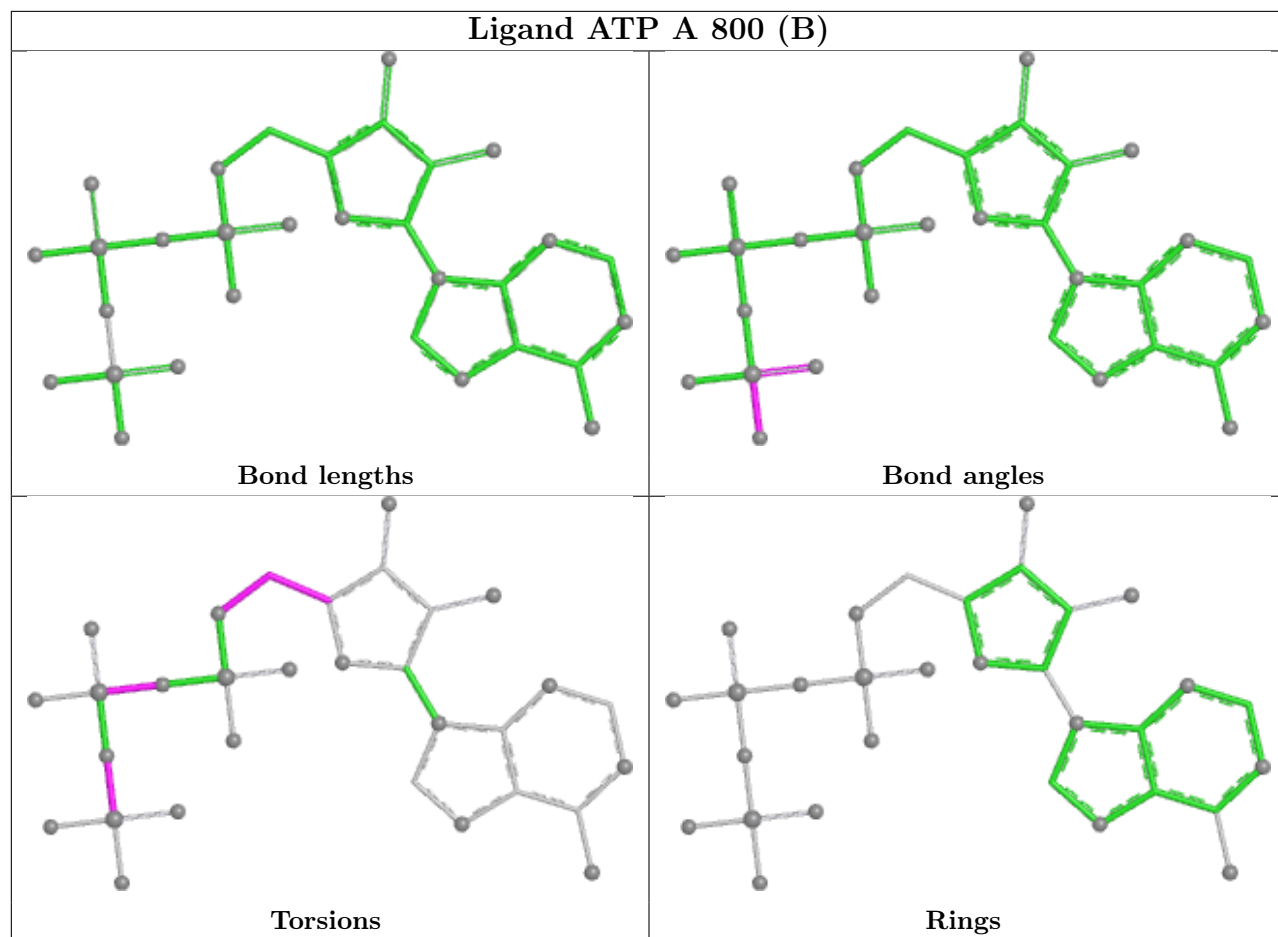
Mol	Chain	Res	Type	Atoms
3	E	804[B]	ATP	PB-O3B-PG-O2G
3	B	801[B]	ATP	C4'-C5'-O5'-PA
3	A	800[B]	ATP	PA-O3A-PB-O2B
3	D	803[B]	ATP	PA-O3A-PB-O1B
3	A	800[B]	ATP	C4'-C5'-O5'-PA
3	A	800[B]	ATP	C3'-C4'-C5'-O5'
3	A	800[A]	ATP	PB-O3A-PA-O1A

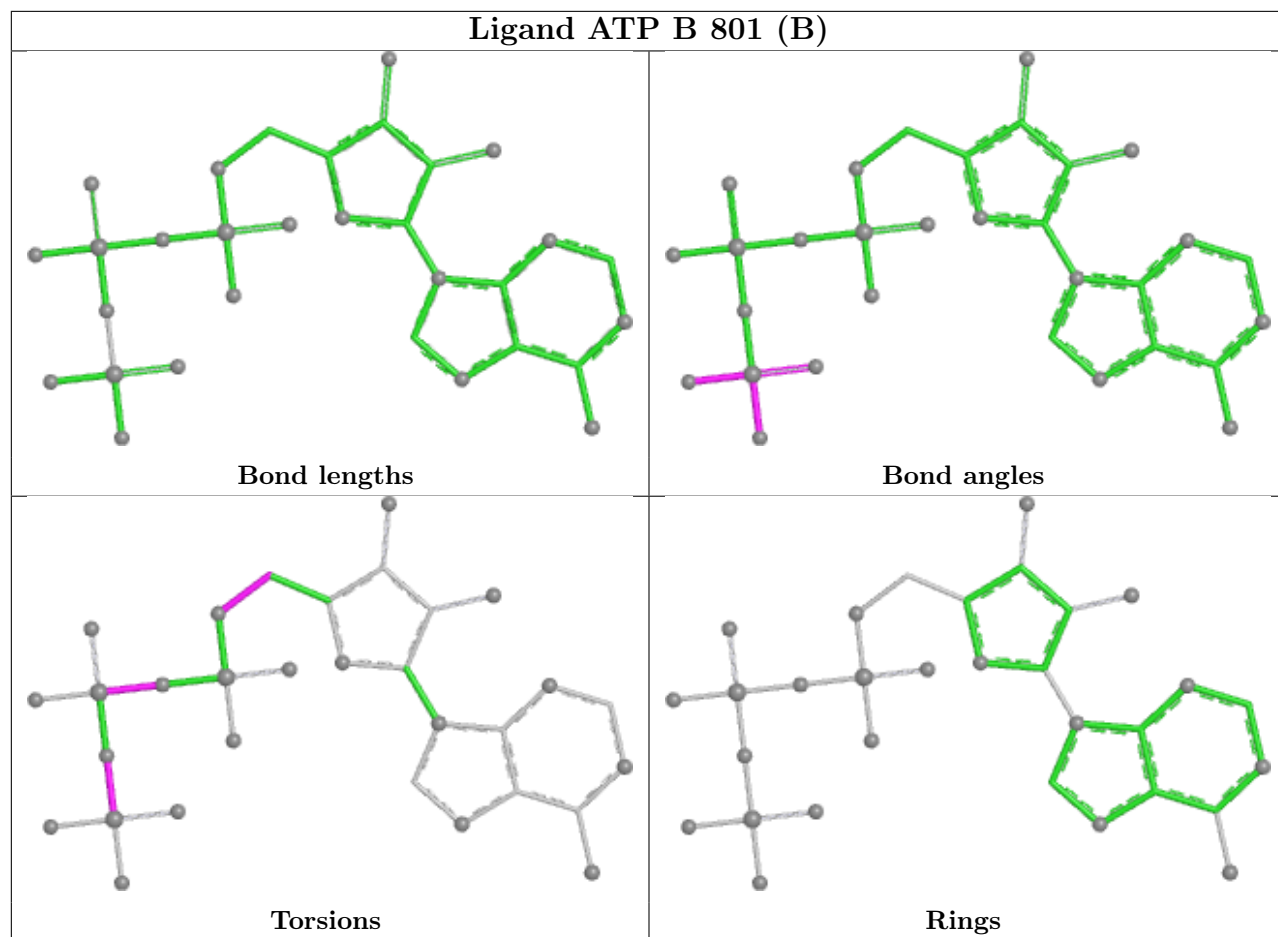
There are no ring outliers.

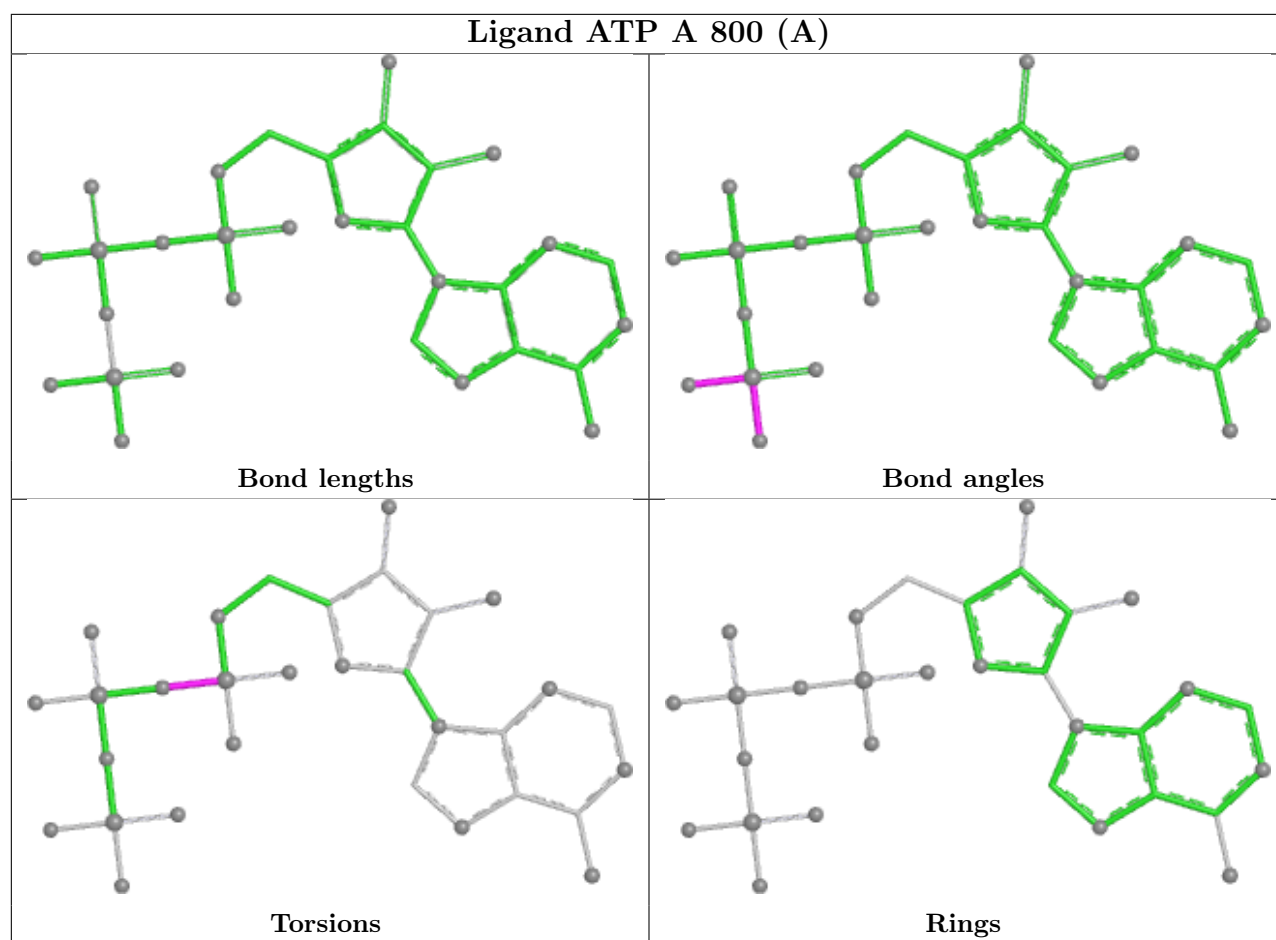
3 monomers are involved in 4 short contacts:

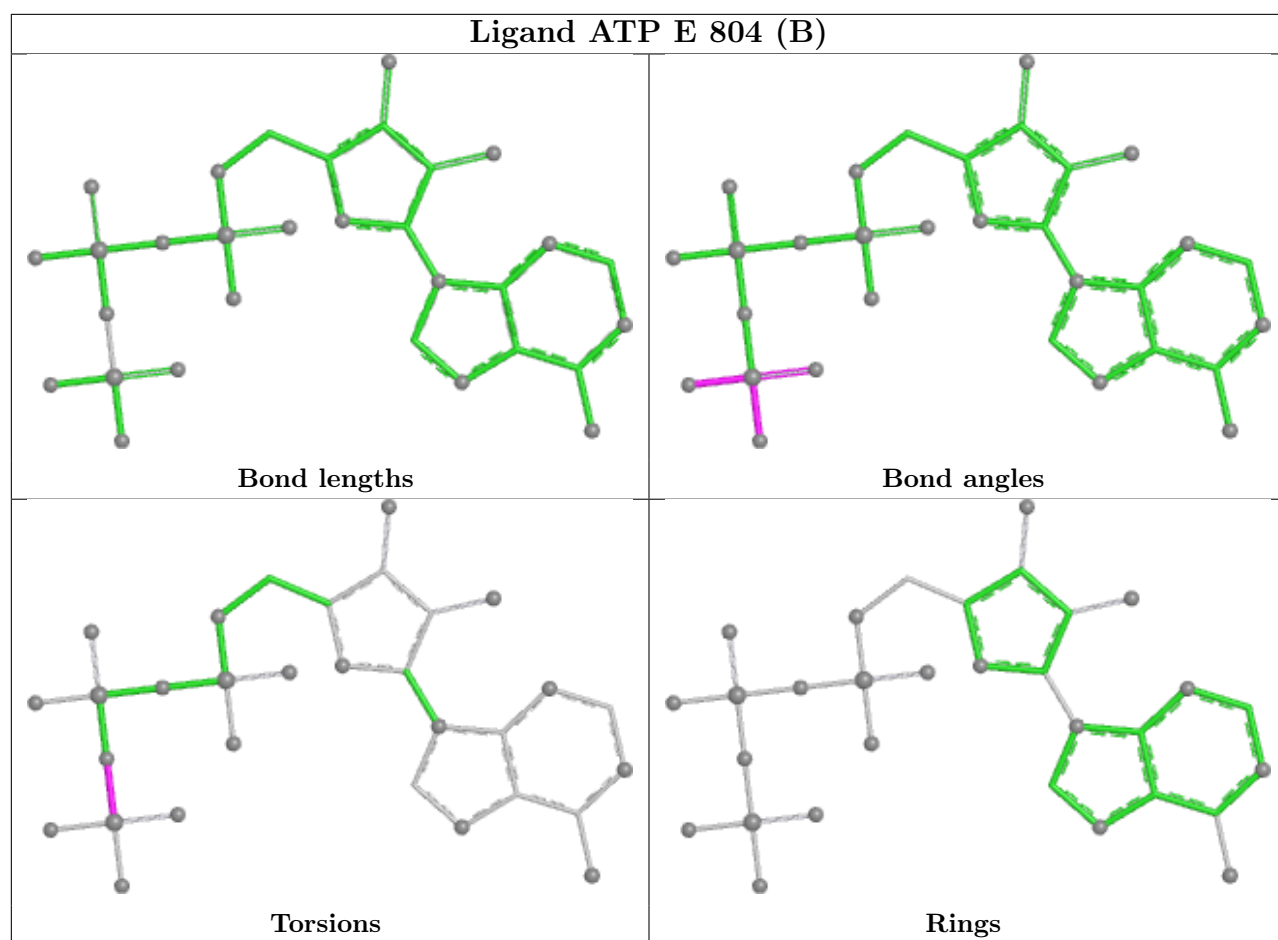
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	800[B]	ATP	1	0
3	B	801[B]	ATP	1	0
3	D	803[B]	ATP	2	0

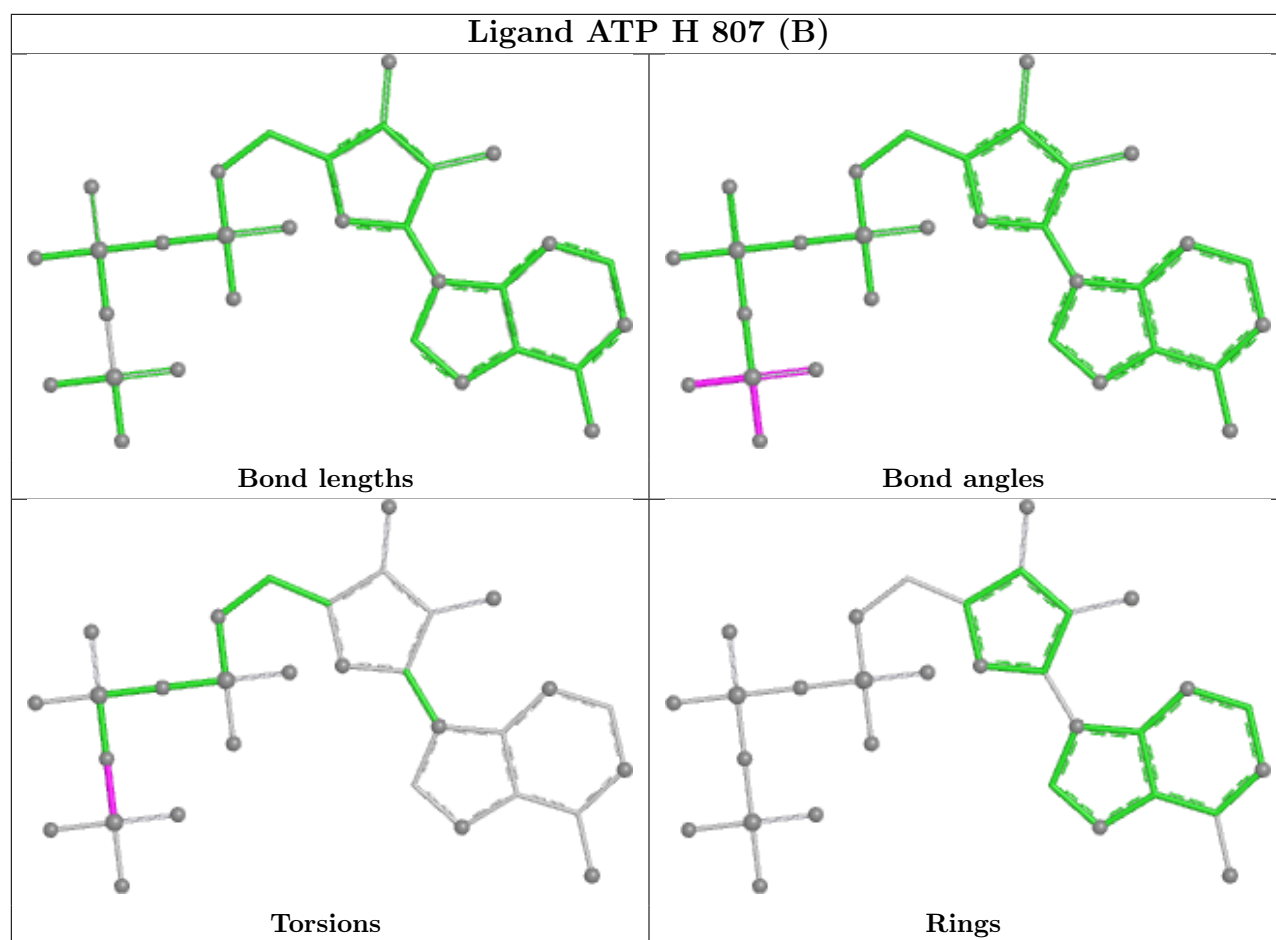
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



