Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2024 – 02:20 am GMT

PDB ID	:	8OOZ
Title	:	Glutamine synthetase from Methermicoccus shengliensis in complex with MgATP at 2.7 A resolution
Authors	:	Mueller, M.-C.; Lemaire, O.N.; Wagner, T.
Deposited on	:	2023-04-06
Resolution	:	2.70 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:

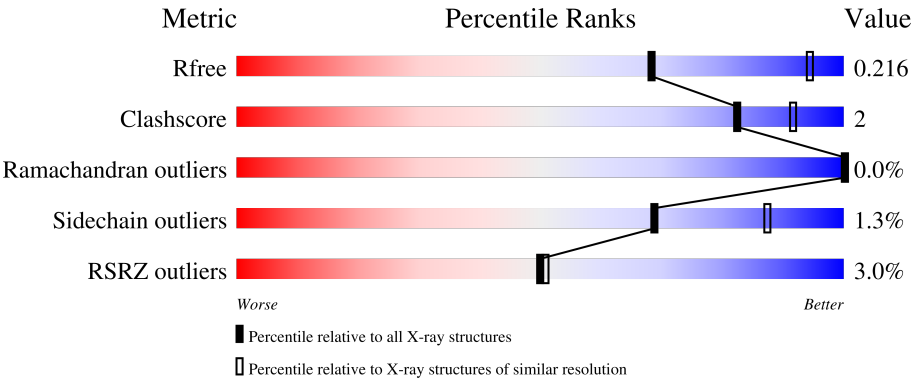
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	442	91% 6%
1	B	442	4% 93% 5%
1	C	442	2% 91% 6%
1	D	442	93% 5%
1	E	442	4% 91% 7%

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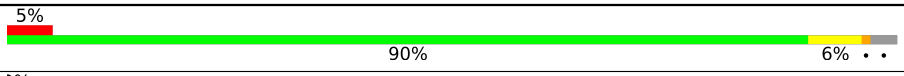
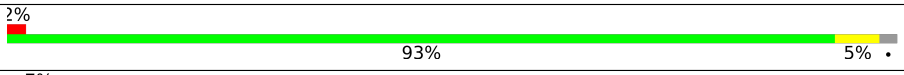
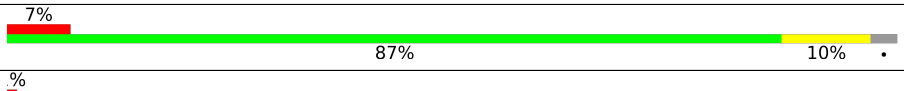
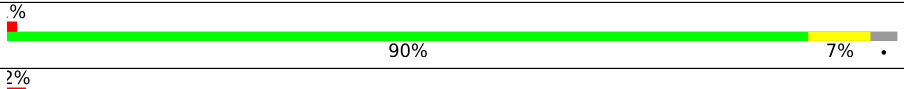
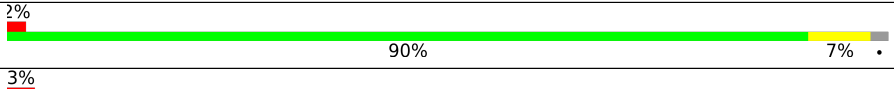
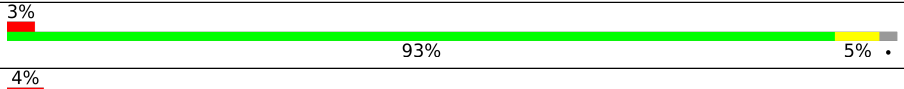
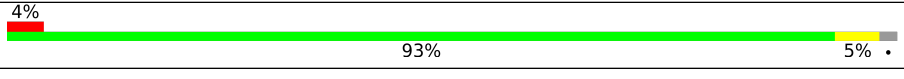
Mol	Chain	Length	Quality of chain
1	F	442	
1	G	442	
1	H	442	
1	I	442	
1	J	442	
1	K	442	
1	L	442	

2 Entry composition (i)

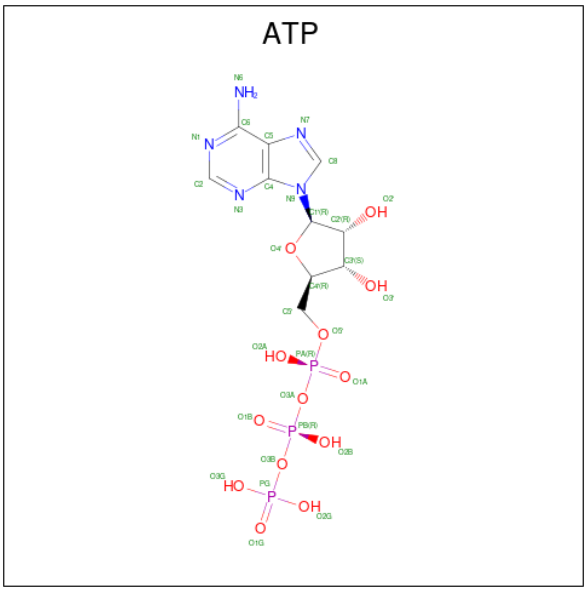
There are 6 unique types of molecules in this entry. The entry contains 41279 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamine synthetase.

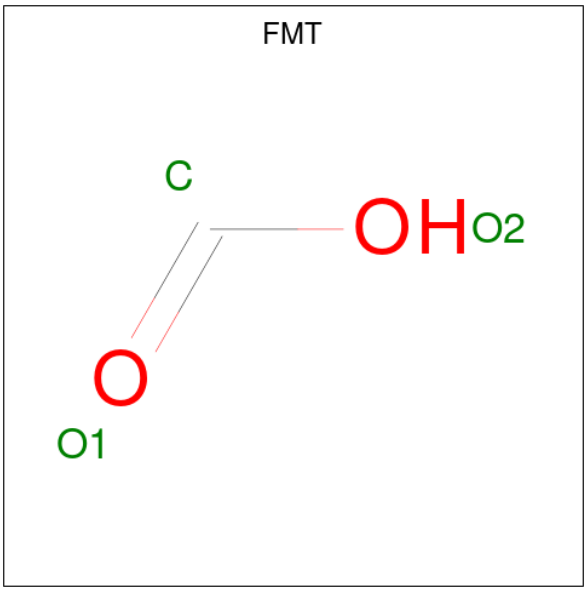
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3397	2168	576	638	15			
1	B	435	Total	C	N	O	S	0	0	0
			3431	2186	582	648	15			
1	C	428	Total	C	N	O	S	0	0	0
			3385	2162	574	634	15			
1	D	433	Total	C	N	O	S	0	0	0
			3418	2179	580	644	15			
1	E	434	Total	C	N	O	S	0	0	0
			3416	2178	578	645	15			
1	F	430	Total	C	N	O	S	0	0	0
			3391	2165	573	638	15			
1	G	432	Total	C	N	O	S	0	0	0
			3399	2169	575	640	15			
1	H	428	Total	C	N	O	S	0	0	0
			3378	2158	571	634	15			
1	I	429	Total	C	N	O	S	0	0	0
			3380	2157	573	635	15			
1	J	431	Total	C	N	O	S	0	0	0
			3395	2167	574	639	15			
1	K	432	Total	C	N	O	S	0	0	0
			3399	2169	575	640	15			
1	L	435	Total	C	N	O	S	0	0	0
			3426	2183	582	646	15			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	I	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	J	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	K	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	L	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).

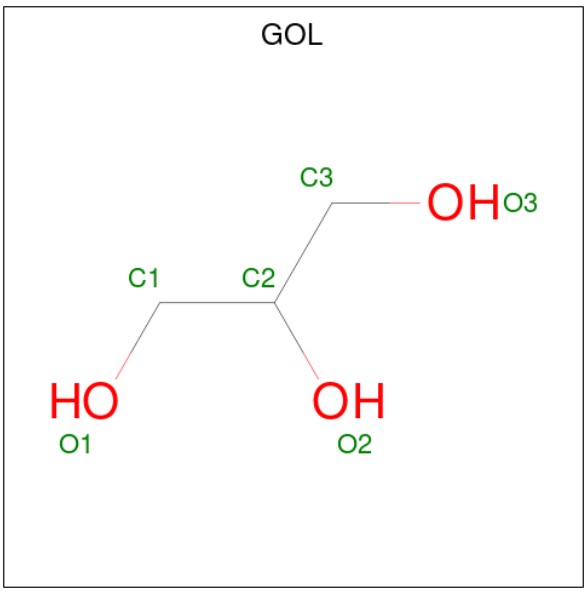


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	E	1	Total C O 3 1 2	0	0
3	G	1	Total C O 3 1 2	0	0
3	G	1	Total C O 3 1 2	0	0
3	J	1	Total C O 3 1 2	0	0
3	J	1	Total C O 3 1 2	0	0
3	K	1	Total C O 3 1 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	2	Total Mg 2 2	0	0
4	D	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0
4	F	2	Total Mg 2 2	0	0
4	G	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0
4	I	1	Total Mg 1 1	0	0
4	J	1	Total Mg 1 1	0	0
4	K	1	Total Mg 1 1	0	0
4	L	1	Total Mg 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

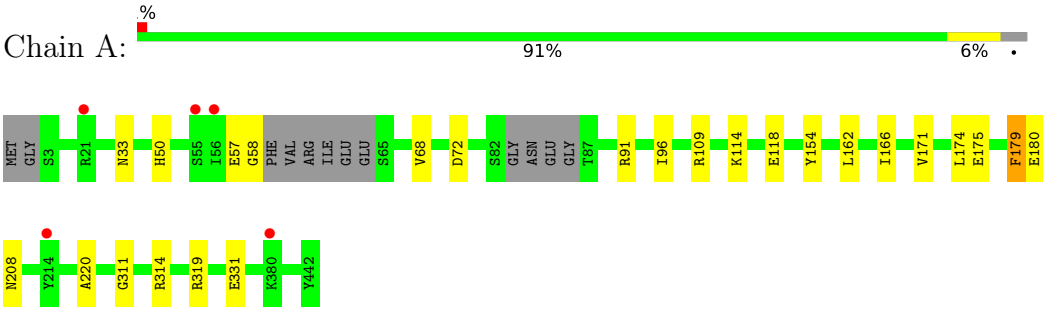
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	4	Total O 4 4	0	0
6	B	3	Total O 3 3	0	0
6	C	3	Total O 3 3	0	0
6	D	7	Total O 7 7	0	0
6	E	4	Total O 4 4	0	0
6	F	1	Total O 1 1	0	0
6	G	1	Total O 1 1	0	0
6	H	2	Total O 2 2	0	0
6	J	2	Total O 2 2	0	0
6	L	6	Total O 6 6	0	0

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.

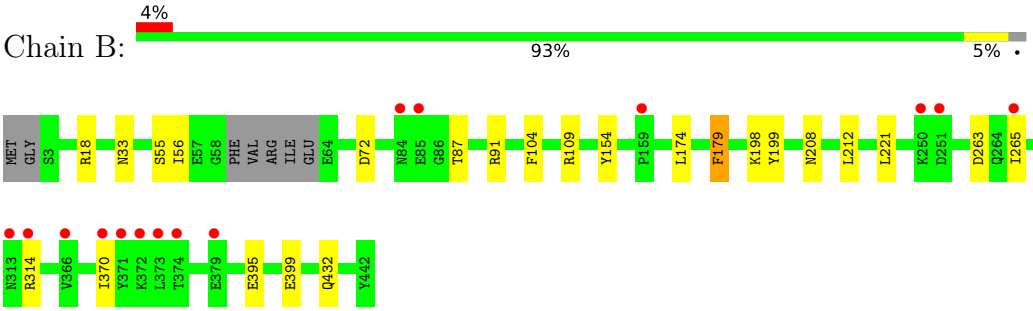
• Molecule 1: Glutamine synthetase

Chain A:



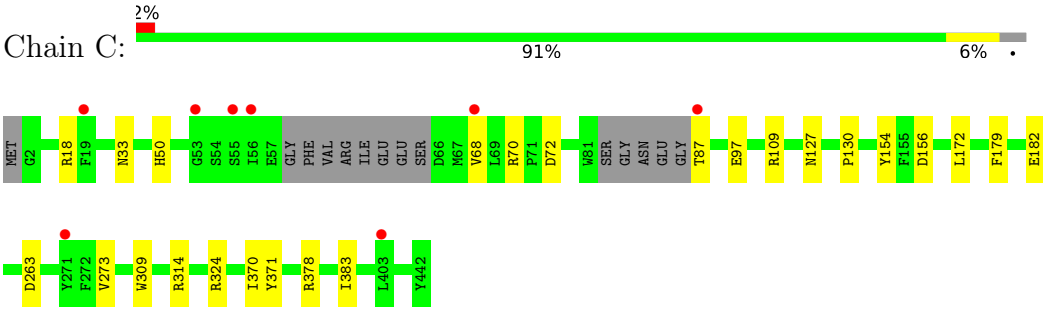
• Molecule 1: Glutamine synthetase

Chain B:



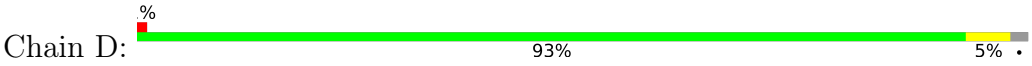
• Molecule 1: Glutamine synthetase

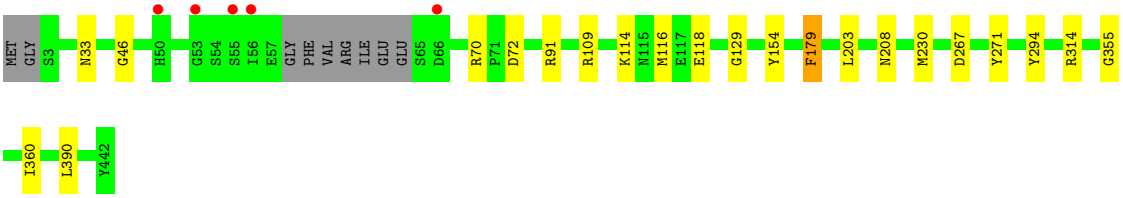
Chain C:



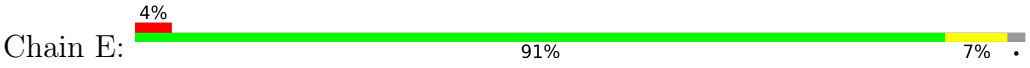
• Molecule 1: Glutamine synthetase

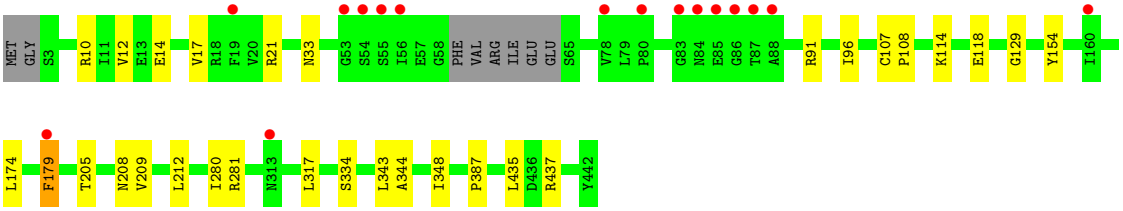
Chain D:



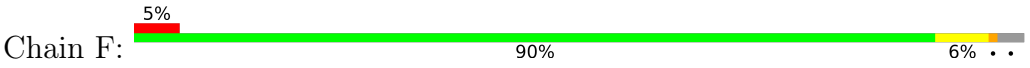


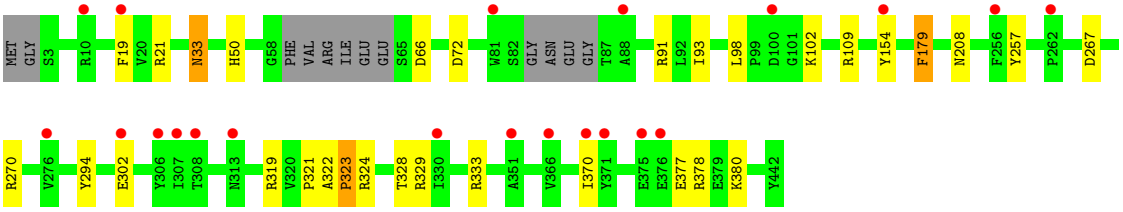
• Molecule 1: Glutamine synthetase



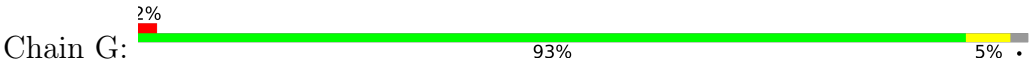


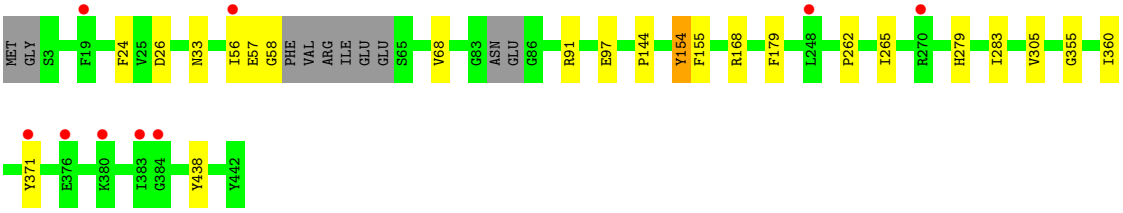
• Molecule 1: Glutamine synthetase



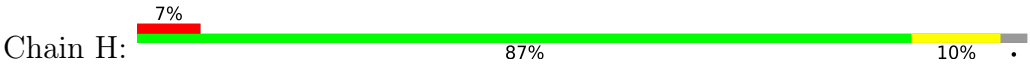


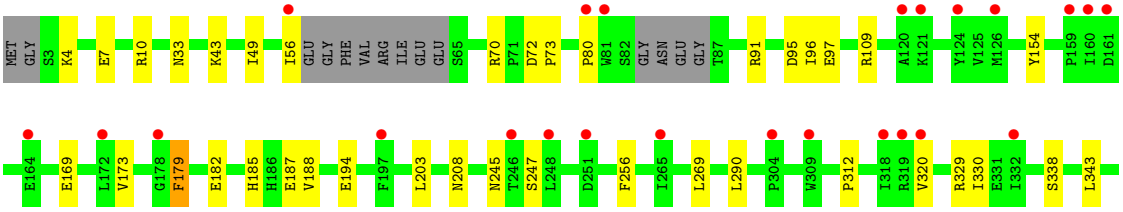
• Molecule 1: Glutamine synthetase

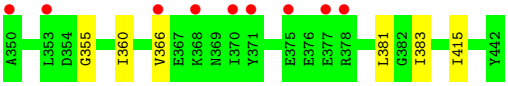




• Molecule 1: Glutamine synthetase

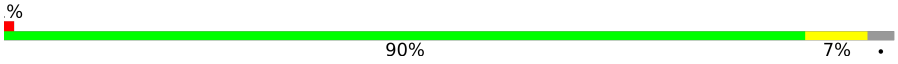


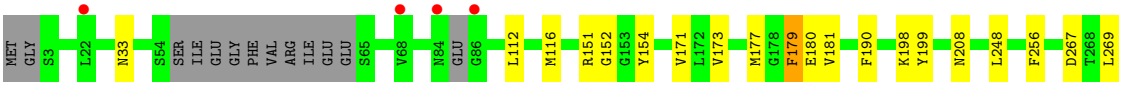


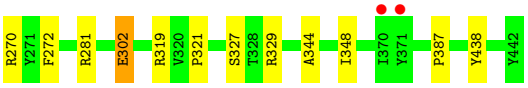


• Molecule 1: Glutamine synthetase

Chain I:

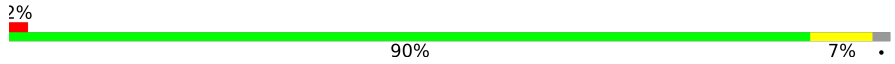


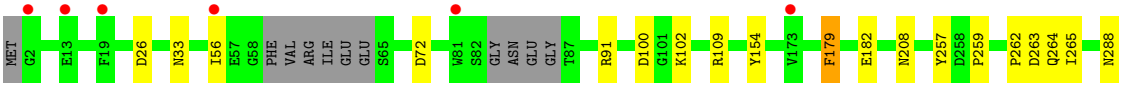


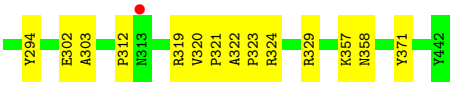


• Molecule 1: Glutamine synthetase

Chain J:

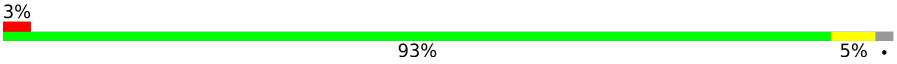


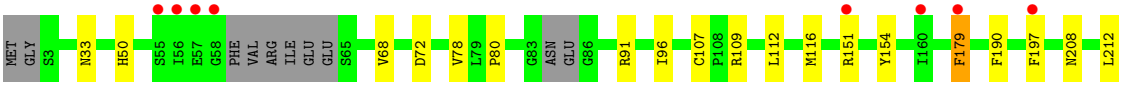


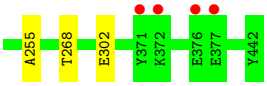


• Molecule 1: Glutamine synthetase

Chain K:

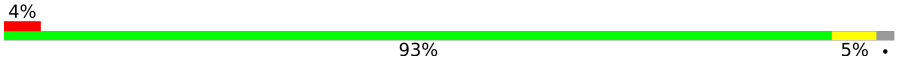


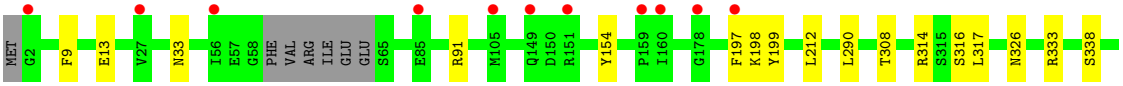


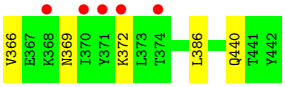


• Molecule 1: Glutamine synthetase

Chain L:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	131.55Å 197.40Å 135.17Å 90.00° 94.89° 90.00°	Depositor
Resolution (Å)	49.10 – 2.70 78.84 – 2.70	Depositor EDS
% Data completeness (in resolution range)	68.5 (49.10-2.70) 68.5 (78.84-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.196 , 0.217 0.198 , 0.216	Depositor DCC
R_{free} test set	6731 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å^2)	65.7	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 28.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	41279	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.39	0/3475	0.55	0/4708
1	B	0.38	0/3510	0.54	0/4756
1	C	0.39	0/3463	0.56	0/4692
1	D	0.38	0/3497	0.54	0/4739
1	E	0.39	0/3495	0.56	0/4737
1	F	0.38	0/3469	0.55	0/4701
1	G	0.39	0/3477	0.54	0/4711
1	H	0.41	0/3456	0.57	0/4684
1	I	0.39	0/3458	0.56	0/4686
1	J	0.38	0/3473	0.55	0/4706
1	K	0.39	0/3477	0.55	0/4711
1	L	0.39	0/3505	0.56	0/4749
All	All	0.39	0/41755	0.55	0/56580

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3397	0	3366	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3431	0	3391	18	0
1	C	3385	0	3356	16	0
1	D	3418	0	3382	12	0
1	E	3416	0	3374	17	0
1	F	3391	0	3355	23	0
1	G	3399	0	3361	16	0
1	H	3378	0	3346	27	0
1	I	3380	0	3342	18	0
1	J	3395	0	3358	21	0
1	K	3399	0	3361	12	0
1	L	3426	0	3388	14	0
2	A	31	0	12	0	0
2	B	31	0	12	1	0
2	C	31	0	12	1	0
2	D	31	0	12	1	0
2	E	31	0	12	1	0
2	F	31	0	12	0	0
2	G	31	0	12	0	0
2	H	31	0	12	3	0
2	I	31	0	12	0	0
2	J	31	0	12	1	0
2	K	31	0	12	0	0
2	L	31	0	12	0	0
3	A	6	0	2	0	0
3	B	3	0	1	1	0
3	C	9	0	3	0	0
3	D	3	0	1	0	0
3	E	3	0	1	0	0
3	G	6	0	2	0	0
3	J	6	0	2	0	0
3	K	3	0	1	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	2	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	1	0	0	0	0
5	G	6	0	8	0	0
6	A	4	0	0	0	0
6	B	3	0	0	0	0
6	C	3	0	0	0	0
6	D	7	0	0	0	0
6	E	4	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	2	0	0	0	0
6	J	2	0	0	2	0
6	L	6	0	0	0	0
All	All	41279	0	40545	204	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 2.

All (204) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:PHE:CZ	1:A:208:ASN:HB3	2.28	0.69
1:J:179:PHE:CZ	1:J:208:ASN:HB3	2.29	0.68
1:B:179:PHE:CZ	1:B:208:ASN:HB3	2.30	0.67
1:F:179:PHE:CZ	1:F:208:ASN:HB3	2.36	0.61
1:I:267:ASP:HA	1:I:270:ARG:HE	1.67	0.60
1:J:264:GLN:HB2	1:J:324:ARG:HD2	1.84	0.58
1:J:257:TYR:CZ	1:J:259:PRO:HG3	2.38	0.58
1:H:185:HIS:NE2	1:H:194:GLU:OE1	2.37	0.57
1:D:179:PHE:CZ	1:D:208:ASN:HB3	2.40	0.57
1:G:24:PHE:CE2	1:G:56:ILE:HD11	2.40	0.57
1:L:197:PHE:HZ	1:L:212:LEU:HG	1.69	0.57
1:J:100:ASP:OD2	1:J:102:LYS:HE3	2.04	0.57
1:J:312:PRO:HD3	1:J:320:VAL:O	2.04	0.57
1:A:162:LEU:HD21	1:B:221:LEU:HD11	1.86	0.57
1:I:344:ALA:O	1:I:348:ILE:HG12	2.05	0.57
1:F:302:GLU:HG2	1:F:333:ARG:HH22	1.71	0.56
1:K:179:PHE:CZ	1:K:208:ASN:HB3	2.40	0.56
1:L:314:ARG:HD2	1:L:369:ASN:HA	1.86	0.56
1:E:281:ARG:HD2	1:E:387:PRO:HD3	1.87	0.56
1:F:98:LEU:HD12	1:F:102:LYS:O	2.06	0.55
1:G:154:TYR:CZ	1:G:155:PHE:HE1	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:290:LEU:HD13	1:L:338:SER:OG	2.06	0.55
1:A:114:LYS:O	1:A:118:GLU:HG2	2.07	0.55
1:G:24:PHE:CE2	1:G:56:ILE:CD1	2.90	0.55
1:H:245:ASN:HB3	1:H:329:ARG:HD2	1.87	0.55
1:B:179:PHE:CE2	1:B:208:ASN:HB3	2.41	0.55
1:E:344:ALA:O	1:E:348:ILE:HD12	2.07	0.54
1:H:179:PHE:CZ	1:H:208:ASN:HB3	2.41	0.54
1:J:357:LYS:HD3	1:J:358:ASN:OD1	2.06	0.54
1:J:182:GLU:OE1	2:J:501:ATP:H5'1	2.08	0.54
1:H:7:GLU:HG3	1:H:10:ARG:NH1	2.22	0.53
1:E:179:PHE:CZ	1:E:208:ASN:HB3	2.44	0.53
1:I:281:ARG:HD2	1:I:387:PRO:HD3	1.91	0.53
1:D:355:GLY:HA2	1:D:360:ILE:CD1	2.39	0.53
1:J:26:ASP:HB2	1:J:56:ILE:O	2.10	0.52
1:K:197:PHE:CZ	1:K:212:LEU:HD22	2.45	0.52
1:H:182:GLU:HG3	2:H:501:ATP:H5'2	1.92	0.52
1:D:355:GLY:HA2	1:D:360:ILE:HD12	1.92	0.52
1:H:256:PHE:HB3	1:H:269:LEU:HD13	1.92	0.52
1:C:18:ARG:HG3	1:C:87:THR:HG21	1.92	0.51
1:B:263:ASP:HB3	1:B:265:ILE:HG12	1.91	0.51
1:J:179:PHE:CE2	1:J:208:ASN:HB3	2.45	0.51
1:H:355:GLY:HA2	1:H:360:ILE:HD12	1.91	0.51
1:B:18:ARG:HG3	1:B:87:THR:HB	1.92	0.51
1:F:321:PRO:HD2	1:F:329:ARG:O	2.09	0.51
1:C:127:ASN:HB3	1:C:199:TYR:HD2	1.76	0.51
1:G:305:VAL:CG1	1:G:371:TYR:HE1	2.23	0.51
1:H:7:GLU:HG3	1:H:10:ARG:HH12	1.75	0.51
1:I:112:LEU:O	1:I:116:MET:HG3	2.10	0.51
1:F:321:PRO:HG2	1:F:329:ARG:NH1	2.26	0.50
1:J:263:ASP:O	1:J:265:ILE:HG23	2.11	0.50
1:G:262:PRO:O	1:G:265:ILE:HG12	2.10	0.50
1:G:279:HIS:O	1:G:283:ILE:HG13	2.12	0.50
1:B:314:ARG:HD2	1:B:370:ILE:HD12	1.93	0.50
1:F:322:ALA:O	1:F:324:ARG:HG2	2.12	0.50
1:H:290:LEU:HD23	1:I:438:TYR:CG	2.46	0.50
1:L:308:THR:HG22	1:L:366:VAL:HG21	1.93	0.50
1:E:12:VAL:HG13	1:E:17:VAL:HG12	1.93	0.49
1:C:370:ILE:HD11	1:C:383:ILE:HD13	1.94	0.49
1:E:129:GLY:HA3	2:E:501:ATP:O2'	2.12	0.49
1:I:171:VAL:HG13	1:I:181:VAL:HG11	1.94	0.49
1:K:255:ALA:O	1:K:268:THR:OG1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:HD22	1:A:179:PHE:HD2	1.77	0.49
1:I:248:LEU:HD11	1:I:272:PHE:CD2	2.47	0.49
1:A:180:GLU:HB3	1:A:198:LYS:HD3	1.94	0.49
1:E:114:LYS:O	1:E:118:GLU:HG2	2.13	0.49
1:F:322:ALA:O	1:F:323:PRO:C	2.51	0.49
1:H:247:SER:OG	2:H:501:ATP:N1	2.43	0.48
1:F:322:ALA:N	1:F:323:PRO:HD2	2.27	0.48
1:C:172:LEU:HD13	1:F:19:PHE:CE1	2.48	0.48
1:C:370:ILE:CD1	1:C:383:ILE:HD13	2.43	0.48
1:H:269:LEU:HD11	1:H:330:ILE:HG23	1.94	0.48
1:K:50:HIS:CD2	1:K:68:VAL:HG22	2.48	0.48
1:E:280:ILE:HG12	1:E:317:LEU:HD21	1.95	0.48
1:G:438:TYR:CD1	1:L:290:LEU:HD23	2.49	0.48
1:H:290:LEU:HD13	1:H:338:SER:OG	2.13	0.48
1:G:26:ASP:HB2	1:G:56:ILE:O	2.13	0.48
1:L:198:LYS:HE3	1:L:199:TYR:CD2	2.48	0.48
1:H:70:ARG:HG3	1:H:97:GLU:CD	2.34	0.48
1:I:198:LYS:HG3	1:I:199:TYR:H	1.79	0.48
1:A:319:ARG:HG2	1:A:319:ARG:HH11	1.78	0.47
1:I:256:PHE:CE1	1:I:269:LEU:HA	2.49	0.47
1:F:72:ASP:OD2	1:F:109:ARG:NH2	2.47	0.47
1:H:381:LEU:HD23	1:H:383:ILE:HD11	1.95	0.47
1:K:179:PHE:HZ	1:K:197:PHE:CD2	2.32	0.47
1:C:182:GLU:H	1:C:197:PHE:HA	1.78	0.47
1:J:319:ARG:O	1:J:321:PRO:HD3	2.14	0.47
1:K:197:PHE:HZ	1:K:212:LEU:HD22	1.78	0.47
1:I:173:VAL:O	1:I:177:MET:HG3	2.14	0.47
1:H:187:GLU:HG3	1:H:188:VAL:H	1.78	0.47
1:C:172:LEU:HD13	1:F:19:PHE:HE1	1.78	0.47
1:D:294:TYR:CE2	1:D:390:LEU:HA	2.50	0.47
1:B:72:ASP:OD2	1:B:109:ARG:NH2	2.48	0.47
1:F:179:PHE:CE2	1:F:208:ASN:HB3	2.49	0.47
1:D:267:ASP:HB3	1:D:271:TYR:CE2	2.49	0.46
1:G:355:GLY:HA2	1:G:360:ILE:HD12	1.96	0.46
1:J:72:ASP:OD2	1:J:109:ARG:NH2	2.48	0.46
1:B:199:TYR:HB3	2:B:501:ATP:C4	2.50	0.46
1:L:317:LEU:HD12	1:L:386:LEU:HD21	1.97	0.46
1:E:174:LEU:HD11	1:E:212:LEU:HD12	1.96	0.46
1:F:319:ARG:O	1:F:321:PRO:HD3	2.15	0.46
1:F:321:PRO:HG2	1:F:329:ARG:HD2	1.98	0.46
1:B:221:LEU:HD23	1:B:221:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:GLU:O	1:B:399:GLU:HG2	2.15	0.46
1:C:273:VAL:HG11	1:C:309:TRP:CE3	2.50	0.46
1:H:4:LYS:HD2	1:H:73:PRO:HB2	1.98	0.46
1:F:267:ASP:OD1	1:F:270:ARG:NH1	2.48	0.45
1:H:56:ILE:HD11	1:H:96:ILE:HD12	1.99	0.45
1:A:154:TYR:HD2	1:B:55:SER:HB3	1.80	0.45
1:B:310:SER:OG	1:B:314:ARG:HB3	2.16	0.45
1:D:116:MET:HE1	1:D:203:LEU:HB2	1.99	0.45
1:D:72:ASP:OD2	1:D:109:ARG:NH2	2.49	0.45
1:F:324:ARG:HD3	1:F:328:THR:HG23	1.98	0.45
1:L:9:PHE:O	1:L:13:GLU:HG2	2.16	0.45
1:A:174:LEU:HB3	1:A:179:PHE:HB3	1.98	0.45
1:G:68:VAL:HB	1:G:97:GLU:HG2	1.97	0.45
1:I:327:SER:O	1:I:329:ARG:HG3	2.16	0.45
1:A:96:ILE:HD12	1:A:96:ILE:N	2.32	0.45
1:D:230:MET:HE1	1:E:435:LEU:HD23	1.98	0.45
1:I:281:ARG:HE	1:I:387:PRO:HG3	1.82	0.45
1:E:205:THR:O	1:E:209:VAL:HG23	2.16	0.45
1:I:179:PHE:CZ	1:I:208:ASN:HB3	2.51	0.45
1:L:197:PHE:CZ	1:L:212:LEU:HG	2.51	0.45
1:A:50:HIS:CE1	1:A:68:VAL:HG22	2.52	0.45
1:F:257:TYR:CE1	1:F:324:ARG:HB3	2.51	0.45
1:G:57:GLU:O	1:G:58:GLY:C	2.55	0.45
1:J:288:ASN:ND2	6:J:601:HOH:O	2.45	0.45
1:J:303:ALA:O	1:J:371:TYR:OH	2.34	0.45
1:A:171:VAL:O	1:A:175:GLU:HG3	2.17	0.45
1:C:130:PRO:HD2	1:C:197:PHE:CE1	2.52	0.44
1:A:72:ASP:OD2	1:A:109:ARG:NH2	2.50	0.44
1:C:370:ILE:HG23	1:C:371:TYR:N	2.32	0.44
1:E:96:ILE:HG12	1:E:107:CYS:SG	2.58	0.44
1:K:151:ARG:HA	1:K:190:PHE:CD1	2.52	0.44
1:D:267:ASP:HB3	1:D:271:TYR:HE2	1.82	0.44
1:K:72:ASP:OD2	1:K:109:ARG:NH2	2.51	0.44
1:A:166:ILE:HD11	1:A:220:ALA:HA	2.00	0.44
1:B:432:GLN:H	3:B:502:FMT:C	2.30	0.44
2:H:501:ATP:O5'	2:H:501:ATP:H8	2.01	0.44
1:I:152:GLY:O	1:I:190:PHE:HD1	2.01	0.44
1:L:369:ASN:CG	1:L:372:LYS:HG3	2.38	0.44
1:E:174:LEU:HD22	1:E:179:PHE:HD2	1.83	0.43
1:H:72:ASP:OD2	1:H:109:ARG:NH2	2.50	0.43
1:F:50:HIS:HD1	1:F:66:ASP:CG	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:80:PRO:HG2	1:H:173:VAL:HG23	2.00	0.43
1:C:370:ILE:HD11	1:C:378:ARG:HG2	2.00	0.43
1:A:154:TYR:CD2	1:B:55:SER:HB3	2.54	0.43
1:A:174:LEU:HD22	1:A:179:PHE:CD2	2.52	0.43
1:J:262:PRO:O	1:J:265:ILE:HG12	2.18	0.43
1:B:56:ILE:HG21	1:B:104:PHE:HE2	1.83	0.43
1:K:179:PHE:HZ	1:K:197:PHE:CE2	2.36	0.43
1:A:311:GLY:O	1:A:319:ARG:HG3	2.19	0.43
1:C:72:ASP:OD2	1:C:109:ARG:NH2	2.51	0.43
1:H:312:PRO:HD3	1:H:320:VAL:O	2.18	0.43
1:H:366:VAL:O	1:H:366:VAL:HG13	2.19	0.43
1:I:319:ARG:O	1:I:321:PRO:HD3	2.19	0.43
1:K:96:ILE:HG12	1:K:107:CYS:SG	2.59	0.43
1:H:7:GLU:HG3	1:H:10:ARG:NH2	2.34	0.43
1:D:114:LYS:O	1:D:118:GLU:HG3	2.18	0.43
1:G:24:PHE:HE2	1:G:56:ILE:HD13	1.83	0.43
1:K:112:LEU:O	1:K:116:MET:HG3	2.18	0.43
2:C:501:ATP:H5'2	2:C:501:ATP:O1G	2.18	0.42
1:F:21:ARG:HG2	1:F:33:ASN:OD1	2.19	0.42
1:H:343:LEU:HD13	1:H:415:ILE:HD11	2.01	0.42
1:F:302:GLU:HG2	1:F:333:ARG:NH2	2.33	0.42
1:B:198:LYS:HG2	1:B:199:TYR:N	2.33	0.42
1:C:130:PRO:HG2	1:C:197:PHE:CZ	2.53	0.42
1:I:248:LEU:HD12	1:I:248:LEU:N	2.35	0.42
1:K:78:VAL:O	1:K:80:PRO:HD3	2.19	0.42
1:B:198:LYS:CG	1:B:199:TYR:N	2.83	0.42
1:E:10:ARG:NH1	1:E:14:GLU:OE1	2.53	0.42
1:E:174:LEU:HD22	1:E:179:PHE:CD2	2.55	0.42
1:J:321:PRO:HD2	1:J:329:ARG:O	2.20	0.42
1:J:322:ALA:O	1:J:324:ARG:HG2	2.19	0.42
1:B:174:LEU:HD11	1:B:212:LEU:HD12	2.02	0.42
1:C:70:ARG:HG3	1:C:97:GLU:HG3	2.02	0.42
1:H:355:GLY:HA2	1:H:360:ILE:CD1	2.49	0.41
1:L:316:SER:O	1:L:333:ARG:HD3	2.20	0.41
1:G:56:ILE:C	1:G:58:GLY:H	2.23	0.41
1:J:302:GLU:HG3	6:J:602:HOH:O	2.20	0.41
1:A:57:GLU:O	1:A:58:GLY:C	2.58	0.41
1:D:129:GLY:HA3	2:D:501:ATP:O2'	2.21	0.41
1:C:50:HIS:CE1	1:C:68:VAL:HG12	2.54	0.41
1:C:263:ASP:O	1:C:324:ARG:NH1	2.54	0.41
1:D:46:GLY:O	1:D:70:ARG:NH1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:PRO:HB3	1:E:343:LEU:HG	2.02	0.41
1:H:169:GLU:O	1:H:173:VAL:HG12	2.20	0.41
1:F:377:GLU:HA	1:F:380:LYS:HE2	2.03	0.41
1:J:321:PRO:HG2	1:J:329:ARG:NE	2.35	0.41
1:J:322:ALA:N	1:J:323:PRO:CD	2.83	0.41
1:E:21:ARG:NH1	1:E:21:ARG:HG2	2.35	0.41
1:H:109:ARG:NH1	1:H:203:LEU:HD11	2.36	0.41
1:G:438:TYR:CG	1:L:290:LEU:HD23	2.55	0.41
1:I:302:GLU:O	1:I:302:GLU:HG2	2.21	0.41
1:A:319:ARG:NH2	1:A:331:GLU:OE1	2.53	0.41
1:F:294:TYR:CD1	1:F:294:TYR:N	2.89	0.41
1:L:369:ASN:HB3	1:L:372:LYS:HD2	2.02	0.41
1:E:317:LEU:HD11	1:E:334:SER:HB3	2.02	0.40
1:G:144:PRO:HG3	1:L:440:GLN:OE1	2.20	0.40
1:J:294:TYR:CD1	1:J:294:TYR:N	2.88	0.40
1:G:24:PHE:CD2	1:G:56:ILE:HD11	2.57	0.40
1:I:198:LYS:CG	1:I:199:TYR:N	2.84	0.40
1:F:370:ILE:HD11	1:F:378:ARG:HD3	2.04	0.40
1:H:43:LYS:HE2	1:H:49:ILE:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	424/442 (96%)	413 (97%)	11 (3%)	0	100	100
1	B	431/442 (98%)	423 (98%)	8 (2%)	0	100	100
1	C	422/442 (96%)	416 (99%)	6 (1%)	0	100	100
1	D	429/442 (97%)	420 (98%)	9 (2%)	0	100	100
1	E	430/442 (97%)	422 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	424/442 (96%)	414 (98%)	9 (2%)	1 (0%)	47 73
1	G	426/442 (96%)	413 (97%)	13 (3%)	0	100 100
1	H	422/442 (96%)	412 (98%)	10 (2%)	0	100 100
1	I	423/442 (96%)	415 (98%)	8 (2%)	0	100 100
1	J	425/442 (96%)	417 (98%)	8 (2%)	0	100 100
1	K	426/442 (96%)	419 (98%)	7 (2%)	0	100 100
1	L	431/442 (98%)	424 (98%)	7 (2%)	0	100 100
All	All	5113/5304 (96%)	5008 (98%)	104 (2%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	323	PRO

