



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 3, 2025 – 08:11 AM EDT

PDB ID : 9O3B / pdb_00009o3b
Title : PKM2 bound to MCTI-566
Authors : Stuckey, J.A.
Deposited on : 2025-04-07
Resolution : 2.42 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

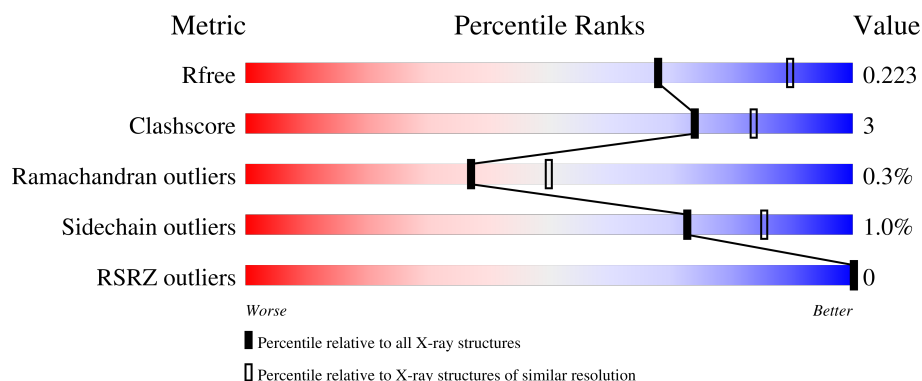
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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}	164625	5670 (2.44-2.40)
Clashscore	180529	6299 (2.44-2.40)
Ramachandran outliers	177936	6232 (2.44-2.40)
Sidechain outliers	177891	6233 (2.44-2.40)
RSRZ outliers	164620	5670 (2.44-2.40)

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	550	
1	B	550	
1	C	550	
1	D	550	
1	E	550	

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Mol	Chain	Length	Quality of chain
1	F	550	
1	G	550	
1	H	550	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	PO4	C	605	-	-	X	-
7	PO4	H	605	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 32262 atoms, of which 297 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 Pyruvate kinase PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	A	519	Total	C	N	O	S	0	0	0	
			3877	2445	680	727	25				
1	B	505	Total	C	N	O	S	0	1	0	
			3738	2349	669	696	24				
1	C	521	Total	C	N	O	S	0	0	0	
			3887	2457	680	725	25				
1	D	502	Total	C	N	O	S	0	0	0	
			3703	2329	656	694	24				
1	E	504	Total	C	N	O	S	0	1	0	
			3744	2351	672	697	24				
1	F	520	Total	C	N	O	S	0	0	0	
			3878	2446	681	726	25				
1	G	503	Total	C	N	O	S	0	0	0	
			3708	2337	656	691	24				
1	H	521	Total	C	H	N	O	S	121	0	0
			3999	2450	121	680	723	25			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP P14618
A	-17	GLY	-	expression tag	UNP P14618
A	-16	SER	-	expression tag	UNP P14618
A	-15	SER	-	expression tag	UNP P14618
A	-14	HIS	-	expression tag	UNP P14618
A	-13	HIS	-	expression tag	UNP P14618
A	-12	HIS	-	expression tag	UNP P14618
A	-11	HIS	-	expression tag	UNP P14618
A	-10	HIS	-	expression tag	UNP P14618
A	-9	HIS	-	expression tag	UNP P14618
A	-8	SER	-	expression tag	UNP P14618
A	-7	SER	-	expression tag	UNP P14618
A	-6	GLY	-	expression tag	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	LEU	-	expression tag	UNP P14618
A	-4	VAL	-	expression tag	UNP P14618
A	-3	PRO	-	expression tag	UNP P14618
A	-2	ARG	-	expression tag	UNP P14618
A	-1	GLY	-	expression tag	UNP P14618
A	0	SER	-	expression tag	UNP P14618
B	-18	MET	-	initiating methionine	UNP P14618
B	-17	GLY	-	expression tag	UNP P14618
B	-16	SER	-	expression tag	UNP P14618
B	-15	SER	-	expression tag	UNP P14618
B	-14	HIS	-	expression tag	UNP P14618
B	-13	HIS	-	expression tag	UNP P14618
B	-12	HIS	-	expression tag	UNP P14618
B	-11	HIS	-	expression tag	UNP P14618
B	-10	HIS	-	expression tag	UNP P14618
B	-9	HIS	-	expression tag	UNP P14618
B	-8	SER	-	expression tag	UNP P14618
B	-7	SER	-	expression tag	UNP P14618
B	-6	GLY	-	expression tag	UNP P14618
B	-5	LEU	-	expression tag	UNP P14618
B	-4	VAL	-	expression tag	UNP P14618
B	-3	PRO	-	expression tag	UNP P14618
B	-2	ARG	-	expression tag	UNP P14618
B	-1	GLY	-	expression tag	UNP P14618
B	0	SER	-	expression tag	UNP P14618
C	-18	MET	-	initiating methionine	UNP P14618
C	-17	GLY	-	expression tag	UNP P14618
C	-16	SER	-	expression tag	UNP P14618
C	-15	SER	-	expression tag	UNP P14618
C	-14	HIS	-	expression tag	UNP P14618
C	-13	HIS	-	expression tag	UNP P14618
C	-12	HIS	-	expression tag	UNP P14618
C	-11	HIS	-	expression tag	UNP P14618
C	-10	HIS	-	expression tag	UNP P14618
C	-9	HIS	-	expression tag	UNP P14618
C	-8	SER	-	expression tag	UNP P14618
C	-7	SER	-	expression tag	UNP P14618
C	-6	GLY	-	expression tag	UNP P14618
C	-5	LEU	-	expression tag	UNP P14618
C	-4	VAL	-	expression tag	UNP P14618
C	-3	PRO	-	expression tag	UNP P14618
C	-2	ARG	-	expression tag	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P14618
C	0	SER	-	expression tag	UNP P14618
D	-18	MET	-	initiating methionine	UNP P14618
D	-17	GLY	-	expression tag	UNP P14618
D	-16	SER	-	expression tag	UNP P14618
D	-15	SER	-	expression tag	UNP P14618
D	-14	HIS	-	expression tag	UNP P14618
D	-13	HIS	-	expression tag	UNP P14618
D	-12	HIS	-	expression tag	UNP P14618
D	-11	HIS	-	expression tag	UNP P14618
D	-10	HIS	-	expression tag	UNP P14618
D	-9	HIS	-	expression tag	UNP P14618
D	-8	SER	-	expression tag	UNP P14618
D	-7	SER	-	expression tag	UNP P14618
D	-6	GLY	-	expression tag	UNP P14618
D	-5	LEU	-	expression tag	UNP P14618
D	-4	VAL	-	expression tag	UNP P14618
D	-3	PRO	-	expression tag	UNP P14618
D	-2	ARG	-	expression tag	UNP P14618
D	-1	GLY	-	expression tag	UNP P14618
D	0	SER	-	expression tag	UNP P14618
E	-18	MET	-	initiating methionine	UNP P14618
E	-17	GLY	-	expression tag	UNP P14618
E	-16	SER	-	expression tag	UNP P14618
E	-15	SER	-	expression tag	UNP P14618
E	-14	HIS	-	expression tag	UNP P14618
E	-13	HIS	-	expression tag	UNP P14618
E	-12	HIS	-	expression tag	UNP P14618
E	-11	HIS	-	expression tag	UNP P14618
E	-10	HIS	-	expression tag	UNP P14618
E	-9	HIS	-	expression tag	UNP P14618
E	-8	SER	-	expression tag	UNP P14618
E	-7	SER	-	expression tag	UNP P14618
E	-6	GLY	-	expression tag	UNP P14618
E	-5	LEU	-	expression tag	UNP P14618
E	-4	VAL	-	expression tag	UNP P14618
E	-3	PRO	-	expression tag	UNP P14618
E	-2	ARG	-	expression tag	UNP P14618
E	-1	GLY	-	expression tag	UNP P14618
E	0	SER	-	expression tag	UNP P14618
F	-18	MET	-	initiating methionine	UNP P14618
F	-17	GLY	-	expression tag	UNP P14618

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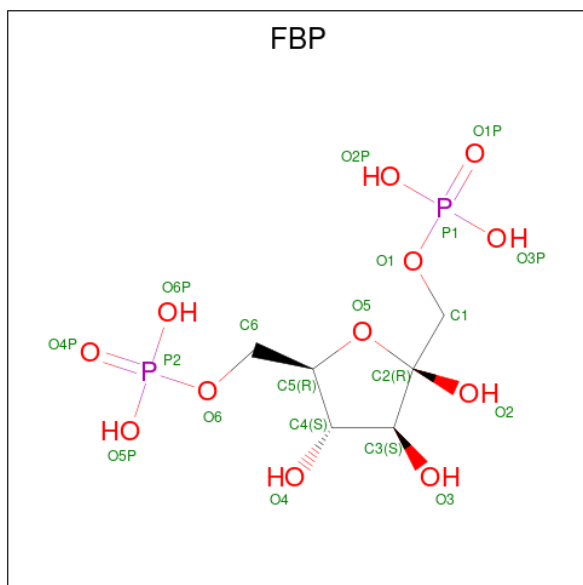
Chain	Residue	Modelled	Actual	Comment	Reference
F	-16	SER	-	expression tag	UNP P14618
F	-15	SER	-	expression tag	UNP P14618
F	-14	HIS	-	expression tag	UNP P14618
F	-13	HIS	-	expression tag	UNP P14618
F	-12	HIS	-	expression tag	UNP P14618
F	-11	HIS	-	expression tag	UNP P14618
F	-10	HIS	-	expression tag	UNP P14618
F	-9	HIS	-	expression tag	UNP P14618
F	-8	SER	-	expression tag	UNP P14618
F	-7	SER	-	expression tag	UNP P14618
F	-6	GLY	-	expression tag	UNP P14618
F	-5	LEU	-	expression tag	UNP P14618
F	-4	VAL	-	expression tag	UNP P14618
F	-3	PRO	-	expression tag	UNP P14618
F	-2	ARG	-	expression tag	UNP P14618
F	-1	GLY	-	expression tag	UNP P14618
F	0	SER	-	expression tag	UNP P14618
G	-18	MET	-	initiating methionine	UNP P14618
G	-17	GLY	-	expression tag	UNP P14618
G	-16	SER	-	expression tag	UNP P14618
G	-15	SER	-	expression tag	UNP P14618
G	-14	HIS	-	expression tag	UNP P14618
G	-13	HIS	-	expression tag	UNP P14618
G	-12	HIS	-	expression tag	UNP P14618
G	-11	HIS	-	expression tag	UNP P14618
G	-10	HIS	-	expression tag	UNP P14618
G	-9	HIS	-	expression tag	UNP P14618
G	-8	SER	-	expression tag	UNP P14618
G	-7	SER	-	expression tag	UNP P14618
G	-6	GLY	-	expression tag	UNP P14618
G	-5	LEU	-	expression tag	UNP P14618
G	-4	VAL	-	expression tag	UNP P14618
G	-3	PRO	-	expression tag	UNP P14618
G	-2	ARG	-	expression tag	UNP P14618
G	-1	GLY	-	expression tag	UNP P14618
G	0	SER	-	expression tag	UNP P14618
H	-18	MET	-	initiating methionine	UNP P14618
H	-17	GLY	-	expression tag	UNP P14618
H	-16	SER	-	expression tag	UNP P14618
H	-15	SER	-	expression tag	UNP P14618
H	-14	HIS	-	expression tag	UNP P14618
H	-13	HIS	-	expression tag	UNP P14618