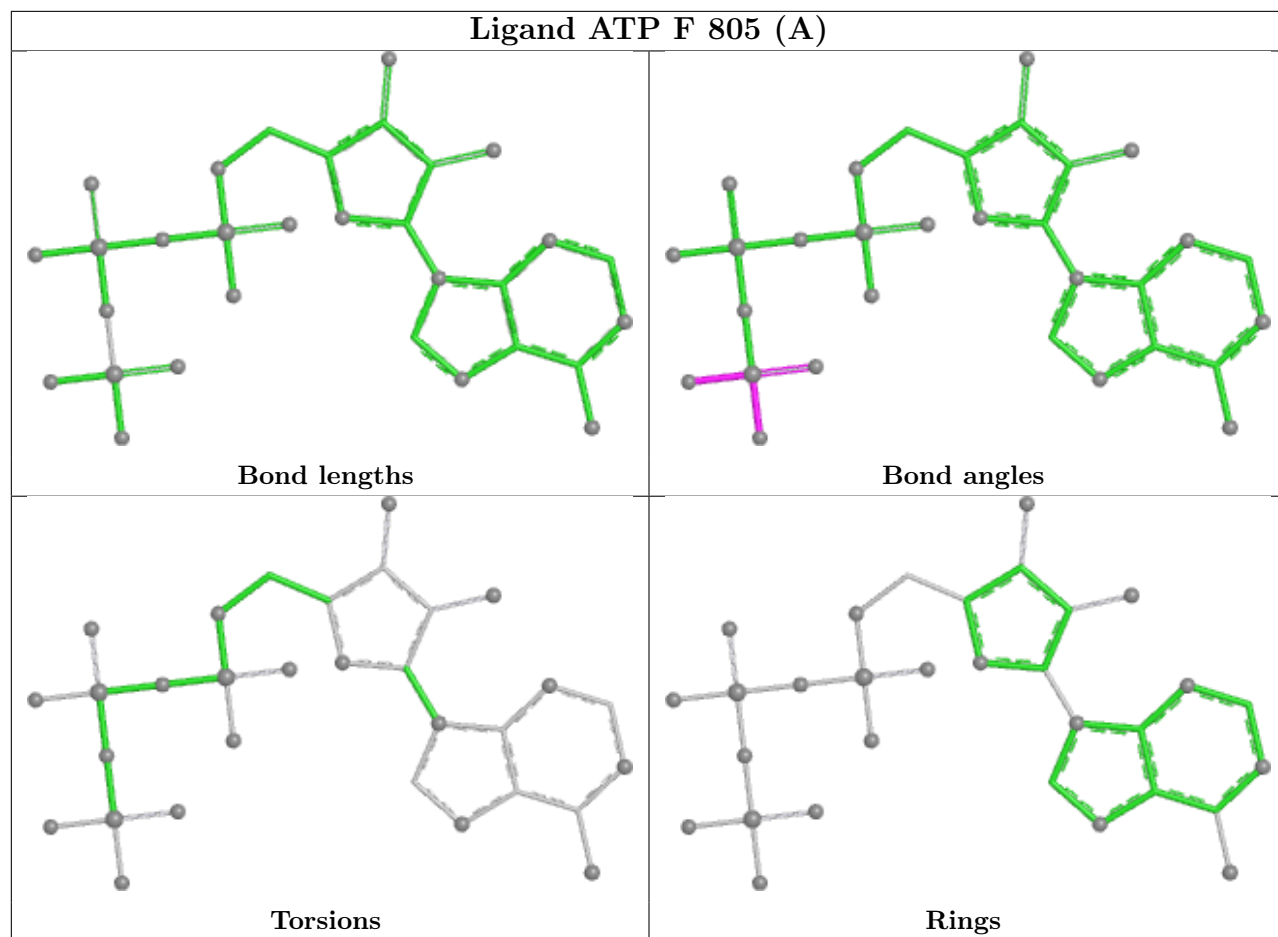


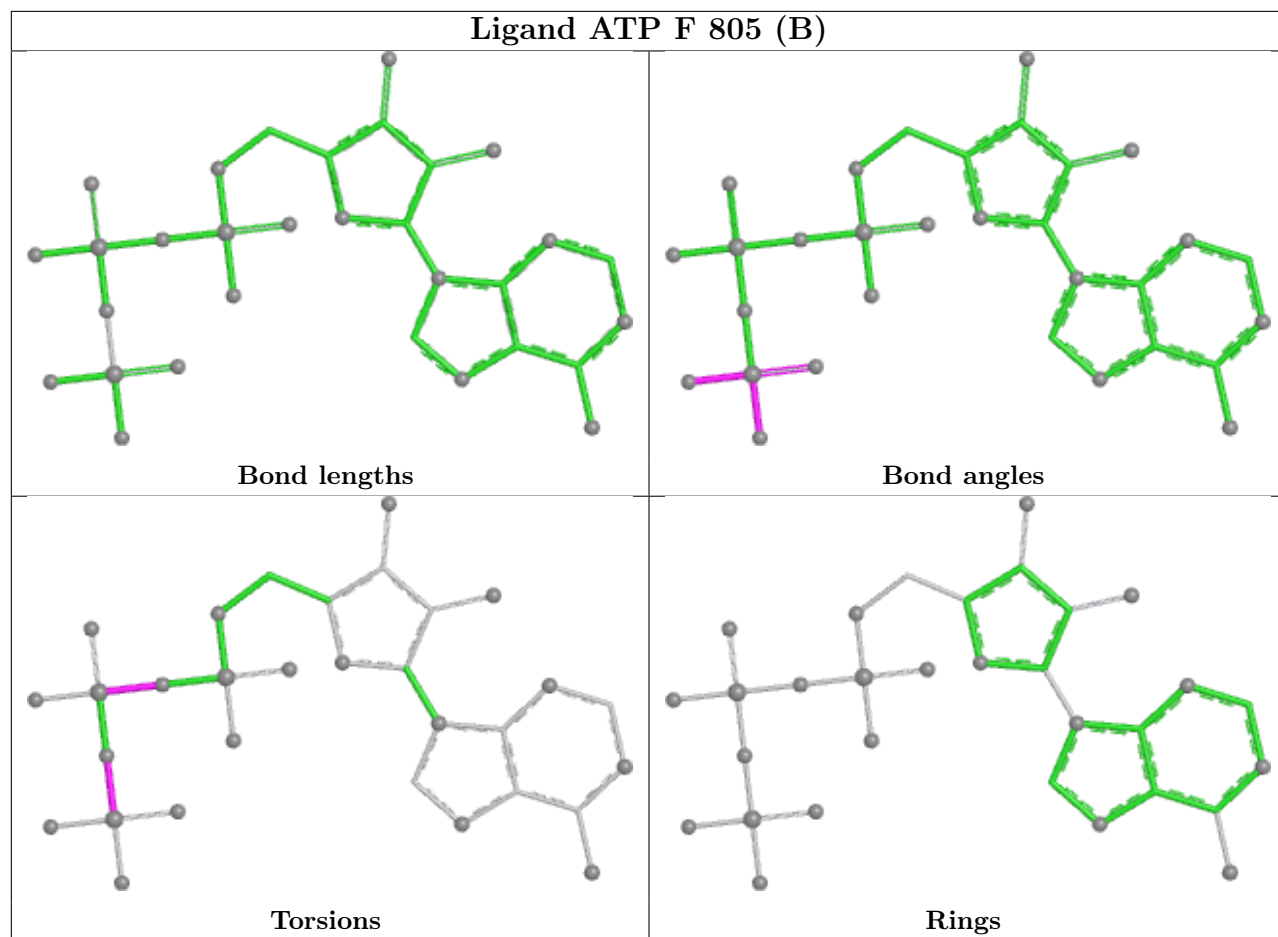


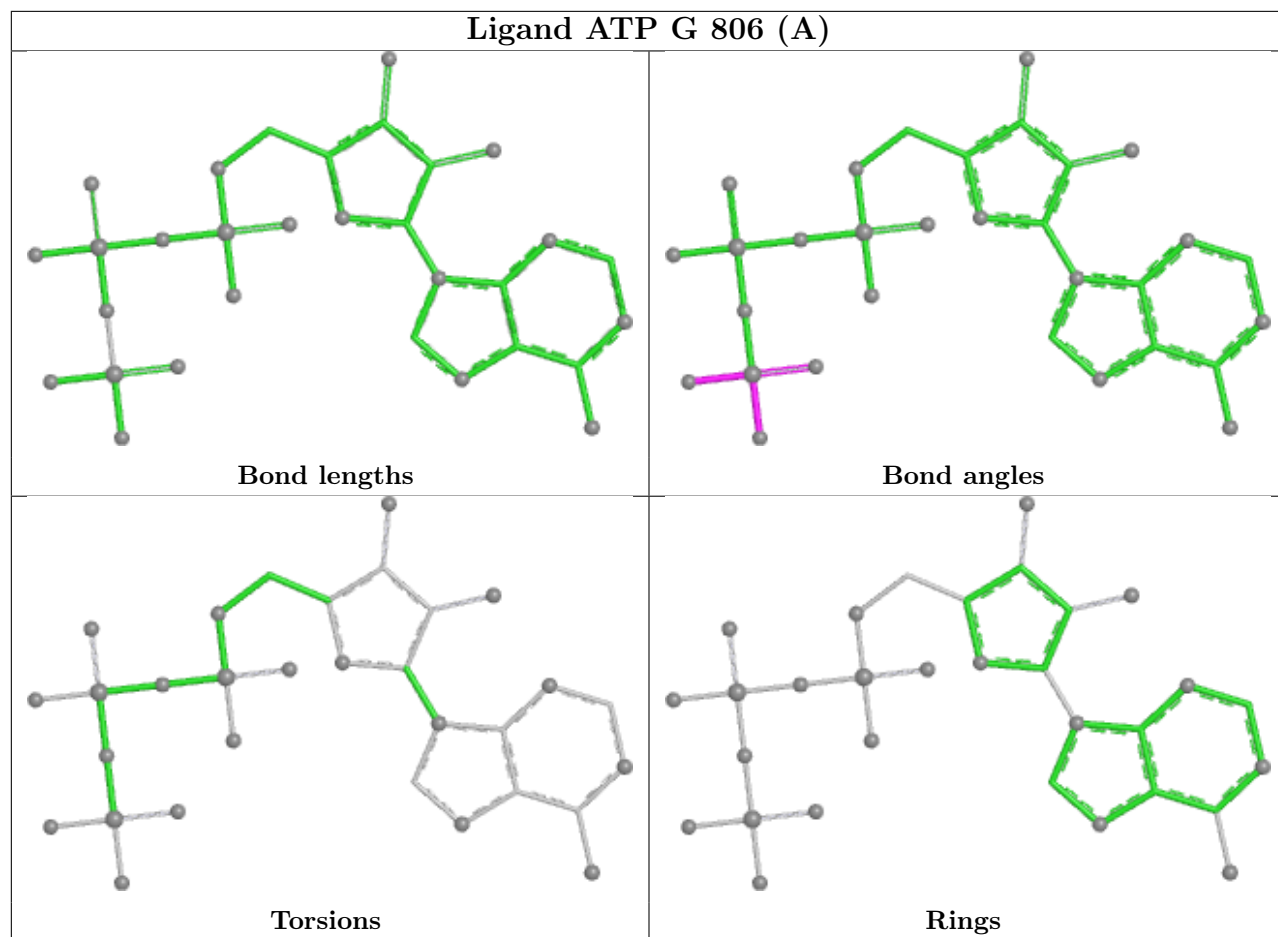


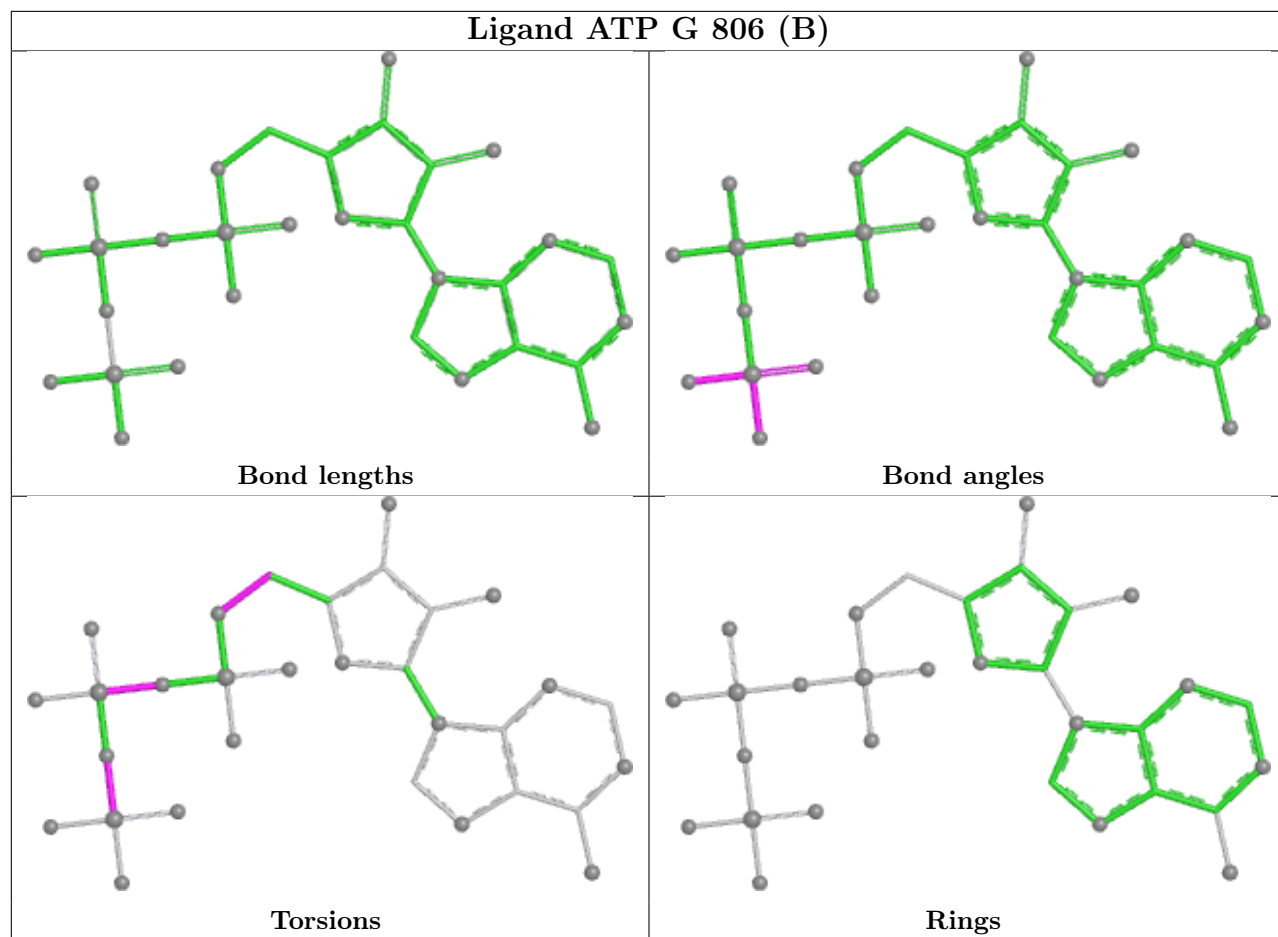


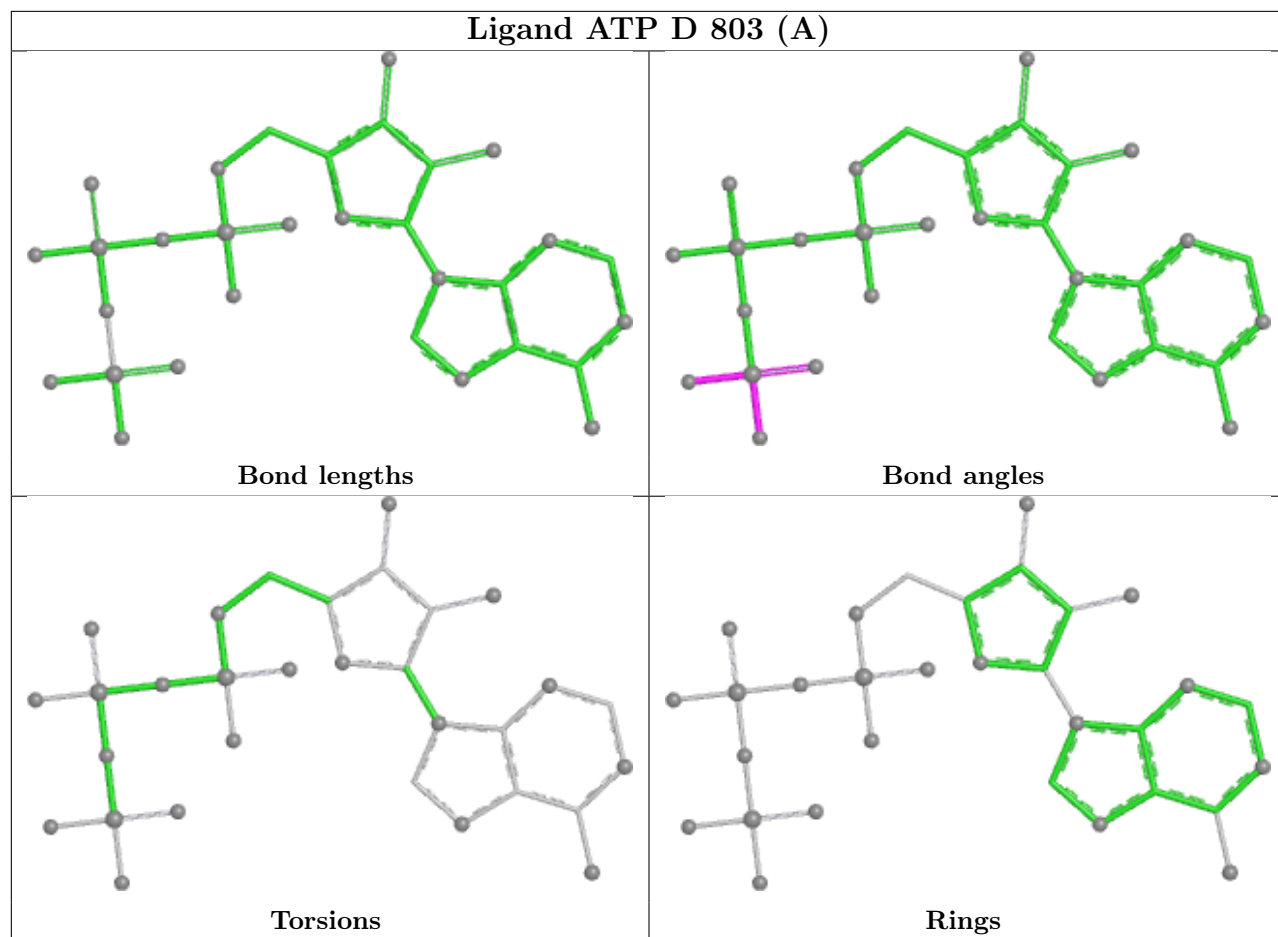
Ligand ATP F 805 (A)

