



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 05:16 PM BST

PDB ID : 5ZWK
Title : Crystal structure of Human liver fructose-1,6-bisphosphatase complex with fructose-1,6-bisphosphate and AMP
Authors : Yunyuan, H.; Zeyuan, G.; Junjie, Y.; Ping, Y.; Jian, W.
Deposited on : 2018-05-15
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.13.1
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) : 2.13.1

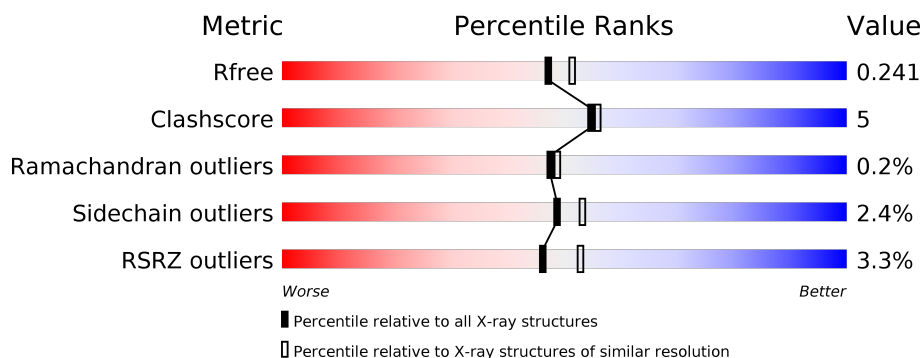
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	348	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>8%</div> </div> </div>
1	B	348	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>8%</div> </div> </div>
1	C	348	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>8%</div> </div> </div>
1	D	348	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10377 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
			2441	1556	409	459	17			
1	B	319	Total	C	N	O	S	0	0	0
			2441	1556	409	459	17			
1	C	319	Total	C	N	O	S	0	0	0
			2441	1556	409	459	17			
1	D	319	Total	C	N	O	S	0	0	0
			2441	1556	409	459	17			

There are 40 discrepancies between the modelled and reference sequences:

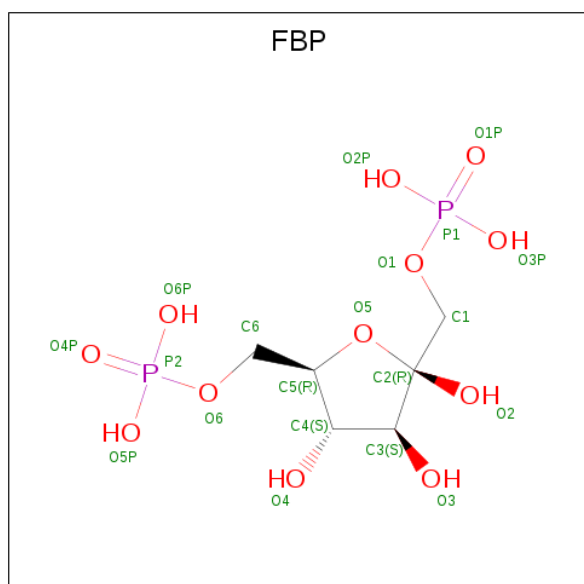
Chain	Residue	Modelled	Actual	Comment	Reference
A	338	LEU	-	expression tag	UNP Q2TU34
A	339	GLU	-	expression tag	UNP Q2TU34
A	340	HIS	-	expression tag	UNP Q2TU34
A	341	HIS	-	expression tag	UNP Q2TU34
A	342	HIS	-	expression tag	UNP Q2TU34
A	343	HIS	-	expression tag	UNP Q2TU34
A	344	HIS	-	expression tag	UNP Q2TU34
A	345	HIS	-	expression tag	UNP Q2TU34
A	346	HIS	-	expression tag	UNP Q2TU34
A	347	HIS	-	expression tag	UNP Q2TU34
B	338	LEU	-	expression tag	UNP Q2TU34
B	339	GLU	-	expression tag	UNP Q2TU34
B	340	HIS	-	expression tag	UNP Q2TU34
B	341	HIS	-	expression tag	UNP Q2TU34
B	342	HIS	-	expression tag	UNP Q2TU34
B	343	HIS	-	expression tag	UNP Q2TU34
B	344	HIS	-	expression tag	UNP Q2TU34
B	345	HIS	-	expression tag	UNP Q2TU34
B	346	HIS	-	expression tag	UNP Q2TU34
B	347	HIS	-	expression tag	UNP Q2TU34
C	338	LEU	-	expression tag	UNP Q2TU34

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	339	GLU	-	expression tag	UNP Q2TU34
C	340	HIS	-	expression tag	UNP Q2TU34
C	341	HIS	-	expression tag	UNP Q2TU34
C	342	HIS	-	expression tag	UNP Q2TU34
C	343	HIS	-	expression tag	UNP Q2TU34
C	344	HIS	-	expression tag	UNP Q2TU34
C	345	HIS	-	expression tag	UNP Q2TU34
C	346	HIS	-	expression tag	UNP Q2TU34
C	347	HIS	-	expression tag	UNP Q2TU34
D	338	LEU	-	expression tag	UNP Q2TU34
D	339	GLU	-	expression tag	UNP Q2TU34
D	340	HIS	-	expression tag	UNP Q2TU34
D	341	HIS	-	expression tag	UNP Q2TU34
D	342	HIS	-	expression tag	UNP Q2TU34
D	343	HIS	-	expression tag	UNP Q2TU34
D	344	HIS	-	expression tag	UNP Q2TU34
D	345	HIS	-	expression tag	UNP Q2TU34
D	346	HIS	-	expression tag	UNP Q2TU34
D	347	HIS	-	expression tag	UNP Q2TU34

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



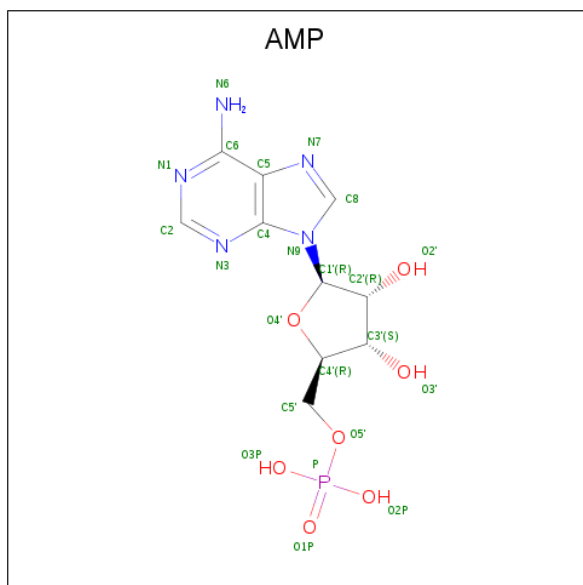
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	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 ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Mg	0	0
			2	2		
4	A	2	Total	Mg	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total 2	Mg 2	0	0
4	C	2	Total 2	Mg 2	0	0

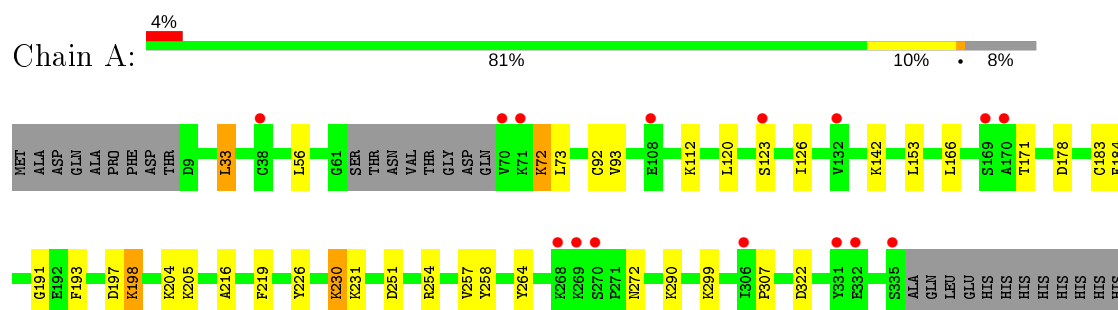
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	117	Total 117	O 117	0	0
5	B	97	Total 97	O 97	0	0
5	C	111	Total 111	O 111	0	0
5	D	108	Total 108	O 108	0	0

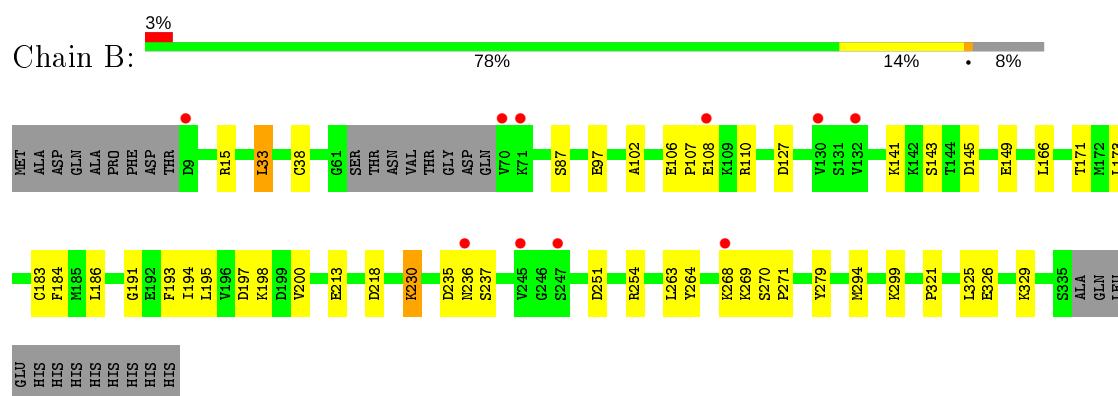
3 Residue-property plots [i](#)

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.

