



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2021 – 12:09 PM JST

PDB ID : 7CVH
Title : Human Fructose-1,6-bisphosphatase 1 in complex with geranylgeranyl diphosphate
Authors : Chen, Y.; Zhang, J.; Li, C.; Cao, Y.
Deposited on : 2020-08-26
Resolution : 2.09 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
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) : 2.23.1

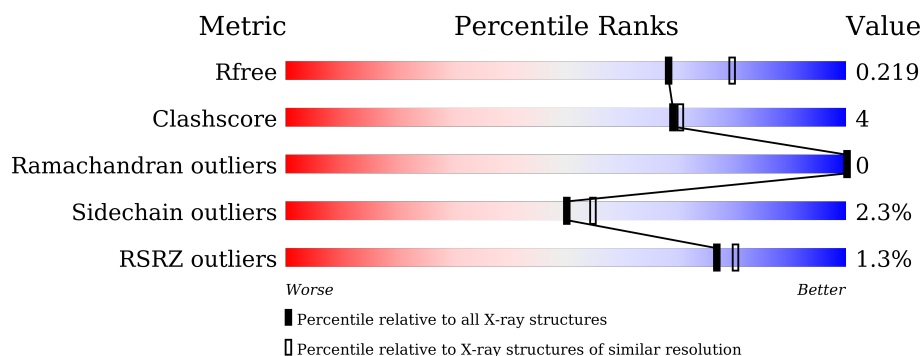
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	338	<div> <div>87%</div> <div>7% • 6%</div> </div>
1	B	338	<div> <div>84%</div> <div>10% 6%</div> </div>
1	C	338	<div> <div>84%</div> <div>9% • 6%</div> </div>
1	D	338	<div> <div>90%</div> <div>5% 5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GRG	D	601[A]	-	-	-	X
5	GRG	D	601[B]	-	-	-	X

2 Entry composition [i](#)

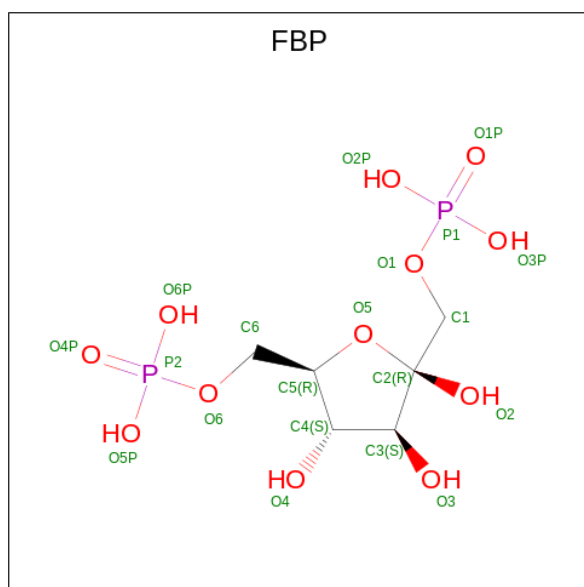
There are 6 unique types of molecules in this entry. The entry contains 11079 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fructose-1,6-bisphosphatase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2443	1556	411	459	17			
1	C	318	Total	C	N	O	S	5	1	0
			2437	1554	410	456	17			
1	B	319	Total	C	N	O	S	0	0	0
			2443	1556	411	459	17			
1	D	322	Total	C	N	O	S	0	1	0
			2464	1568	415	463	18			

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (three-letter code: FBP) (formula: $C_6H_{14}O_{12}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		

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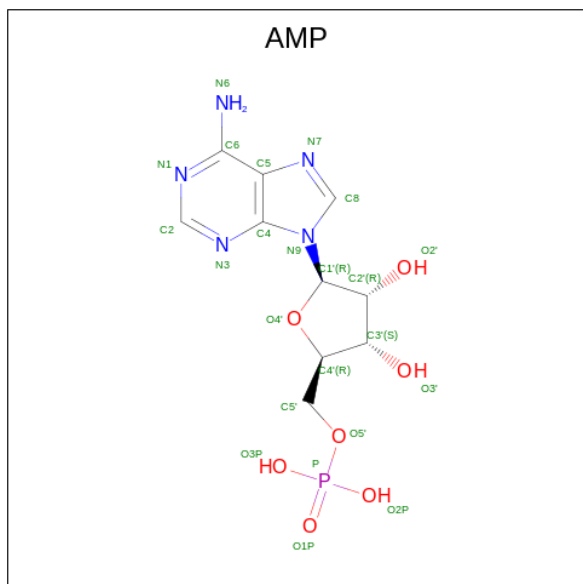
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



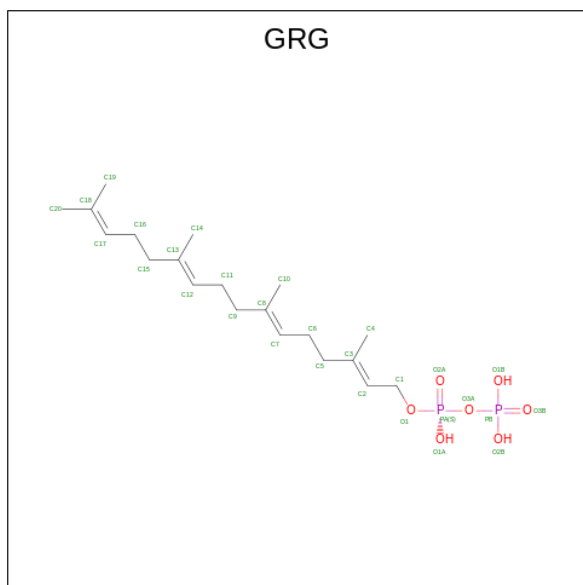
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 5 is GERANYLGERANYL DIPHOSPHATE (three-letter code: GRG) (formula: $C_{20}H_{36}O_7P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	O	P	0	1
			58	40	14	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	292	Total	O	0	0
			292	292		
6	C	252	Total	O	0	0
			252	252		
6	B	271	Total	O	0	0
			271	271		
6	D	239	Total	O	0	0
			239	239		

G1N

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.39Å 83.43Å 277.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.25 – 2.09 41.25 – 2.09	Depositor EDS
% Data completeness (in resolution range)	95.5 (41.25-2.09) 95.5 (41.25-2.09)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.178 , 0.218 0.178 , 0.219	Depositor DCC
R_{free} test set	2000 reflections (2.25%)	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11079	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FBP, AMP, MG, GRG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/2486	0.49	0/3357
1	B	0.26	0/2486	0.49	0/3357
1	C	0.26	0/2483	0.50	2/3353 (0.1%)
1	D	0.25	0/2510	0.48	0/3390
All	All	0.26	0/9965	0.49	2/13457 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	34[A]	LEU	CA-CB-CG	5.08	126.98	115.30
1	C	34[B]	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2443	0	2491	20	0
1	B	2443	0	2491	22	0
1	C	2437	0	2489	19	0
1	D	2464	0	2512	13	0
2	A	20	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	20	0	9	0	0
2	C	20	0	9	0	0
2	D	20	0	9	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	23	0	12	0	0
4	B	23	0	12	0	0
4	C	23	0	12	0	0
4	D	23	0	12	0	0
5	D	58	0	66	25	0
6	A	292	0	0	0	0
6	B	271	0	0	1	0
6	C	252	0	0	2	0
6	D	239	0	0	1	0
All	All	11079	0	10133	74	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 4.