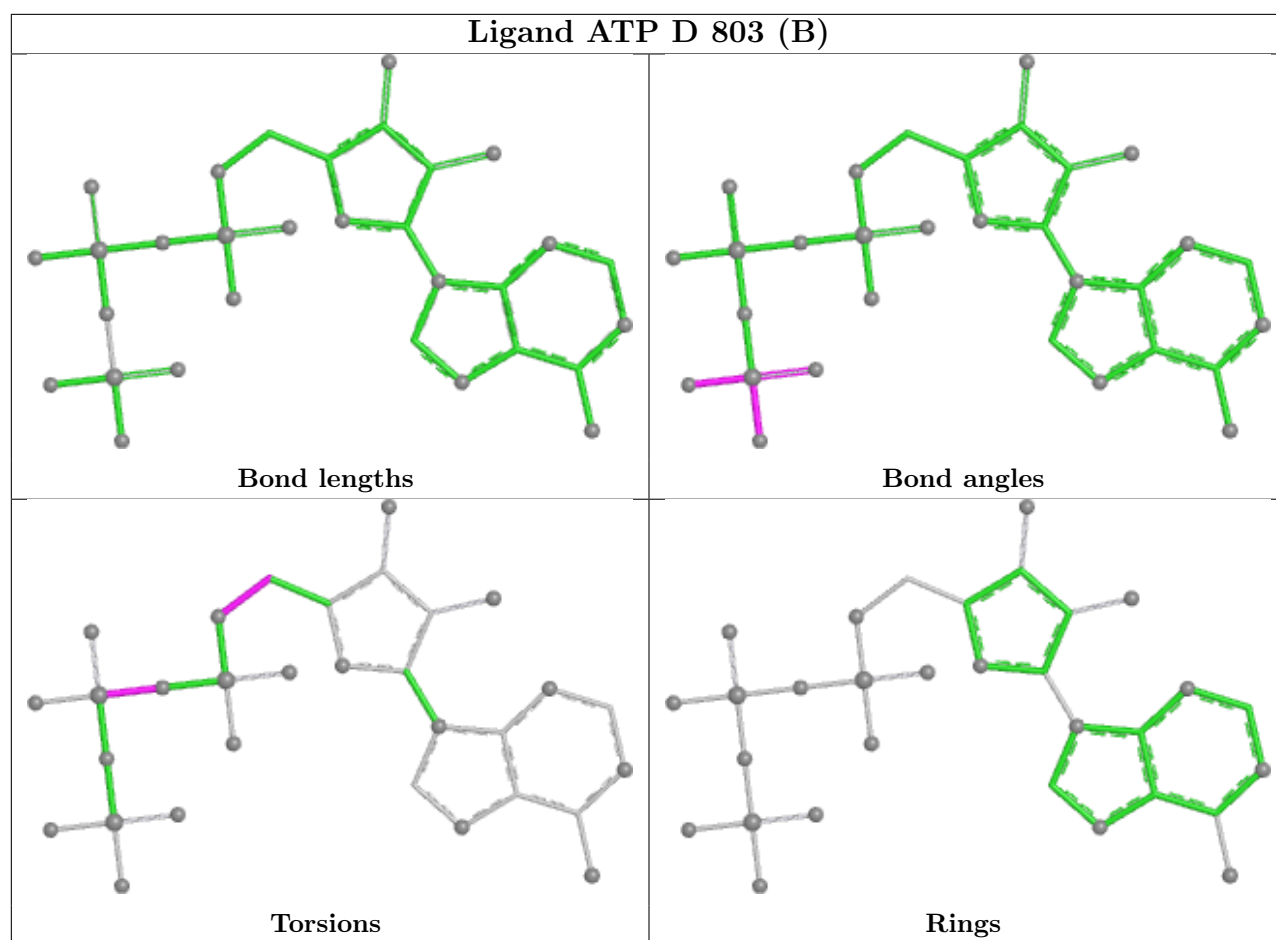


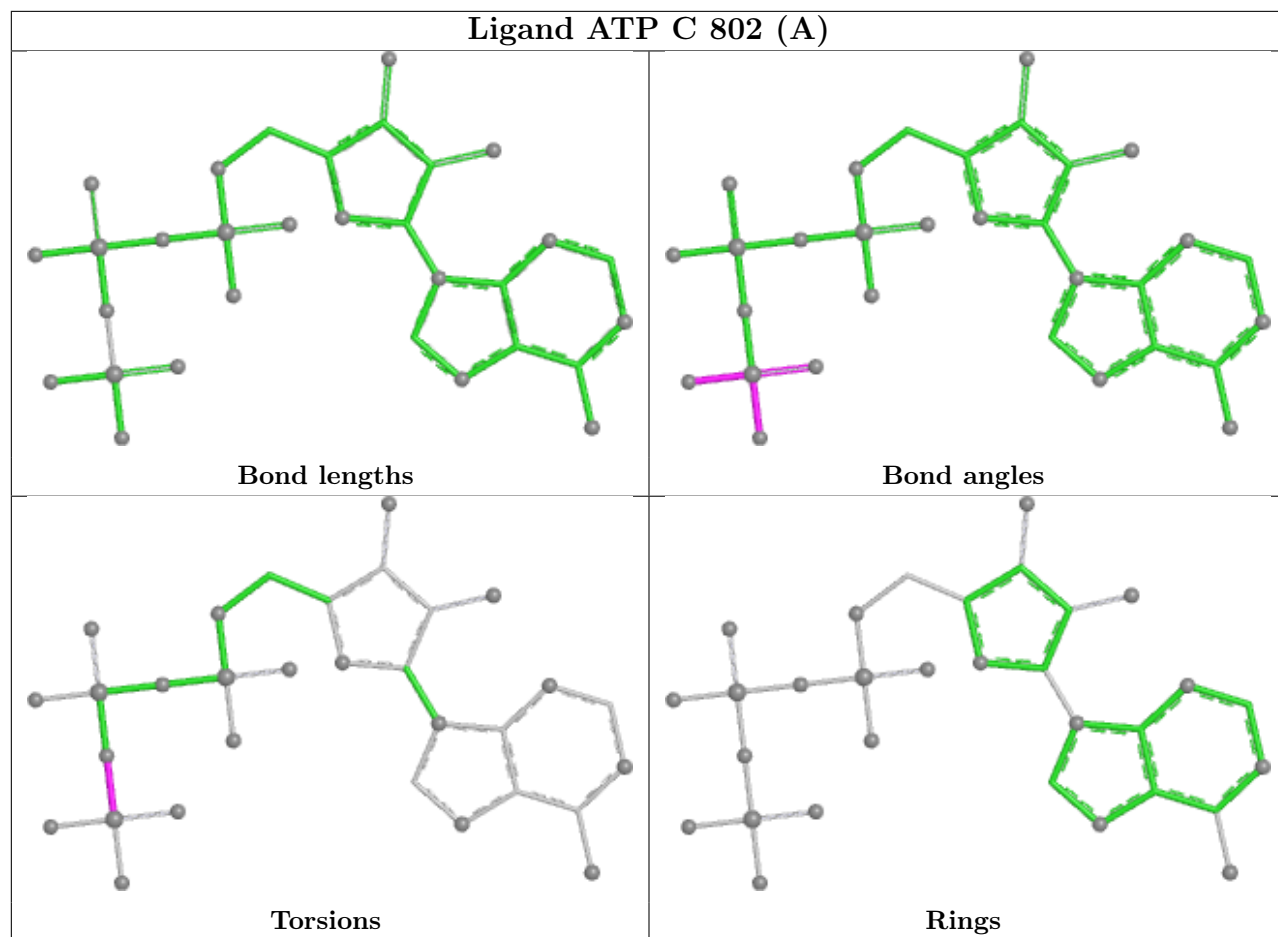


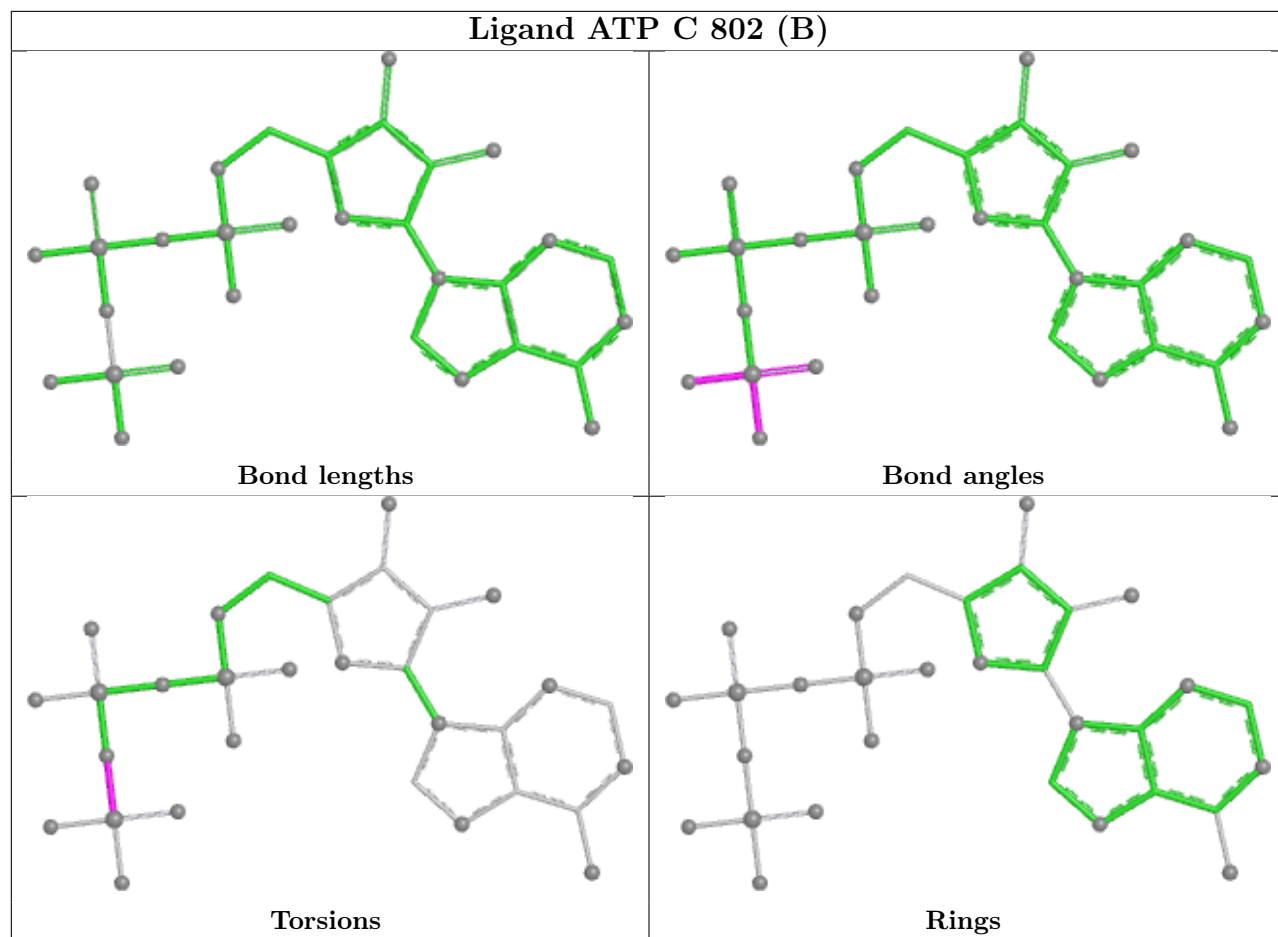