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	367/376 (98%)	362 (99%)	5 (1%)	67 86
1	B	370/376 (98%)	366 (99%)	4 (1%)	73 90
1	C	365/376 (97%)	360 (99%)	5 (1%)	67 86
1	D	369/376 (98%)	364 (99%)	5 (1%)	67 86
1	E	368/376 (98%)	363 (99%)	5 (1%)	67 86
1	F	366/376 (97%)	361 (99%)	5 (1%)	67 86
1	G	366/376 (97%)	361 (99%)	5 (1%)	67 86
1	H	365/376 (97%)	360 (99%)	5 (1%)	67 86
1	I	364/376 (97%)	358 (98%)	6 (2%)	62 85
1	J	366/376 (97%)	362 (99%)	4 (1%)	73 90
1	K	366/376 (97%)	361 (99%)	5 (1%)	67 86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	369/376 (98%)	365 (99%)	4 (1%)	73 90
All	All	4401/4512 (98%)	4343 (99%)	58 (1%)	69 87

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

Mol	Chain	Res	Type
1	A	33	ASN
1	A	91	ARG
1	A	179	PHE
1	A	197	PHE
1	A	314	ARG
1	B	33	ASN
1	B	91	ARG
1	B	154	TYR
1	B	179	PHE
1	C	33	ASN
1	C	154	TYR
1	C	156	ASP
1	C	179	PHE
1	C	314	ARG
1	D	33	ASN
1	D	91	ARG
1	D	154	TYR
1	D	179	PHE
1	D	314	ARG
1	E	33	ASN
1	E	91	ARG
1	E	154	TYR
1	E	179	PHE
1	E	437	ARG
1	F	33	ASN
1	F	91	ARG
1	F	93	ILE
1	F	154	TYR
1	F	179	PHE
1	G	33	ASN
1	G	91	ARG
1	G	154	TYR
1	G	168	ARG
1	G	179	PHE
1	H	33	ASN
1	H	91	ARG

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Mol	Chain	Res	Type
1	H	95	ASP
1	H	154	TYR
1	H	179	PHE
1	I	33	ASN
1	I	151	ARG
1	I	154	TYR
1	I	179	PHE
1	I	180	GLU
1	I	302	GLU
1	J	33	ASN
1	J	91	ARG
1	J	154	TYR
1	J	179	PHE
1	K	33	ASN
1	K	91	ARG
1	K	154	TYR
1	K	179	PHE
1	K	302	GLU
1	L	33	ASN
1	L	91	ARG
1	L	154	TYR
1	L	326	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 40 ligands modelled in this entry, 14 are monoatomic - leaving 26 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	FMT	K	502	-	2,2,2	0.99	0	1,1,1	0.25	0
2	ATP	K	501	-	26,33,33	0.77	0	31,52,52	1.56	4 (12%)
3	FMT	B	502	-	2,2,2	0.63	0	1,1,1	0.60	0
3	FMT	J	503	-	2,2,2	1.00	0	1,1,1	0.24	0
2	ATP	D	501	-	26,33,33	0.78	0	31,52,52	1.54	4 (12%)
3	FMT	G	502	-	2,2,2	0.64	0	1,1,1	0.61	0
2	ATP	C	501	-	26,33,33	0.77	0	31,52,52	1.52	4 (12%)
2	ATP	H	501	-	26,33,33	0.77	0	31,52,52	1.55	4 (12%)
3	FMT	D	502	-	2,2,2	0.65	0	1,1,1	0.61	0
3	FMT	C	504	-	2,2,2	0.64	0	1,1,1	0.62	0
3	FMT	C	502	-	2,2,2	0.64	0	1,1,1	0.62	0
3	FMT	E	502	-	2,2,2	0.63	0	1,1,1	0.61	0
3	FMT	A	502	-	2,2,2	0.60	0	1,1,1	0.62	0
3	FMT	J	502	-	2,2,2	0.98	0	1,1,1	0.24	0
2	ATP	L	501	-	26,33,33	0.77	0	31,52,52	1.53	4 (12%)
3	FMT	A	503	-	2,2,2	0.64	0	1,1,1	0.61	0
2	ATP	E	501	-	26,33,33	0.78	0	31,52,52	1.52	4 (12%)
2	ATP	I	501	-	26,33,33	0.77	0	31,52,52	1.56	4 (12%)
2	ATP	F	501	-	26,33,33	0.78	0	31,52,52	1.52	4 (12%)
3	FMT	G	504	-	2,2,2	0.64	0	1,1,1	0.60	0
2	ATP	B	501	-	26,33,33	0.78	0	31,52,52	1.57	4 (12%)
3	FMT	C	503	-	2,2,2	0.64	0	1,1,1	0.59	0
5	GOL	G	503	-	5,5,5	0.08	0	5,5,5	0.33	0
2	ATP	A	501	-	26,33,33	0.77	0	31,52,52	1.53	4 (12%)
2	ATP	G	501	-	26,33,33	0.77	0	31,52,52	1.57	4 (12%)
2	ATP	J	501	-	26,33,33	0.78	0	31,52,52	1.54	4 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	B	501	-	-	4/18/38/38	0/3/3/3
2	ATP	K	501	-	-	5/18/38/38	0/3/3/3
5	GOL	G	503	-	-	4/4/4/4	-
2	ATP	A	501	-	-	3/18/38/38	0/3/3/3
2	ATP	G	501	-	-	6/18/38/38	0/3/3/3
2	ATP	H	501	-	-	4/18/38/38	0/3/3/3
2	ATP	L	501	-	-	8/18/38/38	0/3/3/3
2	ATP	J	501	-	-	4/18/38/38	0/3/3/3
2	ATP	E	501	-	-	4/18/38/38	0/3/3/3
2	ATP	I	501	-	-	1/18/38/38	0/3/3/3
2	ATP	D	501	-	-	5/18/38/38	0/3/3/3
2	ATP	F	501	-	-	7/18/38/38	0/3/3/3
2	ATP	C	501	-	-	4/18/38/38	0/3/3/3

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	501	ATP	N3-C2-N1	-4.22	122.08	128.68
2	E	501	ATP	N3-C2-N1	-4.13	122.22	128.68
2	G	501	ATP	N3-C2-N1	-4.09	122.28	128.68
2	J	501	ATP	N3-C2-N1	-4.07	122.32	128.68
2	B	501	ATP	N3-C2-N1	-4.05	122.35	128.68
2	K	501	ATP	N3-C2-N1	-4.04	122.37	128.68
2	L	501	ATP	N3-C2-N1	-4.01	122.41	128.68
2	G	501	ATP	PA-O3A-PB	-4.00	119.09	132.83
2	D	501	ATP	N3-C2-N1	-4.00	122.43	128.68
2	B	501	ATP	PA-O3A-PB	-3.99	119.14	132.83
2	I	501	ATP	N3-C2-N1	-3.97	122.47	128.68
2	A	501	ATP	N3-C2-N1	-3.97	122.47	128.68
2	C	501	ATP	N3-C2-N1	-3.97	122.47	128.68
2	H	501	ATP	PA-O3A-PB	-3.92	119.39	132.83
2	K	501	ATP	PB-O3B-PG	-3.91	119.39	132.83
2	I	501	ATP	PA-O3A-PB	-3.91	119.41	132.83
2	F	501	ATP	PA-O3A-PB	-3.90	119.45	132.83
2	F	501	ATP	N3-C2-N1	-3.88	122.62	128.68
2	K	501	ATP	PA-O3A-PB	-3.87	119.54	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	501	ATP	PA-O3A-PB	-3.86	119.58	132.83
2	C	501	ATP	PB-O3B-PG	-3.84	119.64	132.83
2	D	501	ATP	PB-O3B-PG	-3.84	119.65	132.83
2	G	501	ATP	PB-O3B-PG	-3.81	119.75	132.83
2	I	501	ATP	PB-O3B-PG	-3.80	119.79	132.83
2	A	501	ATP	PA-O3A-PB	-3.75	119.97	132.83
2	E	501	ATP	PA-O3A-PB	-3.71	120.08	132.83
2	J	501	ATP	PA-O3A-PB	-3.71	120.09	132.83
2	D	501	ATP	PA-O3A-PB	-3.71	120.10	132.83
2	A	501	ATP	PB-O3B-PG	-3.67	120.25	132.83
2	E	501	ATP	PB-O3B-PG	-3.66	120.26	132.83
2	H	501	ATP	PB-O3B-PG	-3.66	120.27	132.83
2	B	501	ATP	PB-O3B-PG	-3.64	120.32	132.83
2	J	501	ATP	PB-O3B-PG	-3.58	120.54	132.83
2	C	501	ATP	PA-O3A-PB	-3.50	120.80	132.83
2	B	501	ATP	C3'-C2'-C1'	3.48	106.21	100.98
2	D	501	ATP	C3'-C2'-C1'	3.46	106.19	100.98
2	F	501	ATP	C3'-C2'-C1'	3.44	106.16	100.98
2	A	501	ATP	C3'-C2'-C1'	3.40	106.09	100.98
2	J	501	ATP	C3'-C2'-C1'	3.39	106.08	100.98
2	F	501	ATP	PB-O3B-PG	-3.38	121.23	132.83
2	L	501	ATP	C3'-C2'-C1'	3.37	106.05	100.98
2	L	501	ATP	PB-O3B-PG	-3.37	121.26	132.83
2	H	501	ATP	C3'-C2'-C1'	3.35	106.03	100.98
2	C	501	ATP	C3'-C2'-C1'	3.35	106.03	100.98
2	K	501	ATP	C3'-C2'-C1'	3.34	106.01	100.98
2	I	501	ATP	C3'-C2'-C1'	3.30	105.94	100.98
2	G	501	ATP	C3'-C2'-C1'	3.13	105.69	100.98
2	E	501	ATP	C3'-C2'-C1'	2.98	105.47	100.98