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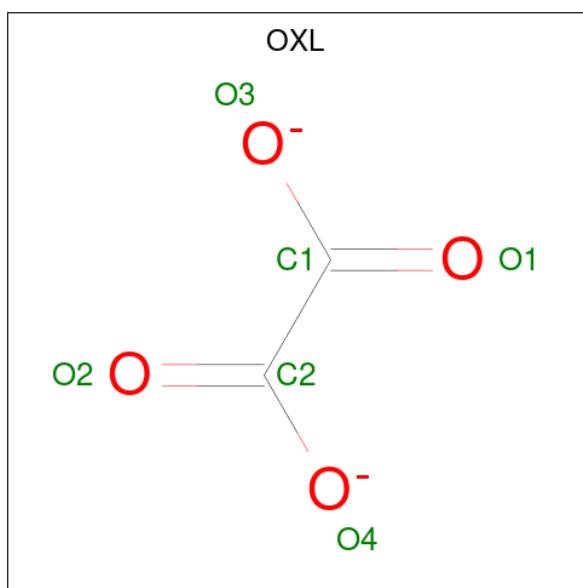
Chain	Residue	Modelled	Actual	Comment	Reference
H	-12	HIS	-	expression tag	UNP P14618
H	-11	HIS	-	expression tag	UNP P14618
H	-10	HIS	-	expression tag	UNP P14618
H	-9	HIS	-	expression tag	UNP P14618
H	-8	SER	-	expression tag	UNP P14618
H	-7	SER	-	expression tag	UNP P14618
H	-6	GLY	-	expression tag	UNP P14618
H	-5	LEU	-	expression tag	UNP P14618
H	-4	VAL	-	expression tag	UNP P14618
H	-3	PRO	-	expression tag	UNP P14618
H	-2	ARG	-	expression tag	UNP P14618
H	-1	GLY	-	expression tag	UNP P14618
H	0	SER	-	expression tag	UNP P14618

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



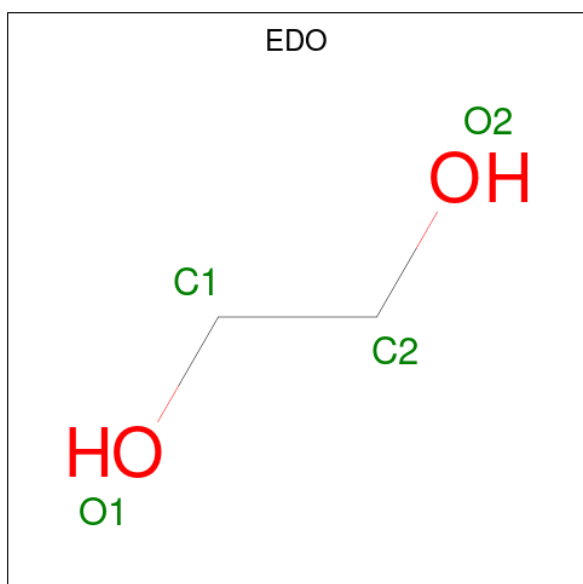
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	E	1	Total	C	O	P	0	0
			20	6	12	2		
2	F	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 3 is OXALATE ION (CCD ID: OXL) (formula: C_2O_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	2	4		
3	C	1	Total	C	O	0	0
			6	2	4		
3	F	1	Total	C	O	0	0
			6	2	4		
3	H	1	Total	C	O	0	0
			6	2	4		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).

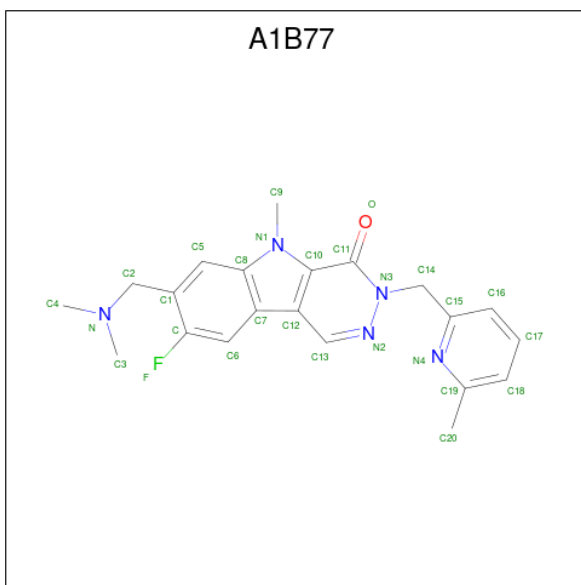


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

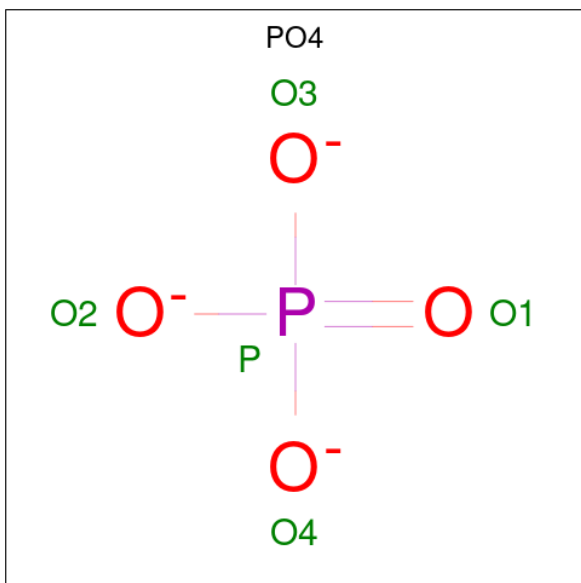
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	B	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0
5	E	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0
5	G	1	Total Mg 1 1	0	0
5	H	1	Total Mg 1 1	0	0

- Molecule 6 is 7-[(dimethylamino)methyl]-8-fluoro-5-methyl-3-[(6-methylpyridin-2-yl)methyl]-3,5-dihydro-4H-pyridazino[4,5-b]indol-4-one (CCD ID: A1B77) (formula: C₂₁H₂₂FN₅O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total 100	C 42	F 2	H 44	N 10	O 2	44	1
6	C	1	Total 100	C 42	F 2	H 44	N 10	O 2	44	1
6	F	1	Total 100	C 42	F 2	H 44	N 10	O 2	44	1
6	H	1	Total 100	C 42	F 2	H 44	N 10	O 2	44	1

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total O P 5 4 1	0	0
7	D	1	Total O P 5 4 1	0	0
7	G	1	Total O P 5 4 1	0	0
7	H	1	Total O P 5 4 1	0	0

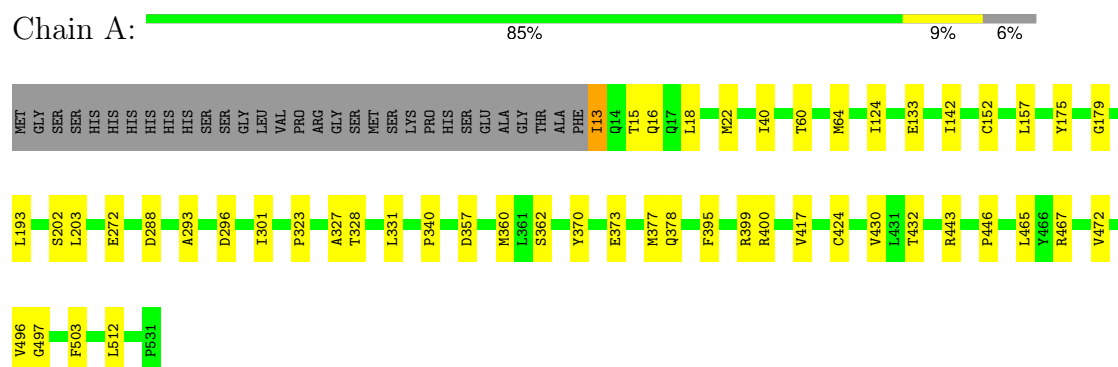
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	167	Total O 167 167	0	0
8	B	182	Total O 182 182	0	0
8	C	117	Total O 117 117	0	0
8	D	127	Total O 127 127	0	0
8	E	168	Total O 168 168	0	0
8	F	165	Total O 165 165	0	0
8	G	128	Total O 128 128	0	0
8	H	118	Total O 118 118	0	0

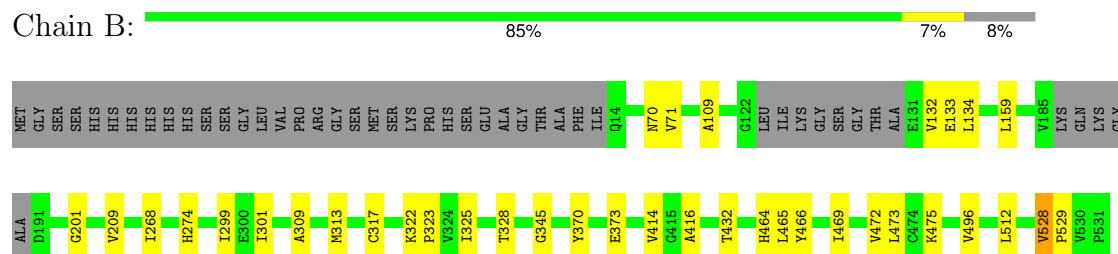
3 Residue-property plots [i](#)

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.