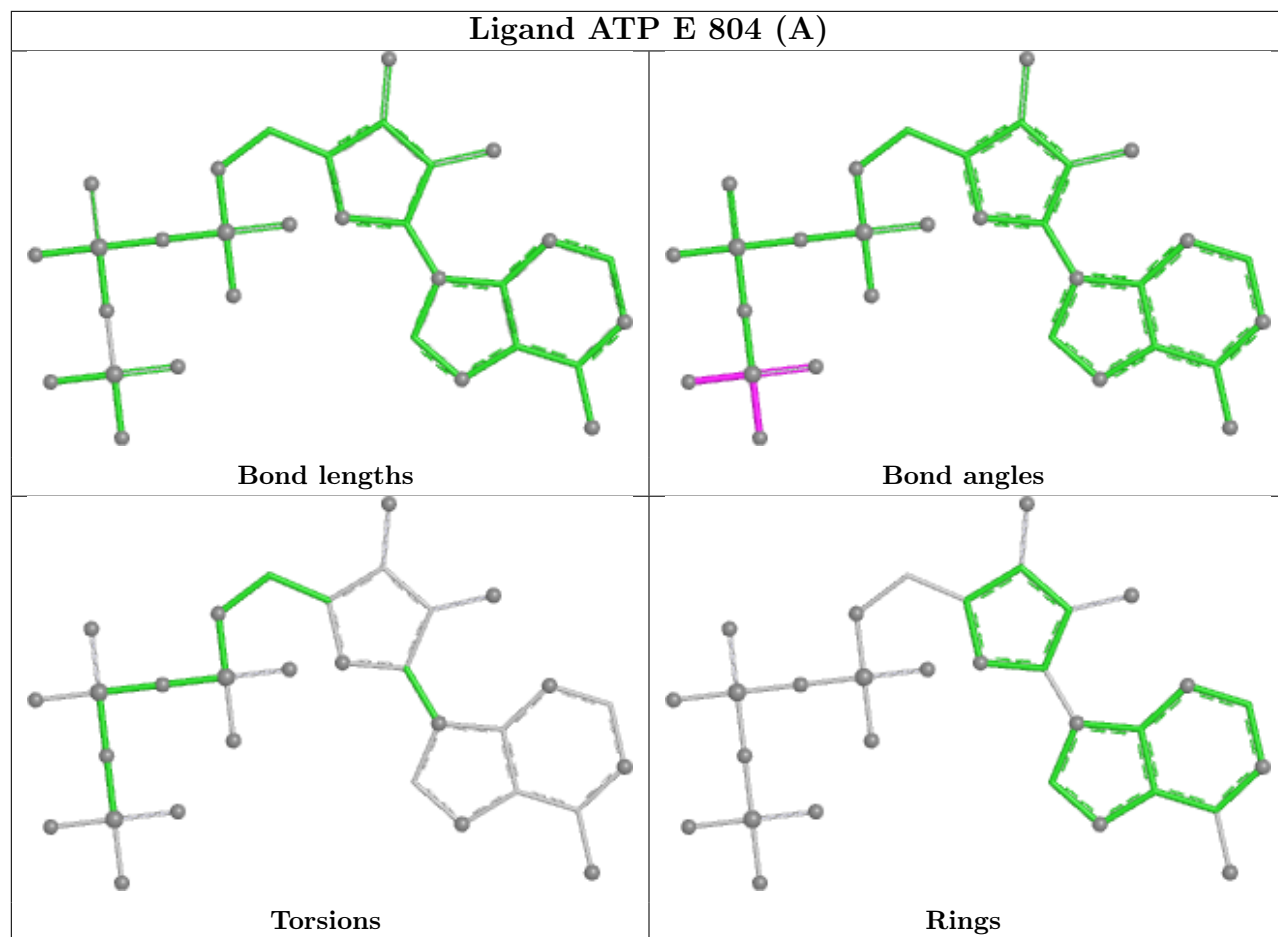


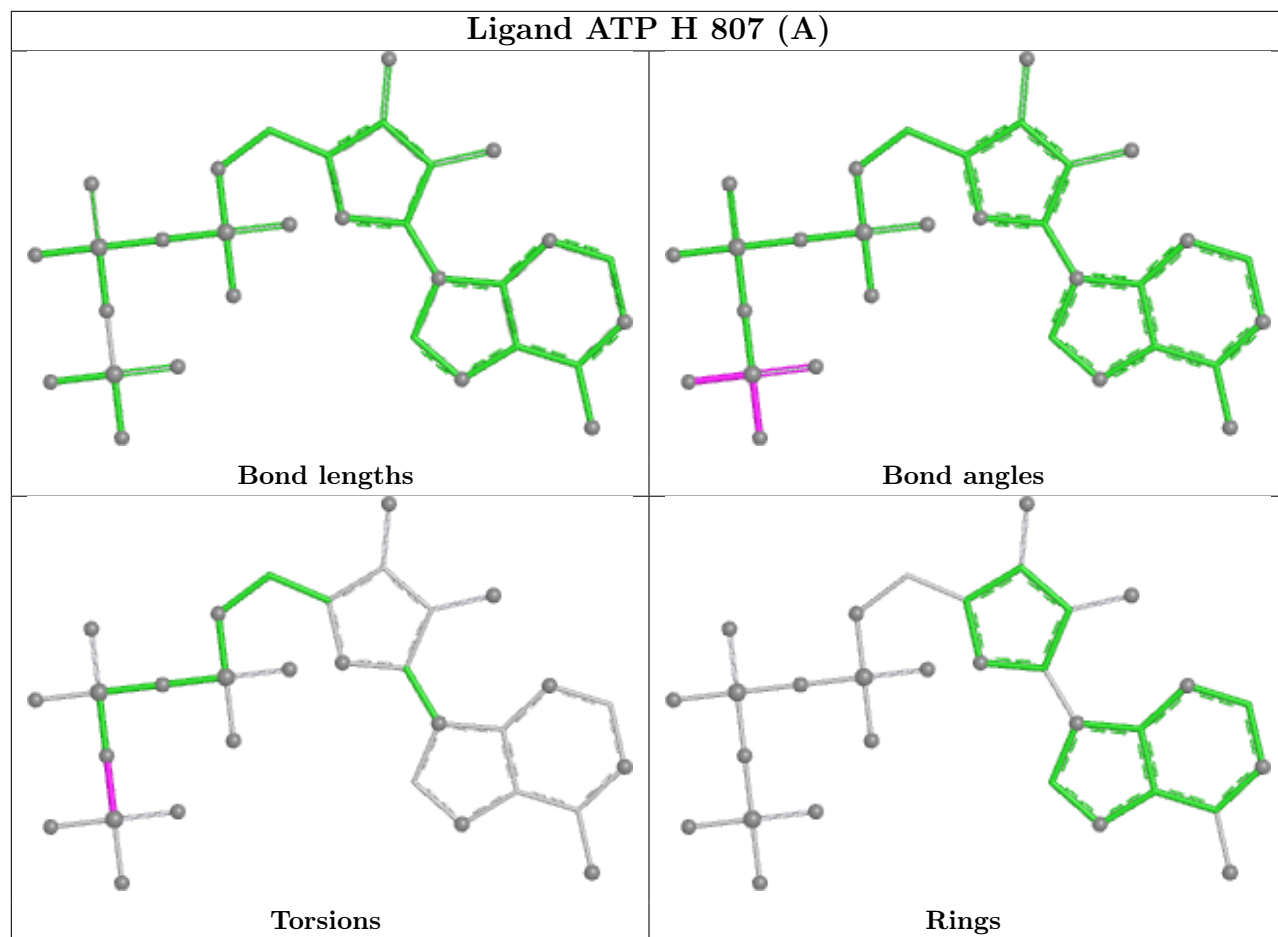


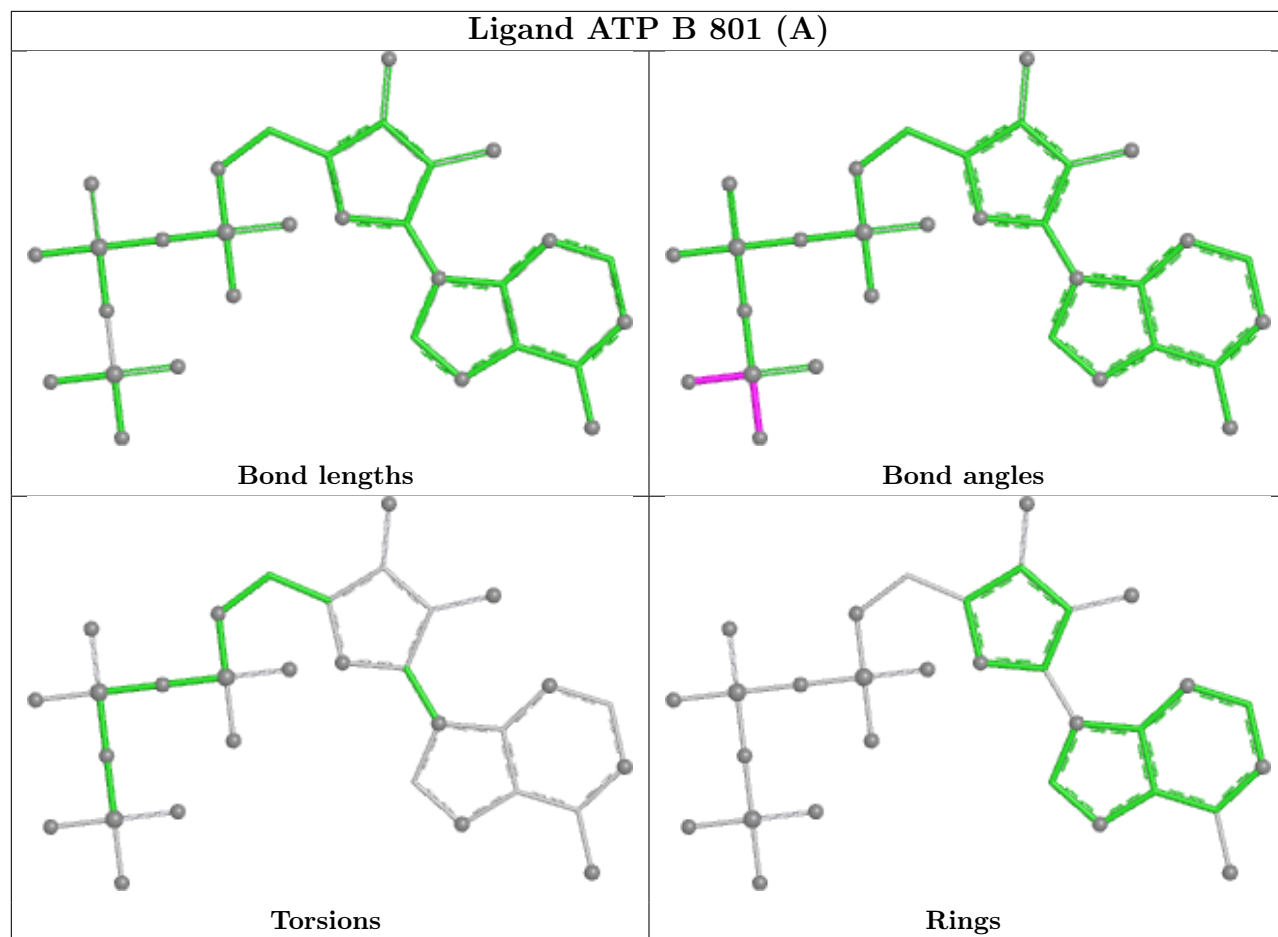




Ligand ATP E 804 (A)