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	ATP	C5'-O5'-PA-O3A
2	C	501	ATP	C5'-O5'-PA-O1A
2	C	501	ATP	C5'-O5'-PA-O3A
2	D	501	ATP	C5'-O5'-PA-O2A
2	D	501	ATP	C5'-O5'-PA-O3A
2	F	501	ATP	PB-O3B-PG-O2G
2	G	501	ATP	PB-O3B-PG-O3G
2	G	501	ATP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	G	501	ATP	C3'-C4'-C5'-O5'
2	J	501	ATP	C5'-O5'-PA-O2A
2	J	501	ATP	C5'-O5'-PA-O3A
2	K	501	ATP	C5'-O5'-PA-O2A
2	K	501	ATP	O4'-C4'-C5'-O5'
2	K	501	ATP	C3'-C4'-C5'-O5'
2	L	501	ATP	PB-O3B-PG-O2G
2	L	501	ATP	PB-O3B-PG-O3G
2	L	501	ATP	C5'-O5'-PA-O1A
2	L	501	ATP	C5'-O5'-PA-O2A
2	L	501	ATP	C3'-C4'-C5'-O5'
5	G	503	GOL	C1-C2-C3-O3
2	B	501	ATP	O4'-C4'-C5'-O5'
2	L	501	ATP	O4'-C4'-C5'-O5'
2	B	501	ATP	C3'-C4'-C5'-O5'
2	H	501	ATP	O4'-C4'-C5'-O5'
5	G	503	GOL	O1-C1-C2-C3
2	H	501	ATP	C3'-C4'-C5'-O5'
2	F	501	ATP	C3'-C4'-C5'-O5'
2	J	501	ATP	PB-O3A-PA-O1A
2	F	501	ATP	O4'-C4'-C5'-O5'
2	F	501	ATP	PB-O3A-PA-O5'
2	H	501	ATP	PB-O3A-PA-O5'
2	L	501	ATP	PB-O3A-PA-O5'
2	K	501	ATP	C5'-O5'-PA-O3A
2	L	501	ATP	C5'-O5'-PA-O3A
5	G	503	GOL	O1-C1-C2-O2
2	A	501	ATP	PG-O3B-PB-O2B
2	B	501	ATP	C5'-O5'-PA-O1A
2	D	501	ATP	C5'-O5'-PA-O1A
2	J	501	ATP	C5'-O5'-PA-O1A
2	K	501	ATP	C5'-O5'-PA-O1A
2	C	501	ATP	C3'-C4'-C5'-O5'
5	G	503	GOL	O2-C2-C3-O3
2	A	501	ATP	PB-O3A-PA-O1A
2	E	501	ATP	PB-O3A-PA-O1A
2	F	501	ATP	PA-O3A-PB-O1B
2	G	501	ATP	PB-O3A-PA-O2A
2	E	501	ATP	PB-O3A-PA-O2A
2	C	501	ATP	O4'-C4'-C5'-O5'
2	G	501	ATP	PB-O3B-PG-O1G
2	E	501	ATP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	D	501	ATP	PB-O3B-PG-O2G
2	E	501	ATP	PB-O3B-PG-O3G
2	F	501	ATP	PB-O3B-PG-O3G
2	A	501	ATP	PB-O3A-PA-O2A
2	G	501	ATP	PB-O3A-PA-O1A
2	H	501	ATP	C5'-O5'-PA-O1A
2	I	501	ATP	C5'-O5'-PA-O1A
2	D	501	ATP	C3'-C4'-C5'-O5'
2	F	501	ATP	PB-O3B-PG-O1G

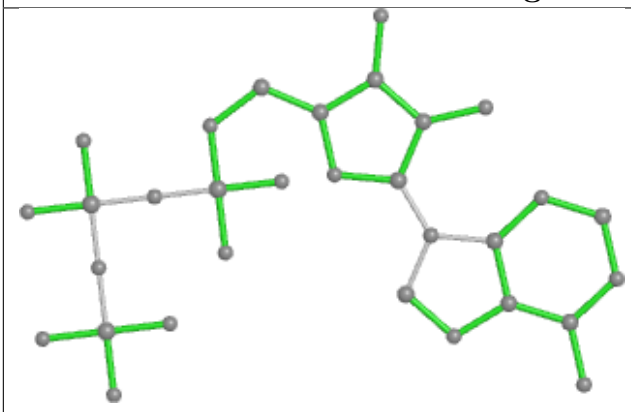
There are no ring outliers.

7 monomers are involved in 9 short contacts:

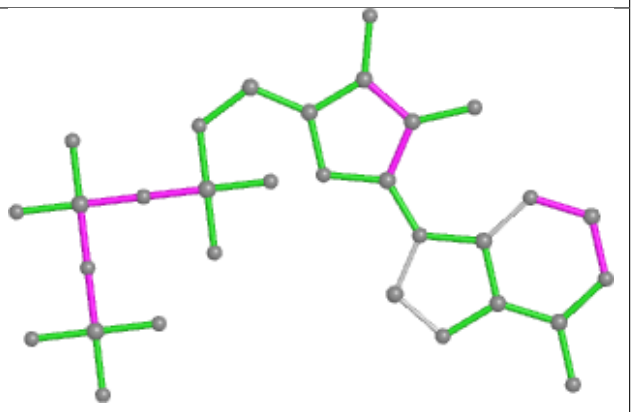
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	FMT	1	0
2	D	501	ATP	1	0
2	C	501	ATP	1	0
2	H	501	ATP	3	0
2	E	501	ATP	1	0
2	B	501	ATP	1	0
2	J	501	ATP	1	0

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.

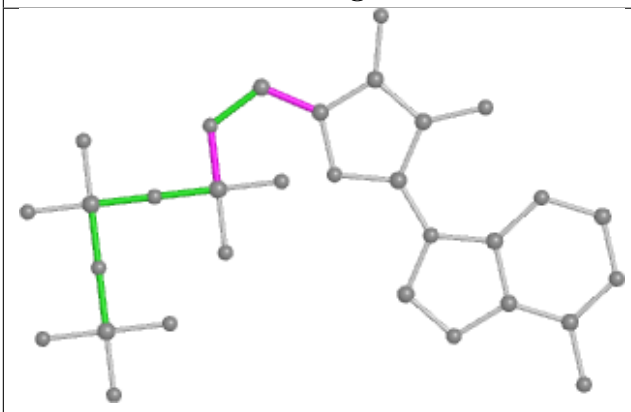
Ligand ATP K 501



Bond lengths



Bond angles



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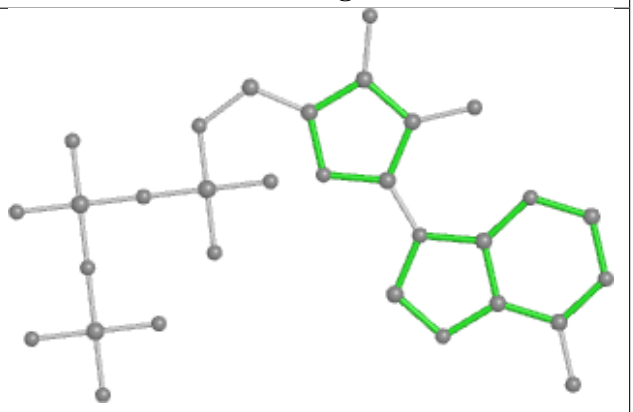
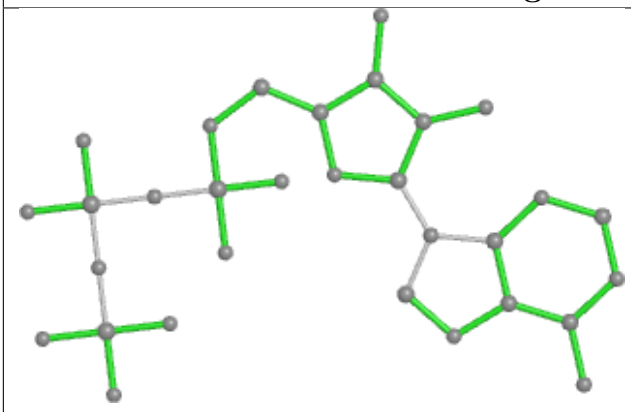
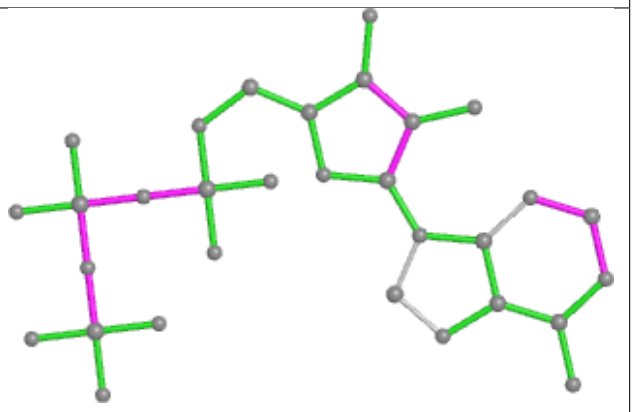