All (74) 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:71:VAL:HG12	1:A:72:LYS:H	1.39	0.88
1:C:50:ARG:HB3	5:D:601[A]:GRG:H12	1.63	0.81
1:B:50:ARG:O	5:D:601[B]:GRG:H141	1.86	0.75
1:B:50:ARG:HB3	5:D:601[B]:GRG:H12	1.70	0.74
5:D:601[A]:GRG:H162	5:D:601[A]:GRG:H111	1.70	0.73
1:C:50:ARG:HB3	5:D:601[A]:GRG:C12	2.18	0.72
1:A:192:GLY:HA3	1:B:192:GLY:HA3	1.71	0.71
1:C:50:ARG:O	5:D:601[A]:GRG:H141	1.95	0.65
1:C:189:PRO:HB2	5:D:601[A]:GRG:HC62	1.79	0.65
1:D:189:PRO:HB3	5:D:601[B]:GRG:H191	1.79	0.65
1:B:50:ARG:HB3	5:D:601[B]:GRG:C12	2.31	0.60
1:B:268:ASN:OD1	1:B:271:SER:N	2.36	0.59
1:D:189:PRO:HG3	5:D:601[B]:GRG:H12	1.85	0.59
1:A:189:PRO:HB3	5:D:601[A]:GRG:H191	1.85	0.58
1:A:109:GLU:H	1:A:109:GLU:CD	2.09	0.56
1:C:30:GLU:OE2	1:C:113:LYS:HG3	2.05	0.56
1:A:205:LYS:HE3	1:A:323:ASP:OD2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:SER:HA	1:A:127:ILE:HD12	1.87	0.56
1:D:258:VAL:HG12	1:D:259:TYR:CD1	2.42	0.55
1:B:205:LYS:HE3	1:B:323:ASP:OD2	2.06	0.55
1:C:192:GLY:HA3	1:D:192:GLY:HA3	1.89	0.55
1:A:187:LEU:HD21	5:D:601[A]:GRG:H193	1.87	0.55
1:A:50:ARG:HE	5:D:601[A]:GRG:H161	1.74	0.53
1:C:110:LYS:HE2	1:D:10:ASP:OD2	2.07	0.53
1:C:147:GLU:OE2	6:C:501:HOH:O	2.19	0.53
1:A:187:LEU:CD2	5:D:601[A]:GRG:H193	2.40	0.52
1:D:187:LEU:CD2	5:D:601[B]:GRG:H193	2.38	0.52
1:B:11:VAL:HG11	1:D:60:ILE:HA	1.92	0.52
5:D:601[B]:GRG:C11	5:D:601[B]:GRG:H162	2.40	0.52
1:C:197:VAL:HG23	1:C:198:ASP:OD2	2.10	0.52
1:A:71:VAL:HG12	1:A:72:LYS:N	2.19	0.52
1:A:189:PRO:HG3	5:D:601[A]:GRG:H12	1.92	0.51
1:D:268:ASN:OD1	1:D:271:SER:N	2.37	0.51
1:A:278:LEU:HD23	1:A:308:PRO:HB3	1.94	0.50
1:D:327:GLU:HA	1:D:330:LYS:HE3	1.92	0.50
1:C:122:ASP:OD2	1:C:250:VAL:HG23	2.12	0.50
1:B:217:ALA:HA	1:B:220:PHE:CD2	2.47	0.50
1:A:71:VAL:CG1	1:A:72:LYS:H	2.19	0.50
1:B:329:LEU:O	1:B:333:GLU:HG3	2.12	0.49
1:A:149:SER:OG	1:A:151:LYS:HD2	2.13	0.49
1:B:278:LEU:HD23	1:B:308:PRO:HB3	1.95	0.48
1:B:124:SER:HA	1:B:127:ILE:HD11	1.95	0.48
1:C:258:VAL:HG12	1:C:259:TYR:CD1	2.49	0.48
1:B:111:ARG:HD3	1:B:148:PRO:HG3	1.94	0.48
1:D:187:LEU:HD21	5:D:601[B]:GRG:H193	1.96	0.47
1:A:50:ARG:HE	5:D:601[A]:GRG:C16	2.28	0.47
1:B:310:ASP:HB3	1:B:313:GLN:HB3	1.95	0.47
1:C:150:GLU:HG2	1:C:311:ILE:HG21	1.97	0.47
1:C:16:ARG:NH2	6:C:505:HOH:O	2.41	0.46
1:C:217:ALA:HA	1:C:220:PHE:CD2	2.51	0.45
1:B:124:SER:O	1:B:127:ILE:HD12	2.18	0.45
1:A:50:ARG:HD2	1:C:170:SER:O	2.17	0.44
1:D:46:SER:OG	5:D:601[B]:GRG:H161	2.17	0.44
1:B:208:LYS:NZ	6:B:504:HOH:O	2.40	0.44
1:D:189:PRO:HB2	5:D:601[B]:GRG:HC52	1.99	0.44
1:A:236:ASP:HB2	1:A:238:SER:OG	2.18	0.44
1:B:258:VAL:HG12	1:B:259:TYR:CD1	2.53	0.44
1:C:46:SER:O	1:C:50:ARG:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:VAL:HG12	1:A:259:TYR:CD1	2.54	0.42
1:C:56:HIS:HA	1:C:60:ILE:HG22	2.01	0.42
1:B:182:VAL:HB	1:B:201:VAL:HG22	2.01	0.42
1:B:46:SER:O	1:B:50:ARG:HD3	2.19	0.42
1:A:122:ASP:OD2	1:A:250:VAL:HG23	2.20	0.42
1:B:184:CYS:HB2	1:B:198:ASP:HB2	2.01	0.42
1:B:226:GLU:OE2	1:B:334:LYS:NZ	2.33	0.42
5:D:601[A]:GRG:H162	5:D:601[A]:GRG:C11	2.46	0.42
1:A:185:PHE:HB3	1:A:194:PHE:HB3	2.01	0.42
1:B:127:ILE:HA	6:D:706:HOH:O	2.20	0.41
5:D:601[B]:GRG:H162	5:D:601[B]:GRG:H111	2.02	0.41
1:C:121:LEU:HD12	1:C:121:LEU:HA	1.92	0.41
1:D:172:THR:H	5:D:601[B]:GRG:H143	1.86	0.41
5:D:601[B]:GRG:HC61	5:D:601[B]:GRG:H101	1.36	0.41
1:C:103:ALA:CB	1:C:150:GLU:HG3	2.50	0.41
1:B:329:LEU:HD23	1:B:329:LEU:HA	1.98	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	315/338 (93%)	313 (99%)	2 (1%)	0	100	100
1	B	315/338 (93%)	312 (99%)	3 (1%)	0	100	100
1	C	315/338 (93%)	315 (100%)	0	0	100	100
1	D	319/338 (94%)	316 (99%)	3 (1%)	0	100	100
All	All	1264/1352 (94%)	1256 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	266/281 (95%)	262 (98%)	4 (2%)	65	71
1	B	266/281 (95%)	260 (98%)	6 (2%)	50	55
1	C	265/281 (94%)	254 (96%)	11 (4%)	30	30
1	D	269/281 (96%)	263 (98%)	6 (2%)	52	57
All	All	1066/1124 (95%)	1039 (98%)	27 (2%)	50	52

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LYS
1	A	151	LYS
1	A	265	TYR
1	A	277	ARG
1	C	34[A]	LEU
1	C	34[B]	LEU
1	C	39	CYS
1	C	50	ARG
1	C	143	LYS
1	C	151	LYS
1	C	174	LEU
1	C	179	ASP
1	C	265	TYR
1	C	300	LYS
1	C	336	SER
1	B	10	ASP
1	B	26	ARG
1	B	50	ARG
1	B	125	SER
1	B	179	ASP
1	B	221	ASP
1	D	39[A]	CYS
1	D	39[B]	CYS
1	D	70	GLN

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Mol	Chain	Res	Type
1	D	75	ASP
1	D	179	ASP
1	D	265	TYR

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

Mol	Chain	Res	Type
1	C	229	GLN
1	B	126	ASN
1	D	229	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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
5	GRG	D	601[A]	-	26,28,28	1.00	1 (3%)	33,37,37	3.53	11 (33%)
4	AMP	A	404	-	22,25,25	0.89	1 (4%)	25,38,38	1.17	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FBP	C	401	3	18,20,20	3.47	6 (33%)	23,32,32	0.67	0
2	FBP	D	602	3	18,20,20	3.47	5 (27%)	23,32,32	0.70	0
2	FBP	A	401	3	18,20,20	3.46	5 (27%)	23,32,32	0.67	0
4	AMP	D	605	-	22,25,25	0.89	1 (4%)	25,38,38	1.16	2 (8%)
4	AMP	B	404	-	22,25,25	0.87	1 (4%)	25,38,38	1.20	2 (8%)
5	GRG	D	601[B]	-	26,28,28	1.16	3 (11%)	33,37,37	2.62	13 (39%)
4	AMP	C	404	-	22,25,25	0.89	1 (4%)	25,38,38	1.17	2 (8%)
2	FBP	B	401	3	18,20,20	3.47	5 (27%)	23,32,32	0.69	0

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
5	GRG	D	601[A]	-	-	13/31/31/31	-
4	AMP	A	404	-	-	0/6/26/26	0/3/3/3
2	FBP	C	401	3	-	0/13/32/32	0/1/1/1
2	FBP	D	602	3	-	4/13/32/32	0/1/1/1
2	FBP	A	401	3	-	3/13/32/32	0/1/1/1
4	AMP	D	605	-	-	0/6/26/26	0/3/3/3
4	AMP	B	404	-	-	1/6/26/26	0/3/3/3
5	GRG	D	601[B]	-	-	13/31/31/31	-
4	AMP	C	404	-	-	0/6/26/26	0/3/3/3
2	FBP	B	401	3	-	5/13/32/32	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	602	FBP	O5-C2	-8.64	1.30	1.43
2	A	401	FBP	O5-C2	-8.61	1.30	1.43
2	B	401	FBP	O5-C2	-8.57	1.30	1.43
2	C	401	FBP	O5-C2	-8.57	1.30	1.43
2	C	401	FBP	O5-C5	8.16	1.61	1.43
2	A	401	FBP	O5-C5	8.16	1.61	1.43
2	D	602	FBP	O5-C5	8.14	1.61	1.43
2	B	401	FBP	O5-C5	8.10	1.61	1.43
2	C	401	FBP	C4-C5	-6.93	1.35	1.53
2	B	401	FBP	C4-C5	-6.93	1.35	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	602	FBP	C4-C5	-6.91	1.35	1.53
2	A	401	FBP	C4-C5	-6.83	1.35	1.53
2	B	401	FBP	O3-C3	-3.24	1.36	1.42
2	C	401	FBP	O3-C3	-3.23	1.36	1.42
2	D	602	FBP	O3-C3	-3.22	1.36	1.42
2	A	401	FBP	O3-C3	-3.18	1.36	1.42
2	B	401	FBP	O4-C4	2.66	1.49	1.43
2	C	401	FBP	O4-C4	2.66	1.49	1.43
2	D	602	FBP	O4-C4	2.65	1.49	1.43
2	A	401	FBP	O4-C4	2.59	1.49	1.43
5	D	601[B]	GRG	PB-O2B	2.59	1.64	1.54
4	D	605	AMP	C5-C4	2.51	1.47	1.40
4	C	404	AMP	C5-C4	2.50	1.47	1.40
4	A	404	AMP	C5-C4	2.49	1.47	1.40
4	B	404	AMP	C5-C4	2.46	1.47	1.40
5	D	601[B]	GRG	C15-C13	2.42	1.56	1.51
5	D	601[A]	GRG	C11-C12	2.26	1.57	1.50
5	D	601[B]	GRG	PB-O1B	-2.13	1.46	1.54
2	C	401	FBP	P1-O1	2.04	1.66	1.60