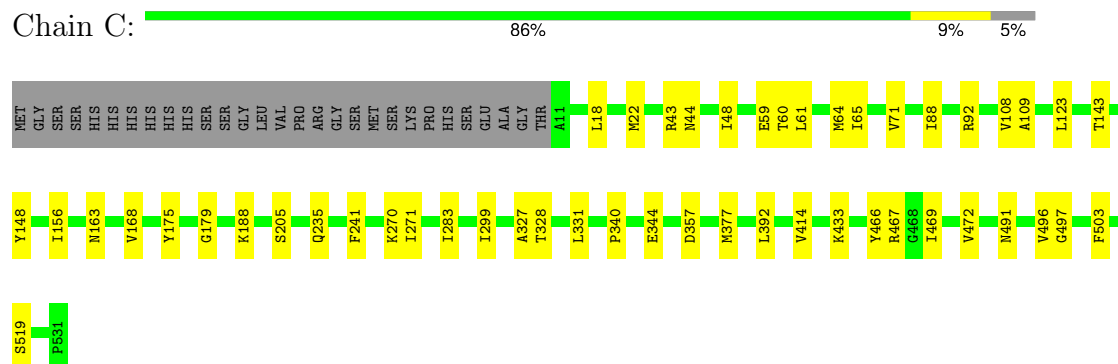
- Molecule 1: Pyruvate kinase PKM




- Molecule 1: Pyruvate kinase PKM

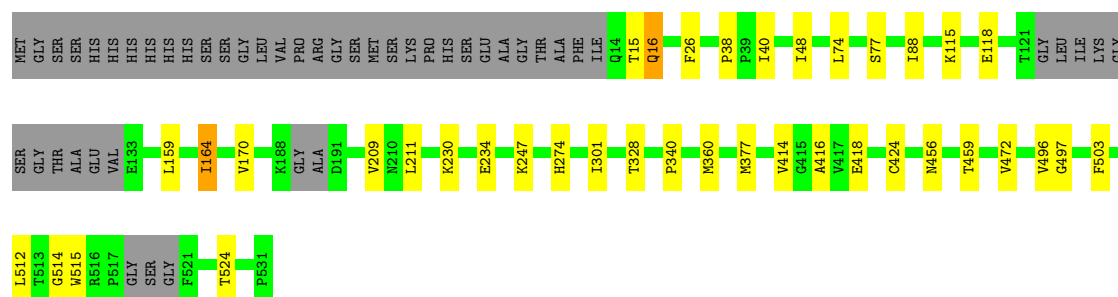


- Molecule 1: Pyruvate kinase PKM




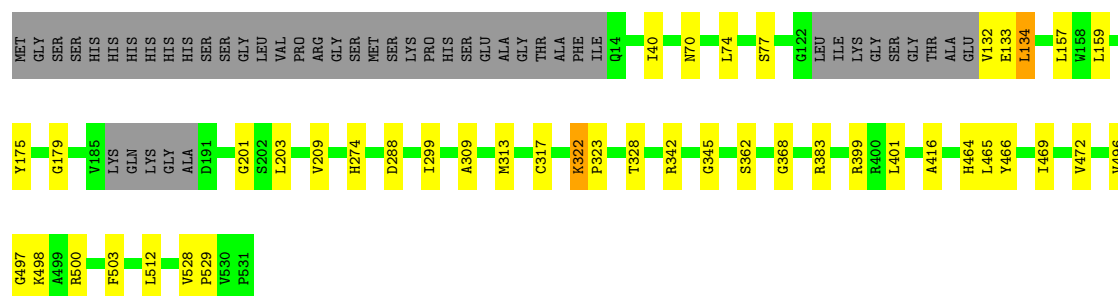
- Molecule 1: Pyruvate kinase PKM

Chain D:  84% 7% 9%




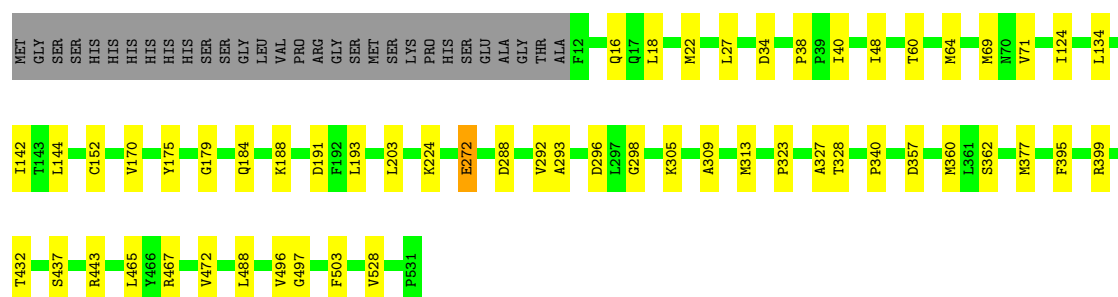
• Molecule 1: Pyruvate kinase PKM

Chain E:  84% 8% 8%




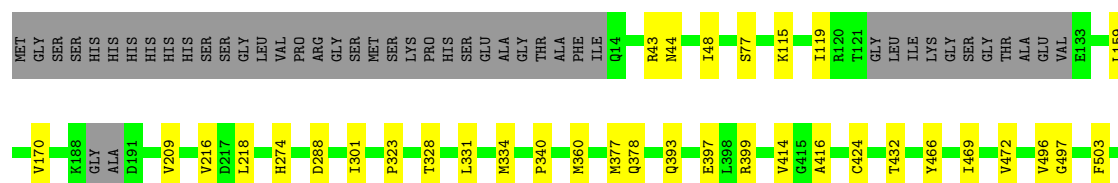
• Molecule 1: Pyruvate kinase PKM

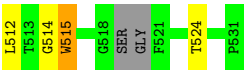
Chain F:  84% 10% 5%



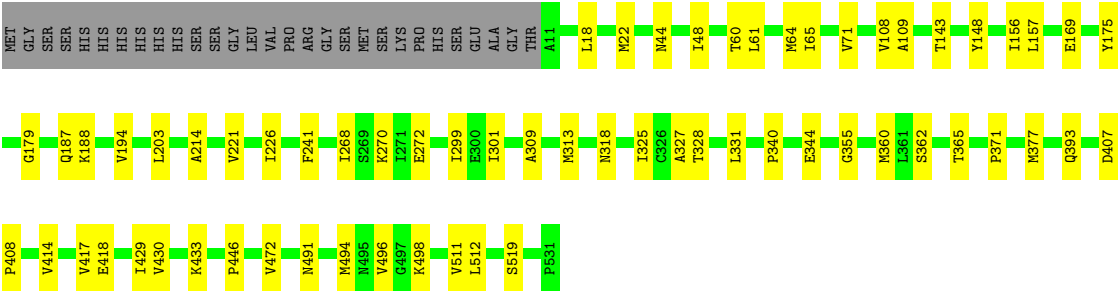
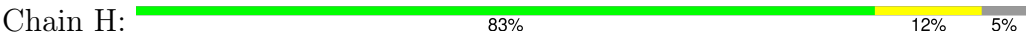
• Molecule 1: Pyruvate kinase PKM

Chain G:  84% 7% 9%





● Molecule 1: Pyruvate kinase PKM



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.81Å 93.86Å 153.66Å 89.73° 89.68° 75.79°	Depositor
Resolution (Å)	45.49 – 2.42 45.49 – 2.42	Depositor EDS
% Data completeness (in resolution range)	92.9 (45.49-2.42) 91.6 (45.49-2.42)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.42Å)	Xtriage
Refinement program	BUSTER 2.10.4 (8-JUN-2022)	Depositor
R, R_{free}	0.186 , 0.226 0.180 , 0.223	Depositor DCC
R_{free} test set	7818 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.429 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32262	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: A1B77, MG, FBP, PO4, EDO, OXL

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	0.71	2/3941 (0.1%)	1.03	2/5341 (0.0%)
1	B	0.71	0/3801	1.05	3/5152 (0.1%)
1	C	0.67	0/3952	1.05	8/5356 (0.1%)
1	D	0.67	0/3762	1.02	1/5104 (0.0%)
1	E	0.72	1/3807 (0.0%)	1.06	4/5158 (0.1%)
1	F	0.72	1/3942 (0.0%)	1.03	2/5343 (0.0%)
1	G	0.67	0/3769	1.03	3/5114 (0.1%)
1	H	0.68	1/3942 (0.0%)	1.05	7/5343 (0.1%)
All	All	0.69	5/30916 (0.0%)	1.04	30/41911 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	362	SER	CA-C	5.56	1.55	1.52
1	F	362	SER	CA-C	5.48	1.55	1.52
1	H	362	SER	CA-C	5.41	1.55	1.52
1	A	301	ILE	CA-C	5.12	1.56	1.52
1	E	362	SER	CA-C	5.11	1.55	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	43	ARG	CA-C-N	6.88	129.49	120.28
1	C	43	ARG	C-N-CA	6.88	129.49	120.28
1	G	43	ARG	CA-C-N	6.39	129.37	120.29
1	G	43	ARG	C-N-CA	6.39	129.37	120.29
1	E	299	ILE	N-CA-C	-6.36	105.54	111.45