Rings

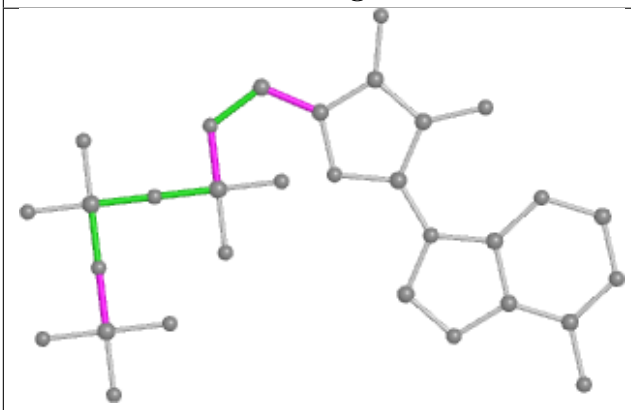
Ligand ATP D 501



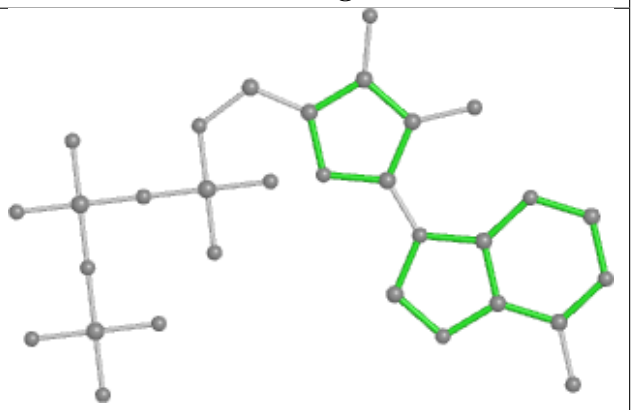
Bond lengths



Bond angles

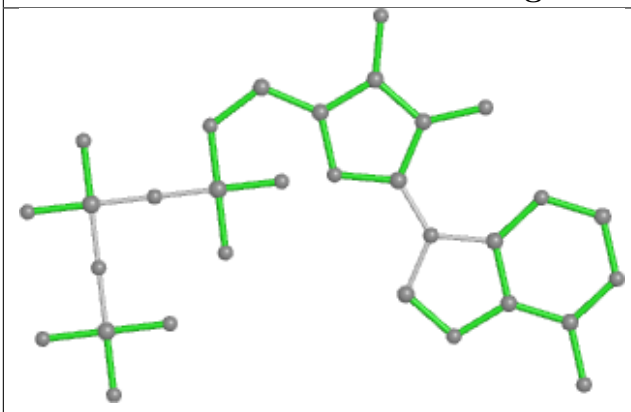


Torsions

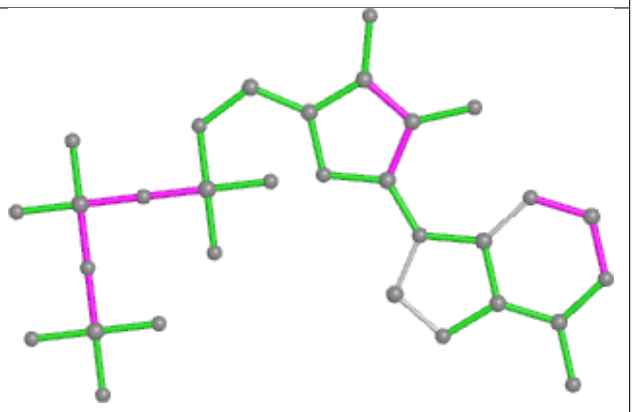


Rings

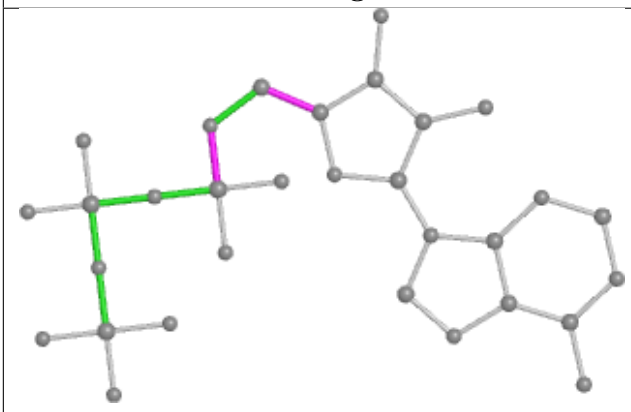
Ligand ATP C 501



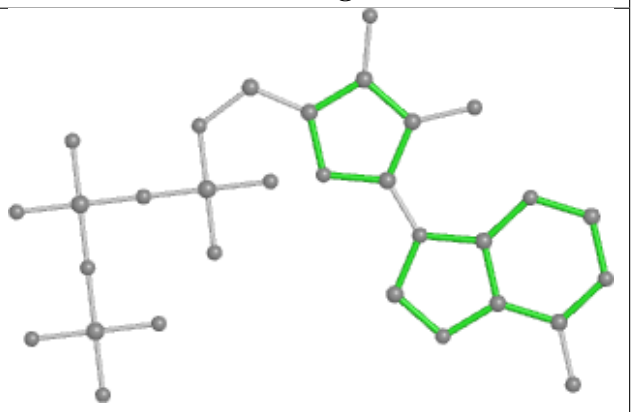
Bond lengths



Bond angles

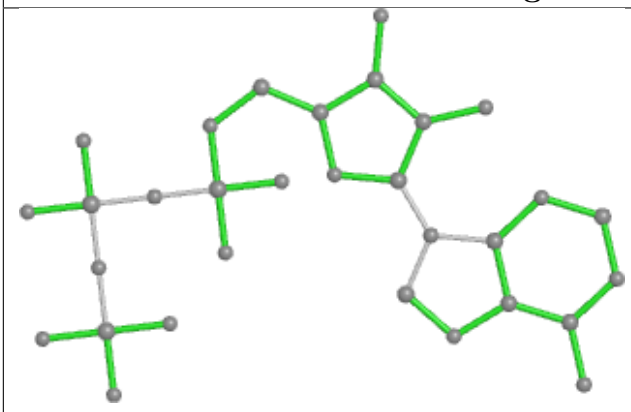


Torsions

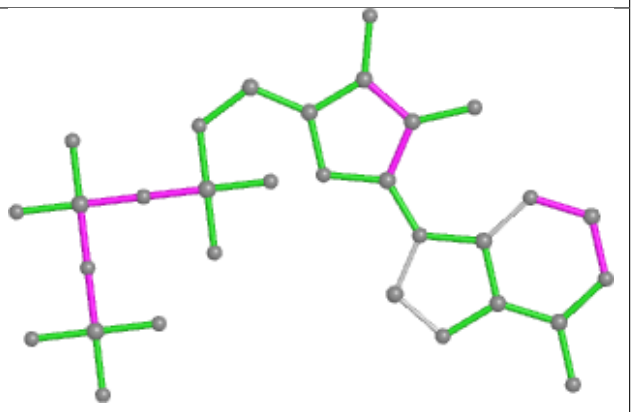


Rings

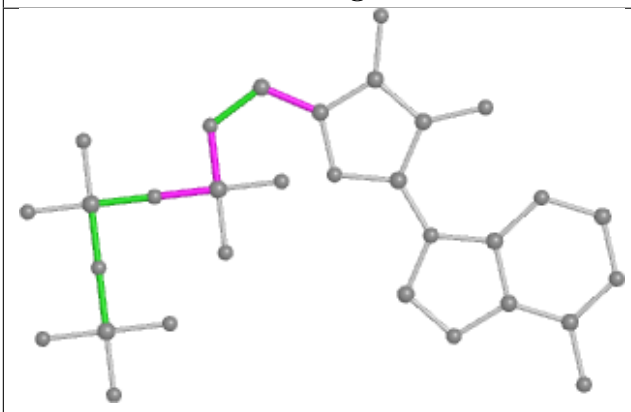
Ligand ATP H 501



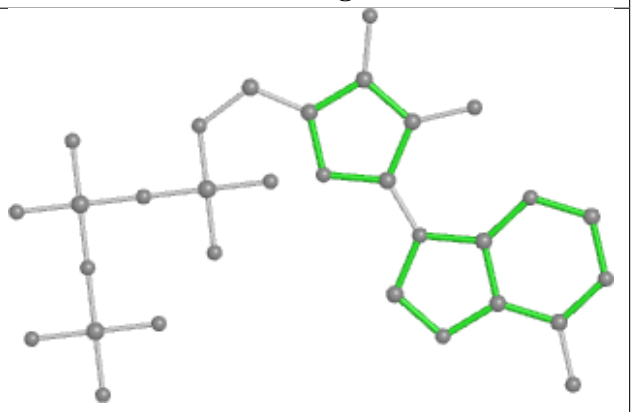
Bond lengths



Bond angles

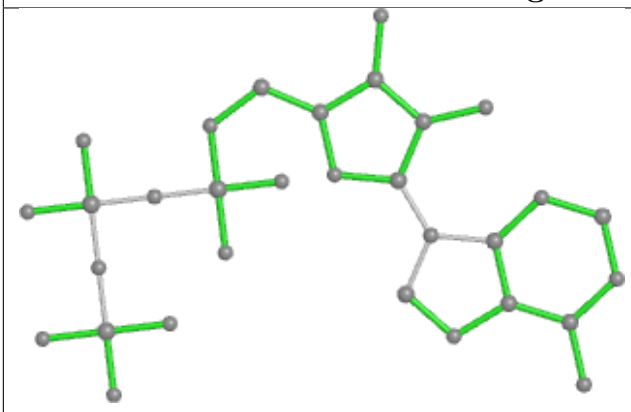


Torsions

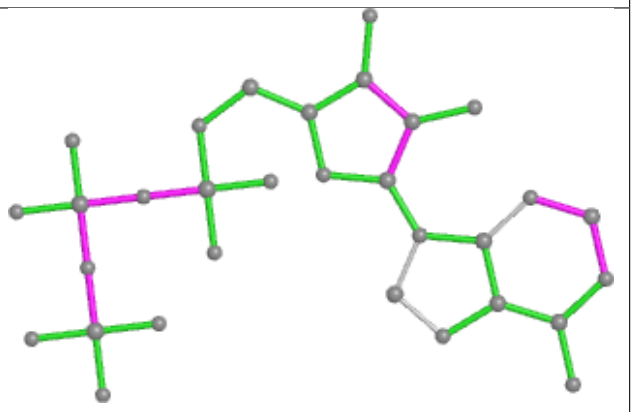


Rings

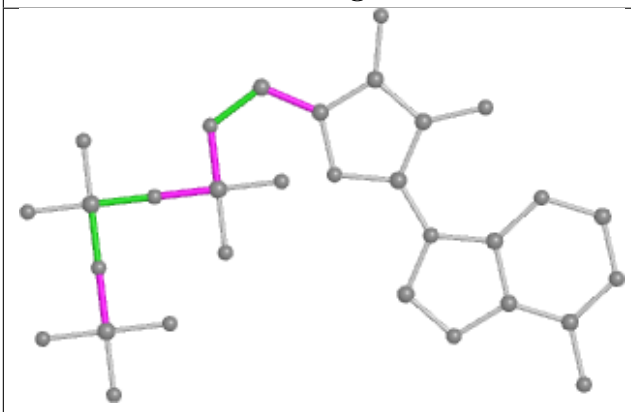
Ligand ATP L 501



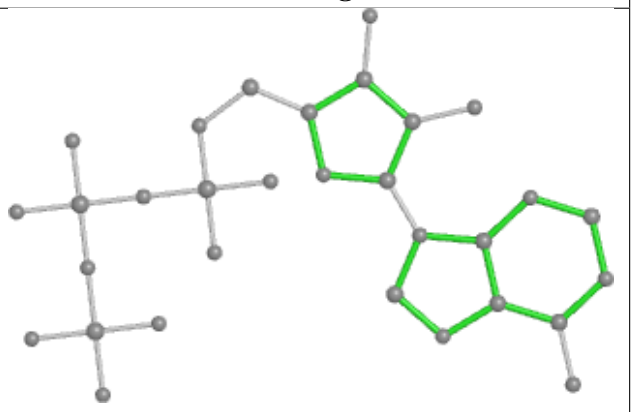
Bond lengths



Bond angles

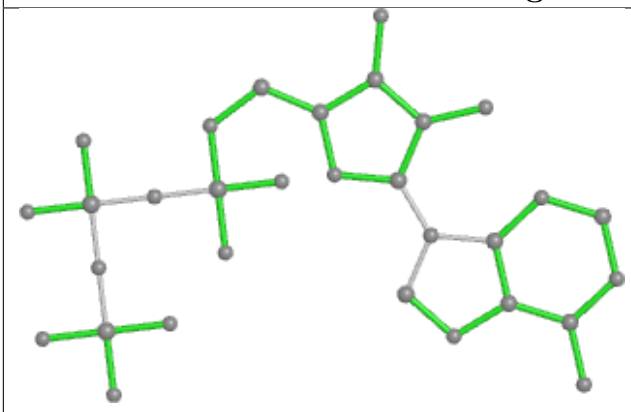


Torsions

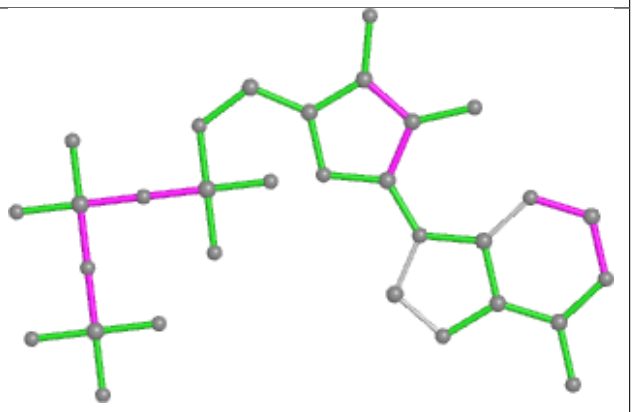


Rings

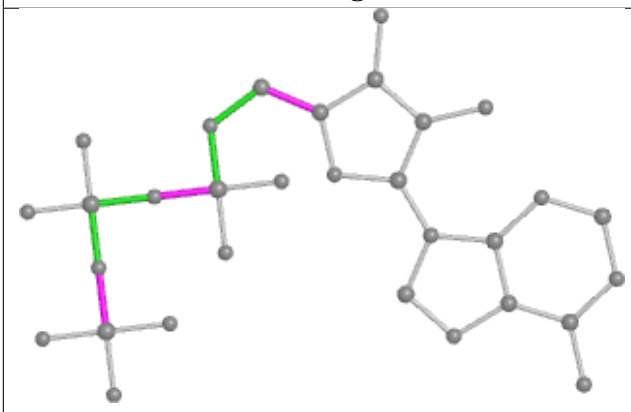
Ligand ATP E 501



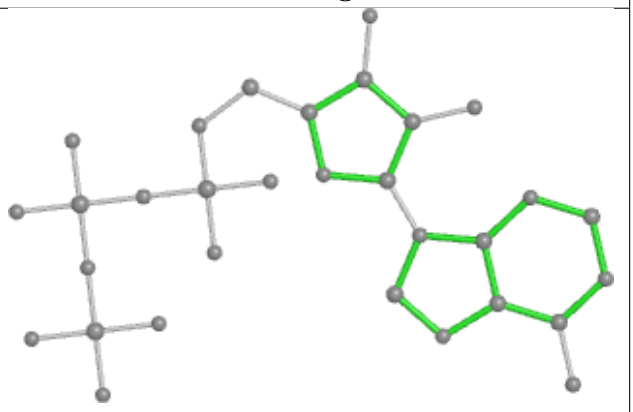
Bond lengths



Bond angles

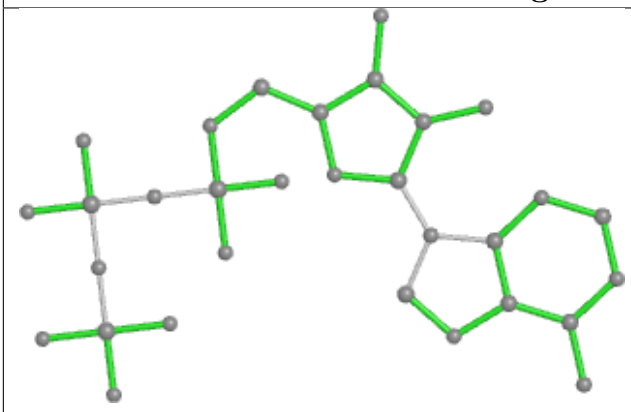


Torsions

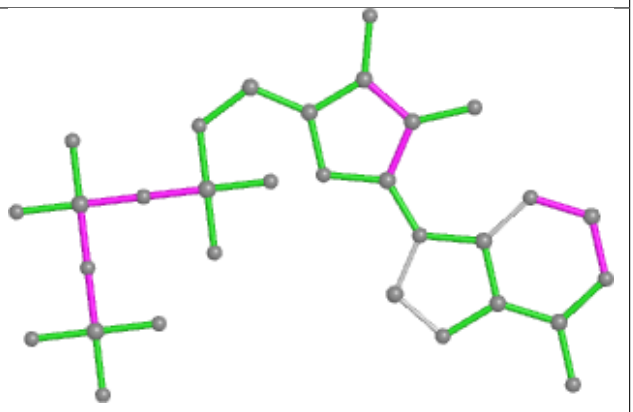


Rings

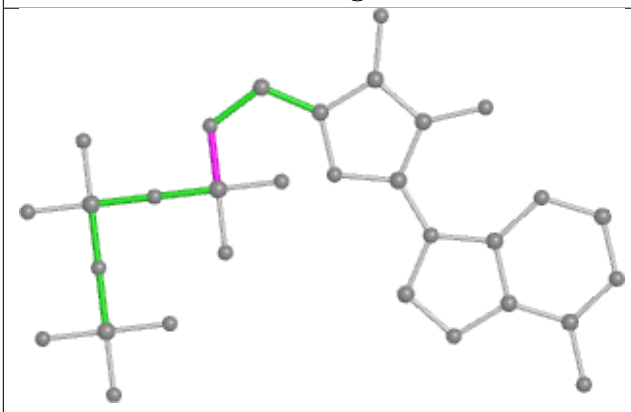
Ligand ATP I 501



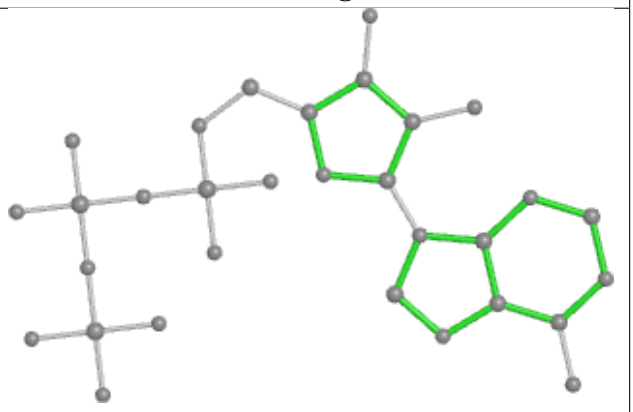
Bond lengths



Bond angles

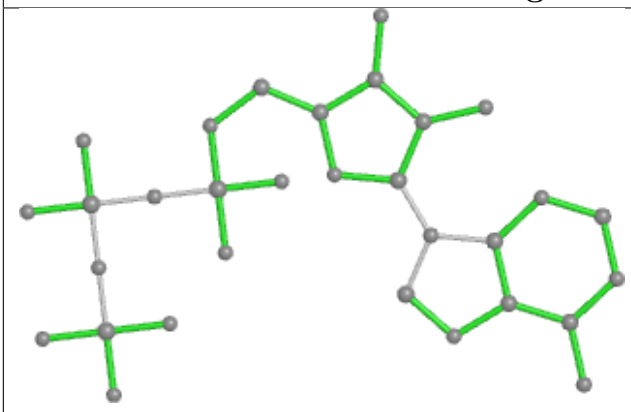


Torsions

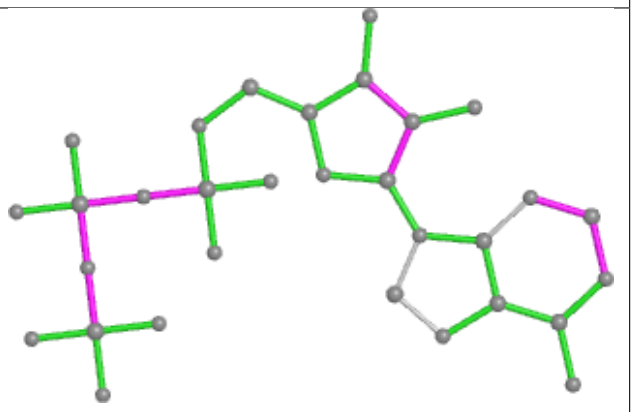


Rings

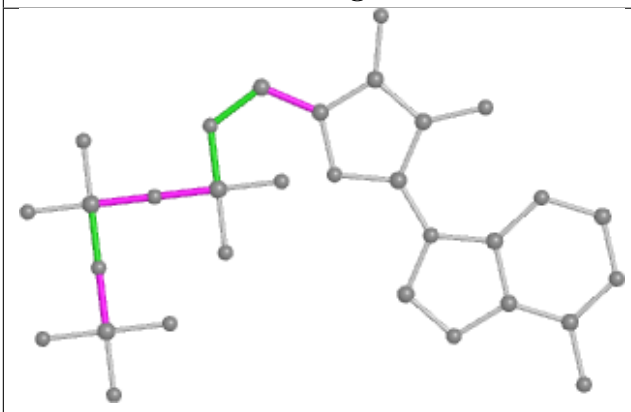
Ligand ATP F 501



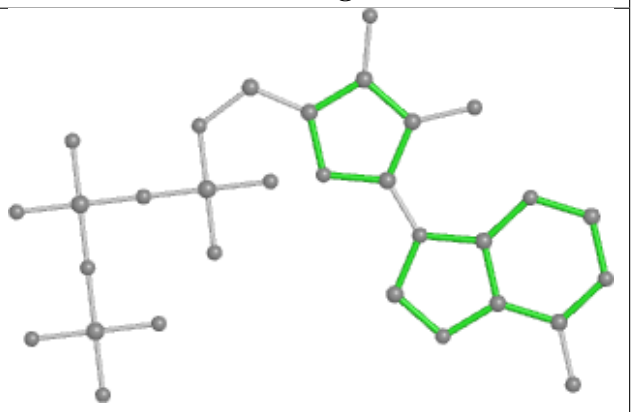
Bond lengths



Bond angles

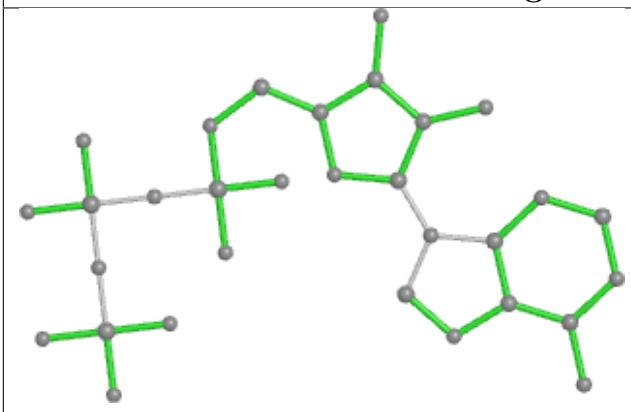


Torsions

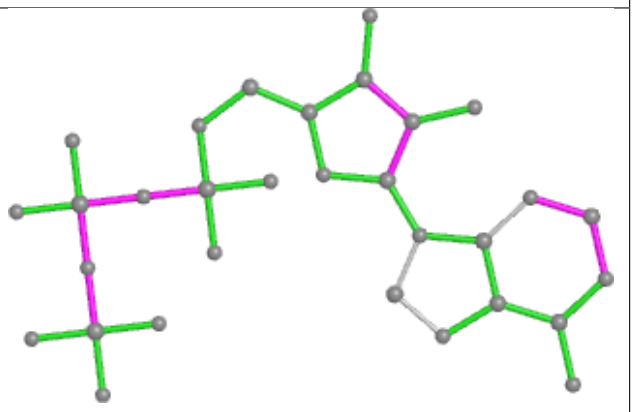


Rings

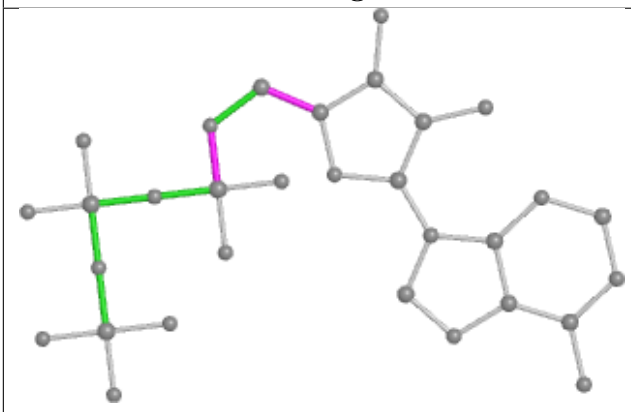
Ligand ATP B 501



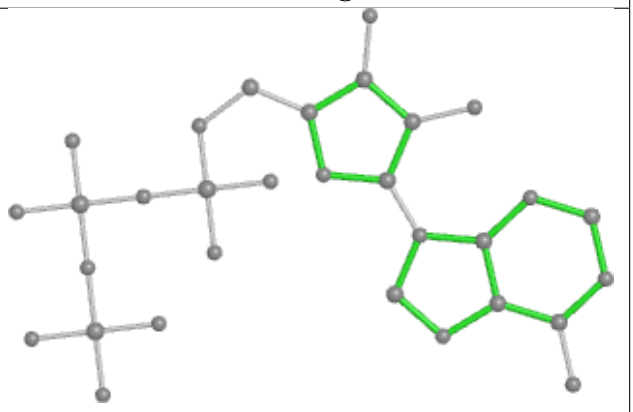
Bond lengths



Bond angles

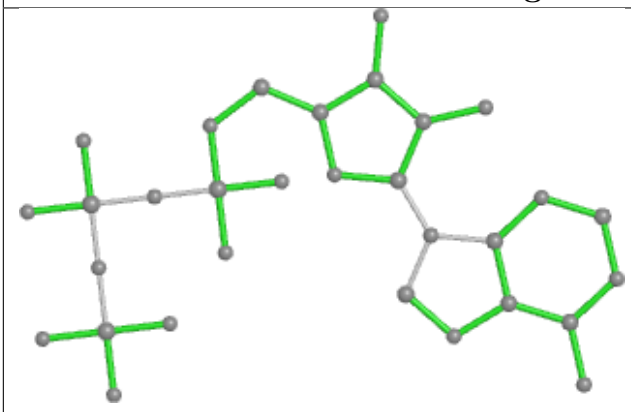


Torsions

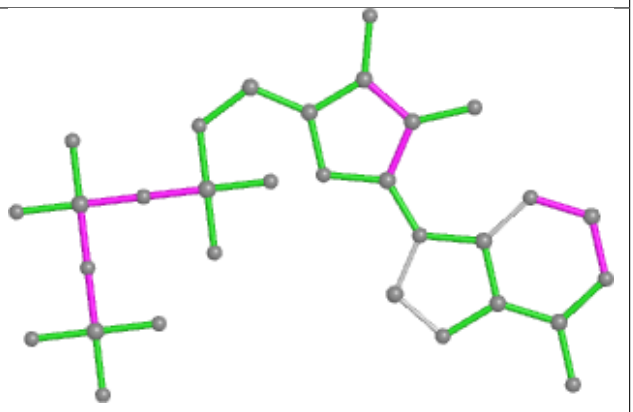


Rings

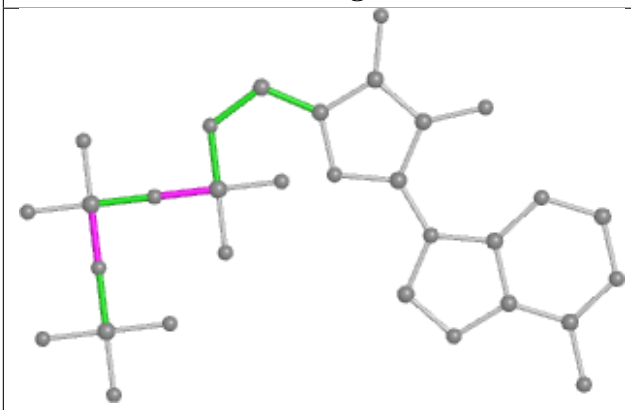
Ligand ATP A 501



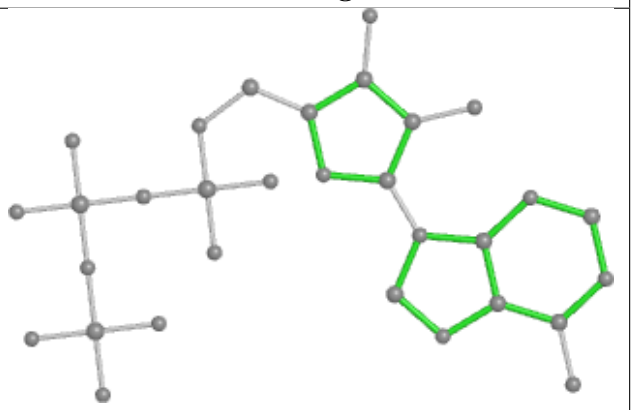
Bond lengths



Bond angles

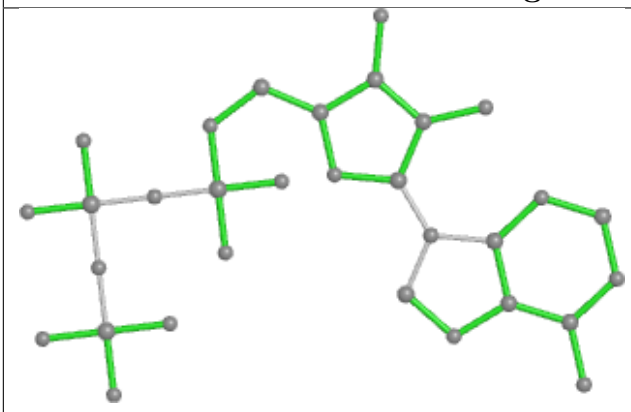


Torsions

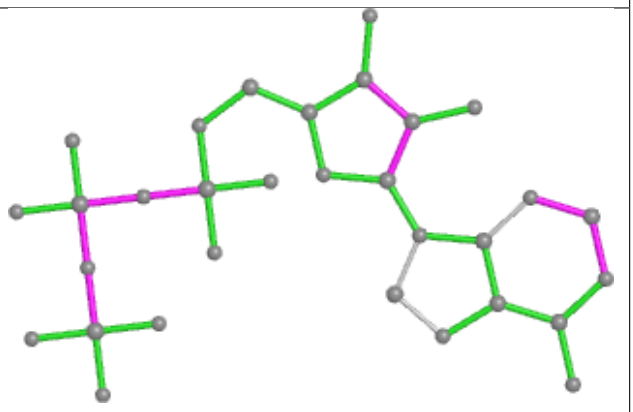


Rings

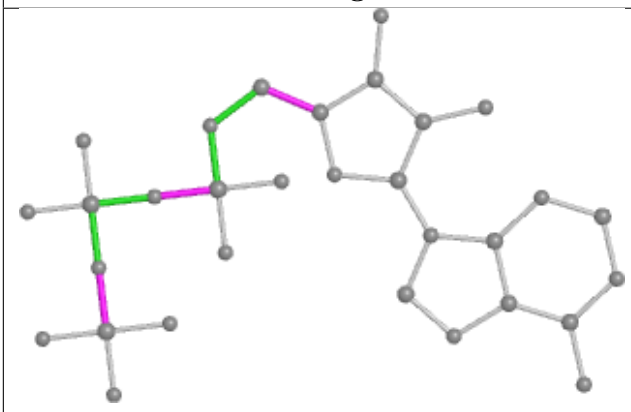
Ligand ATP G 501



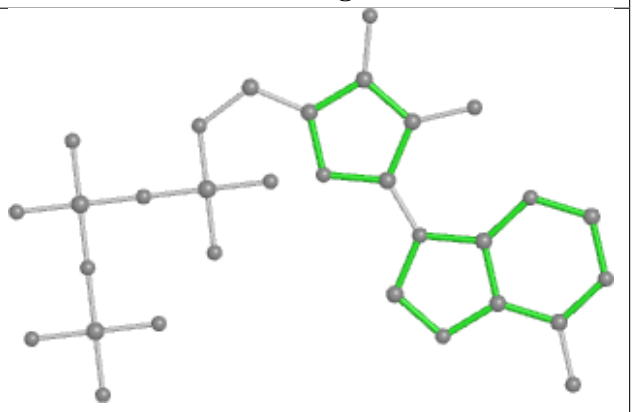
Bond lengths



Bond angles

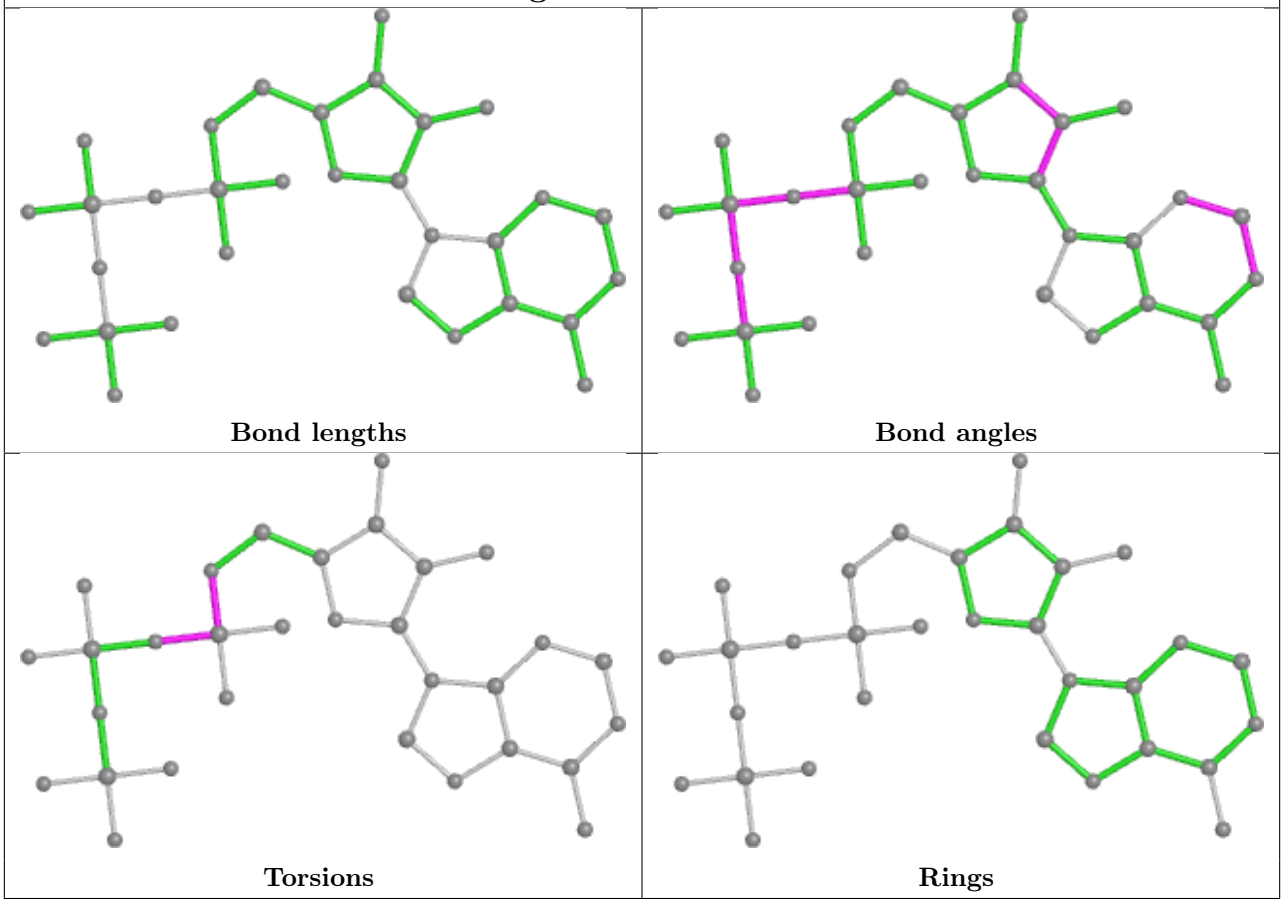


Torsions



Rings

Ligand ATP J 501



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, 95^{th} 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	430/442 (97%)	0.22	5 (1%)	79	80	37, 59, 102, 154	0
1	B	435/442 (98%)	0.17	16 (3%)	41	41	34, 59, 110, 172	0
1	C	428/442 (96%)	0.21	9 (2%)	63	65	36, 64, 109, 145	0
1	D	433/442 (97%)	0.13	5 (1%)	79	80	33, 61, 110, 174	0
1	E	434/442 (98%)	0.14	16 (3%)	41	41	35, 62, 107, 180	0
1	F	430/442 (97%)	0.25	21 (4%)	29	28	37, 66, 113, 147	0
1	G	432/442 (97%)	0.16	9 (2%)	63	65	44, 68, 106, 145	0
1	H	428/442 (96%)	0.46	33 (7%)	13	11	48, 84, 126, 164	0
1	I	429/442 (97%)	0.05	6 (1%)	75	77	50, 72, 110, 158	0
1	J	431/442 (97%)	0.11	7 (1%)	72	74	39, 66, 102, 172	0
1	K	432/442 (97%)	0.16	12 (2%)	53	54	39, 63, 107, 155	0