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	601[A]	GRG	C10-C8-C9	-11.71	95.57	115.27
5	D	601[A]	GRG	C15-C13-C12	8.96	139.24	121.12
5	D	601[A]	GRG	C14-C13-C15	-8.02	101.78	115.27
5	D	601[B]	GRG	C6-C7-C8	-6.84	111.19	127.66
5	D	601[A]	GRG	C9-C8-C7	6.61	134.49	121.12
5	D	601[B]	GRG	C14-C13-C15	-6.51	104.33	115.27
5	D	601[B]	GRG	C15-C13-C12	6.13	133.52	121.12
5	D	601[A]	GRG	C15-C16-C17	4.42	126.41	111.88
5	D	601[B]	GRG	C15-C16-C17	4.35	126.16	111.88
5	D	601[A]	GRG	C11-C9-C8	-3.87	100.24	112.98
5	D	601[B]	GRG	C9-C11-C12	3.44	123.18	111.88
4	B	404	AMP	N3-C2-N1	-3.26	123.59	128.68
4	C	404	AMP	N3-C2-N1	-3.16	123.74	128.68
4	A	404	AMP	N3-C2-N1	-3.15	123.75	128.68
4	D	605	AMP	N3-C2-N1	-3.14	123.76	128.68
5	D	601[B]	GRG	C9-C8-C7	3.07	127.32	121.12
5	D	601[A]	GRG	C6-C7-C8	-2.98	120.49	127.66
5	D	601[A]	GRG	PA-O3A-PB	-2.81	123.17	132.83
5	D	601[B]	GRG	O1B-PB-O3B	-2.79	99.75	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	601[B]	GRG	PA-O3A-PB	-2.65	123.74	132.83
4	B	404	AMP	C4-C5-N7	-2.65	106.64	109.40
5	D	601[B]	GRG	C5-C6-C7	-2.64	103.20	111.88
4	C	404	AMP	C4-C5-N7	-2.58	106.71	109.40
4	D	605	AMP	C4-C5-N7	-2.53	106.77	109.40
5	D	601[A]	GRG	C5-C6-C7	-2.46	103.80	111.88
4	A	404	AMP	C4-C5-N7	-2.45	106.85	109.40
5	D	601[A]	GRG	C10-C8-C7	2.42	129.90	123.68
5	D	601[A]	GRG	C11-C12-C13	-2.31	122.11	127.66
5	D	601[B]	GRG	C6-C5-C3	-2.22	105.66	112.98
5	D	601[B]	GRG	O2B-PB-O3A	2.21	112.05	104.64
5	D	601[B]	GRG	C10-C8-C9	-2.13	111.69	115.27
5	D	601[B]	GRG	C11-C9-C8	-2.02	106.33	112.98

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	FBP	C6-O6-P2-O5P
2	B	401	FBP	C6-O6-P2-O6P
2	D	602	FBP	C1-O1-P1-O1P
2	D	602	FBP	C6-O6-P2-O5P
2	D	602	FBP	C6-O6-P2-O6P
5	D	601[A]	GRG	C16-C17-C18-C20
5	D	601[A]	GRG	C15-C16-C17-C18
5	D	601[A]	GRG	C1-O1-PA-O1A
5	D	601[A]	GRG	PA-O3A-PB-O2B
5	D	601[B]	GRG	C16-C17-C18-C20
5	D	601[B]	GRG	C15-C16-C17-C18
5	D	601[B]	GRG	PA-O3A-PB-O2B
5	D	601[A]	GRG	C16-C17-C18-C19
5	D	601[B]	GRG	C16-C17-C18-C19
5	D	601[A]	GRG	C12-C11-C9-C8
5	D	601[B]	GRG	C11-C12-C13-C14
5	D	601[B]	GRG	C12-C11-C9-C8
5	D	601[B]	GRG	C11-C12-C13-C15
5	D	601[B]	GRG	C13-C15-C16-C17
5	D	601[A]	GRG	C10-C8-C9-C11
5	D	601[B]	GRG	C10-C8-C9-C11
2	A	401	FBP	C1-O1-P1-O1P
2	B	401	FBP	C6-O6-P2-O4P
4	B	404	AMP	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
5	D	601[A]	GRG	C7-C8-C9-C11
5	D	601[B]	GRG	C7-C8-C9-C11
5	D	601[A]	GRG	PA-O3A-PB-O3B
5	D	601[A]	GRG	C1-O1-PA-O3A
2	B	401	FBP	C4-C5-C6-O6
5	D	601[A]	GRG	C1-O1-PA-O2A
5	D	601[B]	GRG	C3-C5-C6-C7
5	D	601[A]	GRG	C13-C15-C16-C17
2	B	401	FBP	O5-C5-C6-O6
2	A	401	FBP	C1-O1-P1-O2P
2	A	401	FBP	C6-O6-P2-O5P
2	D	602	FBP	C1-O1-P1-O2P
5	D	601[A]	GRG	O1-C1-C2-C3
5	D	601[B]	GRG	O1-C1-C2-C3
5	D	601[B]	GRG	PA-O3A-PB-O1B

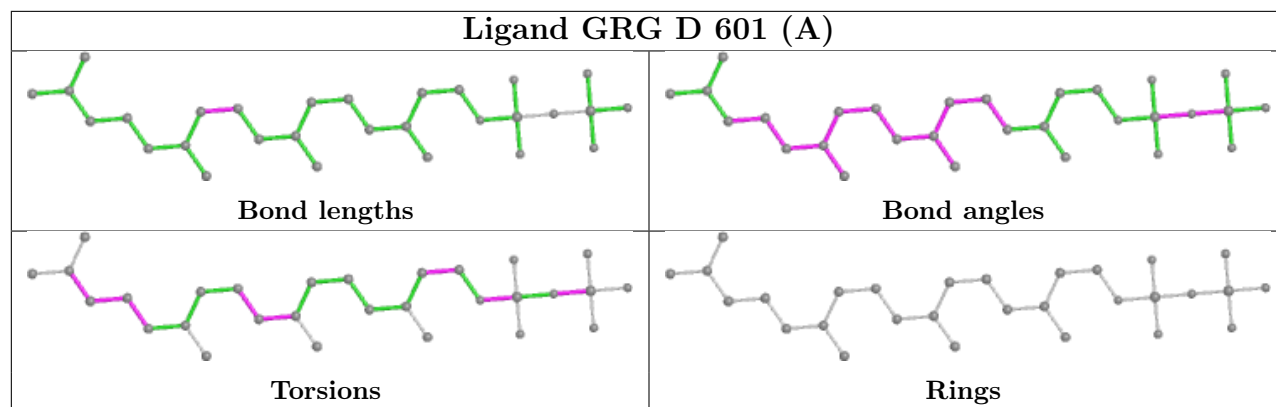
There are no ring outliers.

2 monomers are involved in 25 short contacts:

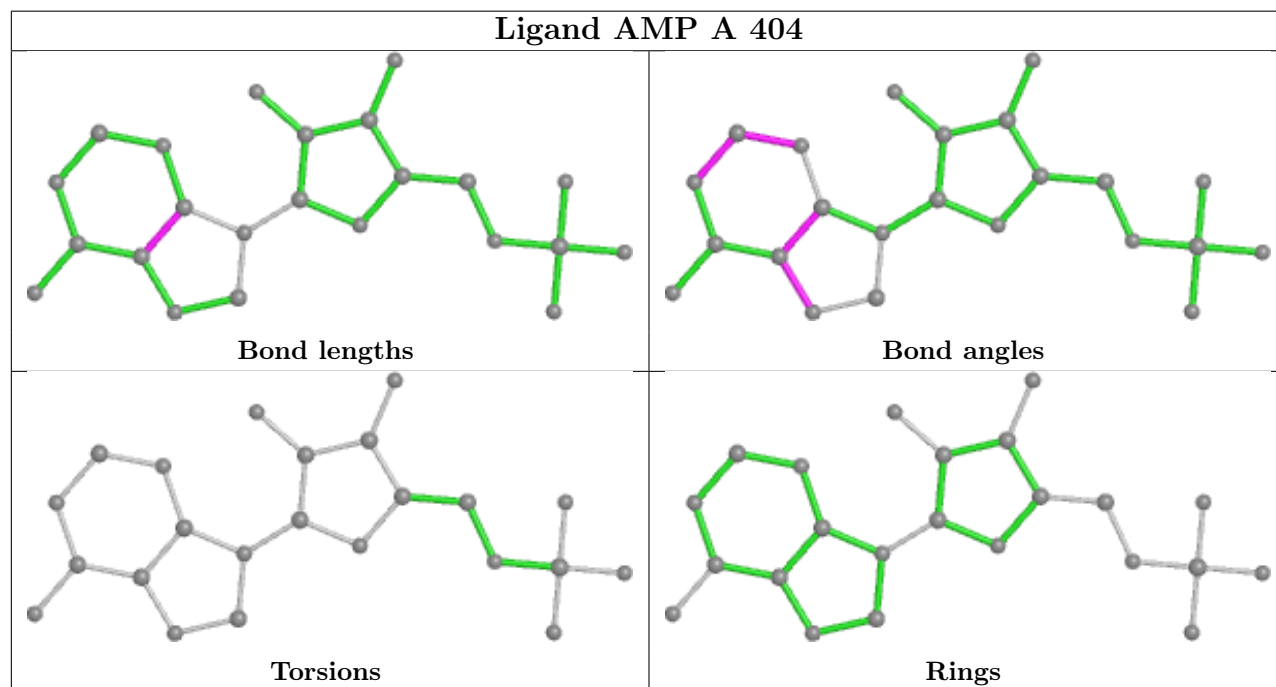
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	601[A]	GRG	12	0
5	D	601[B]	GRG	13	0

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.