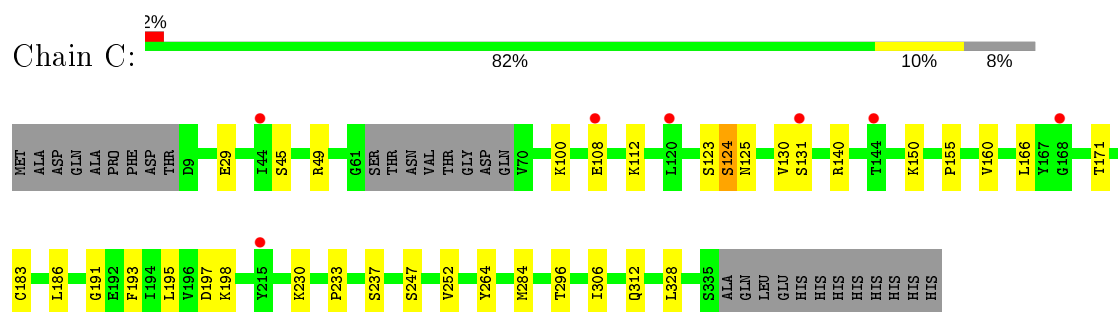
• Molecule 1: Fructose-1,6-bisphosphatase 1



• Molecule 1: Fructose-1,6-bisphosphatase 1

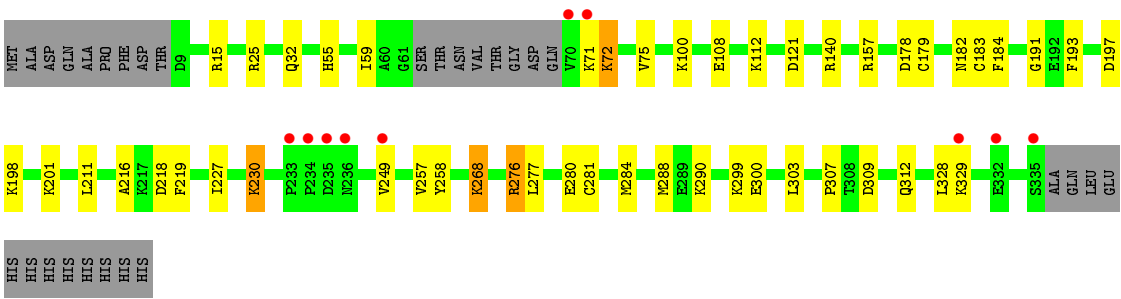


• Molecule 1: Fructose-1,6-bisphosphatase 1



• Molecule 1: Fructose-1,6-bisphosphatase 1





HIS
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.01Å 155.75Å 76.08Å 90.00° 115.54° 90.00°	Depositor
Resolution (Å)	39.13 – 2.10 39.13 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (39.13-2.10) 97.2 (39.13-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.194 , 0.241 0.194 , 0.241	Depositor DCC
R_{free} test set	3770 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.003 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10377	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.40	0/2484	0.58	2/3354 (0.1%)
1	B	0.40	0/2484	0.58	1/3354 (0.0%)
1	C	0.40	0/2484	0.55	0/3354
1	D	0.42	0/2484	0.56	0/3354
All	All	0.40	0/9936	0.57	3/13416 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	33	LEU	CA-CB-CG	7.45	132.42	115.30
1	B	33	LEU	CA-CB-CG	6.82	130.97	115.30
1	A	33	LEU	CB-CG-CD1	5.15	119.76	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	124	SER	Peptide

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	2441	0	2491	28	0
1	B	2441	0	2491	30	0
1	C	2441	0	2491	22	0
1	D	2441	0	2491	30	0
2	A	20	0	9	0	0
2	B	20	0	9	0	0
2	C	20	0	9	0	0
2	D	20	0	10	0	0
3	A	23	0	12	1	0
3	B	23	0	12	0	0
3	C	23	0	12	0	0
3	D	23	0	12	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	117	0	0	2	0
5	B	97	0	0	2	0
5	C	111	0	0	2	0
5	D	108	0	0	3	0
All	All	10377	0	10049	104	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 5.

All (104) 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:B:294:MET:HE3	1:B:321:PRO:HA	1.65	0.77
1:D:211:LEU:HD11	1:D:227:ILE:HD11	1.69	0.74
1:B:102:ALA:HB3	1:B:149:GLU:HG2	1.70	0.74
1:C:252:VAL:HG11	1:C:284:MET:HE2	1.70	0.74
1:A:123:SER:O	1:A:126:ILE:HG12	1.94	0.67
1:B:108:GLU:OE1	5:B:501:HOH:O	2.13	0.65
1:A:251:ASP:OD1	1:A:254:ARG:NH2	2.28	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:CYS:HB2	1:C:197:ASP:HB2	1.79	0.63
1:C:252:VAL:CG1	1:C:284:MET:HE2	2.28	0.63
1:A:123:SER:HA	1:A:126:ILE:HG23	1.82	0.62
1:B:269:LYS:O	1:B:271:PRO:HD3	1.99	0.61
1:D:230:LYS:NZ	5:D:505:HOH:O	2.34	0.60
1:B:251:ASP:OD1	1:B:254:ARG:NH2	2.33	0.60
1:B:191:GLY:HA3	1:D:191:GLY:HA3	1.83	0.60
1:B:230:LYS:NZ	1:B:326:GLU:OE2	2.35	0.60
1:D:183:CYS:HB2	1:D:197:ASP:HB2	1.86	0.58
1:A:226:TYR:CZ	1:A:230:LYS:HD3	2.39	0.57
1:C:123:SER:C	1:C:125:ASN:H	2.07	0.57
1:D:309:ASP:HB3	1:D:312:GLN:HB3	1.85	0.57
1:C:140:ARG:HG2	1:C:160:VAL:HG21	1.85	0.57
1:D:25:ARG:NH1	5:D:506:HOH:O	2.37	0.56
1:C:195:LEU:HD21	1:C:198:LYS:HG2	1.86	0.56
1:A:112:LYS:NZ	3:A:402:AMP:O1P	2.38	0.56
1:A:178:ASP:HA	1:A:290:LYS:HE3	1.88	0.56
1:B:97:GLU:HB2	1:B:279:TYR:CE1	2.42	0.55
1:B:235:ASP:O	1:B:237:SER:N	2.39	0.55
1:B:183:CYS:HB2	1:B:197:ASP:HB2	1.89	0.53
1:D:299:LYS:HG2	1:D:300:GLU:HG3	1.91	0.52
1:B:218:ASP:HB3	1:B:268:LYS:HB2	1.92	0.52
1:D:182:ASN:HD22	1:D:198:LYS:HA	1.75	0.52
1:D:218:ASP:HB3	1:D:268:LYS:HD3	1.92	0.51
1:A:205:LYS:HD2	1:A:322:ASP:HB3	1.93	0.51
1:D:257:VAL:HG12	1:D:258:TYR:CD1	2.46	0.50
1:D:100:LYS:H	1:D:100:LYS:HD3	1.76	0.49
1:A:257:VAL:HG12	1:A:258:TYR:CD1	2.47	0.49
1:D:55:HIS:HA	1:D:59:ILE:HG22	1.95	0.48
1:A:272:ASN:HA	5:A:508:HOH:O	2.12	0.48
1:D:71:LYS:HD3	1:D:75:VAL:HG12	1.96	0.48
1:A:204:LYS:HE2	1:A:322:ASP:OD1	2.15	0.47
1:A:216:ALA:HA	1:A:219:PHE:CD2	2.50	0.47
1:A:184:PHE:HB3	1:A:193:PHE:HB3	1.96	0.47
1:A:254:ARG:HD2	5:A:591:HOH:O	2.14	0.47
1:C:29:GLU:OE2	1:C:112:LYS:HG2	2.15	0.47
1:B:87:SER:OG	1:D:15:ARG:NH2	2.46	0.47
1:C:233:PRO:HG2	1:C:237:SER:O	2.16	0.46
1:B:15:ARG:HG3	1:D:32:GLN:NE2	2.31	0.46
1:D:277:LEU:HD23	1:D:307:PRO:HB3	1.98	0.46
1:B:141:LYS:HZ1	1:B:143:SER:HB2	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:LEU:HD21	1:B:198:LYS:HD2	1.96	0.46
1:B:321:PRO:O	1:B:325:LEU:HB2	2.15	0.46
1:A:142:LYS:HB2	1:A:142:LYS:HE3	1.54	0.45
1:C:155:PRO:HB3	1:C:306:ILE:HD13	1.99	0.45
1:C:108:GLU:CD	1:C:108:GLU:H	2.14	0.45
1:A:72:LYS:HB2	1:A:72:LYS:HE2	1.77	0.45
1:B:106:GLU:OE1	1:B:108:GLU:N	2.43	0.45
1:A:191:GLY:HA3	1:C:191:GLY:HA3	1.99	0.44
1:D:121:ASP:OD2	1:D:249:VAL:HG23	2.17	0.44
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.81	0.44
1:C:112:LYS:NZ	5:C:513:HOH:O	2.49	0.44
1:B:186:LEU:HB2	1:B:193:PHE:CE1	2.51	0.44
1:C:125:ASN:OD1	1:C:130:VAL:HB	2.18	0.44
1:C:140:ARG:HB2	5:C:501:HOH:O	2.18	0.44
1:C:108:GLU:OE2	1:C:108:GLU:N	2.43	0.44
1:B:294:MET:HE1	1:B:325:LEU:HD13	2.00	0.44
1:B:294:MET:HE3	1:B:321:PRO:CA	2.41	0.44
1:C:166:LEU:O	1:C:171:THR:HA	2.18	0.44
1:A:166:LEU:O	1:A:171:THR:HA	2.18	0.44
1:A:56:LEU:O	1:A:56:LEU:HD23	2.17	0.44
1:D:201:LYS:NZ	5:D:510:HOH:O	2.46	0.44
1:C:45:SER:O	1:C:49:ARG:HD3	2.18	0.43
1:D:276:ARG:NH2	1:D:280:GLU:OE2	2.48	0.43
1:A:120:LEU:HD12	1:A:120:LEU:HA	1.80	0.43
1:B:294:MET:CE	1:B:325:LEU:HD13	2.48	0.43
1:C:186:LEU:HB2	1:C:193:PHE:CE1	2.53	0.43
1:A:72:LYS:HD3	1:A:72:LYS:H	1.83	0.43
1:A:92:CYS:SG	1:A:93:VAL:HG23	2.59	0.43
1:D:108:GLU:CD	1:D:108:GLU:H	2.22	0.43
1:A:183:CYS:HB2	1:A:197:ASP:HB2	2.00	0.42
1:B:107:PRO:HA	1:B:110:ARG:HG3	2.02	0.42
1:D:157:ARG:HG2	1:D:303:LEU:O	2.19	0.42
1:B:299:LYS:HB3	1:B:299:LYS:HE3	1.70	0.42
1:C:130:VAL:HG12	1:C:131:SER:N	2.35	0.42
1:C:296:THR:HG21	1:C:328:LEU:HD21	2.01	0.42
1:B:254:ARG:HD2	5:B:551:HOH:O	2.20	0.42
1:A:112:LYS:HB3	1:A:112:LYS:HE3	1.91	0.41
1:B:183:CYS:SG	1:B:200:VAL:HG21	2.61	0.41
1:D:284:MET:O	1:D:288:MET:HG2	2.21	0.41
1:B:235:ASP:C	1:B:237:SER:H	2.23	0.41
1:D:184:PHE:HB3	1:D:193:PHE:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:TYR:OH	1:B:127:ASP:HB2	2.20	0.41
1:C:130:VAL:HG12	1:C:131:SER:H	1.86	0.41
1:D:182:ASN:ND2	1:D:198:LYS:HA	2.36	0.41
1:D:72:LYS:HB2	1:D:72:LYS:HE2	1.83	0.41
1:A:231:LYS:HD3	1:B:213:GLU:O	2.21	0.41
1:D:277:LEU:HA	1:D:281:CYS:HB2	2.02	0.41
1:D:178:ASP:HA	1:D:290:LYS:HE3	2.03	0.41
1:B:166:LEU:O	1:B:171:THR:HA	2.20	0.40
1:C:123:SER:O	1:C:125:ASN:N	2.50	0.40
1:D:216:ALA:HA	1:D:219:PHE:CD2	2.56	0.40
1:B:184:PHE:HA	1:B:194:ILE:O	2.22	0.40
1:A:153:LEU:HA	1:A:307:PRO:HG2	2.04	0.40
1:D:112:LYS:HD2	1:D:140:ARG:HD2	2.04	0.40
1:D:328:LEU:HA	1:D:328:LEU:HD23	1.91	0.40
1:A:198:LYS:HG2	1:A:198:LYS:H	1.68	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	315/348 (90%)	306 (97%)	9 (3%)	0	100	100
1	B	315/348 (90%)	302 (96%)	11 (4%)	2 (1%)	25	21
1	C	315/348 (90%)	308 (98%)	6 (2%)	1 (0%)	41	41
1	D	315/348 (90%)	310 (98%)	5 (2%)	0	100	100
All	All	1260/1392 (90%)	1226 (97%)	31 (2%)	3 (0%)	47	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	236	ASN
1	C	124	SER
1	B	270	SER