1	L	435/442 (98%)	0.21	16 (3%)	41	41	40, 67, 116, 186	0
All	All	5177/5304 (97%)	0.19	155 (2%)	50	51	33, 66, 111, 186	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	371	TYR	9.7
1	C	56	ILE	8.1
1	K	56	ILE	7.9
1	C	55	SER	6.5
1	J	56	ILE	6.2
1	D	56	ILE	5.6
1	A	56	ILE	5.3
1	B	373	LEU	5.1
1	B	85	GLU	5.0
1	E	56	ILE	4.9
1	H	370	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	55	SER	4.5
1	H	371	TYR	4.4
1	B	372	LYS	4.2
1	L	151	ARG	4.1
1	K	371	TYR	4.1
1	K	372	LYS	4.0
1	E	53	GLY	3.9
1	H	248	LEU	3.9
1	H	161	ASP	3.9
1	H	159	PRO	3.9
1	B	370	ILE	3.8
1	F	376	GLU	3.8
1	G	371	TYR	3.8
1	H	377	GLU	3.8
1	E	86	GLY	3.8
1	K	55	SER	3.8
1	A	55	SER	3.7
1	J	313	ASN	3.7
1	L	85	GLU	3.6
1	C	53	GLY	3.6
1	B	374	THR	3.6
1	H	350	ALA	3.6
1	J	2	GLY	3.6
1	G	384	GLY	3.6
1	E	87	THR	3.6
1	E	84	ASN	3.4
1	I	84	ASN	3.4
1	K	151	ARG	3.3
1	H	368	LYS	3.3
1	L	371	TYR	3.2
1	K	160	ILE	3.2
1	F	10	ARG	3.2
1	G	56	ILE	3.2
1	L	160	ILE	3.2
1	D	55	SER	3.2
1	H	81	TRP	3.1
1	F	308	THR	3.1
1	B	159	PRO	3.0
1	A	214	TYR	3.0
1	H	126	MET	3.0
1	F	302	GLU	3.0
1	F	370	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	376	GLU	3.0
1	H	319	ARG	3.0
1	J	81	TRP	3.0
1	B	371	TYR	2.9
1	I	22	LEU	2.9
1	D	53	GLY	2.9
1	G	248	LEU	2.9
1	F	100	ASP	2.9
1	A	21	ARG	2.9
1	F	262	PRO	2.8
1	K	197	PHE	2.8
1	K	57	GLU	2.8
1	H	246	THR	2.8
1	L	178	GLY	2.8
1	L	197	PHE	2.8
1	C	19	PHE	2.7
1	H	320	VAL	2.7
1	I	86	GLY	2.7
1	C	87	THR	2.7
1	E	80	PRO	2.7
1	F	375	GLU	2.7
1	H	318	ILE	2.7
1	J	173	VAL	2.7
1	B	314	ARG	2.7
1	H	197	PHE	2.6
1	H	121	LYS	2.6
1	L	372	LYS	2.6
1	H	172	LEU	2.6
1	L	374	THR	2.6
1	H	124	TYR	2.6
1	E	313	ASN	2.5
1	E	88	ALA	2.5
1	H	309	TRP	2.5
1	C	271	TYR	2.5
1	B	366	VAL	2.5
1	E	83	GLY	2.5
1	G	270	ARG	2.5
1	H	120	ALA	2.5
1	H	304	PRO	2.5
1	D	50	HIS	2.5
1	K	58	GLY	2.5
1	H	160	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	307	ILE	2.4
1	L	27	VAL	2.4
1	G	383	ILE	2.4
1	E	78	VAL	2.4
1	F	276	VAL	2.4
1	E	85	GLU	2.4
1	G	380	LYS	2.4
1	H	80	PRO	2.4
1	K	179	PHE	2.4
1	F	306	TYR	2.4
1	H	378	ARG	2.4
1	H	178	GLY	2.3
1	L	56	ILE	2.3
1	E	179	PHE	2.3
1	H	251	ASP	2.3
1	F	351	ALA	2.3
1	F	256	PHE	2.3
1	J	19	PHE	2.3
1	B	84	ASN	2.3
1	I	68	VAL	2.3
1	B	313	ASN	2.3
1	C	197	PHE	2.3
1	H	366	VAL	2.3
1	K	376	GLU	2.2
1	L	159	PRO	2.2
1	F	330	ILE	2.2
1	H	332	ILE	2.2
1	C	403	LEU	2.2
1	L	149	GLN	2.2
1	B	379	GLU	2.2
1	E	160	ILE	2.2
1	E	19	PHE	2.2
1	B	251	ASP	2.2
1	G	19	PHE	2.2
1	B	250	LYS	2.2
1	F	88	ALA	2.2
1	L	370	ILE	2.1
1	A	380	LYS	2.1
1	C	68	VAL	2.1
1	D	66	ASP	2.1
1	F	81	TRP	2.1
1	H	56	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	265	ILE	2.1
1	K	377	GLU	2.1
1	F	154	TYR	2.1
1	H	164	GLU	2.1
1	B	265	ILE	2.1
1	E	54	SER	2.1
1	H	353	LEU	2.1
1	I	371	TYR	2.1
1	H	375	GLU	2.1
1	F	313	ASN	2.0
1	L	2	GLY	2.0
1	L	105	MET	2.0
1	L	368	LYS	2.0
1	F	366	VAL	2.0
1	F	307	ILE	2.0
1	I	370	ILE	2.0
1	J	13	GLU	2.0
1	F	19	PHE	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, 95^{th} 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
3	FMT	A	503	3/3	0.70	0.37	66,66,70,71	0
5	GOL	G	503	6/6	0.73	0.33	67,70,75,76	0
3	FMT	E	502	3/3	0.75	0.31	59,59,61,61	0
3	FMT	C	503	3/3	0.75	0.25	63,63,64,64	0
4	MG	C	505	1/1	0.76	0.14	74,74,74,74	0