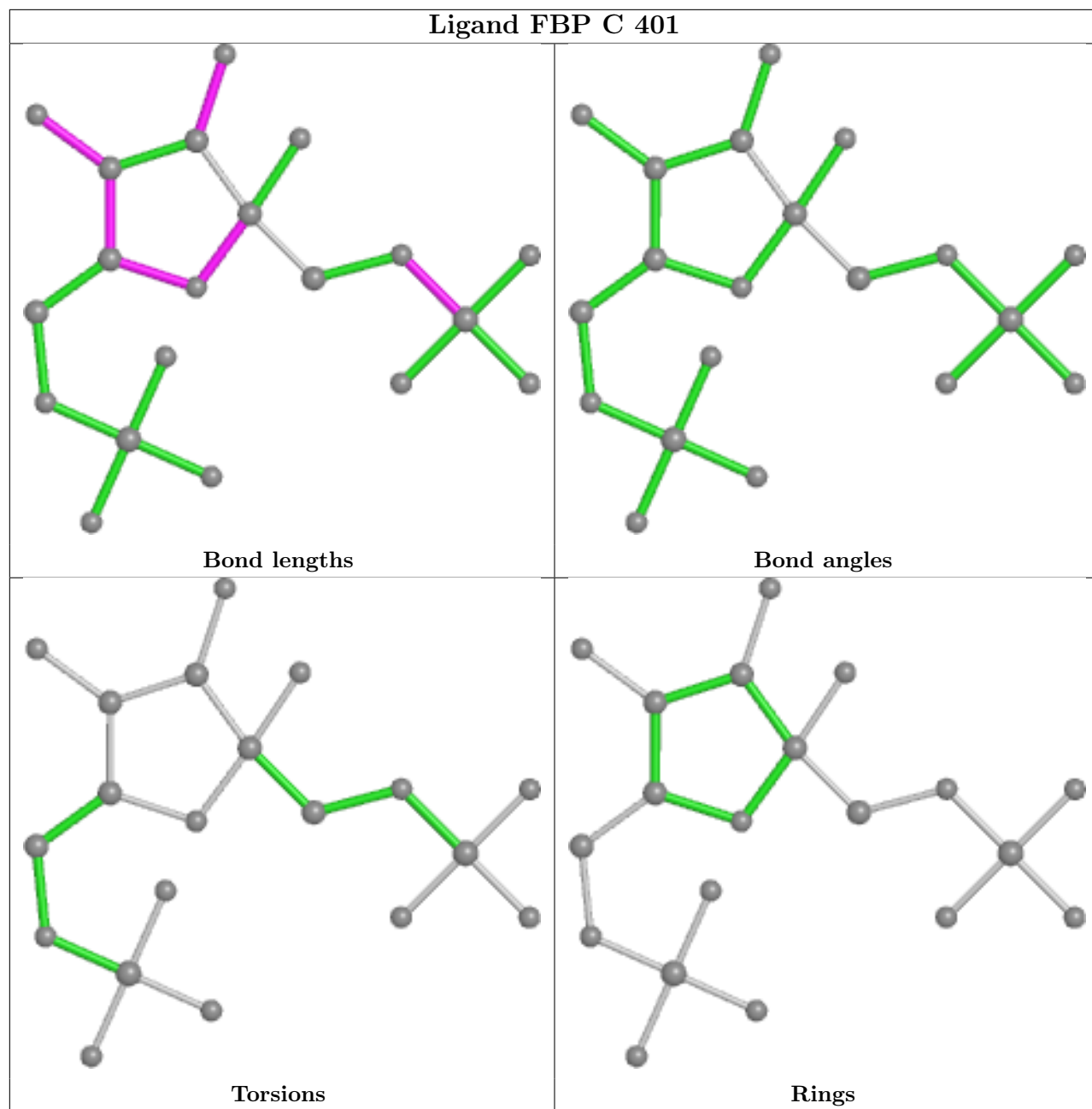
Ligand GRG D 601 (A)