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	3877	0	3853	26	0
1	B	3738	0	3660	17	0
1	C	3887	0	3876	25	0
1	D	3703	0	3599	18	0
1	E	3744	0	3678	22	0
1	F	3878	0	3851	29	0
1	G	3708	0	3599	19	0
1	H	3878	121	3867	30	0
2	A	20	0	10	1	0
2	B	20	0	10	1	0
2	E	20	0	10	0	0
2	F	20	0	10	2	0
3	A	6	0	0	0	0
3	C	6	0	0	0	0
3	F	6	0	0	0	0
3	H	6	0	0	0	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
4	E	4	0	6	0	0
4	G	4	0	6	0	0
4	H	4	0	6	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	B	56	44	0	0	0
6	C	56	44	0	0	0
6	F	56	44	0	0	0
6	H	56	44	0	1	0
7	C	5	0	0	3	0
7	D	5	0	0	0	0
7	G	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	5	0	0	2	0
8	A	167	0	0	0	0
8	B	182	0	0	0	0
8	C	117	0	0	0	0
8	D	127	0	0	0	0
8	E	168	0	0	2	0
8	F	165	0	0	1	0
8	G	128	0	0	0	0
8	H	118	0	0	0	0
All	All	31965	297	30059	180	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 3.

The worst 5 of 180 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:472:VAL:HG11	1:D:496:VAL:HG11	1.72	0.71
1:G:514:GLY:O	1:G:515:TRP:HB3	1.90	0.71
1:H:187:GLN:HB2	1:H:194:VAL:HB	1.73	0.70
1:C:71:VAL:HG22	1:C:109:ALA:HB3	1.73	0.70
1:B:466:TYR:HB2	1:B:469:ILE:HD12	1.74	0.68

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	517/550 (94%)	506 (98%)	10 (2%)	1 (0%)	44 58
1	B	500/550 (91%)	487 (97%)	10 (2%)	3 (1%)	22 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	519/550 (94%)	508 (98%)	10 (2%)	1 (0%)	44	58
1	D	494/550 (90%)	478 (97%)	15 (3%)	1 (0%)	44	58
1	E	499/550 (91%)	489 (98%)	8 (2%)	2 (0%)	30	42
1	F	518/550 (94%)	501 (97%)	16 (3%)	1 (0%)	44	58
1	G	495/550 (90%)	480 (97%)	13 (3%)	2 (0%)	30	42
1	H	519/550 (94%)	504 (97%)	14 (3%)	1 (0%)	44	58
All	All	4061/4400 (92%)	3953 (97%)	96 (2%)	12 (0%)	37	50

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	515	TRP
1	B	134	LEU
1	E	134	LEU
1	B	328	THR
1	D	328	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	397/452 (88%)	395 (100%)	2 (0%)	86	94
1	B	373/452 (82%)	372 (100%)	1 (0%)	91	96
1	C	398/452 (88%)	394 (99%)	4 (1%)	73	85
1	D	368/452 (81%)	362 (98%)	6 (2%)	58	75
1	E	376/452 (83%)	371 (99%)	5 (1%)	65	80
1	F	396/452 (88%)	390 (98%)	6 (2%)	60	77
1	G	367/452 (81%)	364 (99%)	3 (1%)	79	89
1	H	396/452 (88%)	391 (99%)	5 (1%)	65	80
All	All	3071/3616 (85%)	3039 (99%)	32 (1%)	73	85

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	301	ILE
1	H	414	VAL
1	D	424	CYS
1	D	414	VAL
1	H	433	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	210	ASN
1	H	318	ASN
1	E	274	HIS
1	H	458	GLN
1	H	44	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 8 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
6	A1B77	H	602[B]	-	27,31,31	0.68	0	33,46,46	0.74	1 (3%)
7	PO4	C	605	-	4,4,4	0.10	0	6,6,6	0.31	0
7	PO4	D	602	-	4,4,4	0.18	0	6,6,6	0.23	0
6	A1B77	C	602[A]	-	27,31,31	0.67	0	33,46,46	0.75	1 (3%)
7	PO4	H	605	-	4,4,4	0.47	0	6,6,6	0.35	0
2	FBP	B	602	-	18,20,20	0.60	0	21,32,32	1.07	0
2	FBP	A	601	-	18,20,20	0.80	1 (5%)	21,32,32	1.14	1 (4%)
3	OXL	A	602	5	5,5,5	1.70	2 (40%)	6,6,6	1.70	1 (16%)
6	A1B77	C	602[B]	-	27,31,31	0.70	0	33,46,46	0.77	1 (3%)
7	PO4	G	603	-	4,4,4	0.09	0	6,6,6	0.33	0
4	EDO	E	602	-	3,3,3	0.07	0	2,2,2	0.53	0
6	A1B77	B	601[A]	-	27,31,31	0.68	0	33,46,46	0.76	1 (3%)
4	EDO	C	603	-	3,3,3	0.23	0	2,2,2	0.30	0
4	EDO	B	603	-	3,3,3	0.16	0	2,2,2	0.35	0
6	A1B77	F	601[A]	-	27,31,31	0.69	0	33,46,46	0.74	1 (3%)
6	A1B77	B	601[B]	-	27,31,31	0.70	0	33,46,46	0.75	1 (3%)
4	EDO	H	603	-	3,3,3	0.37	0	2,2,2	0.18	0
2	FBP	F	602	-	18,20,20	0.78	1 (5%)	21,32,32	1.12	0
4	EDO	G	601	-	3,3,3	0.12	0	2,2,2	0.38	0
3	OXL	C	601	5	5,5,5	1.72	2 (40%)	6,6,6	1.68	2 (33%)
6	A1B77	H	602[A]	-	27,31,31	0.71	0	33,46,46	0.75	1 (3%)
4	EDO	A	603	-	3,3,3	0.23	0	2,2,2	0.36	0
6	A1B77	F	601[B]	-	27,31,31	0.68	0	33,46,46	0.74	1 (3%)
2	FBP	E	601	-	18,20,20	0.66	0	21,32,32	1.11	1 (4%)
3	OXL	F	603	5	5,5,5	1.76	2 (40%)	6,6,6	1.69	2 (33%)
3	OXL	H	601	5	5,5,5	1.71	2 (40%)	6,6,6	1.69	2 (33%)

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
6	A1B77	H	602[B]	-	-	3/8/8/8	0/4/4/4
6	A1B77	C	602[A]	-	-	2/8/8/8	0/4/4/4
2	FBP	B	602	-	-	3/13/32/32	0/1/1/1
2	FBP	A	601	-	-	6/13/32/32	0/1/1/1
3	OXL	A	602	5	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	A1B77	C	602[B]	-	-	1/8/8/8	0/4/4/4
4	EDO	E	602	-	-	0/1/1/1	-
6	A1B77	B	601[A]	-	-	1/8/8/8	0/4/4/4
4	EDO	C	603	-	-	0/1/1/1	-
4	EDO	B	603	-	-	0/1/1/1	-
6	A1B77	F	601[A]	-	-	1/8/8/8	0/4/4/4
6	A1B77	B	601[B]	-	-	1/8/8/8	0/4/4/4
4	EDO	H	603	-	-	1/1/1/1	-
2	FBP	F	602	-	-	7/13/32/32	0/1/1/1
4	EDO	G	601	-	-	0/1/1/1	-
3	OXL	C	601	5	-	0/4/4/4	-
6	A1B77	H	602[A]	-	-	1/8/8/8	0/4/4/4
4	EDO	A	603	-	-	0/1/1/1	-
6	A1B77	F	601[B]	-	-	0/8/8/8	0/4/4/4
2	FBP	E	601	-	-	2/13/32/32	0/1/1/1
3	OXL	F	603	5	-	0/4/4/4	-
3	OXL	H	601	5	-	0/4/4/4	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	603	OXL	O3-C1	-2.92	1.22	1.30
3	A	602	OXL	O3-C1	-2.89	1.22	1.30
3	C	601	OXL	O4-C2	-2.76	1.23	1.30
3	H	601	OXL	O4-C2	-2.74	1.23	1.30
3	F	603	OXL	O4-C2	-2.49	1.23	1.30

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	602[B]	A1B77	C9-N1-C10	3.00	127.78	124.49
6	B	601[B]	A1B77	C9-N1-C10	2.98	127.75	124.49
6	F	601[A]	A1B77	C9-N1-C10	2.96	127.74	124.49
6	C	602[B]	A1B77	C9-N1-C10	2.96	127.73	124.49
6	C	602[A]	A1B77	C9-N1-C10	2.94	127.72	124.49

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FBP	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	A	601	FBP	O1-C1-C2-C3
2	A	601	FBP	O1-C1-C2-O5
2	F	602	FBP	C1-O1-P1-O2P
2	F	602	FBP	C1-O1-P1-O3P