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	266/291 (91%)	260 (98%)	6 (2%)	50	55
1	B	266/291 (91%)	258 (97%)	8 (3%)	41	44
1	C	266/291 (91%)	260 (98%)	6 (2%)	50	55
1	D	266/291 (91%)	260 (98%)	6 (2%)	50	55
All	All	1064/1164 (91%)	1038 (98%)	26 (2%)	49	53

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	72	LYS
1	A	198	LYS
1	A	230	LYS
1	A	264	TYR
1	A	299	LYS
1	B	33	LEU
1	B	38	CYS
1	B	145	ASP
1	B	173	LEU
1	B	230	LYS
1	B	263	LEU
1	B	264	TYR
1	B	329	LYS
1	C	100	LYS
1	C	150	LYS
1	C	230	LYS
1	C	247	SER
1	C	264	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	312	GLN
1	D	72	LYS
1	D	179	CYS
1	D	230	LYS
1	D	268	LYS
1	D	276	ARG
1	D	329	LYS

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

Mol	Chain	Res	Type
1	A	125	ASN
1	D	182	ASN

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 ⓘ

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	AMP	D	402	-	22,25,25	1.26	3 (13%)	25,38,38	2.21	3 (12%)
2	FBP	C	401	4	18,20,20	3.43	7 (38%)	23,32,32	0.79	0
2	FBP	A	401	4	18,20,20	3.41	7 (38%)	23,32,32	0.85	0
3	AMP	C	402	-	22,25,25	1.21	3 (13%)	25,38,38	2.07	3 (12%)
2	FBP	B	401	4	18,20,20	3.40	7 (38%)	23,32,32	0.93	0
3	AMP	B	402	-	22,25,25	1.20	3 (13%)	25,38,38	1.93	3 (12%)
3	AMP	A	402	-	22,25,25	1.23	3 (13%)	25,38,38	2.06	3 (12%)
2	FBP	D	401	4	18,20,20	3.23	6 (33%)	23,32,32	0.96	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	D	402	-	-	0/6/26/26	0/3/3/3
2	FBP	C	401	4	-	3/13/32/32	0/1/1/1
2	FBP	A	401	4	-	3/13/32/32	0/1/1/1
3	AMP	C	402	-	-	0/6/26/26	0/3/3/3
2	FBP	B	401	4	-	2/13/32/32	0/1/1/1
3	AMP	B	402	-	-	0/6/26/26	0/3/3/3
3	AMP	A	402	-	-	0/6/26/26	0/3/3/3
2	FBP	D	401	4	-	4/13/32/32	0/1/1/1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	FBP	O5-C2	-8.36	1.30	1.43
2	A	401	FBP	O5-C2	-8.20	1.30	1.43
2	B	401	FBP	O5-C2	-8.14	1.30	1.43
2	A	401	FBP	O5-C5	8.05	1.61	1.43
2	B	401	FBP	O5-C5	7.97	1.61	1.43
2	C	401	FBP	O5-C5	7.85	1.61	1.43
2	D	401	FBP	O5-C2	-7.78	1.31	1.43
2	D	401	FBP	O5-C5	7.69	1.60	1.43
2	C	401	FBP	C4-C5	-7.00	1.35	1.53
2	B	401	FBP	C4-C5	-6.67	1.36	1.53
2	A	401	FBP	C4-C5	-6.53	1.36	1.53
2	D	401	FBP	C4-C5	-6.31	1.36	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	AMP	C6-N6	3.44	1.46	1.34
2	C	401	FBP	O3-C3	-3.28	1.36	1.42
2	A	401	FBP	O3-C3	-3.28	1.36	1.42
3	A	402	AMP	C6-N6	3.23	1.45	1.34
3	C	402	AMP	C6-N6	3.22	1.45	1.34
2	B	401	FBP	O3-C3	-3.08	1.36	1.42
3	B	402	AMP	C6-N6	3.02	1.45	1.34
3	A	402	AMP	C2-N3	2.91	1.36	1.32
2	D	401	FBP	O3-C3	-2.81	1.37	1.42
2	B	401	FBP	O4-C4	2.72	1.49	1.43
3	C	402	AMP	C2-N3	2.69	1.36	1.32
3	D	402	AMP	C2-N3	2.67	1.36	1.32
2	C	401	FBP	O4-C4	2.63	1.49	1.43
2	A	401	FBP	O4-C4	2.60	1.49	1.43
3	B	402	AMP	C5-C4	-2.59	1.34	1.40
3	D	402	AMP	C5-C4	-2.56	1.34	1.40
2	D	401	FBP	O4-C4	2.54	1.49	1.43
3	C	402	AMP	C5-C4	-2.49	1.34	1.40
2	A	401	FBP	P2-O6	2.46	1.68	1.60
3	B	402	AMP	C2-N3	2.45	1.36	1.32
2	B	401	FBP	P2-O6	2.36	1.67	1.60
2	C	401	FBP	P1-O1	2.27	1.67	1.60
2	B	401	FBP	P1-O1	2.24	1.67	1.60
3	A	402	AMP	C5-C4	-2.23	1.35	1.40
2	D	401	FBP	P1-O1	2.10	1.67	1.60
2	A	401	FBP	P1-O1	2.06	1.66	1.60
2	C	401	FBP	P2-O6	2.00	1.66	1.60

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	AMP	C5-C6-N6	7.59	131.88	120.35
3	C	402	AMP	C5-C6-N6	6.87	130.80	120.35
3	A	402	AMP	C5-C6-N6	6.86	130.78	120.35
3	B	402	AMP	C5-C6-N6	6.13	129.67	120.35
3	C	402	AMP	N3-C2-N1	-5.45	120.17	128.68
3	D	402	AMP	N3-C2-N1	-5.39	120.25	128.68
3	B	402	AMP	N3-C2-N1	-5.34	120.33	128.68
3	A	402	AMP	N3-C2-N1	-5.27	120.44	128.68
3	D	402	AMP	N6-C6-N1	-4.88	108.45	118.57
3	A	402	AMP	N6-C6-N1	-4.50	109.23	118.57
3	C	402	AMP	N6-C6-N1	-4.25	109.75	118.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	AMP	N6-C6-N1	-4.18	109.89	118.57
2	D	401	FBP	O6P-P2-O6	2.59	113.62	106.73

There are no chirality outliers.