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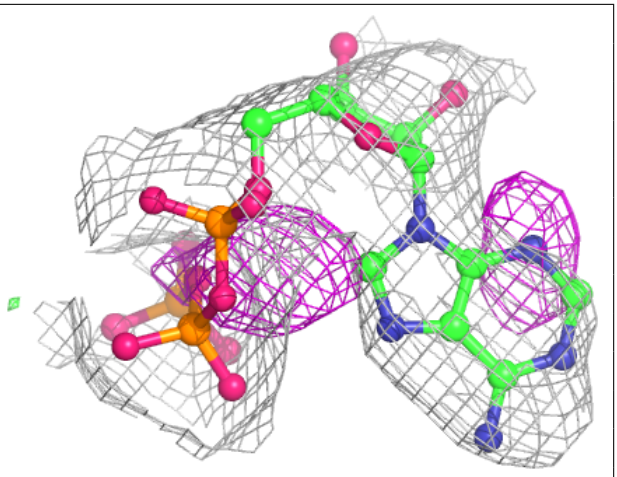
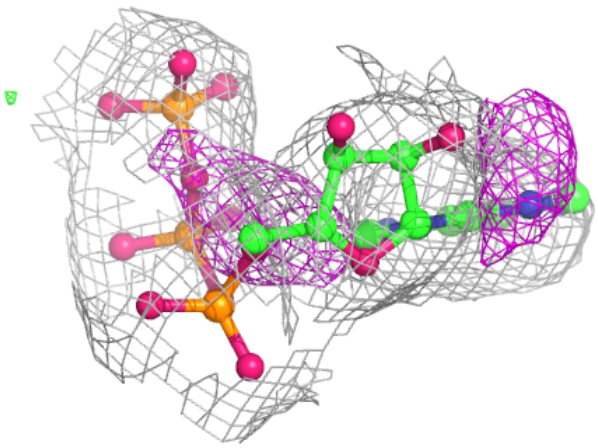
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FMT	G	502	3/3	0.79	0.20	74,74,80,82	0
3	FMT	J	503	3/3	0.79	0.33	54,54,60,63	0
2	ATP	H	501	31/31	0.80	0.22	87,118,149,169	0
3	FMT	B	502	3/3	0.80	0.47	54,54,62,65	0
3	FMT	C	504	3/3	0.81	0.43	56,56,57,61	0
4	MG	H	502	1/1	0.81	0.10	86,86,86,86	0
2	ATP	C	501	31/31	0.81	0.23	79,101,133,142	0
2	ATP	I	501	31/31	0.82	0.18	74,94,136,149	0
3	FMT	C	502	3/3	0.82	0.35	59,59,67,69	0
3	FMT	J	502	3/3	0.83	0.36	64,64,65,68	0
3	FMT	G	504	3/3	0.84	0.21	69,69,73,75	0
2	ATP	J	501	31/31	0.86	0.19	73,87,118,133	0
4	MG	D	503	1/1	0.86	0.12	74,74,74,74	0
3	FMT	A	502	3/3	0.86	0.27	54,54,59,66	0
4	MG	I	502	1/1	0.86	0.23	76,76,76,76	0
2	ATP	G	501	31/31	0.86	0.17	66,88,139,156	0
4	MG	F	503	1/1	0.87	0.15	72,72,72,72	0
2	ATP	L	501	31/31	0.87	0.17	72,92,128,142	0
2	ATP	D	501	31/31	0.88	0.19	67,85,130,139	0
2	ATP	B	501	31/31	0.89	0.30	60,89,134,138	0
3	FMT	D	502	3/3	0.89	0.20	51,51,55,64	0
2	ATP	E	501	31/31	0.89	0.17	60,81,120,138	0
3	FMT	K	502	3/3	0.89	0.41	64,64,68,76	0
2	ATP	A	501	31/31	0.89	0.20	62,79,109,127	0
4	MG	B	503	1/1	0.90	0.08	54,54,54,54	0
4	MG	E	503	1/1	0.90	0.11	66,66,66,66	0
2	ATP	K	501	31/31	0.90	0.19	60,85,133,153	0
2	ATP	F	501	31/31	0.92	0.19	70,88,115,122	0
4	MG	K	503	1/1	0.93	0.11	62,62,62,62	0
4	MG	J	504	1/1	0.93	0.27	60,60,60,60	0
4	MG	L	502	1/1	0.94	0.06	57,57,57,57	0
4	MG	F	502	1/1	0.94	0.10	59,59,59,59	0
4	MG	A	504	1/1	0.95	0.23	62,62,62,62	0
4	MG	G	505	1/1	0.95	0.14	61,61,61,61	0
4	MG	C	506	1/1	0.97	0.15	59,59,59,59	0

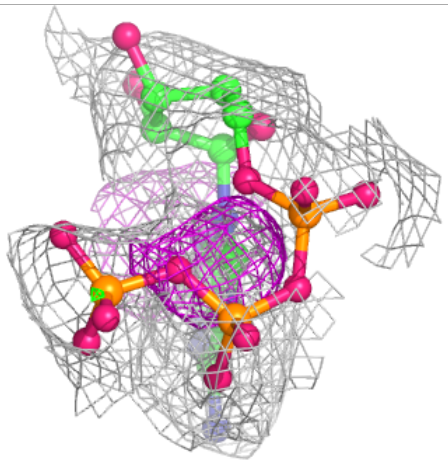
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP H 501:

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

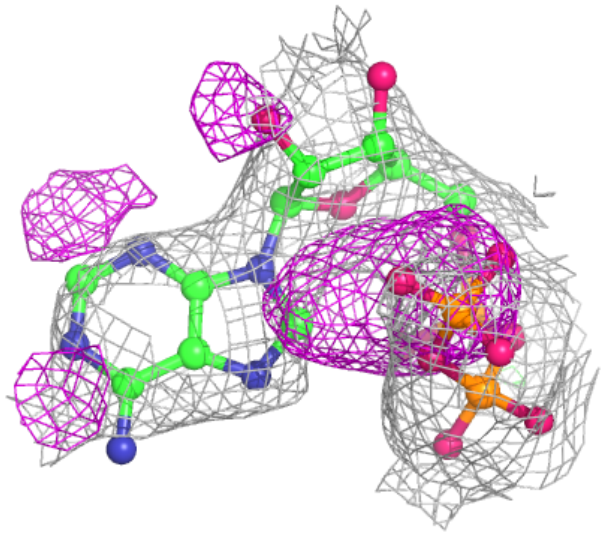


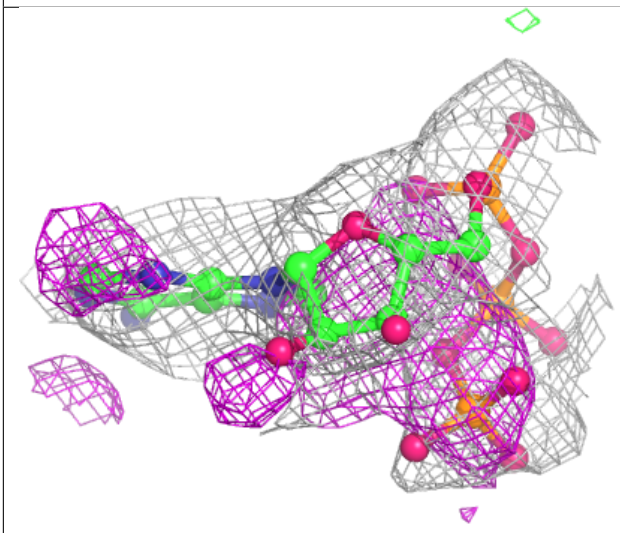


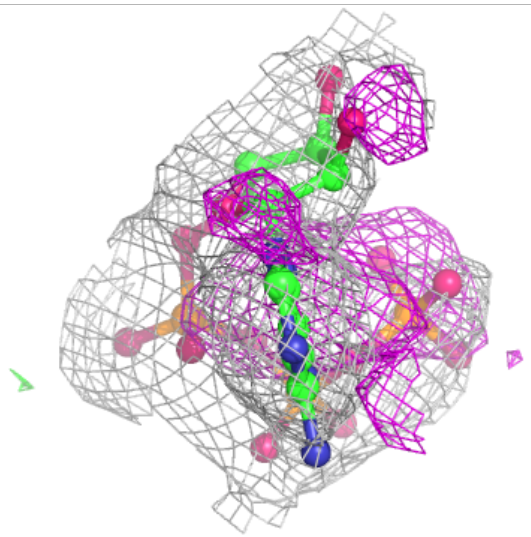


Electron density around ATP C 501:

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

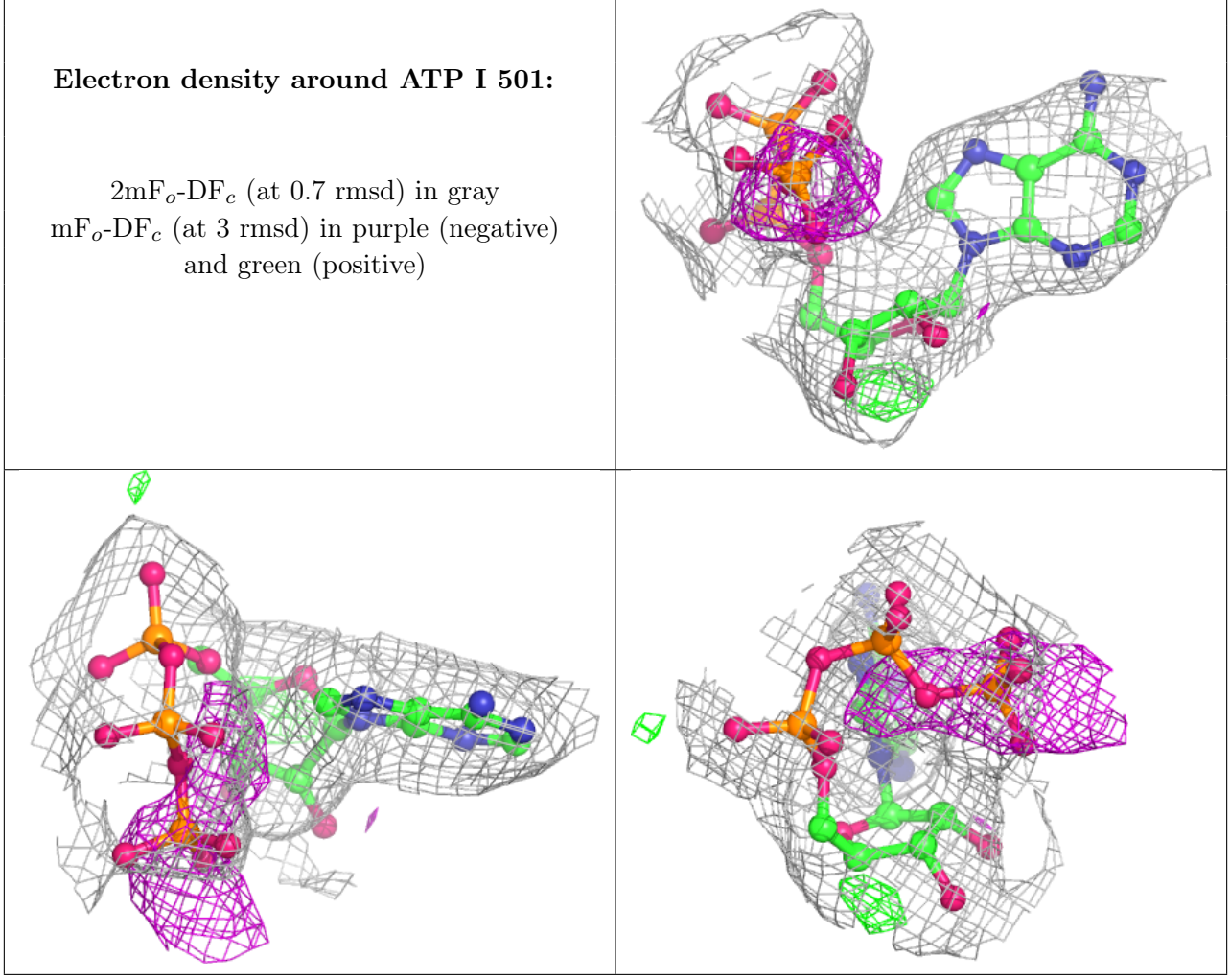






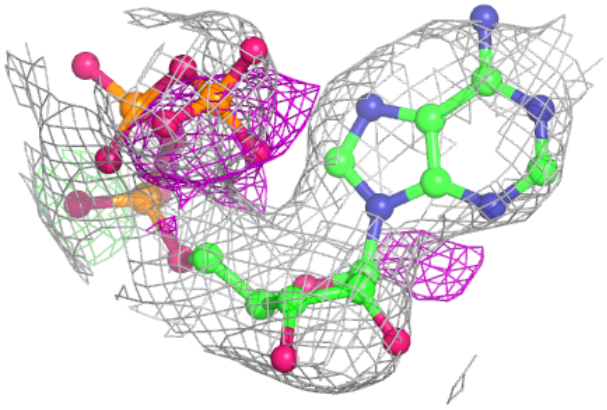
Electron density around ATP I 501:

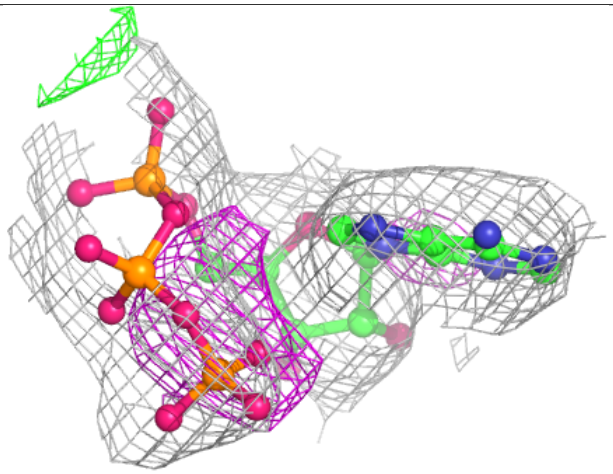
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

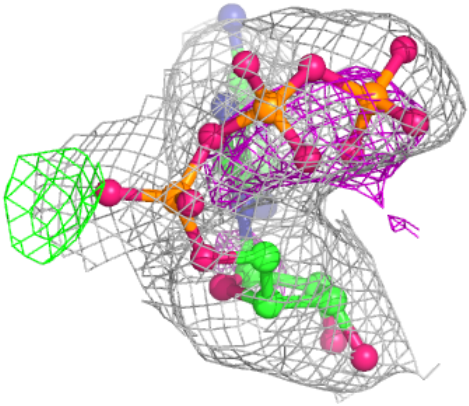


Electron density around ATP J 501:

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

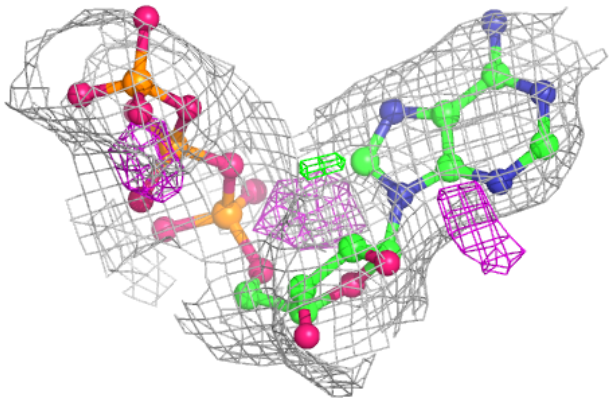


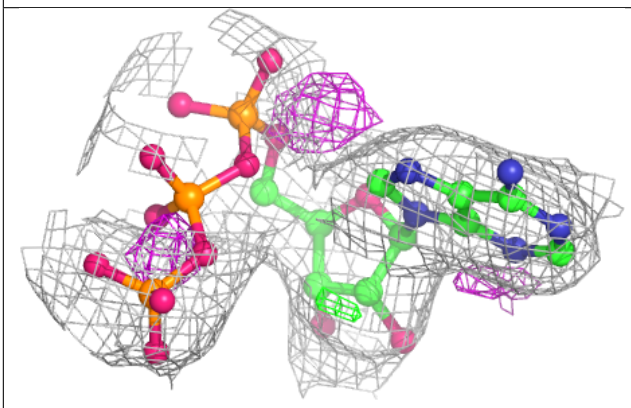


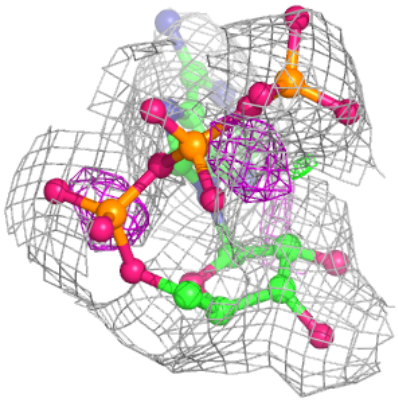


Electron density around ATP G 501:

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

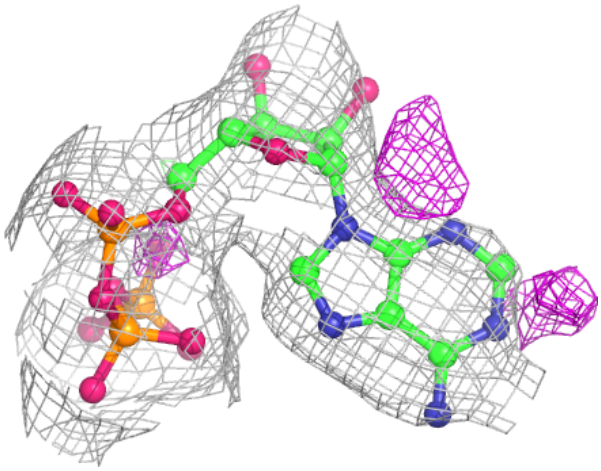


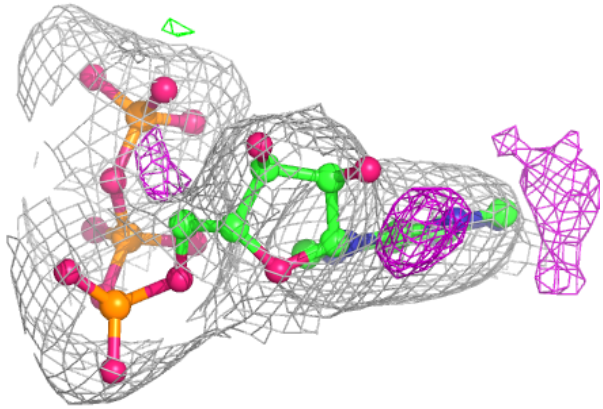


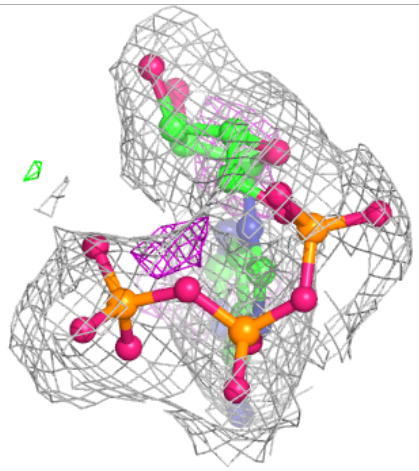


Electron density around ATP L 501:

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

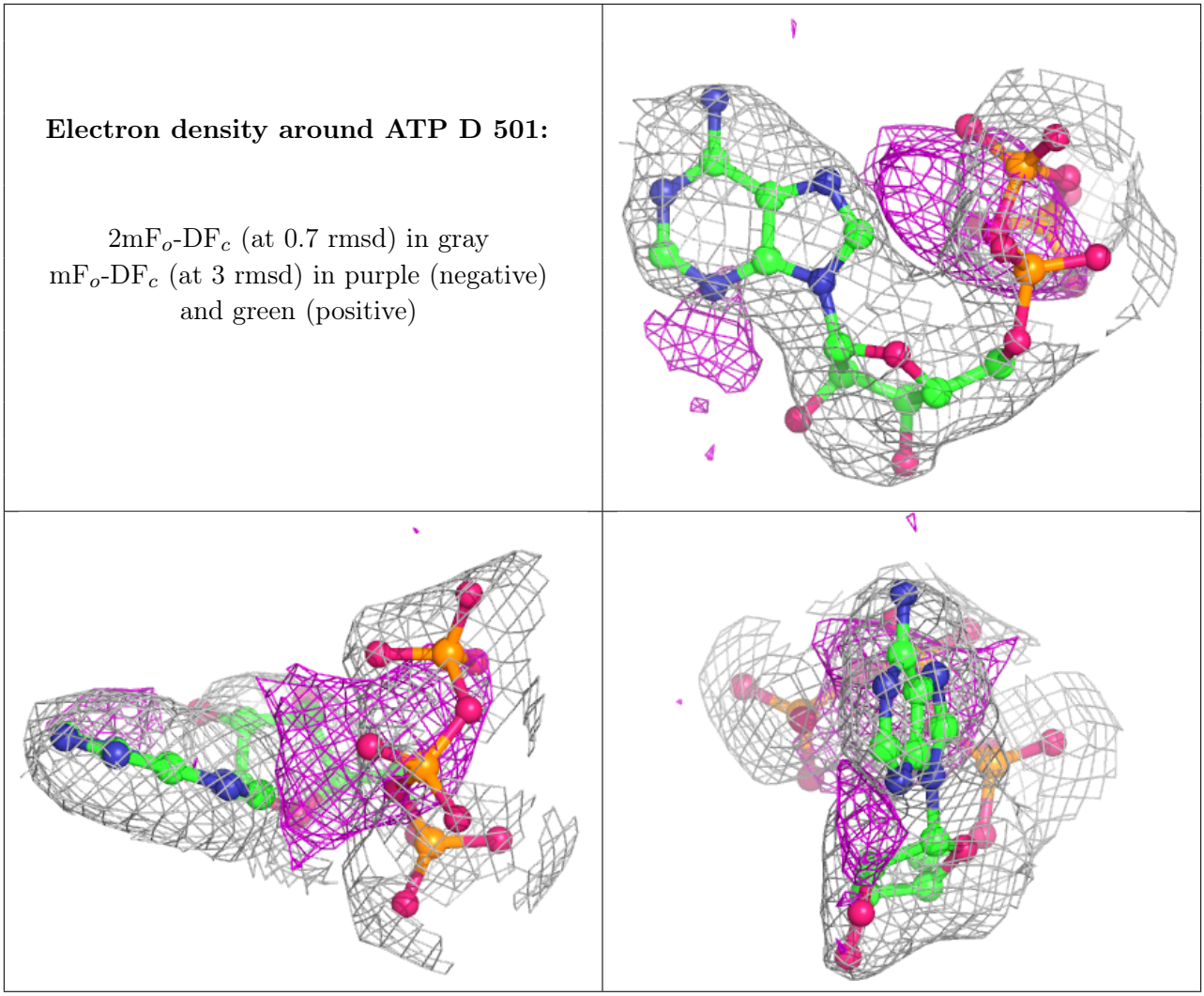






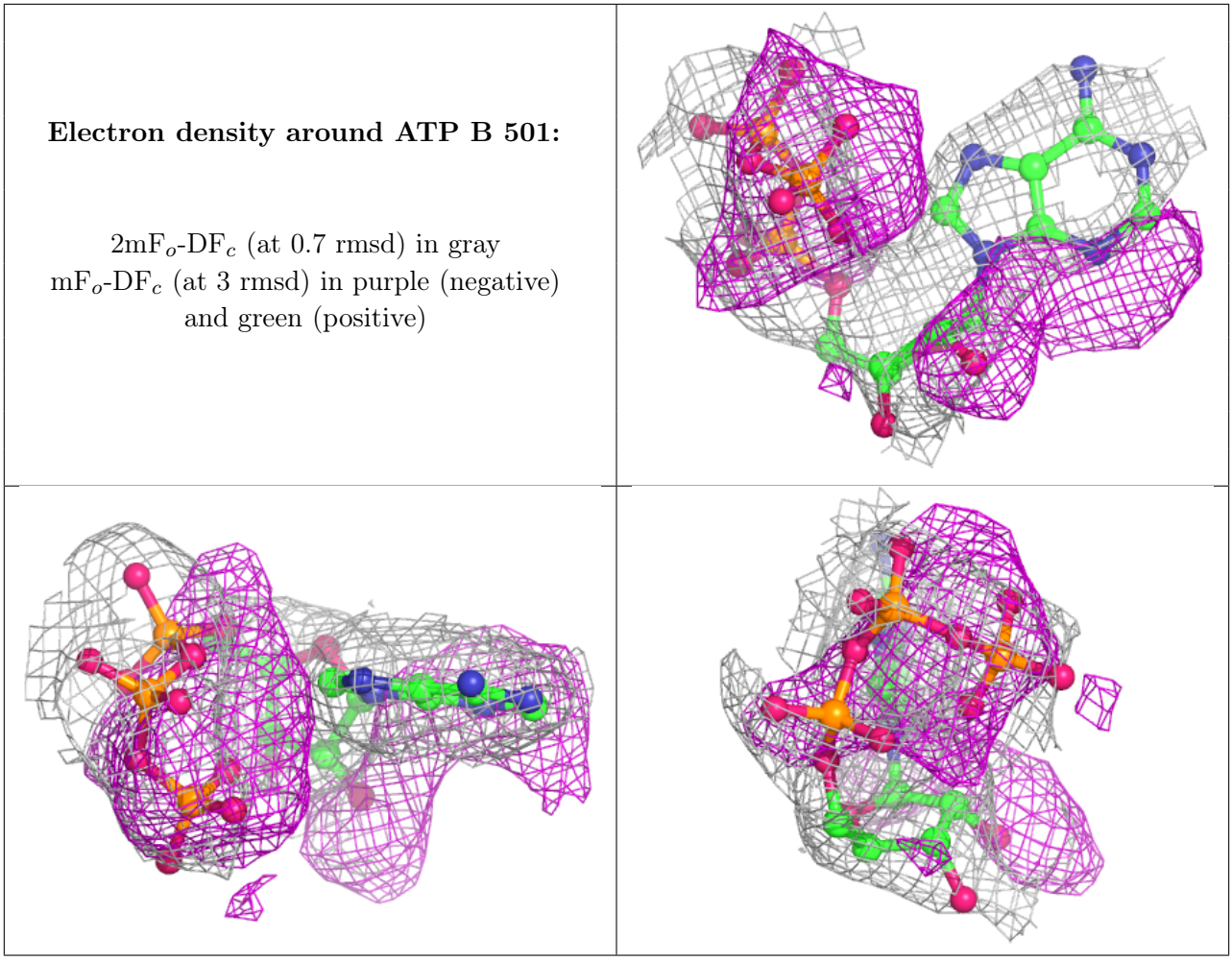
Electron density around ATP D 501:

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



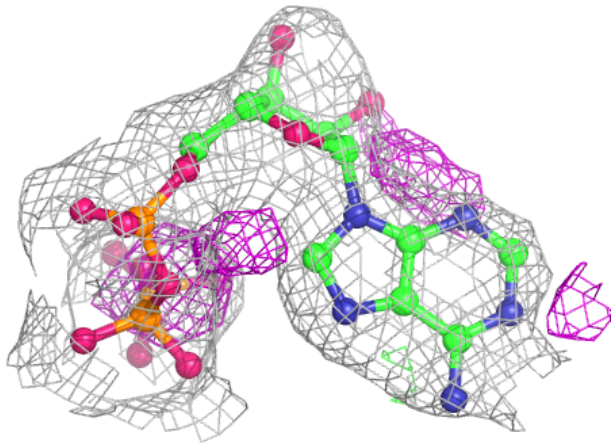
Electron density around ATP B 501:

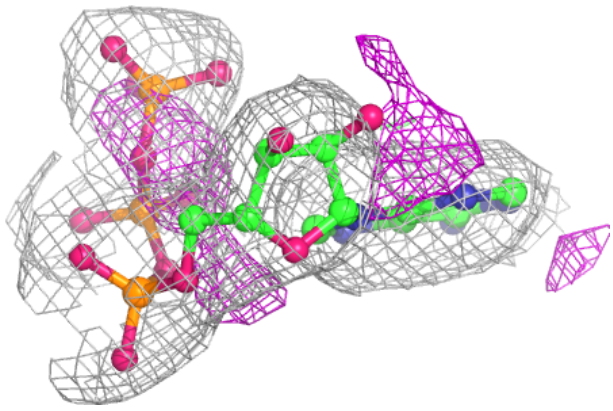
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

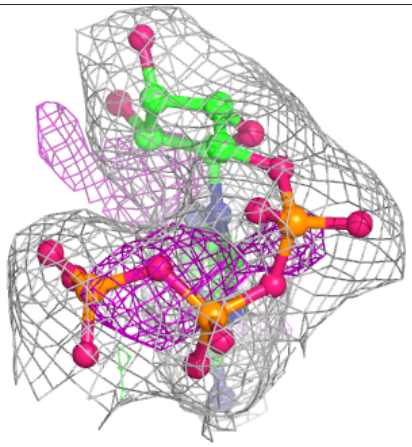


Electron density around ATP E 501:

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

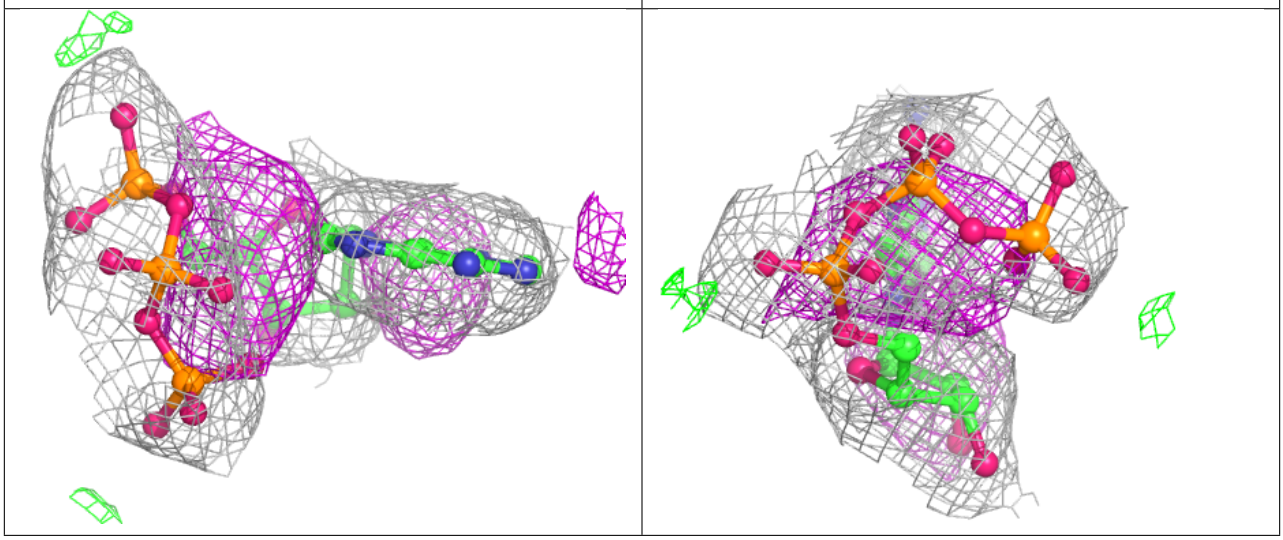






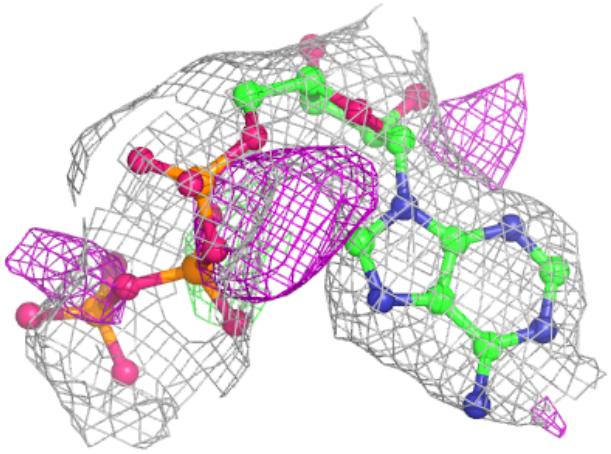
Electron density around ATP A 501:

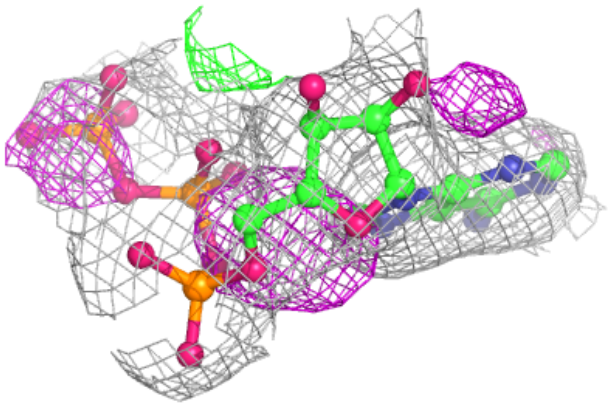
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

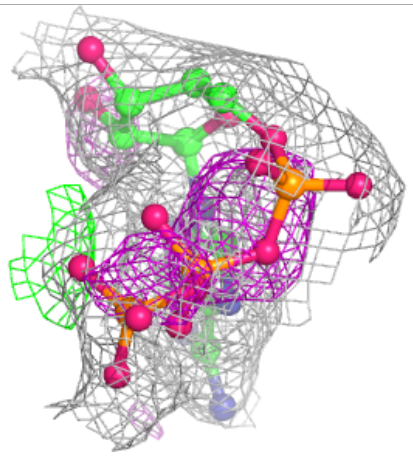


Electron density around ATP K 501:

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

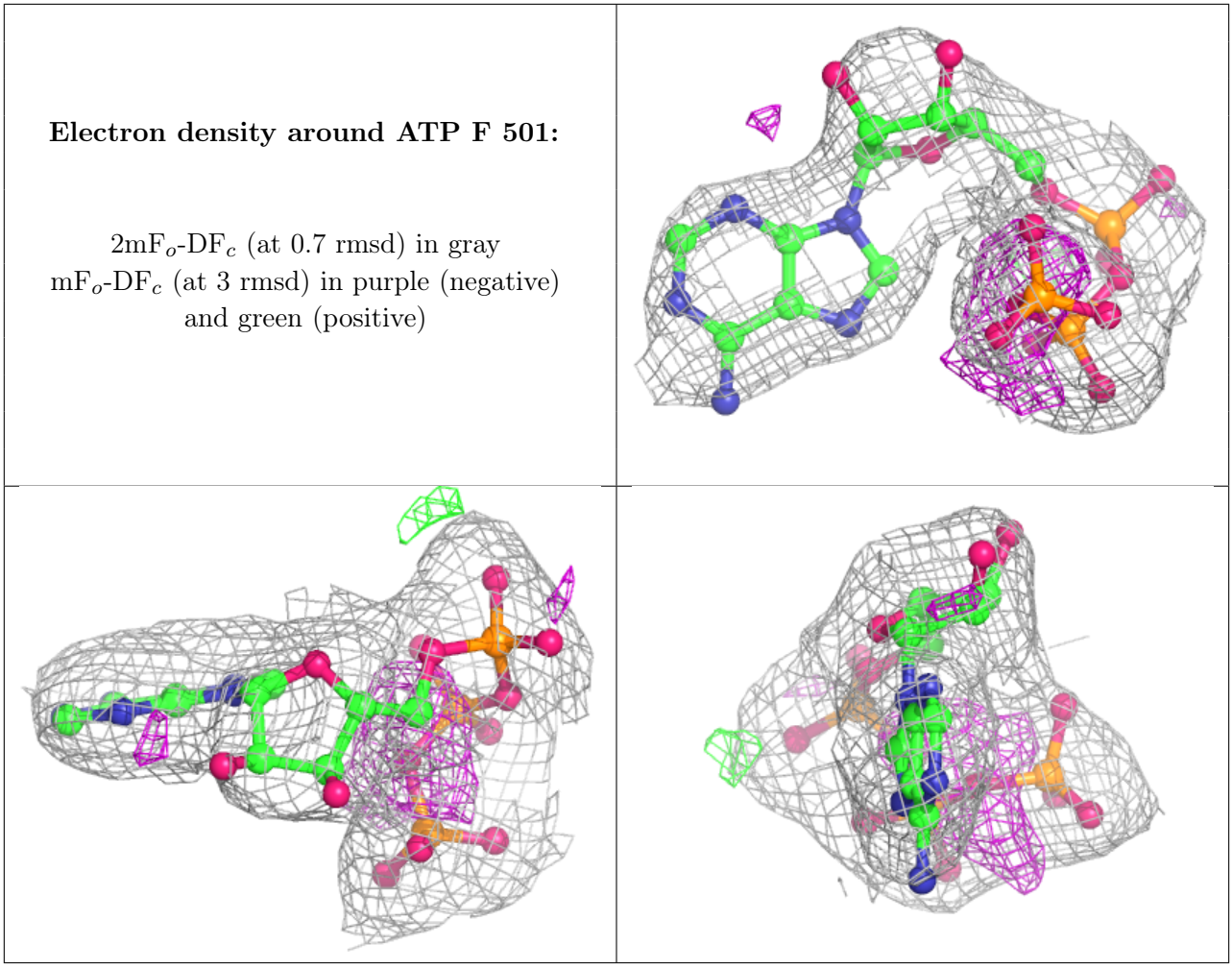






Electron density around ATP F 501:

$2mF_o$-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.