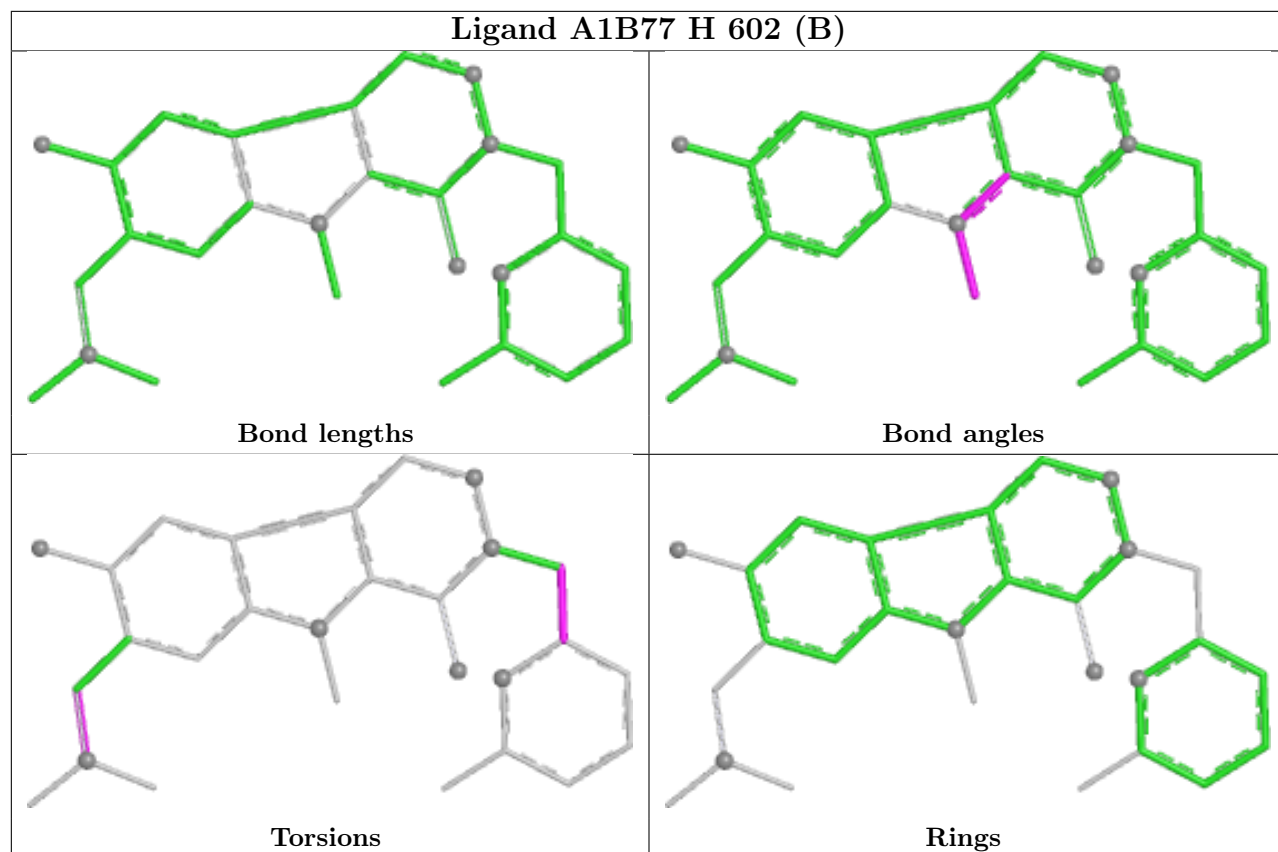
There are no ring outliers.

7 monomers are involved in 11 short contacts:

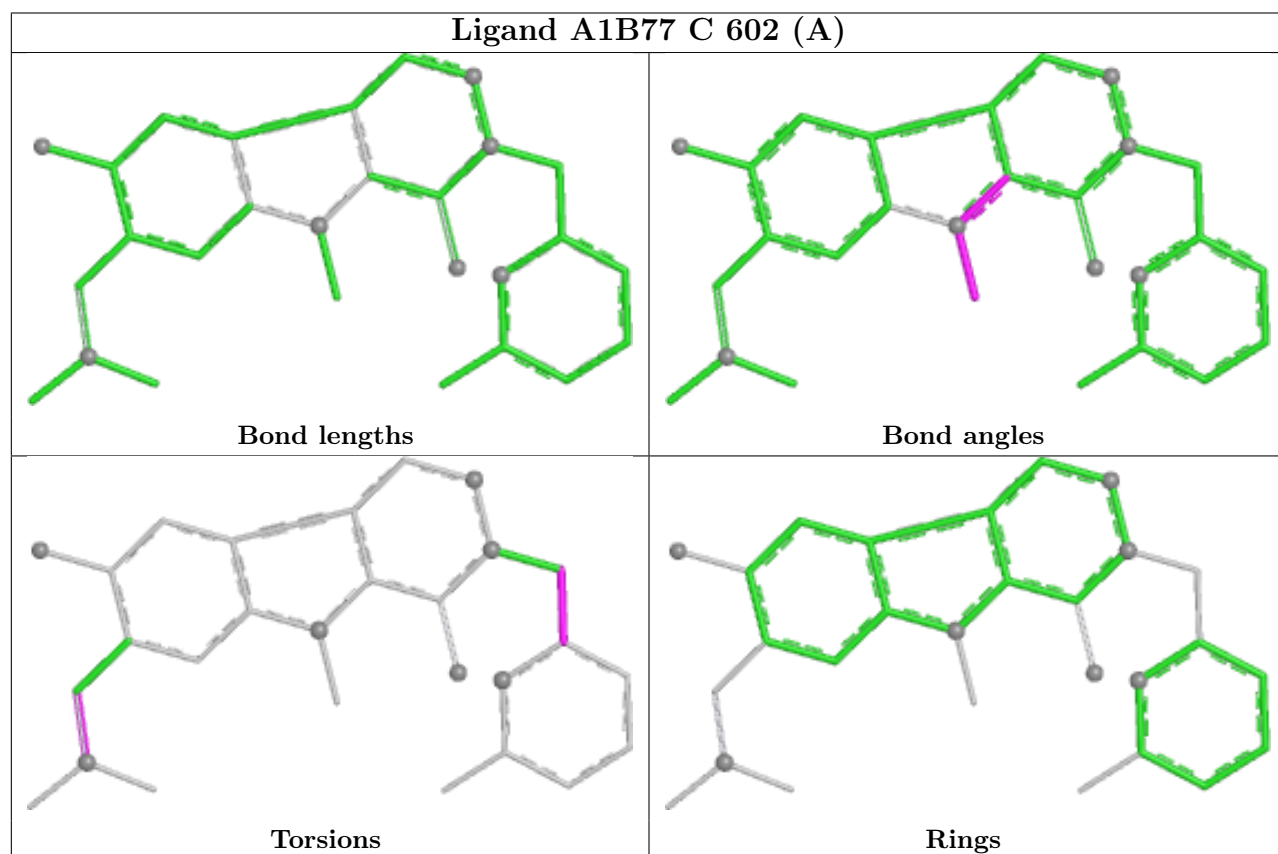
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	602[B]	A1B77	1	0
7	C	605	PO4	3	0
7	H	605	PO4	2	0
2	B	602	FBP	1	0
2	A	601	FBP	1	0
7	G	603	PO4	1	0
2	F	602	FBP	2	0

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

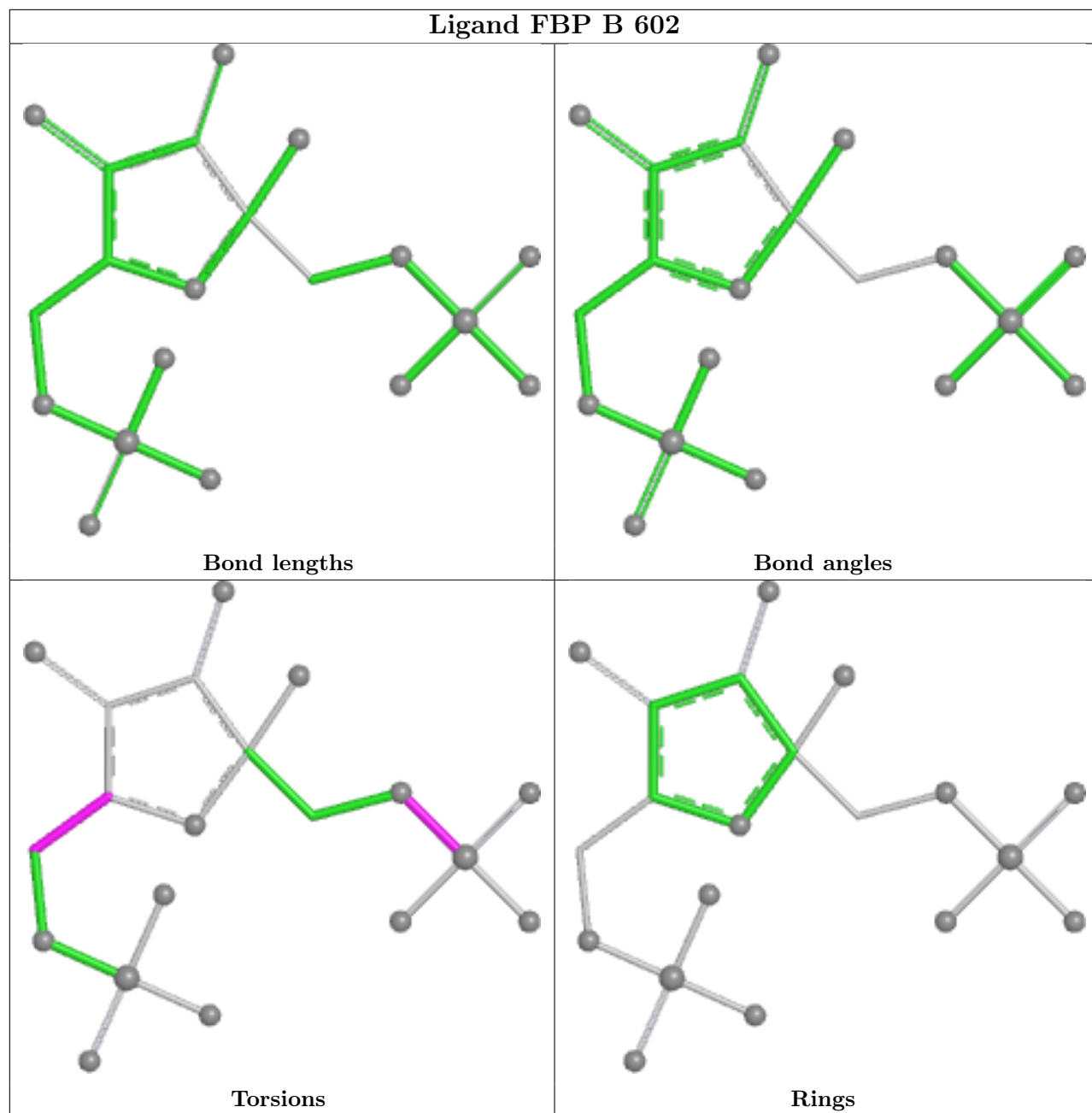
Ligand A1B77 H 602 (B)