All (12) torsion outliers are listed below:

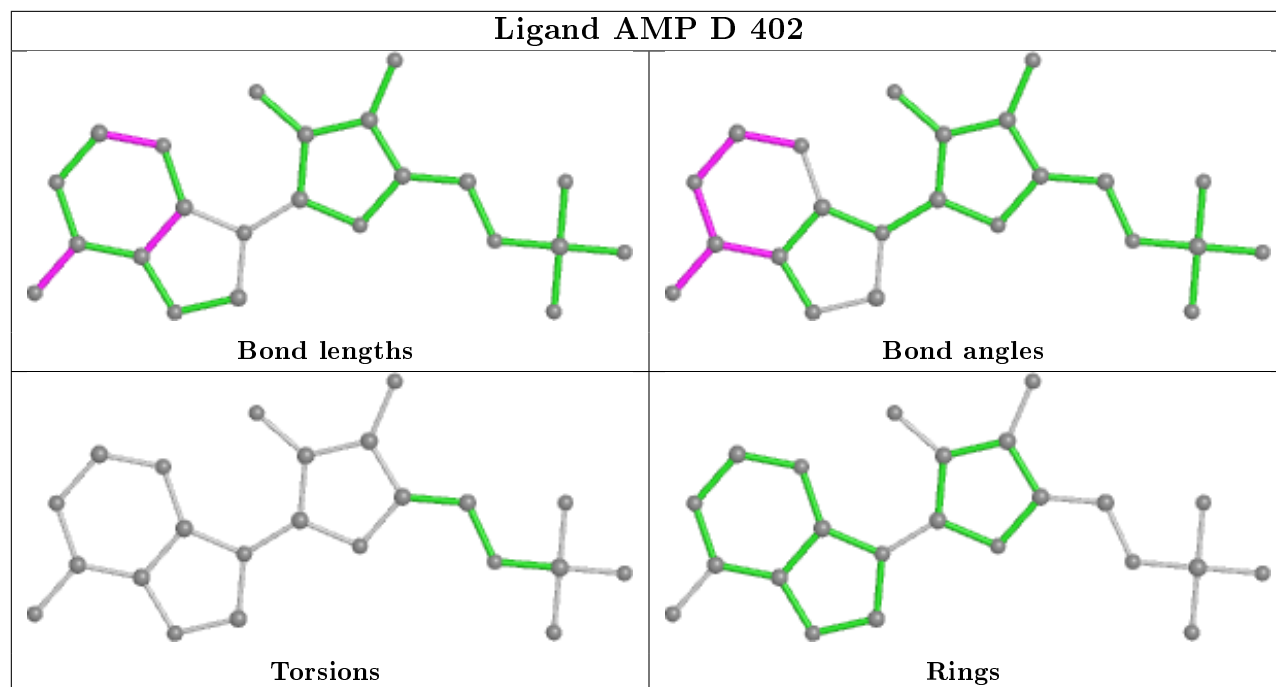
Mol	Chain	Res	Type	Atoms
2	C	401	FBP	C1-O1-P1-O2P
2	C	401	FBP	C1-O1-P1-O3P
2	A	401	FBP	C1-O1-P1-O2P
2	A	401	FBP	C1-O1-P1-O3P
2	D	401	FBP	C6-O6-P2-O5P
2	D	401	FBP	C6-O6-P2-O6P
2	C	401	FBP	C1-O1-P1-O1P
2	D	401	FBP	C6-O6-P2-O4P
2	D	401	FBP	C4-C5-C6-O6
2	A	401	FBP	O1-C1-C2-O2
2	B	401	FBP	C1-O1-P1-O2P
2	B	401	FBP	C6-O6-P2-O5P

There are no ring outliers.

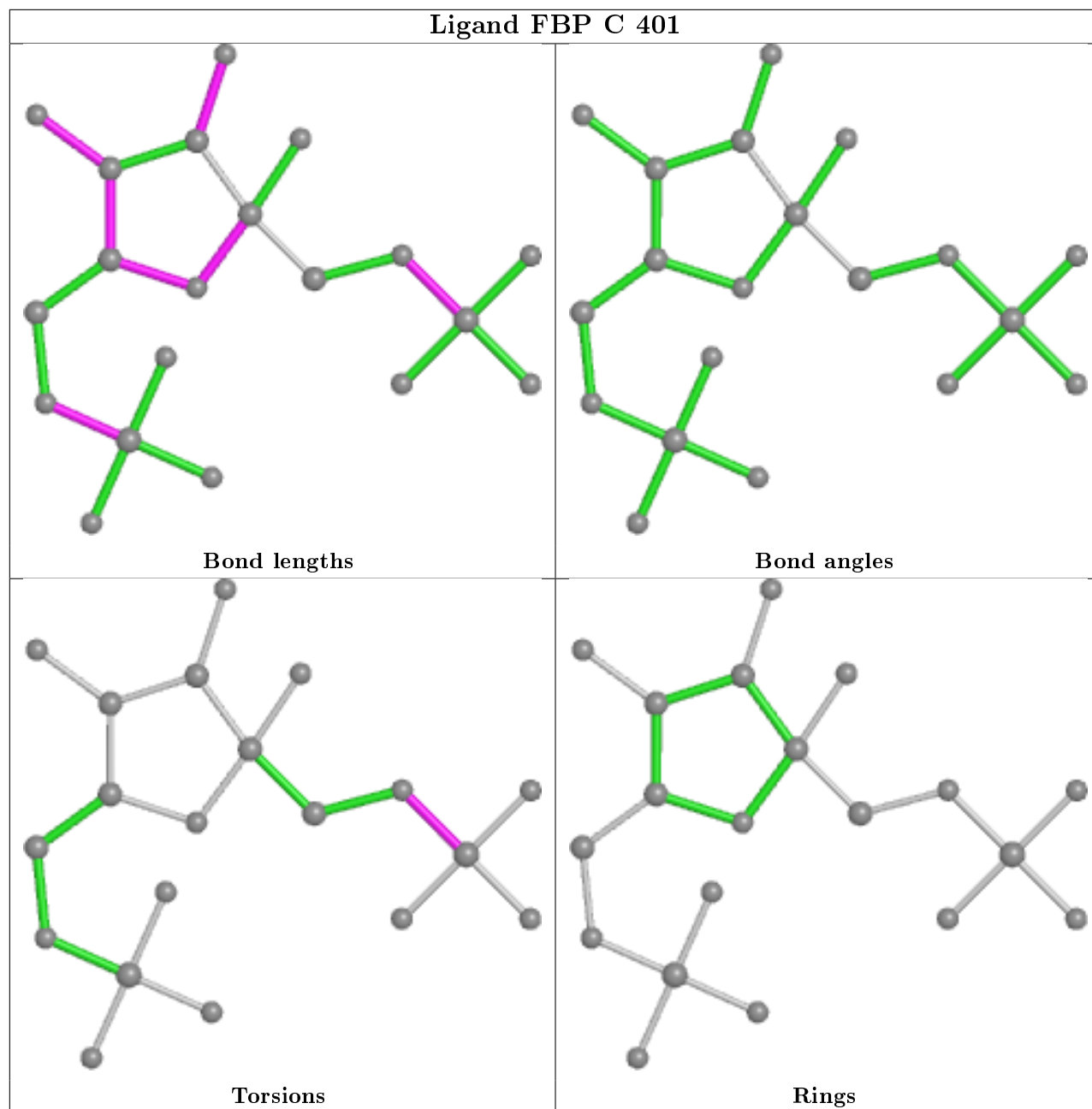
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	AMP	1	0