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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.05	11 (3%)	46	48	11, 23, 46, 69	6 (1%)
1	B	292/422 (69%)	-0.13	8 (2%)	56	59	12, 22, 42, 60	2 (0%)
1	C	285/422 (67%)	0.21	11 (3%)	43	45	16, 30, 56, 82	5 (1%)
1	D	300/422 (71%)	0.48	17 (5%)	29	31	19, 35, 59, 72	2 (0%)
1	E	286/422 (67%)	0.45	12 (4%)	40	42	18, 33, 55, 72	10 (3%)
1	F	286/422 (67%)	0.79	33 (11%)	9	10	19, 38, 66, 83	7 (2%)
1	G	293/422 (69%)	0.38	17 (5%)	29	30	15, 33, 58, 73	1 (0%)
1	H	286/422 (67%)	0.20	6 (2%)	63	66	15, 30, 50, 61	6 (2%)
All	All	2334/3376 (69%)	0.29	115 (4%)	35	37	11, 31, 57, 83	39 (1%)

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	417	ALA	5.7
1	B	417	ALA	5.6
1	G	417	ALA	5.5
1	E	329	THR	5.3
1	C	417	ALA	5.0
1	A	168	LEU	4.8
1	E	337	THR	4.7
1	A	417	ALA	4.6
1	F	417	ALA	4.6
1	A	172	VAL	4.5
1	D	174	VAL	4.3
1	F	329	THR	4.3
1	D	167	VAL	4.2
1	G	331	VAL	4.1
1	E	135	ILE	4.1
1	C	139	ILE	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	416	GLN	4.0
1	F	337	THR	4.0
1	H	329	THR	4.0
1	C	335	TRP	3.8
1	E	137	GLY	3.7
1	D	135	ILE	3.7
1	F	128	LYS	3.6
1	F	127	ALA	3.6
1	C	113	ALA	3.5
1	B	338	ASN	3.5
1	C	134	LYS	3.4
1	G	194	ARG	3.4
1	H	335	TRP	3.3
1	C	175	VAL	3.3
1	F	135	ILE	3.2
1	B	341	SER	3.2
1	D	123	HIS	3.2
1	F	113	ALA	3.1
1	F	344	LEU	3.1
1	F	262	THR	3.1
1	G	334	ASN	3.1
1	A	170	ASN	3.0
1	E	344	LEU	3.0
1	G	342	ALA	3.0
1	E	175	VAL	3.0
1	C	135	ILE	3.0
1	F	412	ASN	3.0
1	E	335	TRP	2.9
1	C	136	HIS	2.9
1	G	330	SER	2.9
1	H	112	ALA	2.9
1	A	340	GLY	2.9
1	F	352	ARG	2.8
1	F	398	HIS	2.8
1	D	127	ALA	2.8
1	D	397	ASP	2.8
1	G	310	ALA	2.8
1	F	136	HIS	2.8
1	F	140	ASP	2.8
1	G	338	ASN	2.7
1	D	112	ALA	2.7
1	F	411	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	123	HIS	2.7
1	D	138	GLU	2.7
1	C	138	GLU	2.7
1	F	401	GLU	2.6
1	G	136	HIS	2.6
1	B	136	HIS	2.6
1	A	169	ARG	2.6
1	F	141	ILE	2.6
1	E	328	ARG	2.6
1	C	123	HIS	2.5
1	B	339	THR	2.5
1	F	177	SER	2.5
1	F	126	TRP	2.5
1	F	131	LYS	2.5
1	G	337	THR	2.4
1	D	325	ALA	2.4
1	F	322	ASN	2.4
1	G	175	VAL	2.4
1	F	327	MET	2.4
1	H	344	LEU	2.4
1	D	137	GLY	2.4
1	F	175	VAL	2.4
1	H	175	VAL	2.4
1	F	348	ALA	2.4
1	D	344	LEU	2.4
1	G	132	GLY	2.4
1	F	397	ASP	2.4
1	F	139	ILE	2.4
1	E	136	HIS	2.4
1	G	416	GLN	2.3
1	G	396	GLY	2.3
1	D	396	GLY	2.3
1	D	377	GLY	2.3
1	E	194	ARG	2.2
1	F	132	GLY	2.2
1	G	139	ILE	2.2
1	A	171	GLY	2.2
1	G	178	LEU	2.2
1	B	416	GLN	2.2
1	C	124	THR	2.2
1	G	113	ALA	2.2
1	H	417	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	359	THR	2.1
1	B	175	VAL	2.1
1	B	340	GLY	2.1
1	D	136	HIS	2.1
1	D	177	SER	2.1
1	A	136	HIS	2.1
1	D	175	VAL	2.1
1	A	416	GLN	2.1
1	F	347	ILE	2.1
1	A	174	VAL	2.1
1	F	143	VAL	2.1
1	F	400	ASP	2.0
1	A	173	LYS	2.0
1	E	112	ALA	2.0
1	E	176	ARG	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 oligosaccharides 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
2	CA	E	817	1/1	0.81	0.12	56,56,56,56	0
2	CA	F	817	1/1	0.85	0.09	48,48,48,48	0
4	EDO	A	818	4/4	0.85	0.12	20,22,26,26	0
3	ATP	C	802[B]	31/31	0.88	0.10	30,33,36,37	31
3	ATP	C	802[A]	31/31	0.88	0.10	21,27,36,37	31
3	ATP	H	807[A]	31/31	0.91	0.09	28,33,43,43	31
3	ATP	H	807[B]	31/31	0.91	0.09	28,31,34,36	31
2	CA	D	817	1/1	0.91	0.06	39,39,39,39	0

Continued on next page...

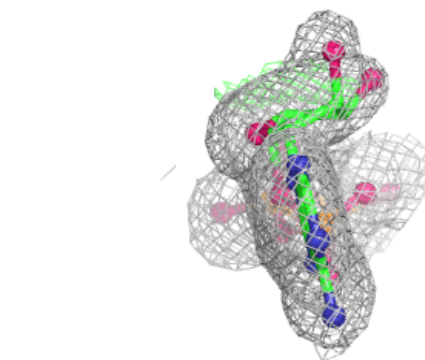
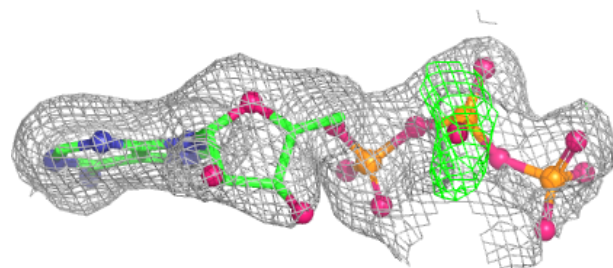
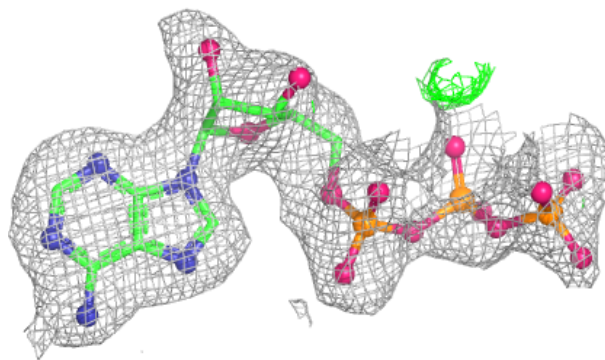
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ATP	E	804[B]	31/31	0.92	0.08	33,35,38,40	31
3	ATP	E	804[A]	31/31	0.92	0.08	28,32,37,39	31
3	ATP	F	805[B]	31/31	0.94	0.08	33,35,37,37	31
3	ATP	G	806[A]	31/31	0.94	0.07	23,26,30,31	31
3	ATP	G	806[B]	31/31	0.94	0.07	24,26,28,28	31
2	CA	G	817	1/1	0.94	0.05	39,39,39,39	0
2	CA	H	817	1/1	0.94	0.05	38,38,38,38	0
3	ATP	F	805[A]	31/31	0.94	0.08	26,35,39,41	31
3	ATP	D	803[B]	31/31	0.95	0.07	27,29,33,33	31
3	ATP	D	803[A]	31/31	0.95	0.07	23,27,30,31	31
4	EDO	B	819	4/4	0.95	0.07	26,28,30,32	0
3	ATP	B	801[A]	31/31	0.96	0.06	15,20,23,23	31
3	ATP	B	801[B]	31/31	0.96	0.06	28,31,32,32	31
2	CA	B	817	1/1	0.96	0.04	28,28,28,28	0
2	CA	A	817	1/1	0.96	0.04	29,29,29,29	0
2	CA	C	817	1/1	0.97	0.04	44,44,44,44	0
3	ATP	A	800[A]	31/31	0.98	0.05	11,19,21,22	31
3	ATP	A	800[B]	31/31	0.98	0.05	21,30,33,33	31

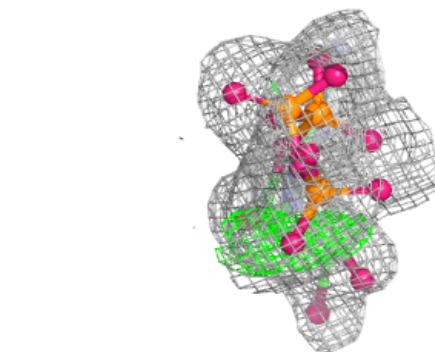
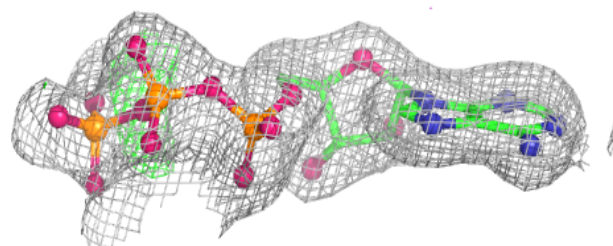
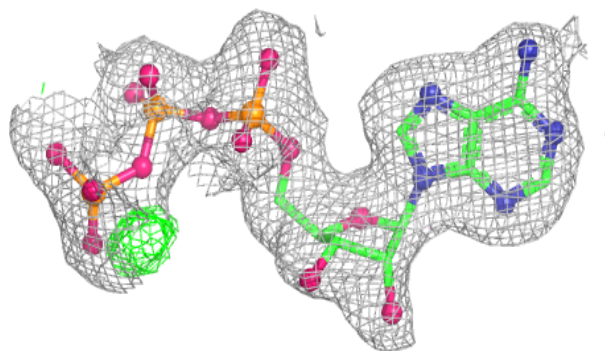
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

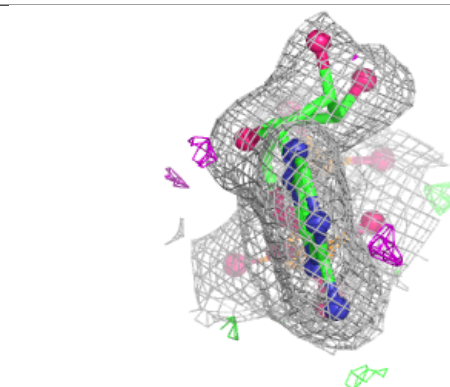
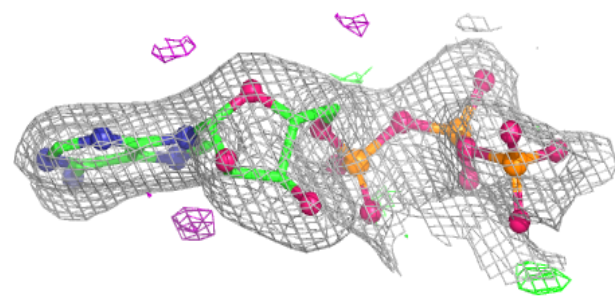
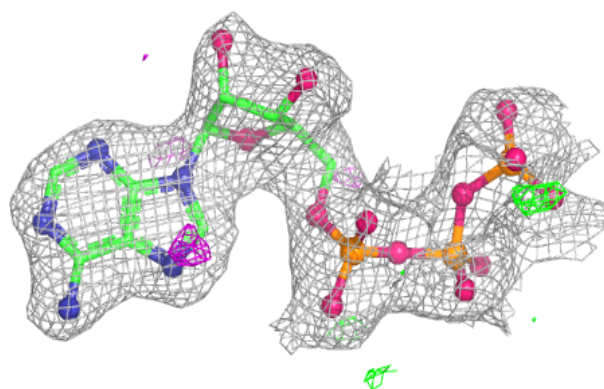
**Electron density around ATP C 802 (A):**