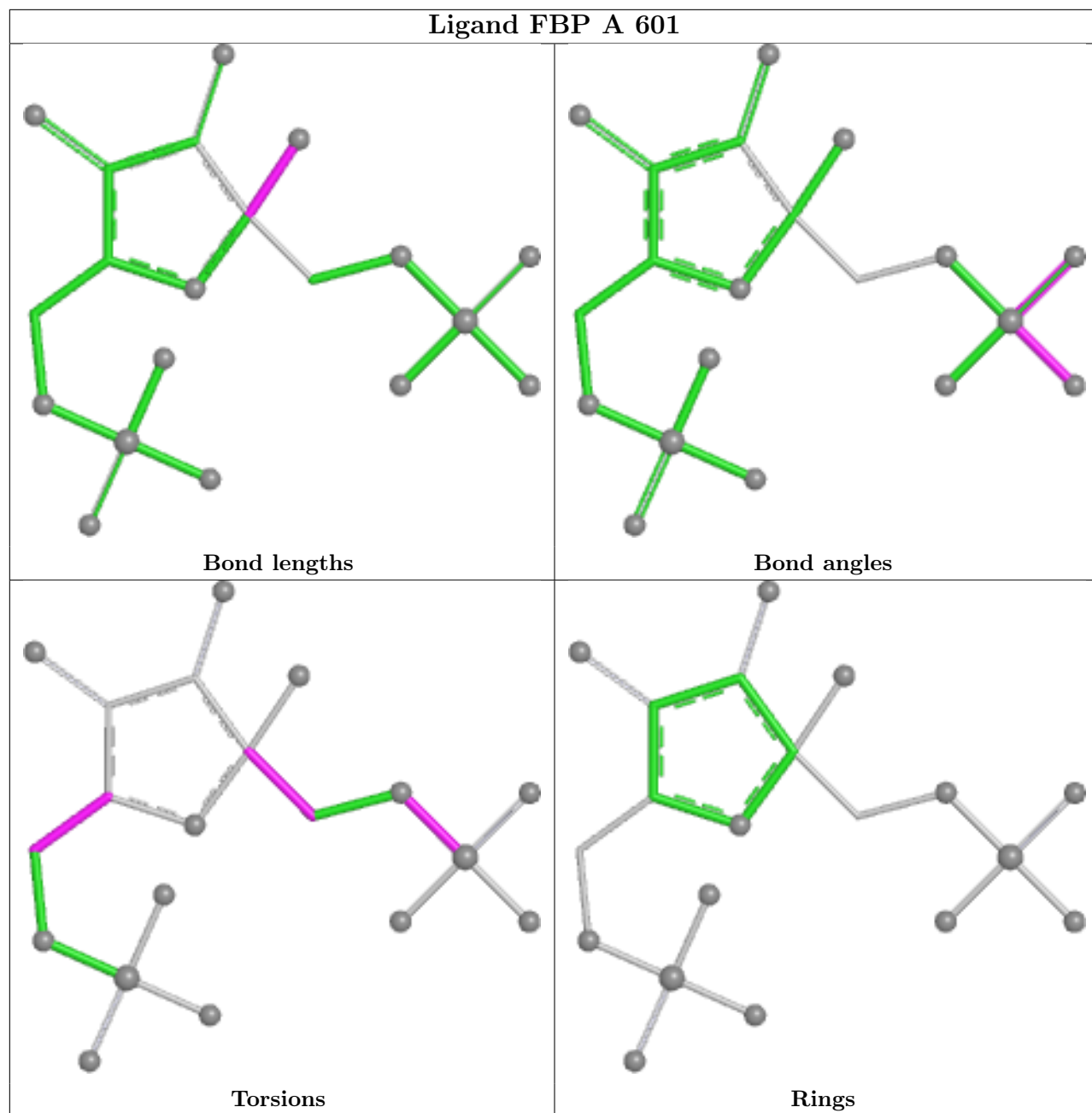
Ligand A1B77 C 602 (A)