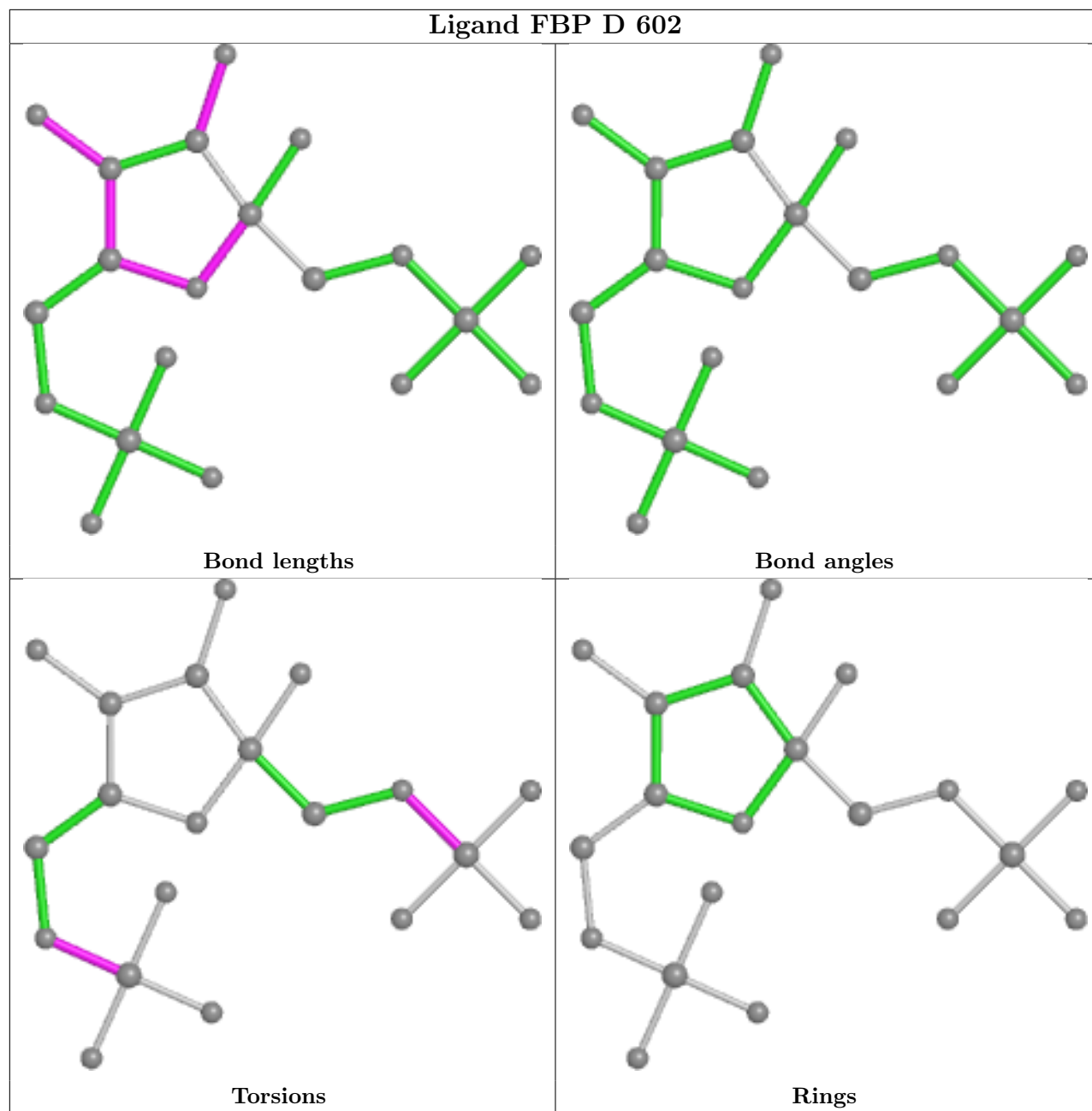


Ligand AMP A 404

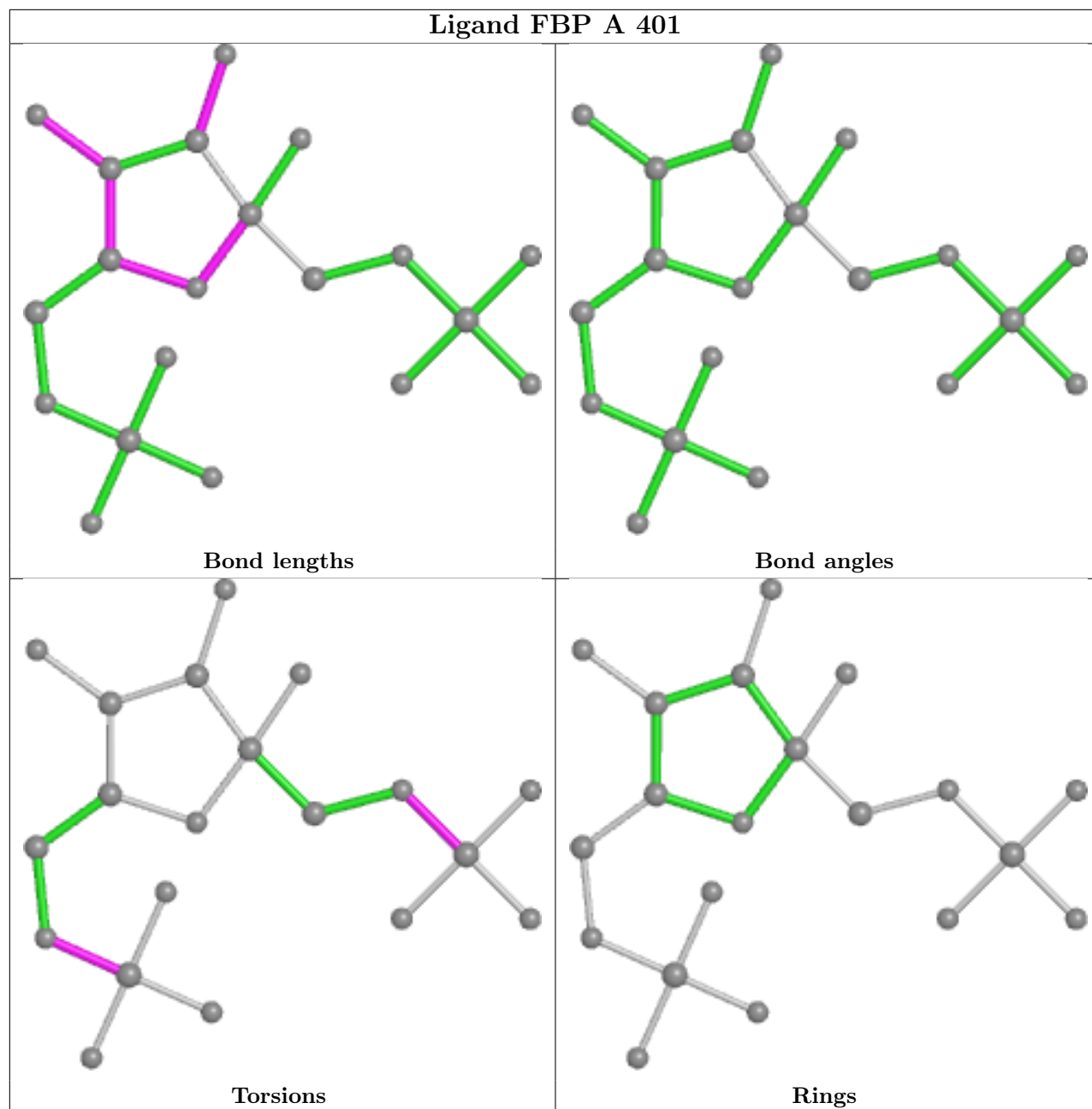


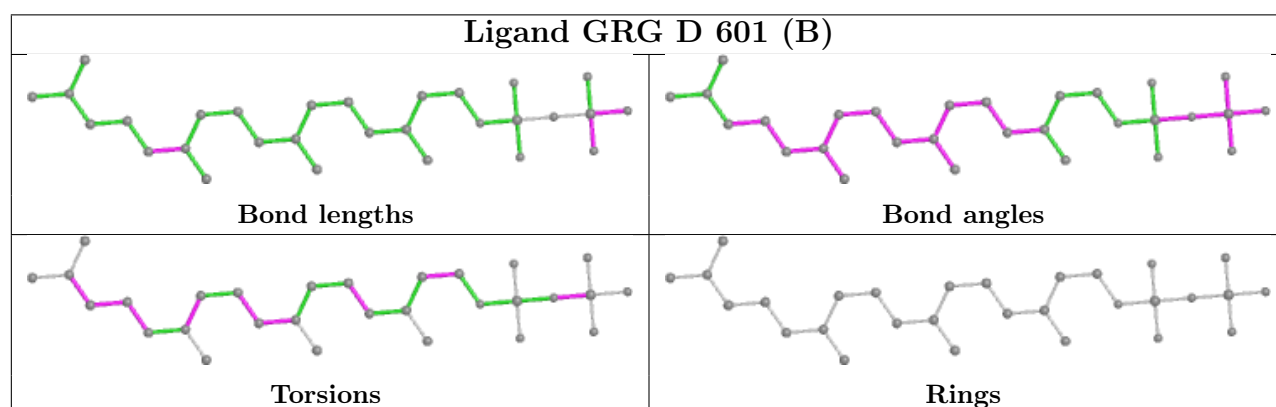
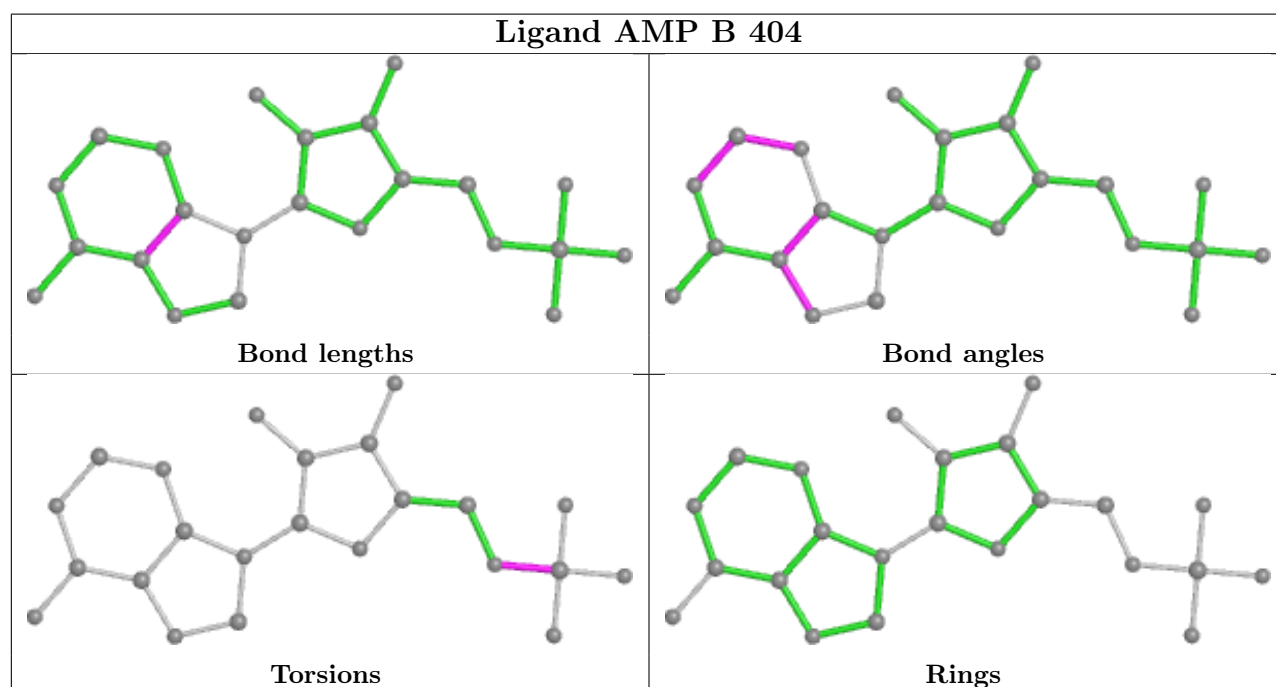
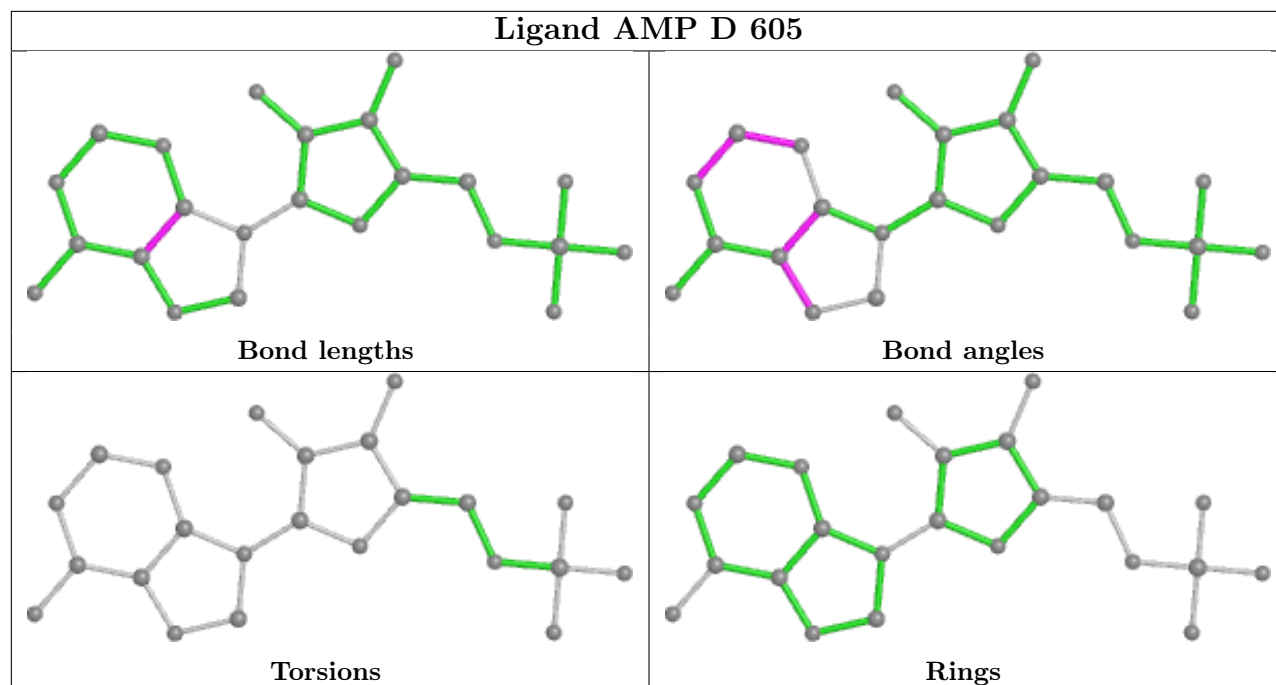
Ligand FBP C 401