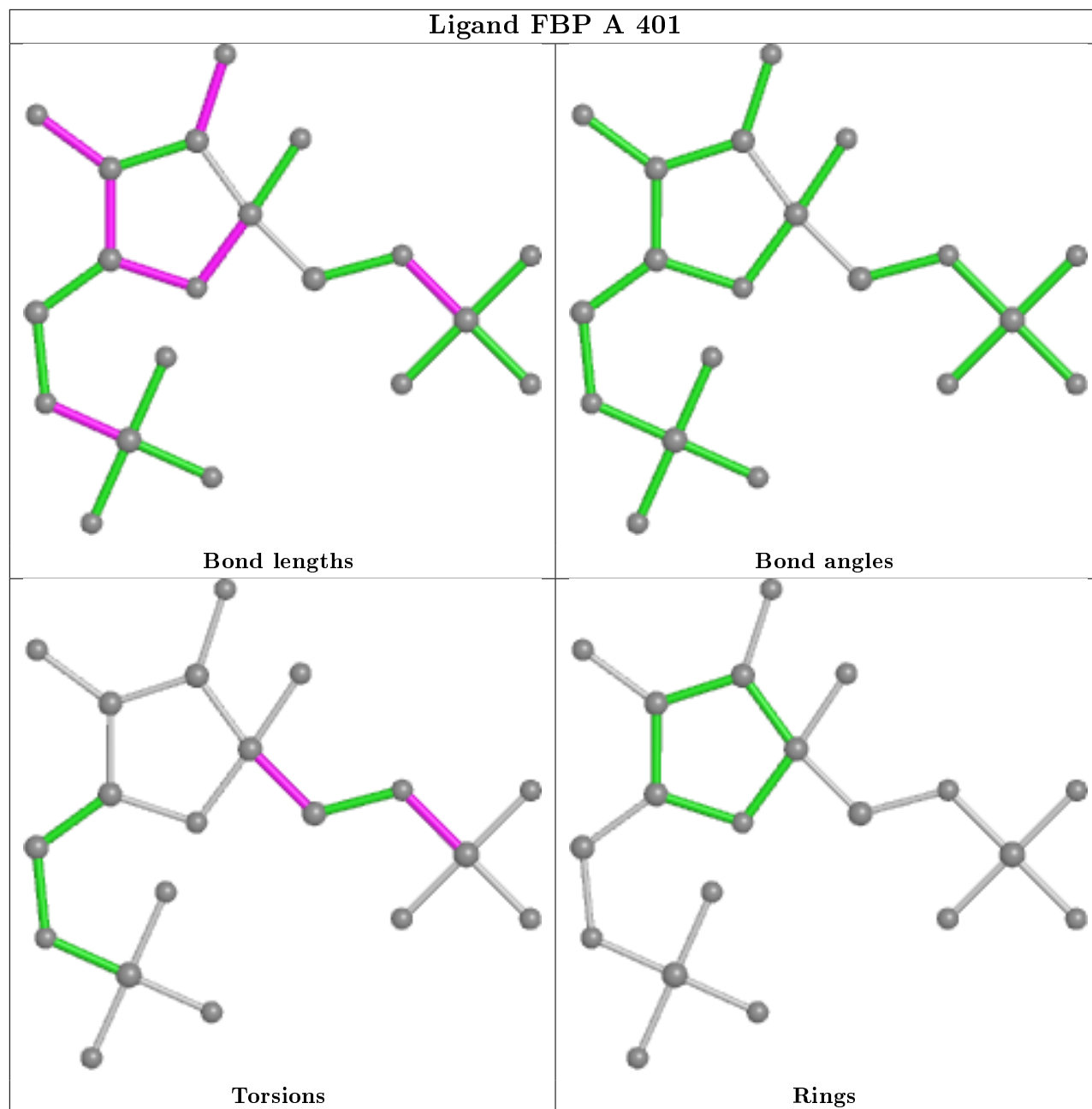
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