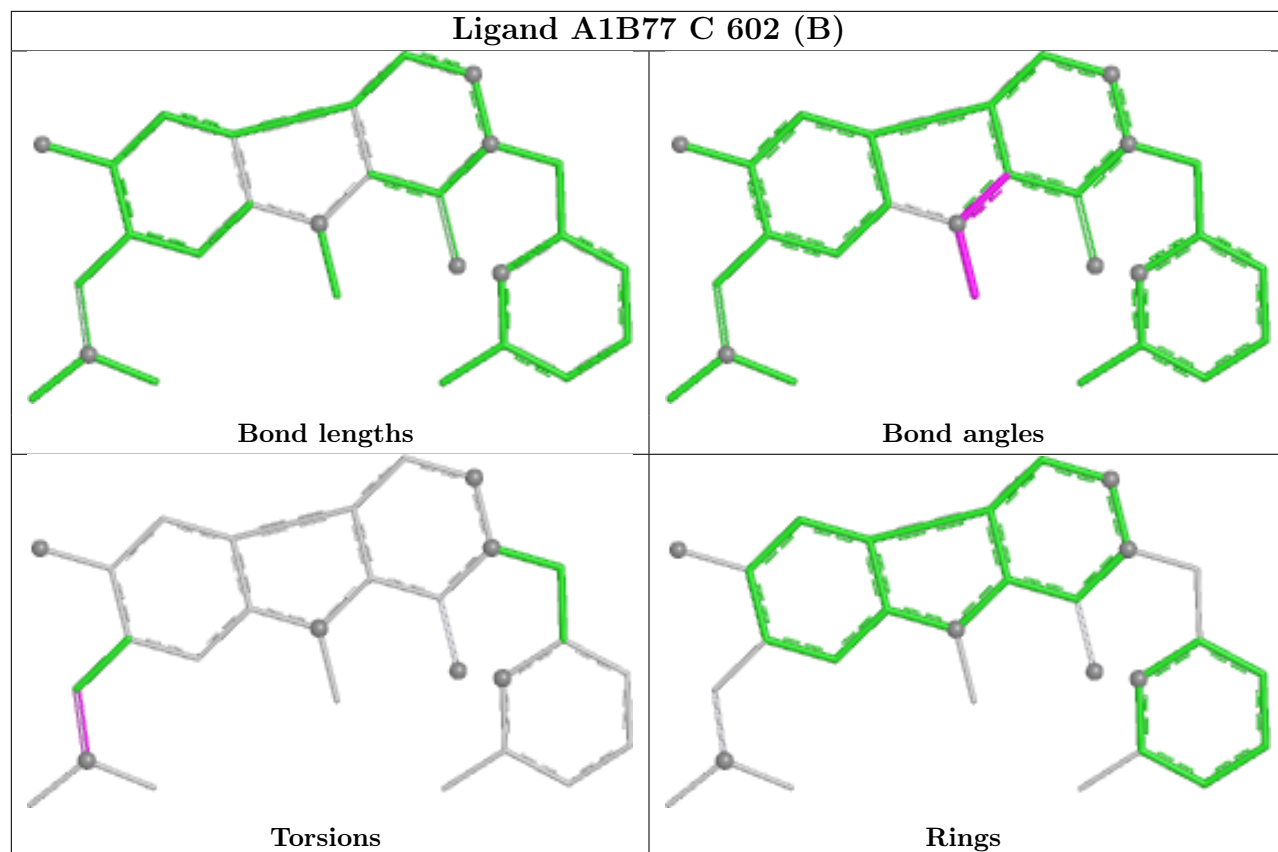
Ligand FBP B 602



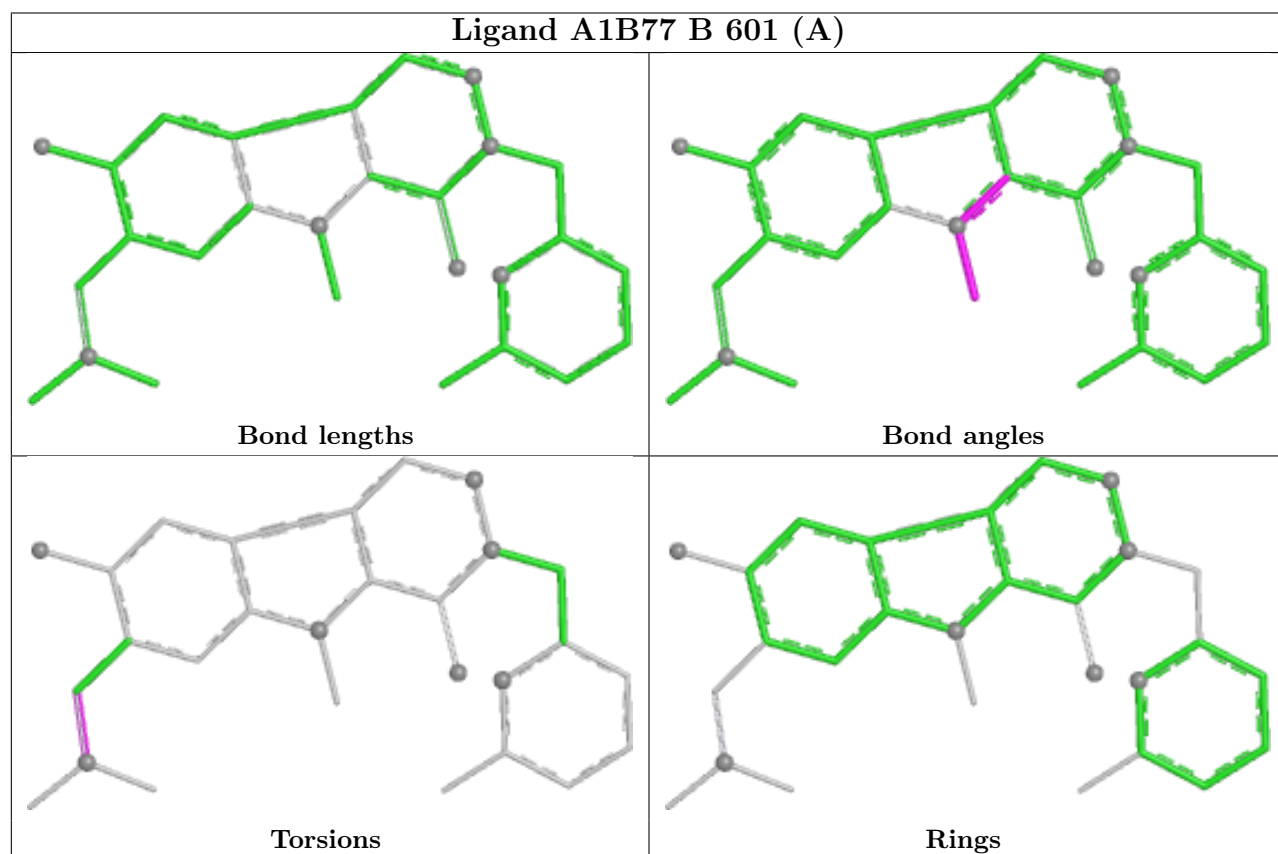
Ligand FBP A 601



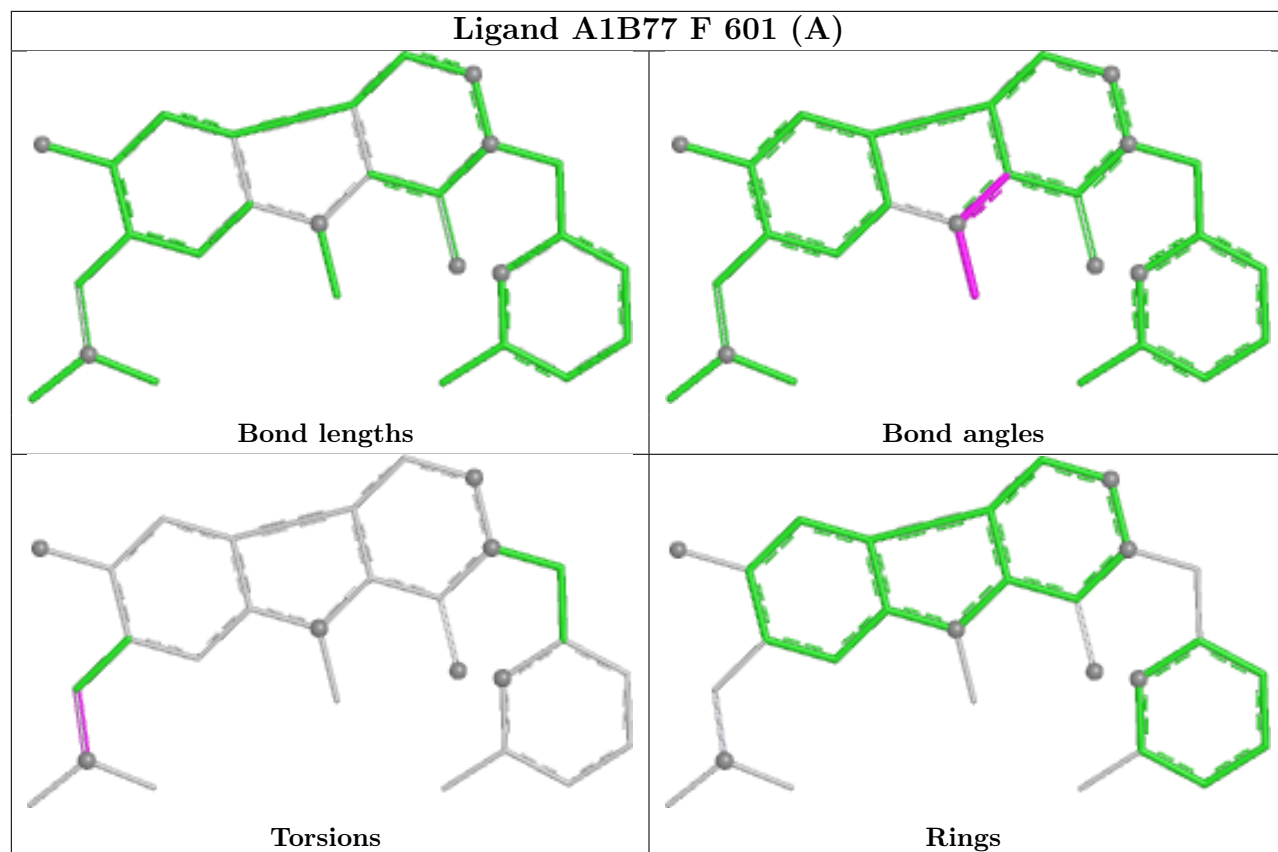
Ligand A1B77 C 602 (B)



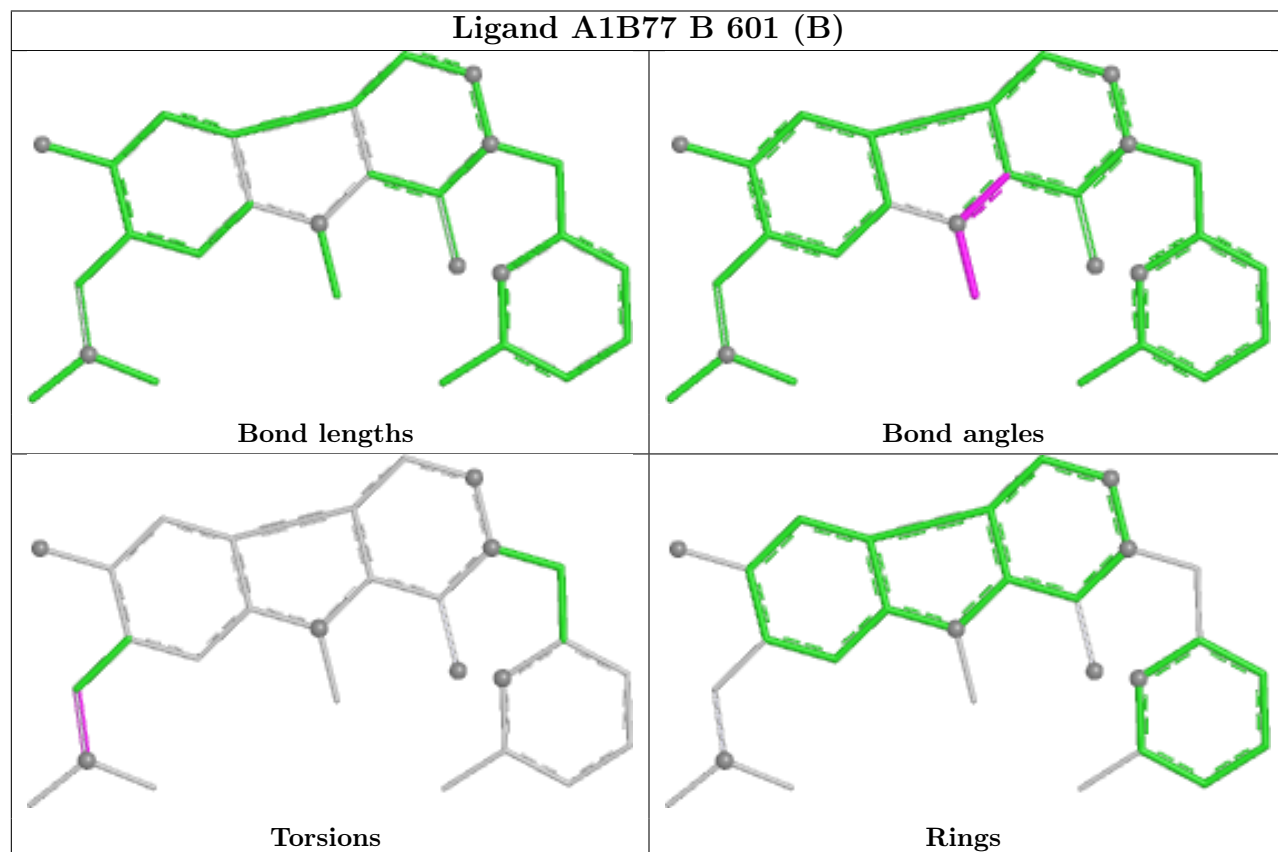
Ligand A1B77 B 601 (A)