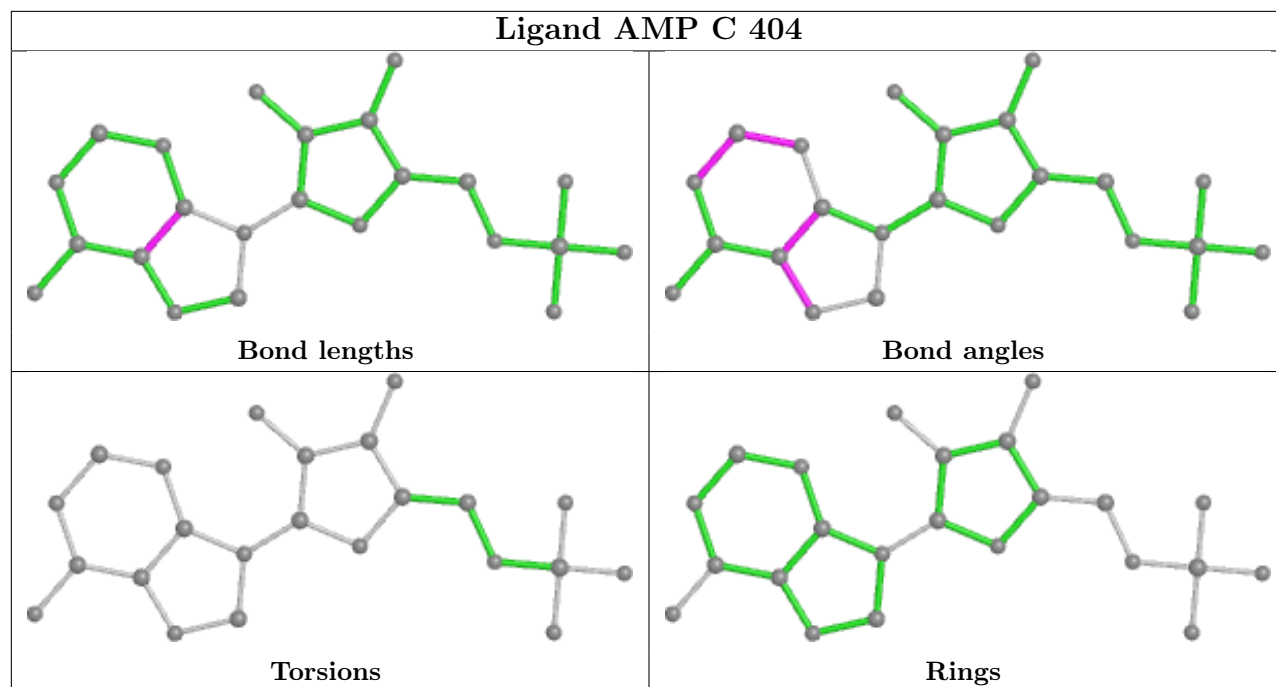


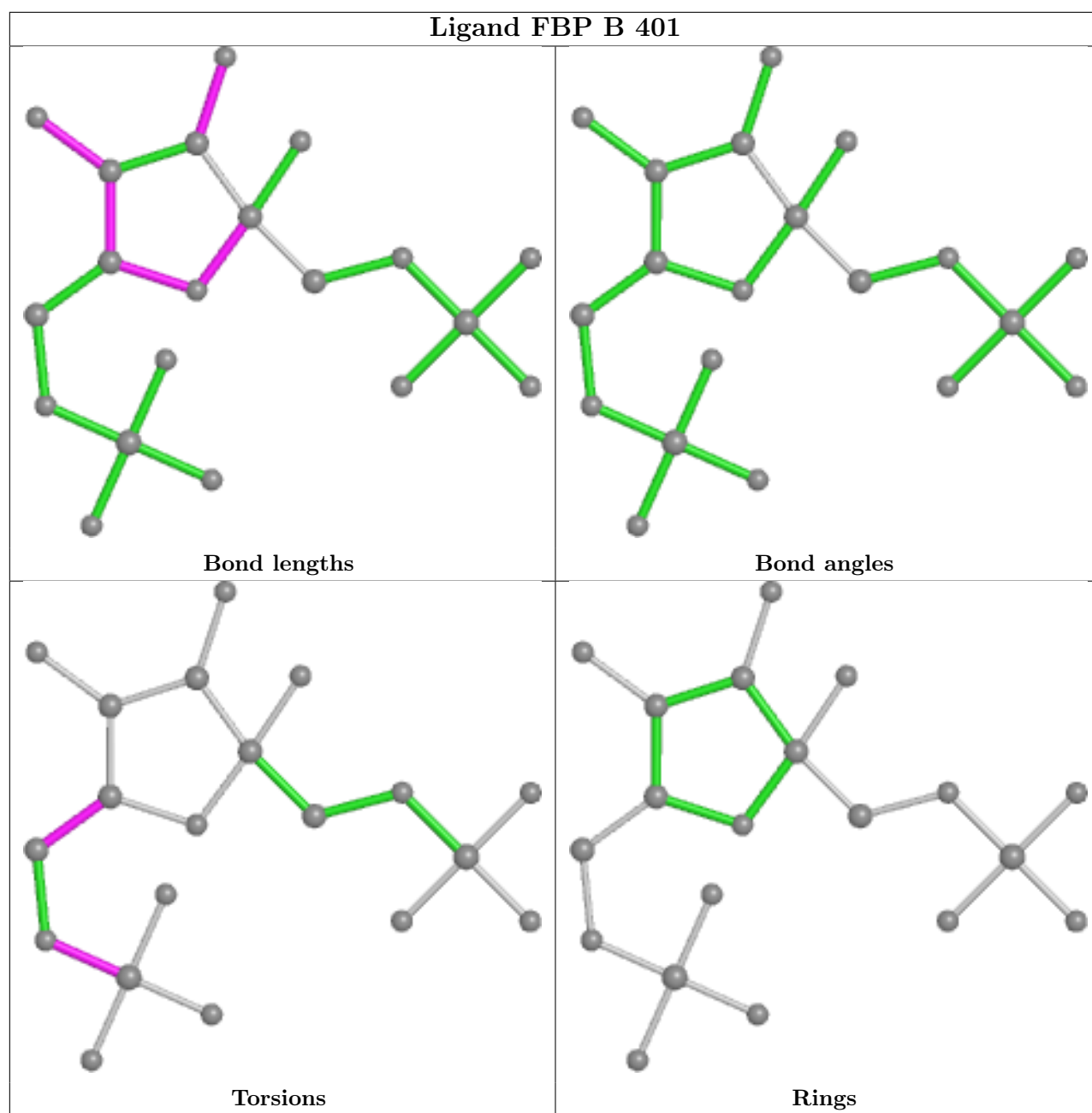


Ligand FBP A 401









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	319/338 (94%)	-0.55	2 (0%) 89 91	7, 13, 30, 64	0
1	B	319/338 (94%)	-0.41	5 (1%) 72 75	8, 16, 36, 66	0
1	C	318/338 (94%)	-0.40	2 (0%) 89 91	9, 16, 33, 72	0
1	D	322/338 (95%)	-0.25	7 (2%) 62 66	10, 20, 43, 63	0
All	All	1278/1352 (94%)	-0.40	16 (1%) 77 80	7, 16, 36, 72	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	71	VAL	5.7
1	B	269	LYS	3.7
1	B	270	LYS	3.7
1	C	237	ASN	3.6
1	B	71	VAL	3.5
1	D	237	ASN	3.5
1	D	64	THR	3.4
1	D	235	PRO	3.2
1	C	235	PRO	3.0
1	B	143	LYS	2.7
1	A	237	ASN	2.6
1	D	236	ASP	2.6
1	B	145	THR	2.5
1	D	238	SER	2.2
1	D	71	VAL	2.2
1	D	145	THR	2.1

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

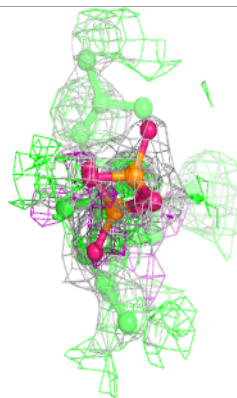
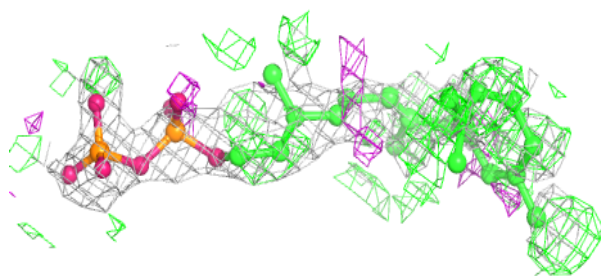
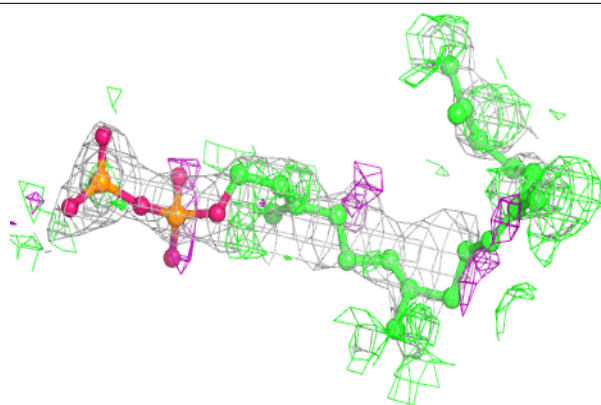
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GRG	D	601[A]	29/29	0.59	0.54	7,17,23,24	29
5	GRG	D	601[B]	29/29	0.59	0.54	9,18,23,23	29
3	MG	D	604	1/1	0.94	0.08	20,20,20,20	0
3	MG	C	402	1/1	0.96	0.10	15,15,15,15	0
3	MG	B	403	1/1	0.96	0.12	14,14,14,14	0
3	MG	D	603	1/1	0.96	0.15	18,18,18,18	0
2	FBP	C	401	20/20	0.97	0.08	13,21,34,41	0
4	AMP	C	404	23/23	0.97	0.08	14,19,24,32	0
4	AMP	B	404	23/23	0.97	0.09	12,16,19,19	0
4	AMP	D	605	23/23	0.97	0.09	15,21,25,29	0
2	FBP	B	401	20/20	0.97	0.08	14,18,25,29	0
2	FBP	D	602	20/20	0.97	0.07	14,21,29,31	0
4	AMP	A	404	23/23	0.98	0.07	10,16,19,20	0
3	MG	C	403	1/1	0.98	0.10	18,18,18,18	0
2	FBP	A	401	20/20	0.98	0.10	10,13,21,22	0
3	MG	B	402	1/1	0.99	0.11	14,14,14,14	0
3	MG	A	402	1/1	0.99	0.10	11,11,11,11	0
3	MG	A	403	1/1	1.00	0.13	6,6,6,6	0