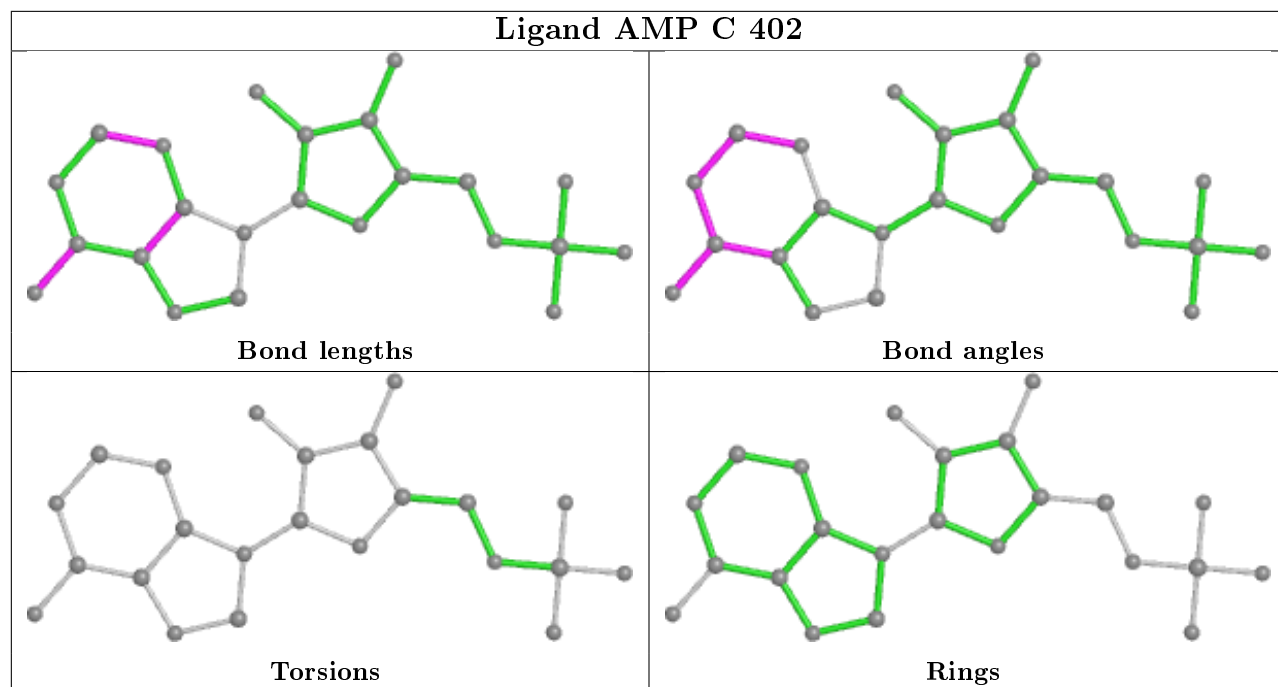


Ligand FBP C 401

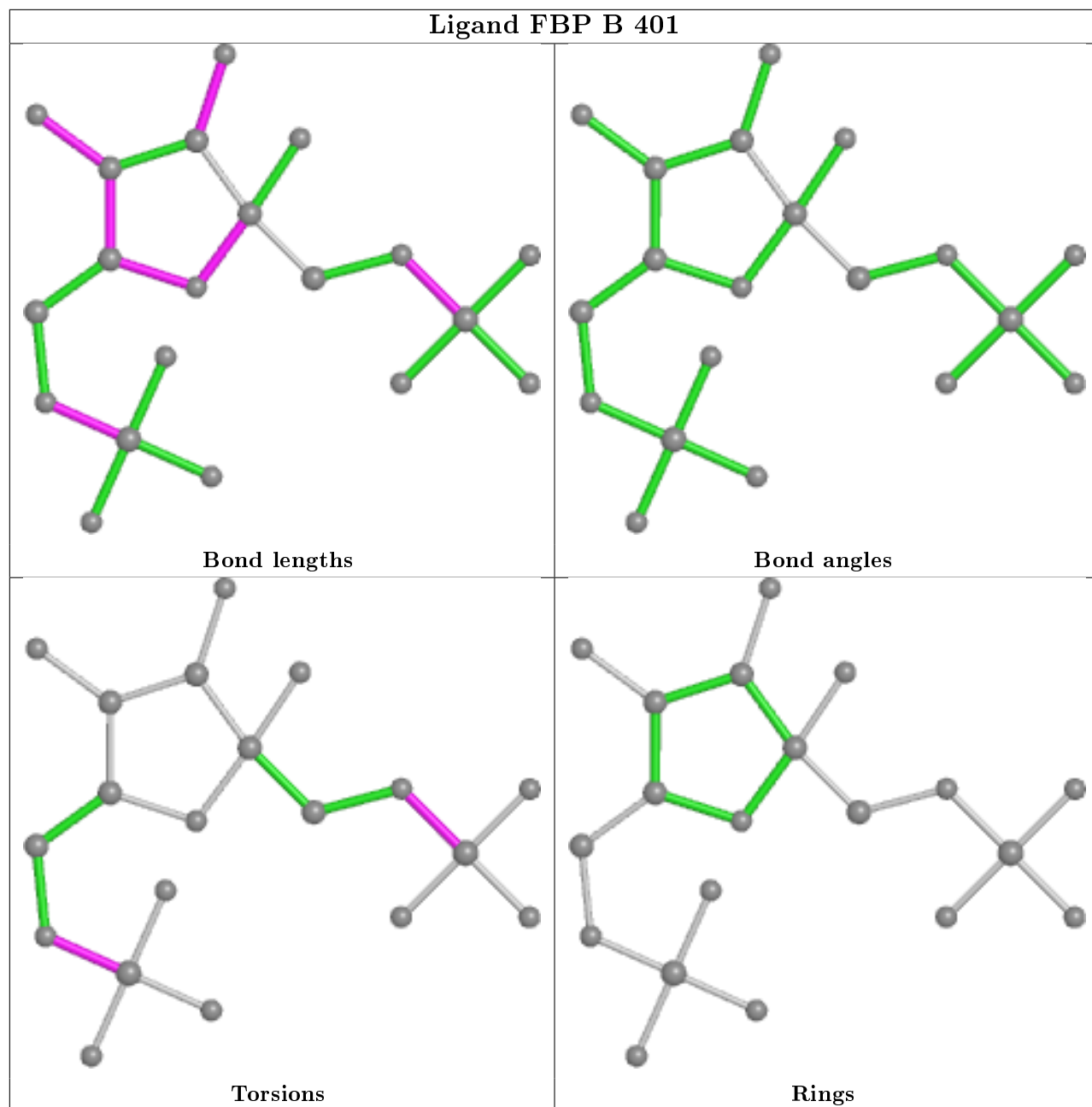


Ligand FBP A 401

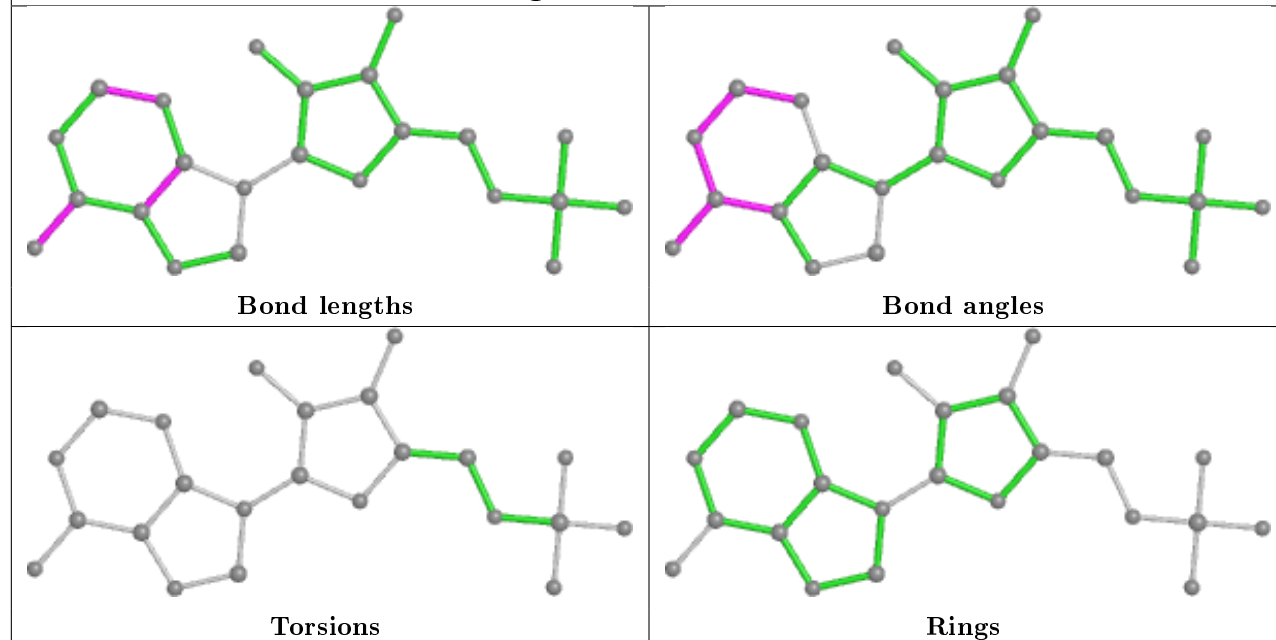




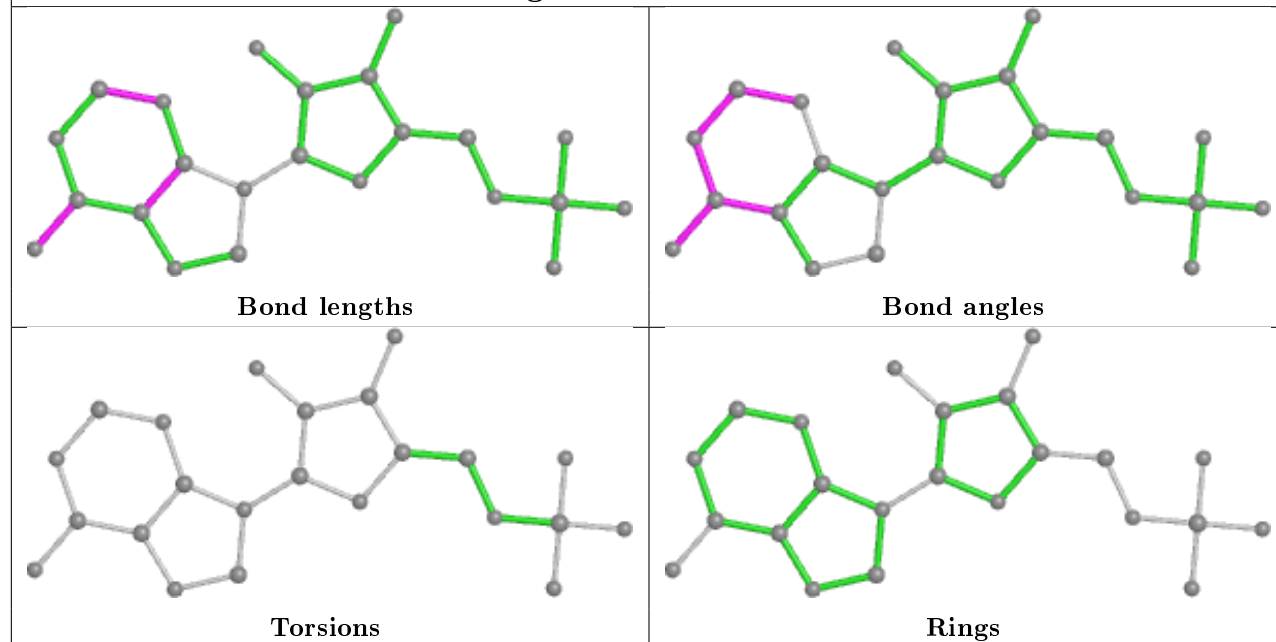
Ligand FBP B 401

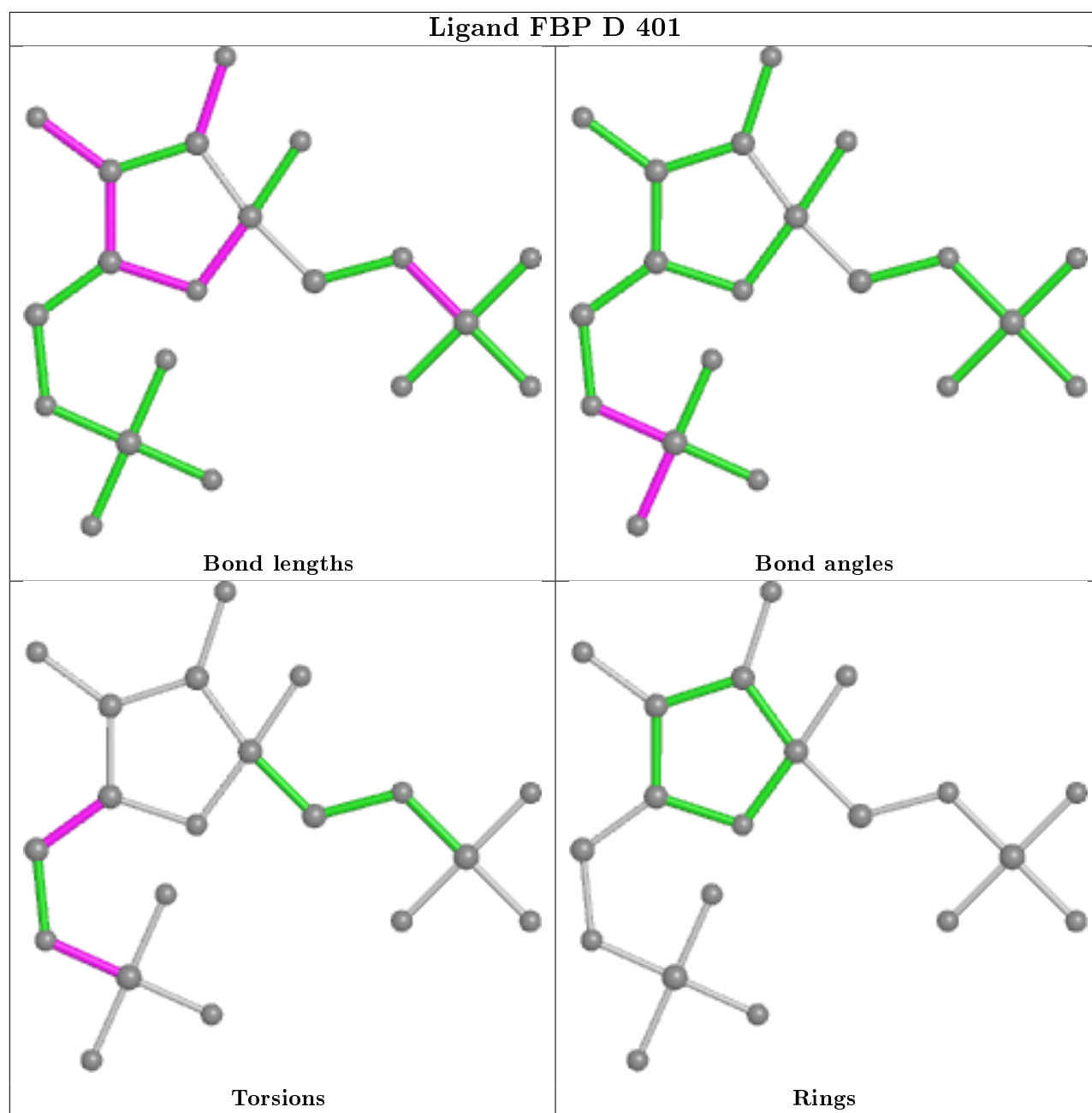


Ligand AMP B 402



Ligand AMP A 402





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	319/348 (91%)	0.09	15 (4%) 31 37	28, 38, 60, 77	0
1	B	319/348 (91%)	0.08	10 (3%) 49 55	28, 38, 64, 82	0
1	C	319/348 (91%)	0.08	7 (2%) 62 66	28, 40, 59, 82	0
1	D	319/348 (91%)	0.13	10 (3%) 49 55	27, 38, 60, 79	0
All	All	1276/1392 (91%)	0.10	42 (3%) 46 53	27, 39, 60, 82	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	70	VAL	9.7
1	A	70	VAL	8.4
1	D	70	VAL	6.3
1	D	335	SER	3.8
1	D	236	ASN	3.5
1	B	268	LYS	3.3
1	A	335	SER	3.3
1	D	234	PRO	3.2
1	A	331	TYR	3.1
1	A	123	SER	3.1
1	D	249	VAL	3.0
1	B	71	LYS	2.9
1	B	236	ASN	2.8
1	B	132	VAL	2.7
1	D	233	PRO	2.7
1	B	130	VAL	2.6
1	A	71	LYS	2.6
1	D	329	LYS	2.6
1	D	332	GLU	2.6
1	B	108	GLU	2.5
1	A	38	CYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	131	SER	2.4
1	D	235	ASP	2.4
1	A	332	GLU	2.3
1	A	306	ILE	2.3
1	B	9	ASP	2.3
1	C	168	GLY	2.3
1	A	132	VAL	2.2
1	A	268	LYS	2.2
1	A	170	ALA	2.2
1	B	245	VAL	2.2
1	C	215	TYR	2.2
1	C	144	THR	2.2
1	A	270	SER	2.2
1	A	108	GLU	2.1
1	C	108	GLU	2.1
1	D	71	LYS	2.1
1	B	247	SER	2.1
1	C	120	LEU	2.0
1	A	169	SER	2.0
1	C	44	ILE	2.0
1	A	269	LYS	2.0

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

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(\AA^2)	Q<0.9
4	MG	B	404	1/1	0.49	0.11	50,50,50,50	0
4	MG	C	404	1/1	0.72	0.06	53,53,53,53	0

Continued on next page...