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

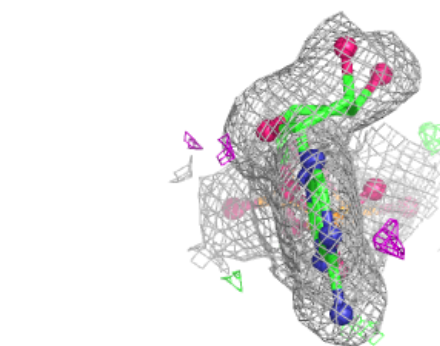
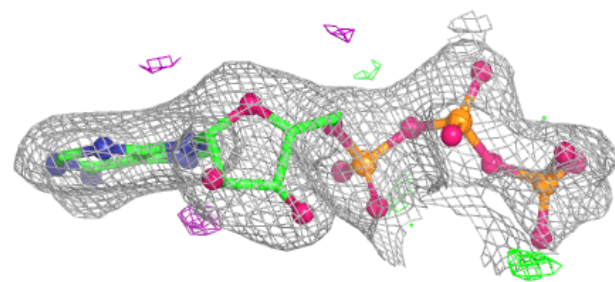
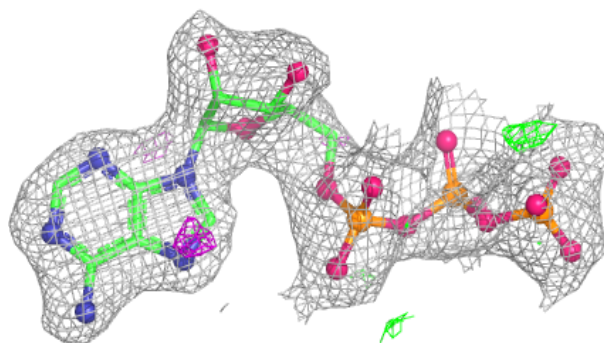


Electron density around ATP H 807 (A):

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

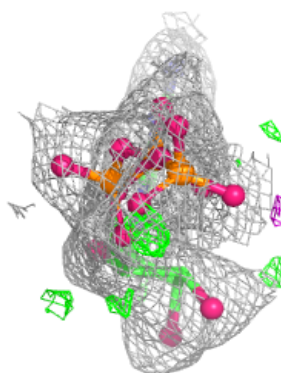
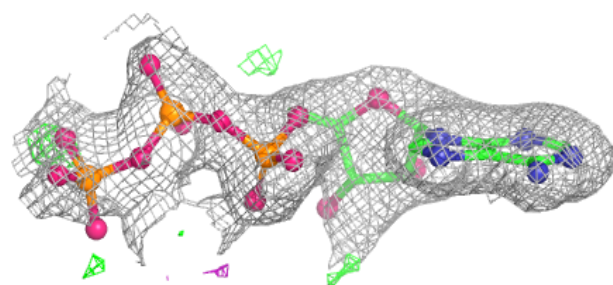
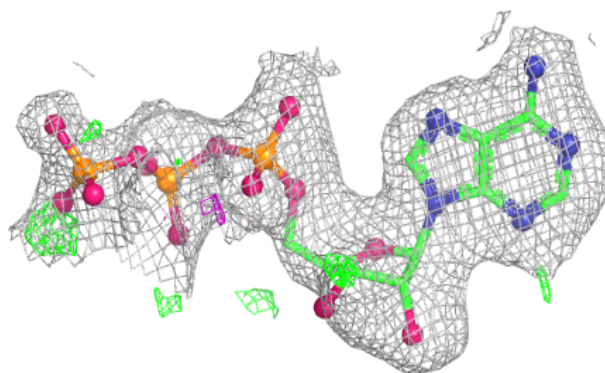
**Electron density around ATP H 807 (B):**

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

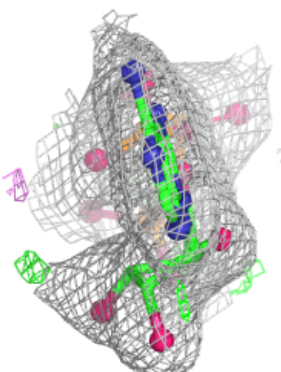
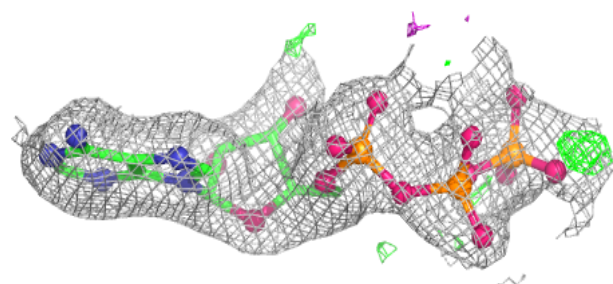
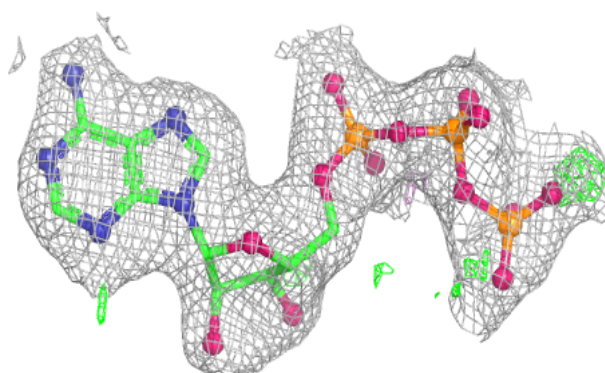


Electron density around ATP E 804 (B):

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

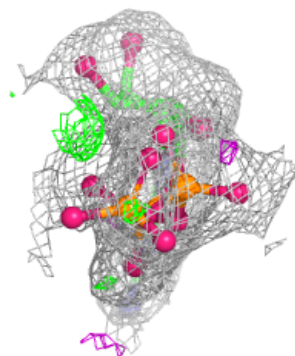
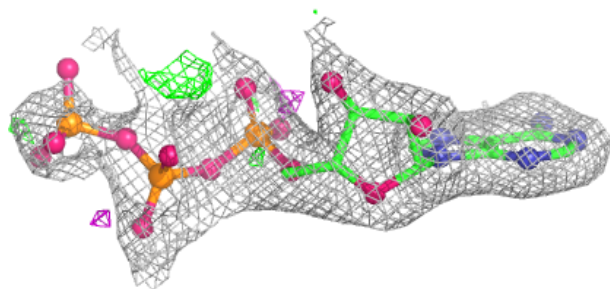
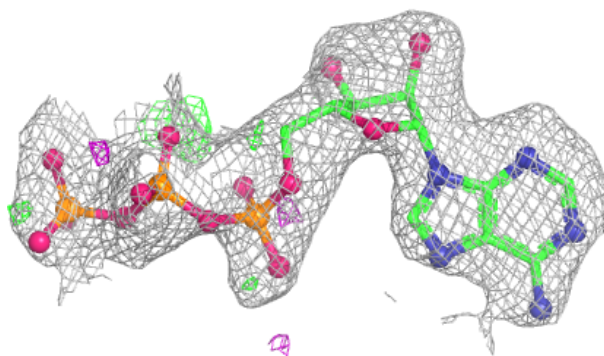
**Electron density around ATP E 804 (A):**

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

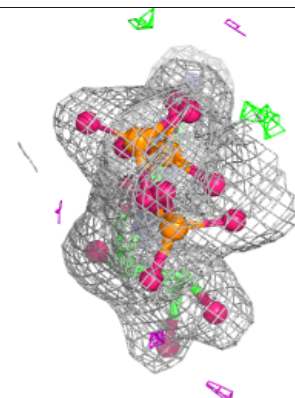
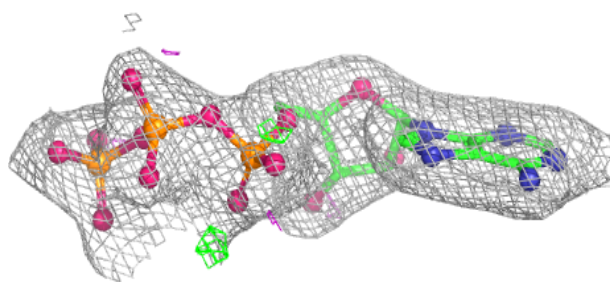
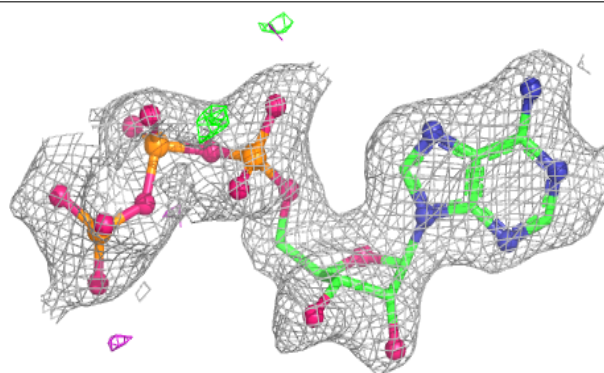


Electron density around ATP F 805 (B):

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

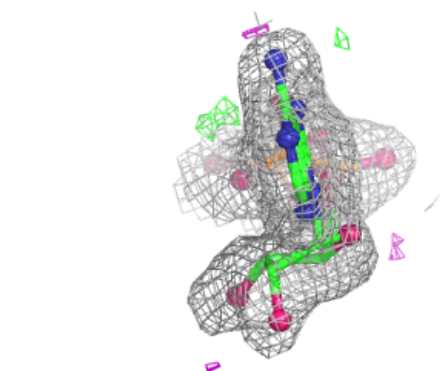
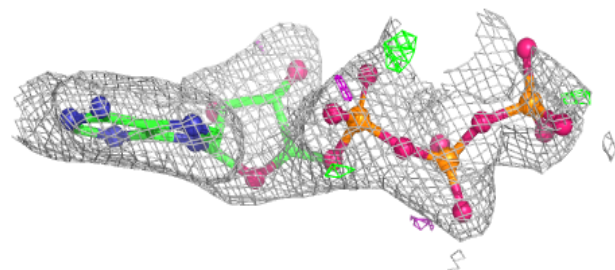
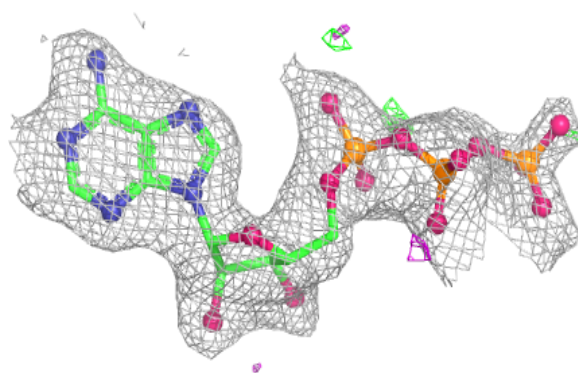
**Electron density around ATP G 806 (A):**

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

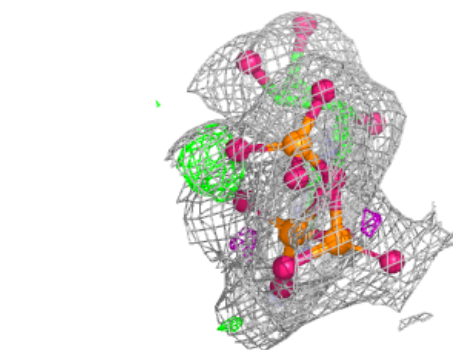
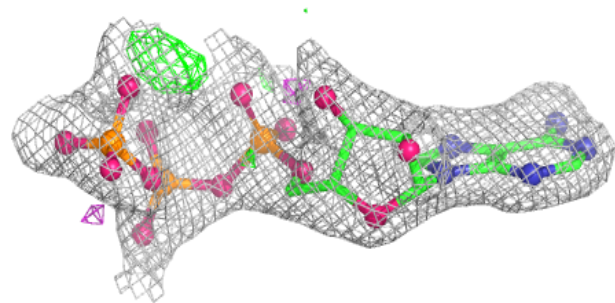
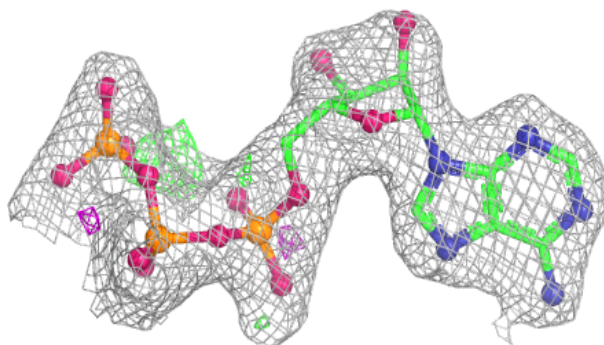