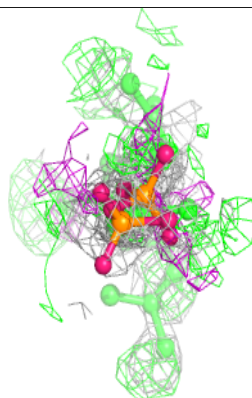
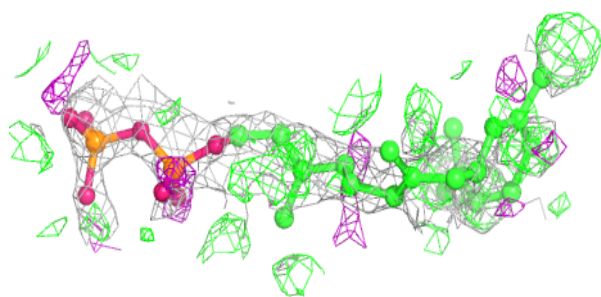
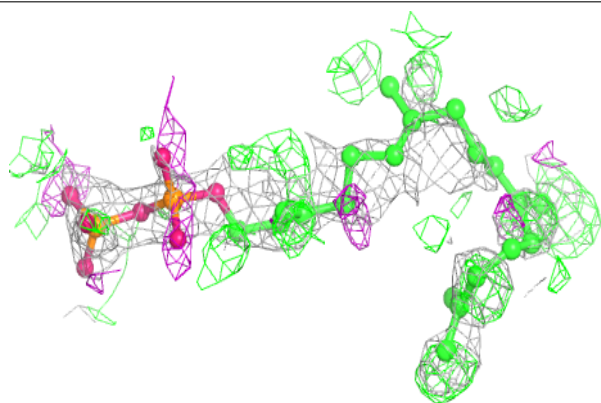
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GRG D 601 (A):

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

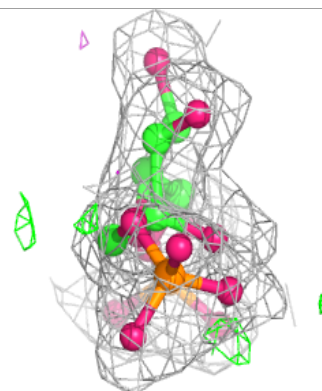
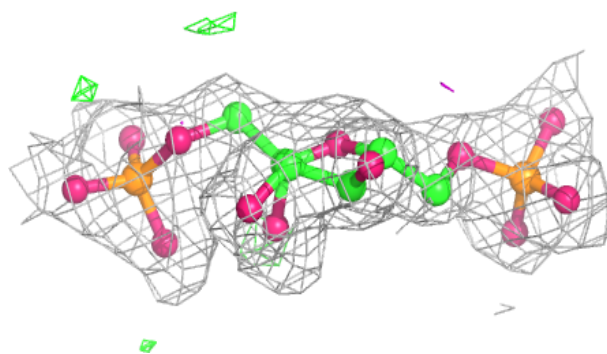
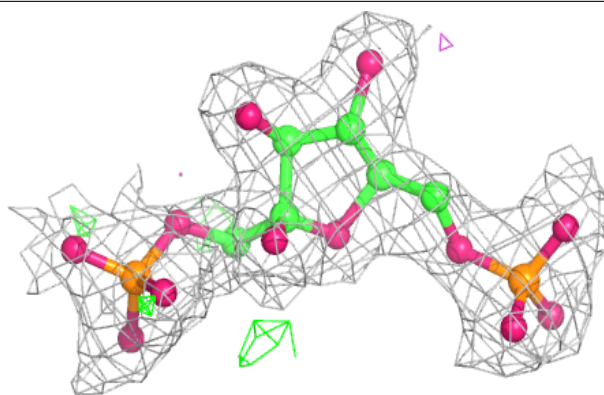
**Electron density around GRG D 601 (B):**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



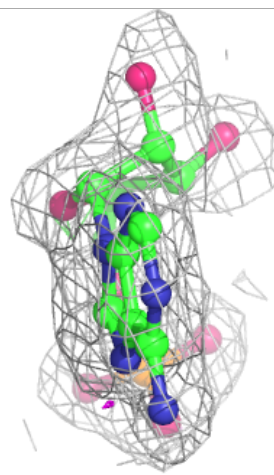
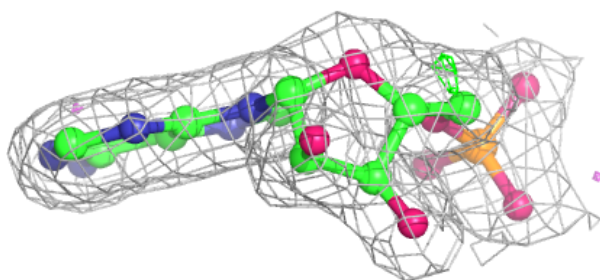
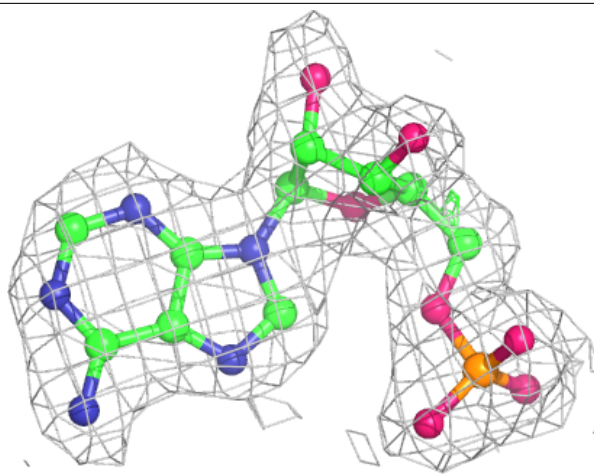
Electron density around FBP C 401:

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



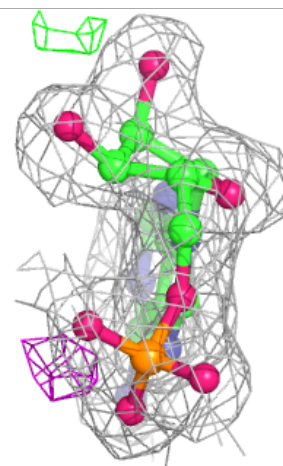
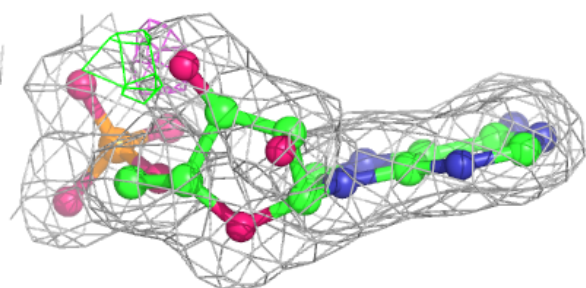
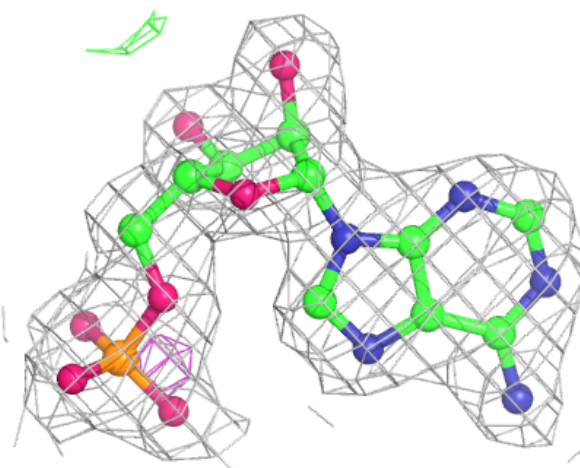
Electron density around AMP C 404:

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and green (positive)



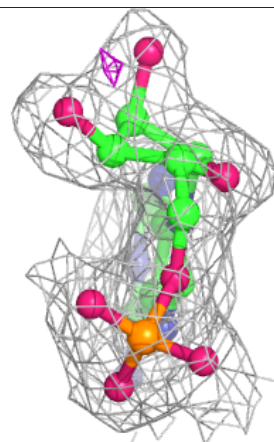
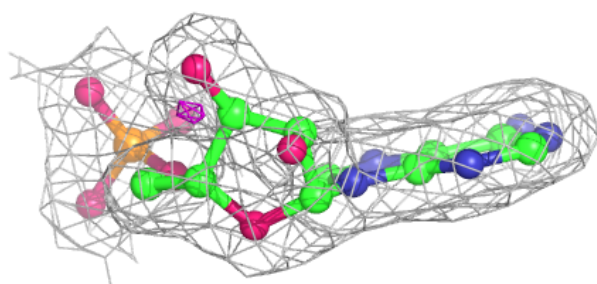
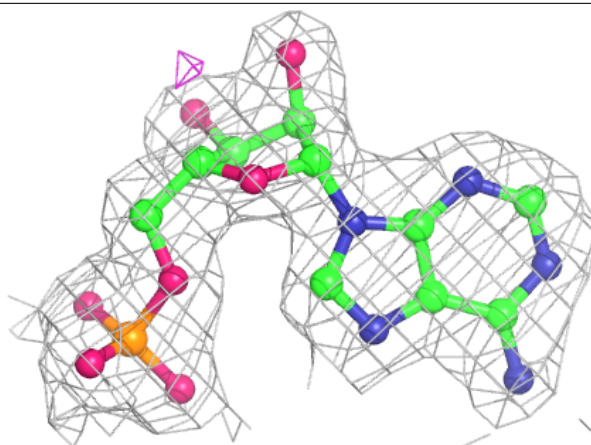
Electron density around AMP B 404:

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

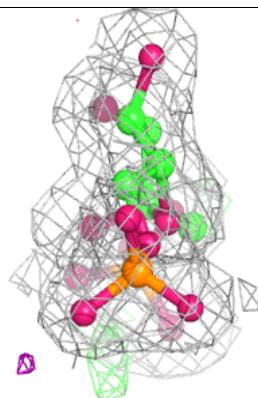
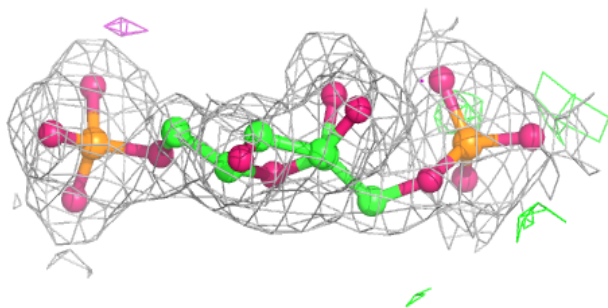
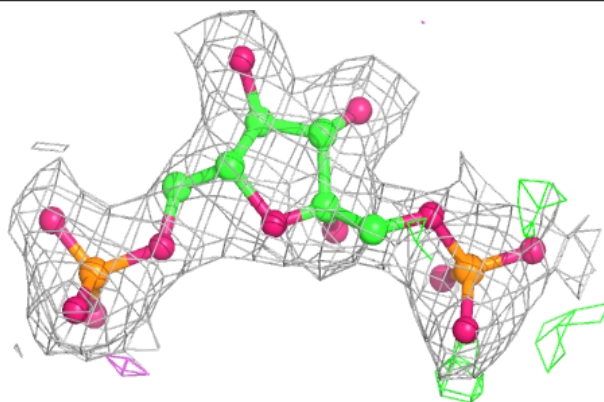


Electron density around AMP D 605:

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

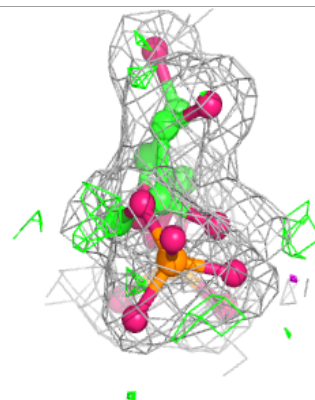
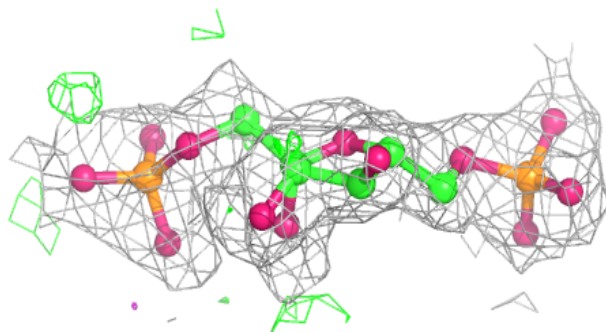
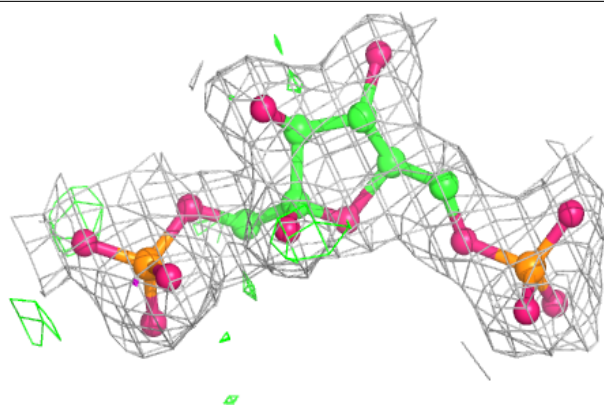
**Electron density around FBP B 401:**

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



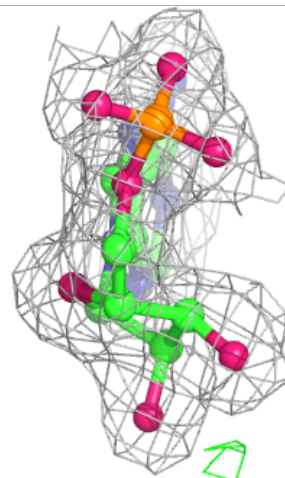
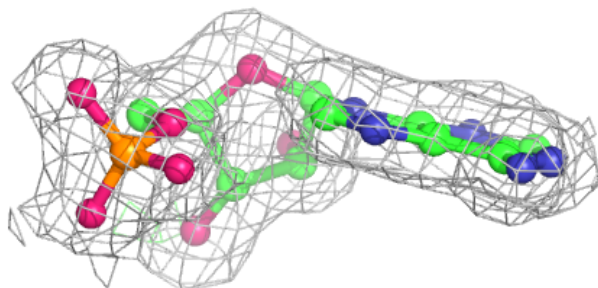
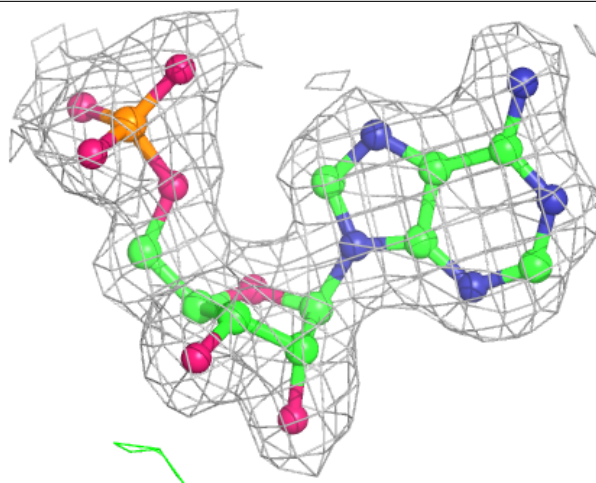
Electron density around FBP D 602:

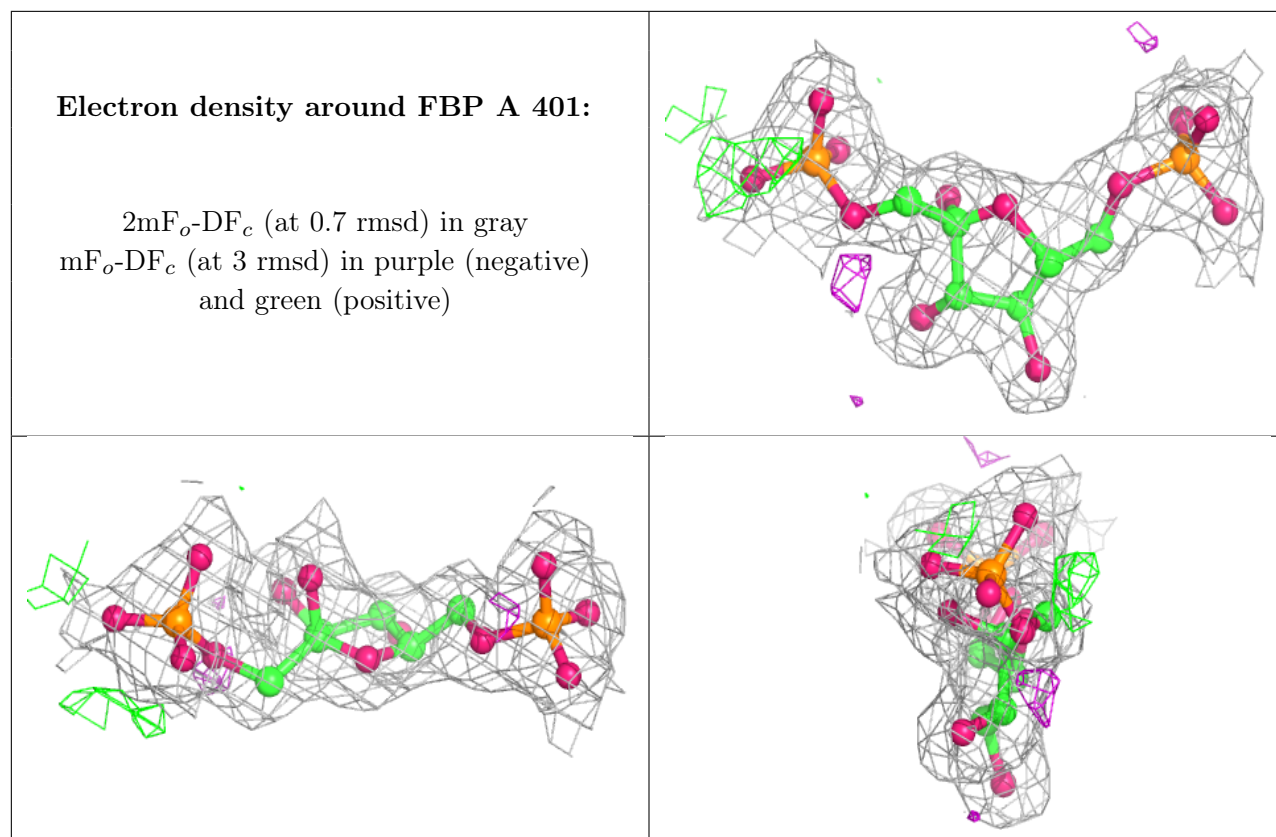
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AMP A 404:

$2mF_o-DF_c$ (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.