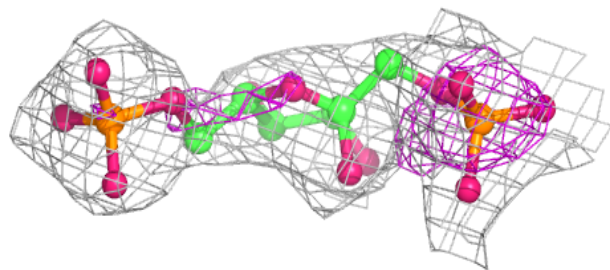
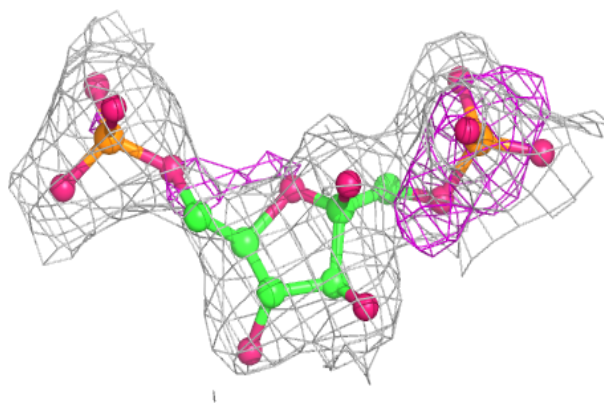
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	C	403	1/1	0.72	0.11	62,62,62,62	0
4	MG	D	403	1/1	0.86	0.31	47,47,47,47	0
4	MG	A	403	1/1	0.88	0.13	56,56,56,56	0
2	FBP	C	401	20/20	0.88	0.13	45,53,66,73	0
4	MG	B	403	1/1	0.90	0.09	37,37,37,37	0
2	FBP	A	401	20/20	0.92	0.12	43,53,65,66	0
3	AMP	D	402	23/23	0.93	0.12	34,38,44,45	0
3	AMP	B	402	23/23	0.94	0.10	35,38,40,41	0
4	MG	D	404	1/1	0.95	0.11	43,43,43,43	0
2	FBP	B	401	20/20	0.97	0.12	35,41,54,55	0
3	AMP	A	402	23/23	0.97	0.08	31,35,38,40	0
3	AMP	C	402	23/23	0.97	0.09	33,40,44,46	0
4	MG	A	404	1/1	0.97	0.20	56,56,56,56	0
2	FBP	D	401	20/20	0.97	0.18	32,37,45,50	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.

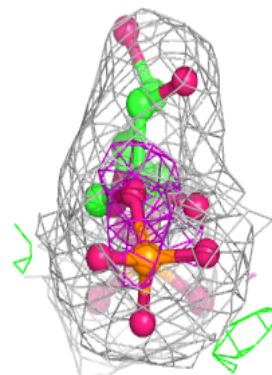
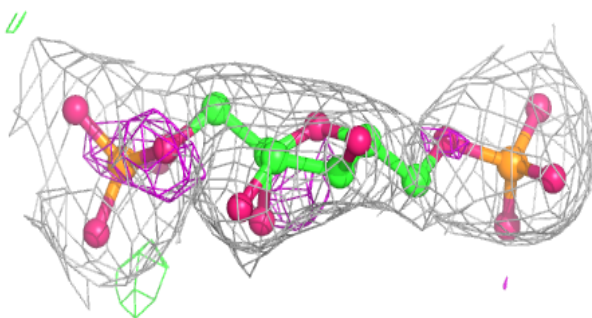
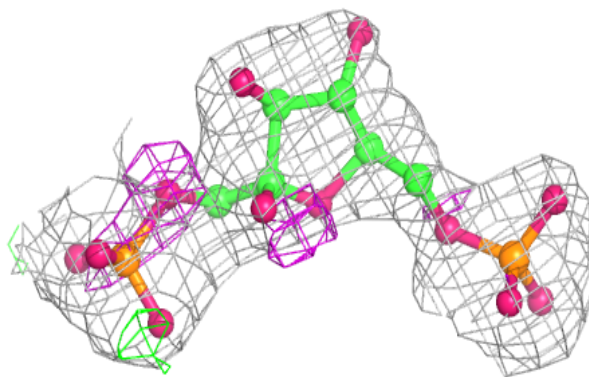
Electron density around FBP C 401:

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



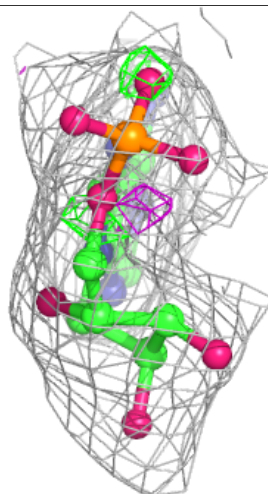
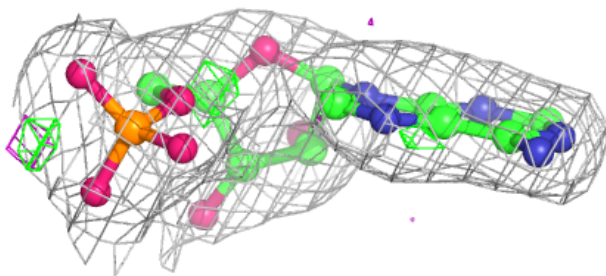
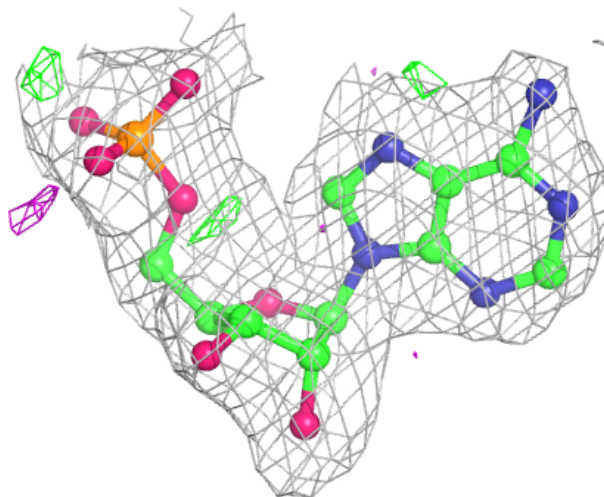
Electron density around FBP A 401:

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



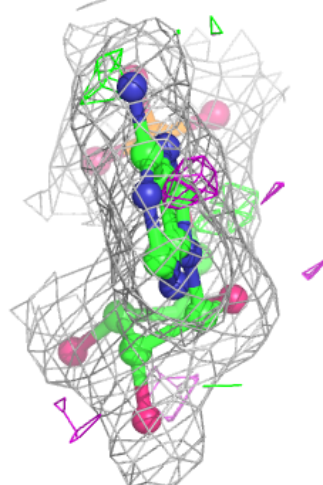
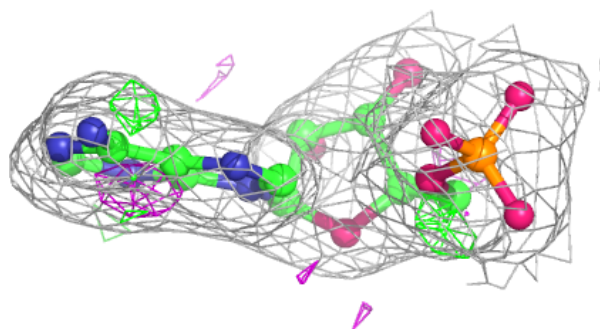
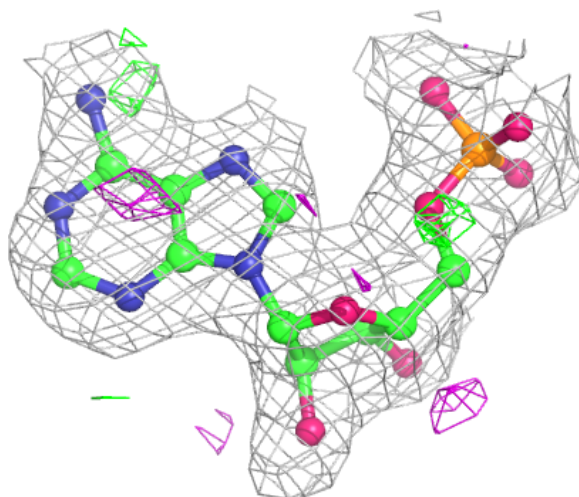
Electron density around AMP D 402:

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



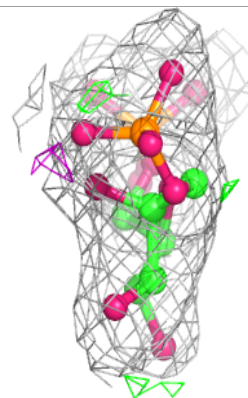
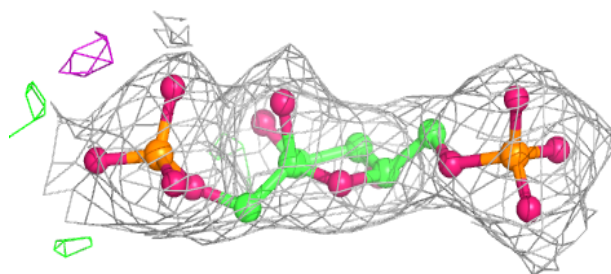
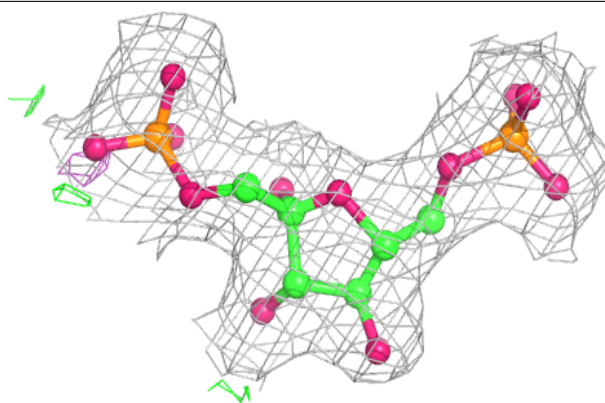
Electron density around AMP B 402:

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



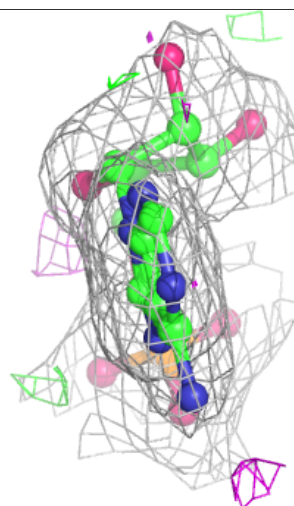
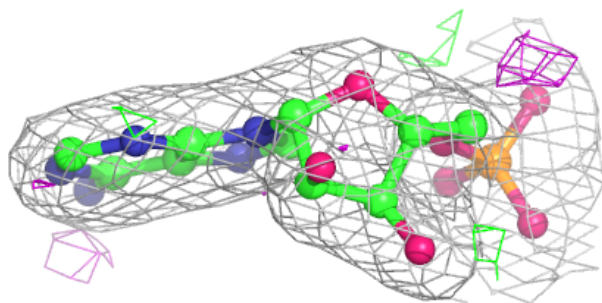
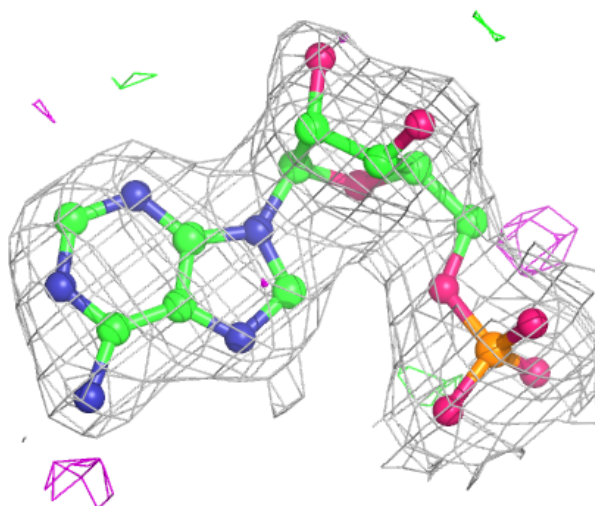
Electron density around FBP B 401:

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



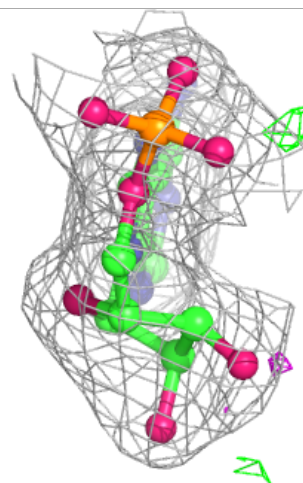
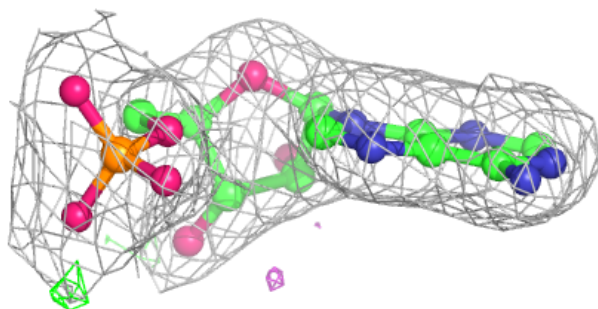
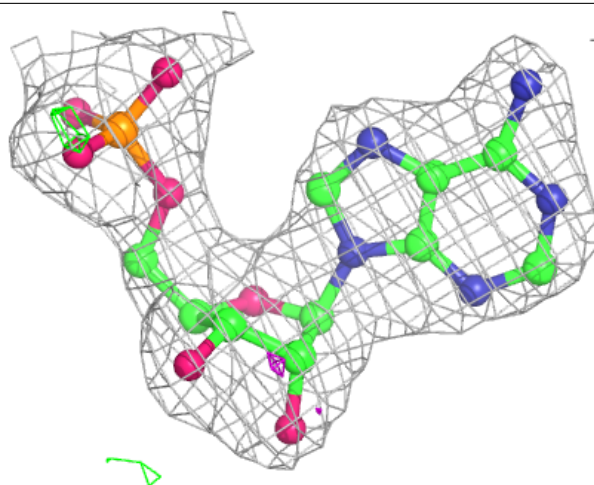
Electron density around AMP A 402:

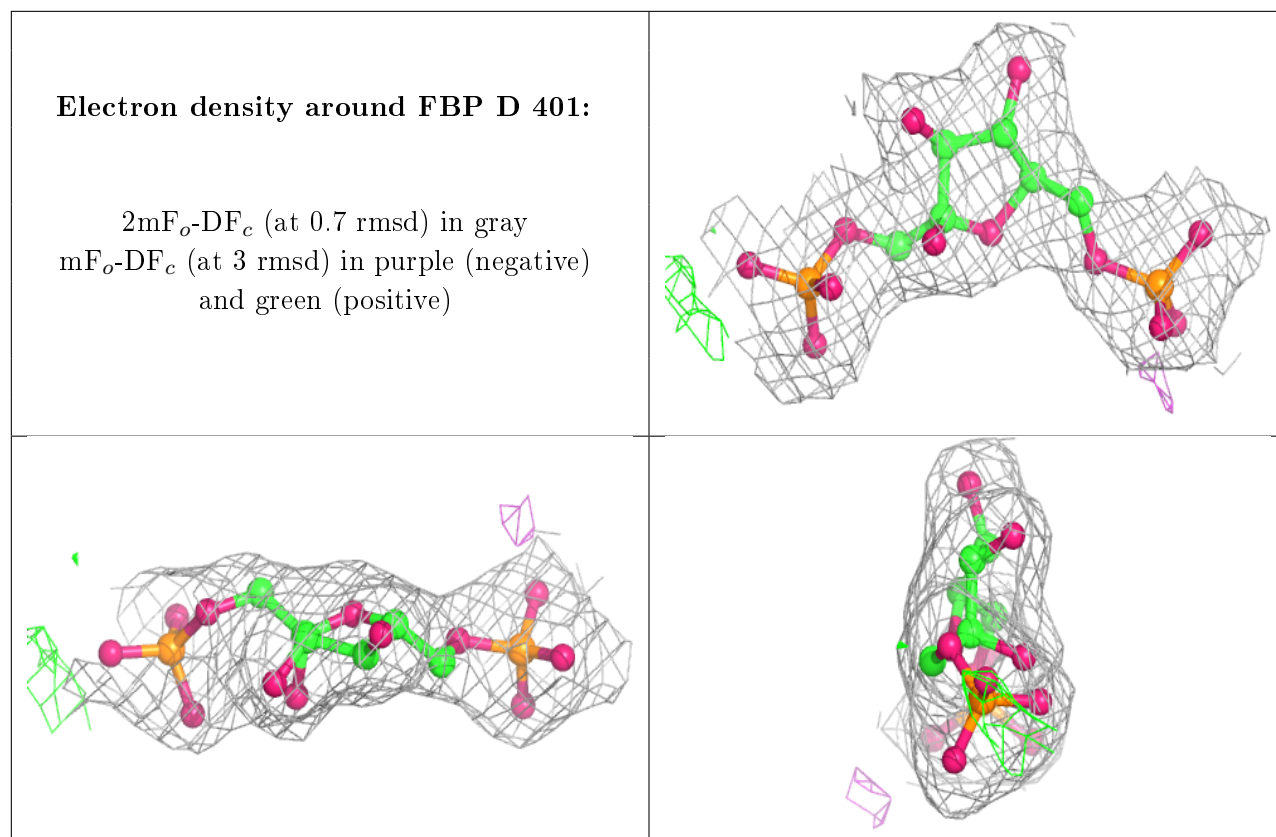
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AMP C 402:

$2mF_o-DF_c$ (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.