Electron density around ATP G 806 (B):

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

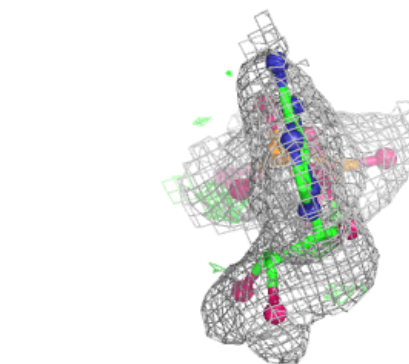
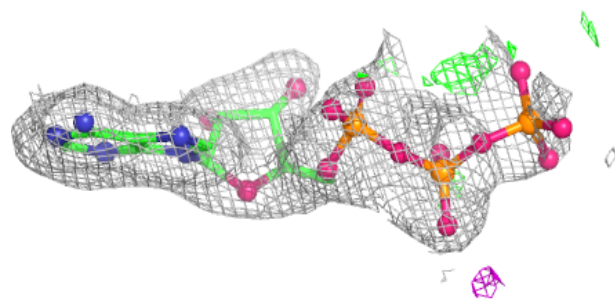
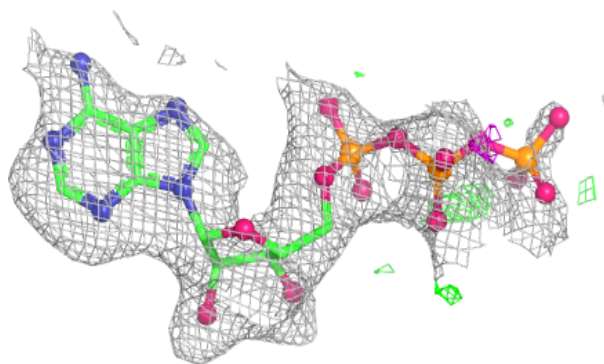
**Electron density around ATP F 805 (A):**

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

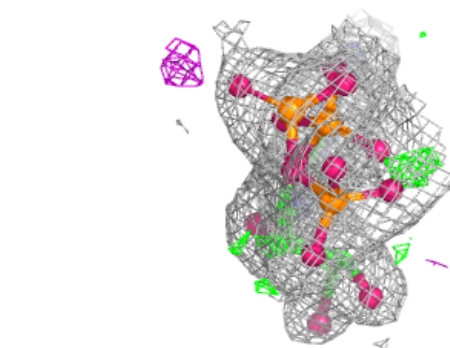
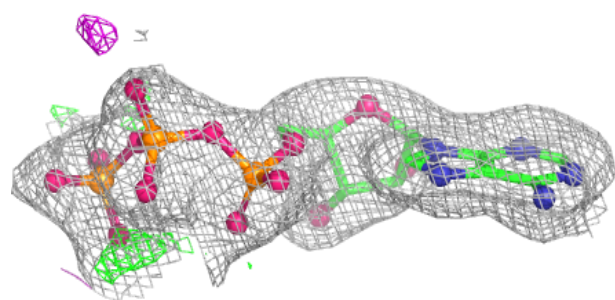
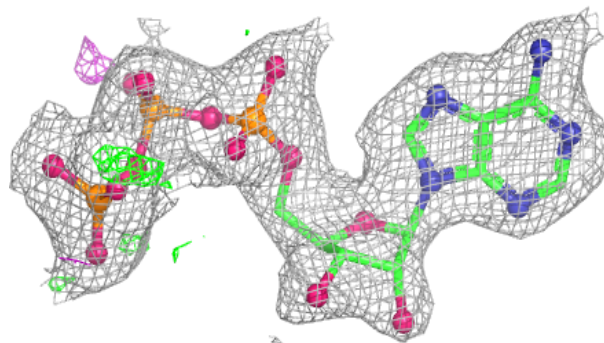


Electron density around ATP D 803 (B):

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

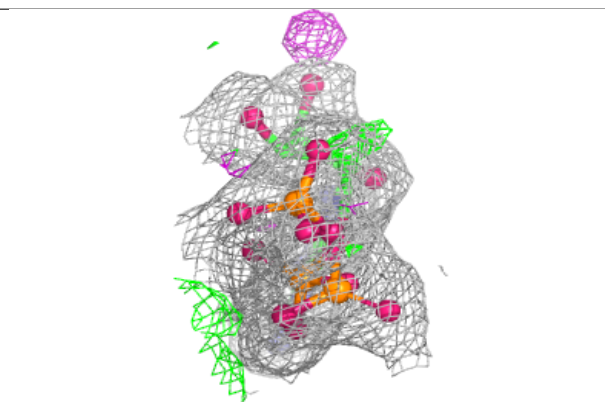
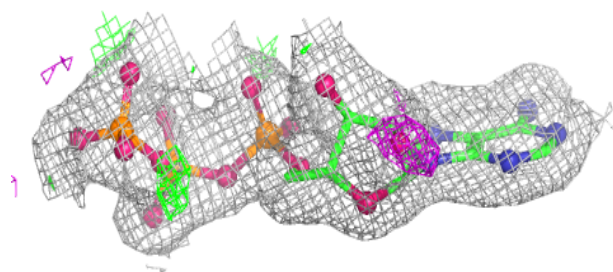
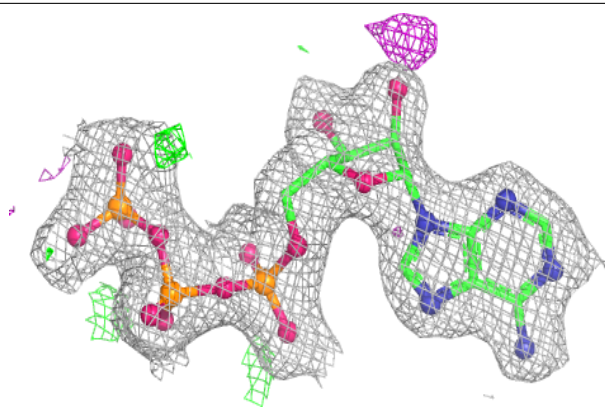
**Electron density around ATP D 803 (A):**

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

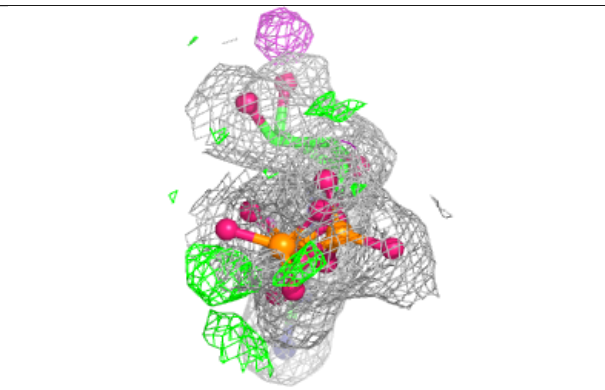
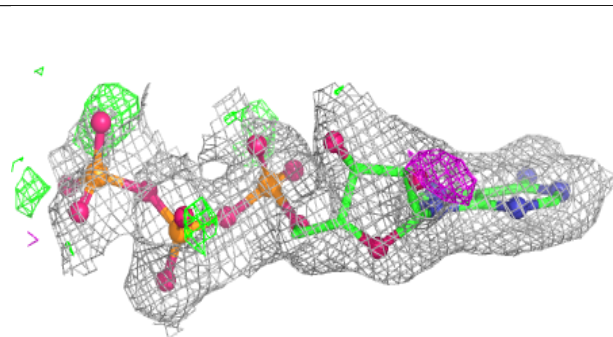
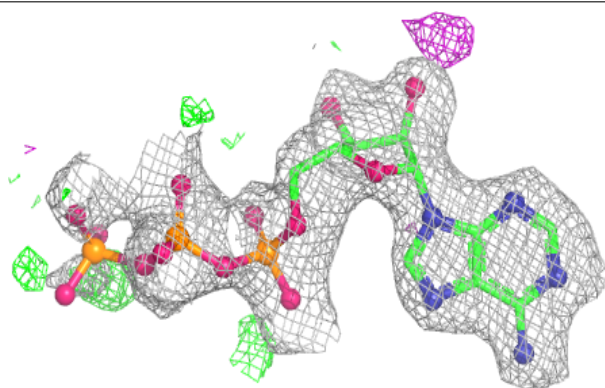


Electron density around ATP B 801 (A):

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

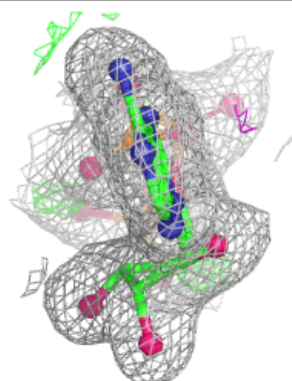
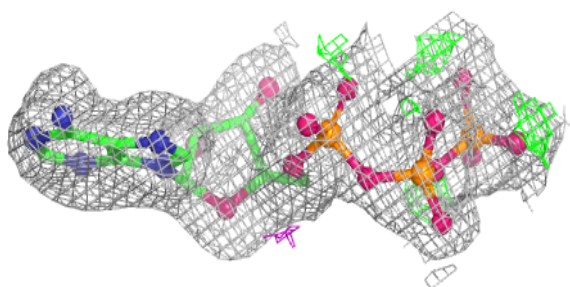
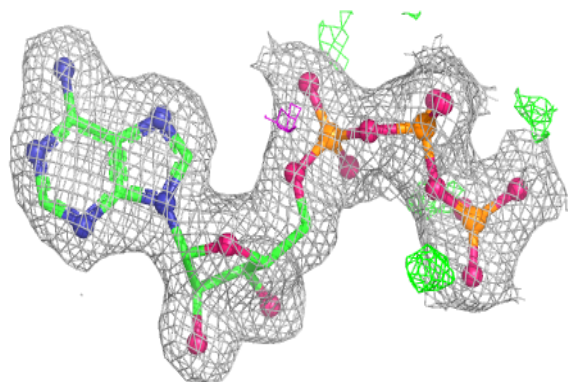
**Electron density around ATP B 801 (B):**

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

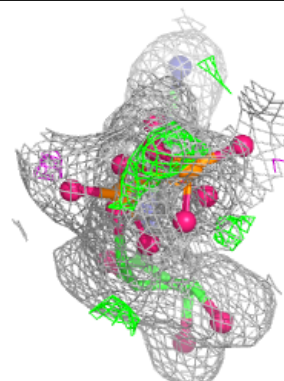
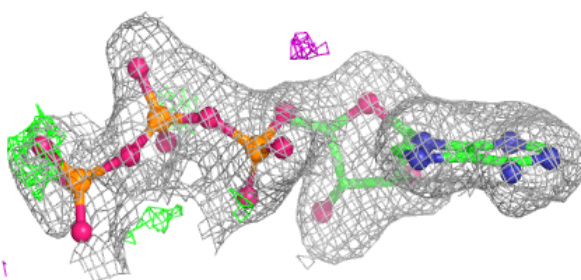
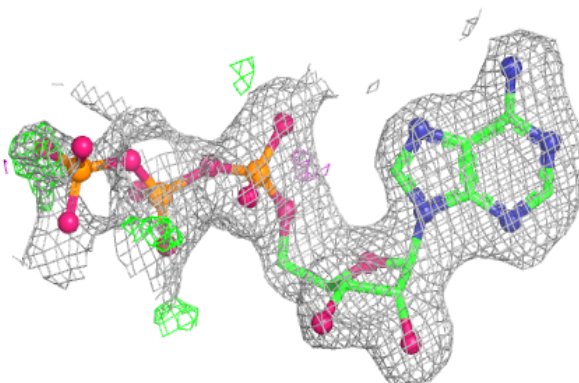


Electron density around ATP A 800 (A):

$2mF_o-DF_c$ (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.