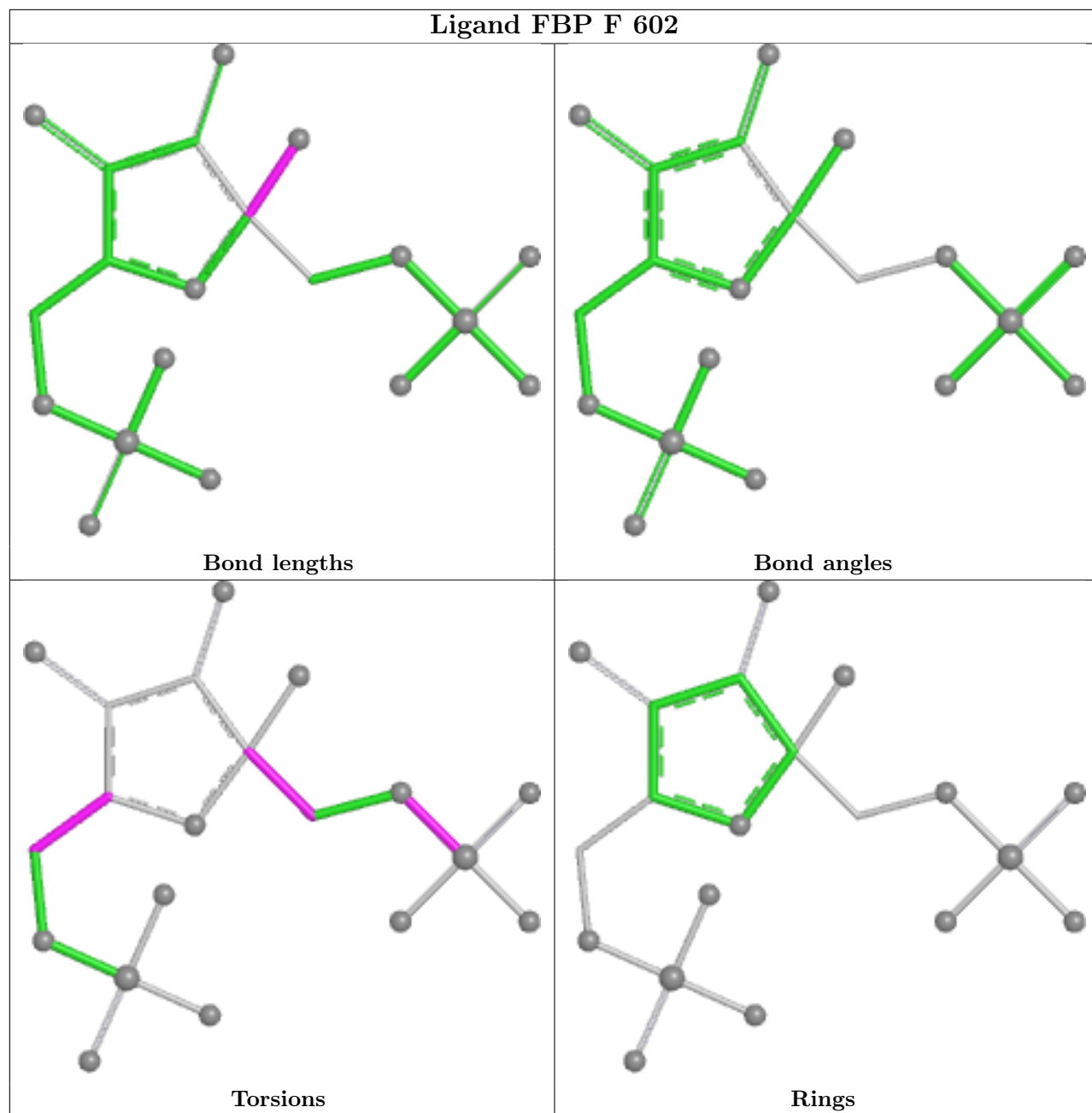
Ligand A1B77 F 601 (A)



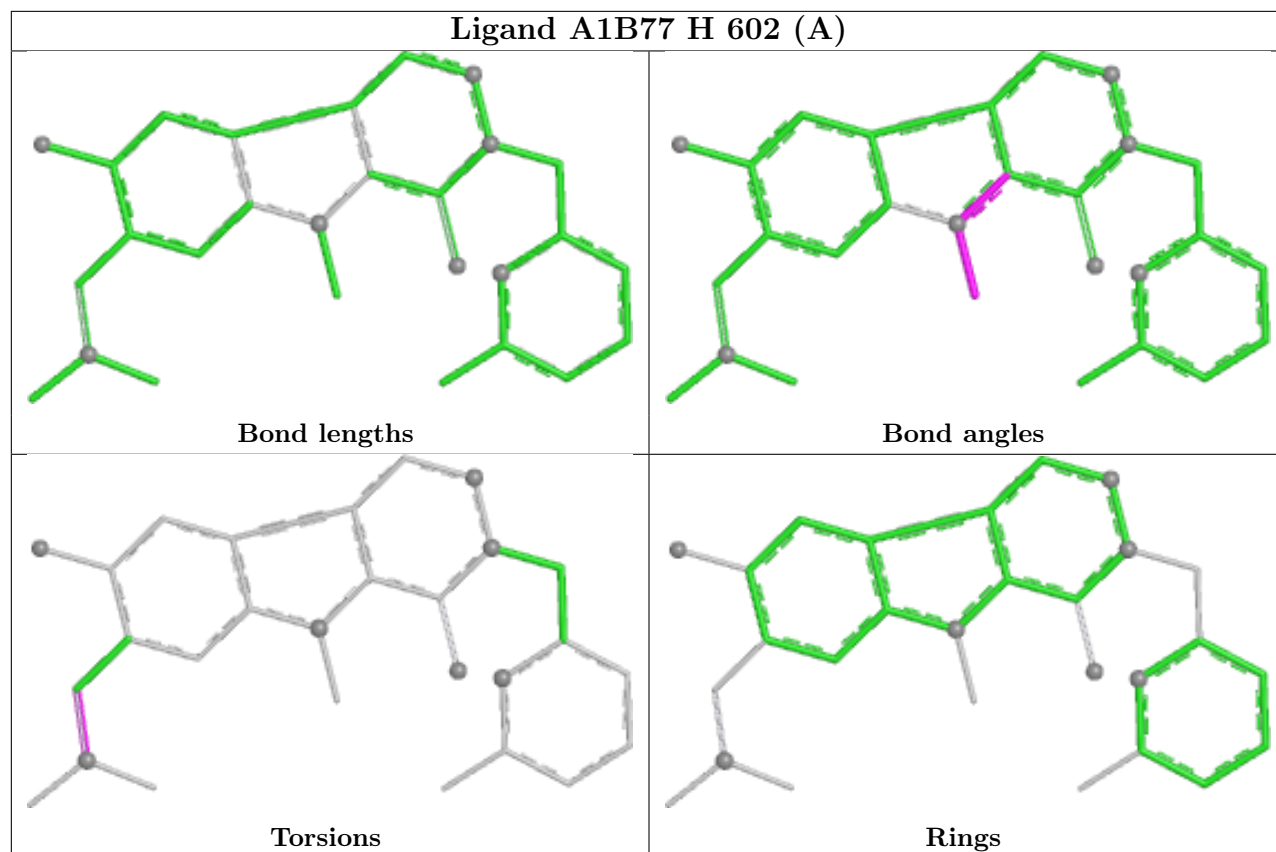
Ligand A1B77 B 601 (B)



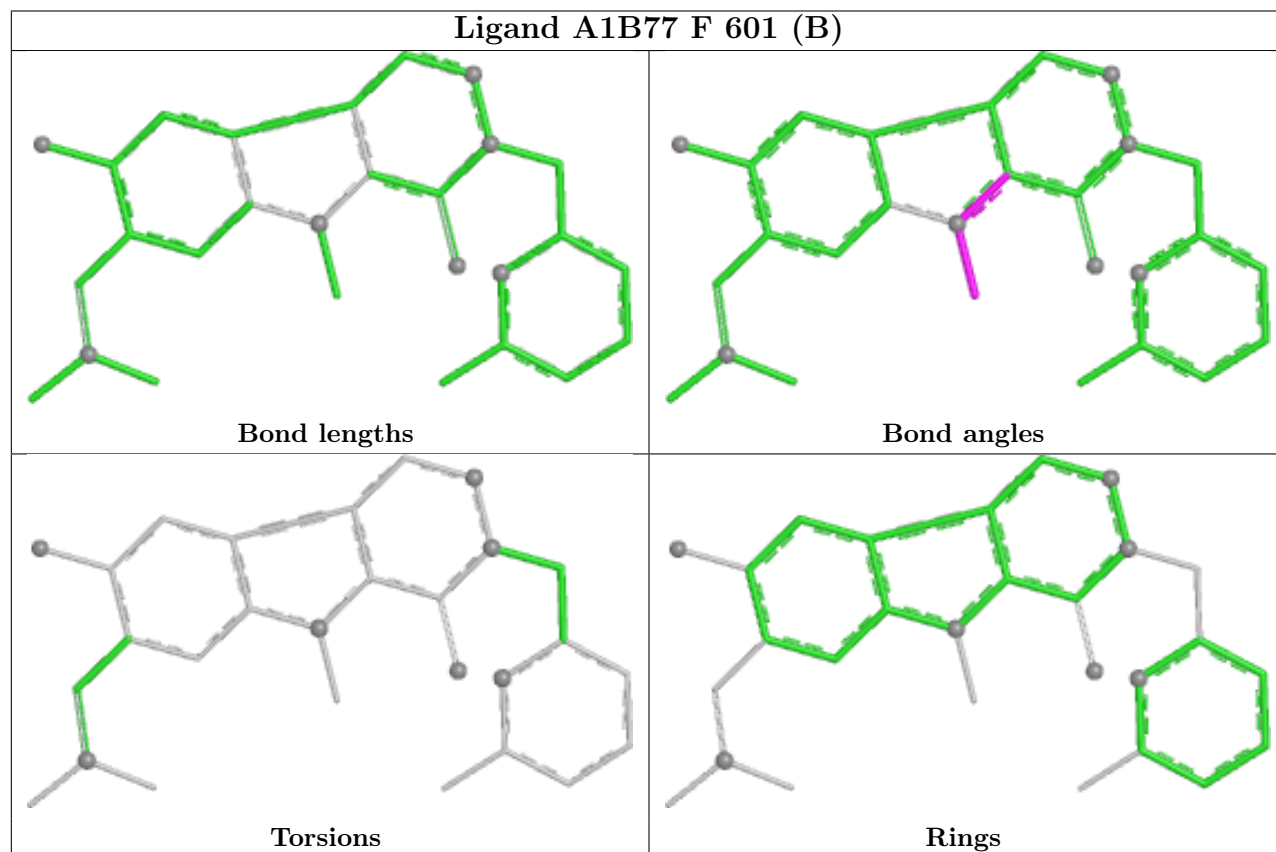
Ligand FBP F 602

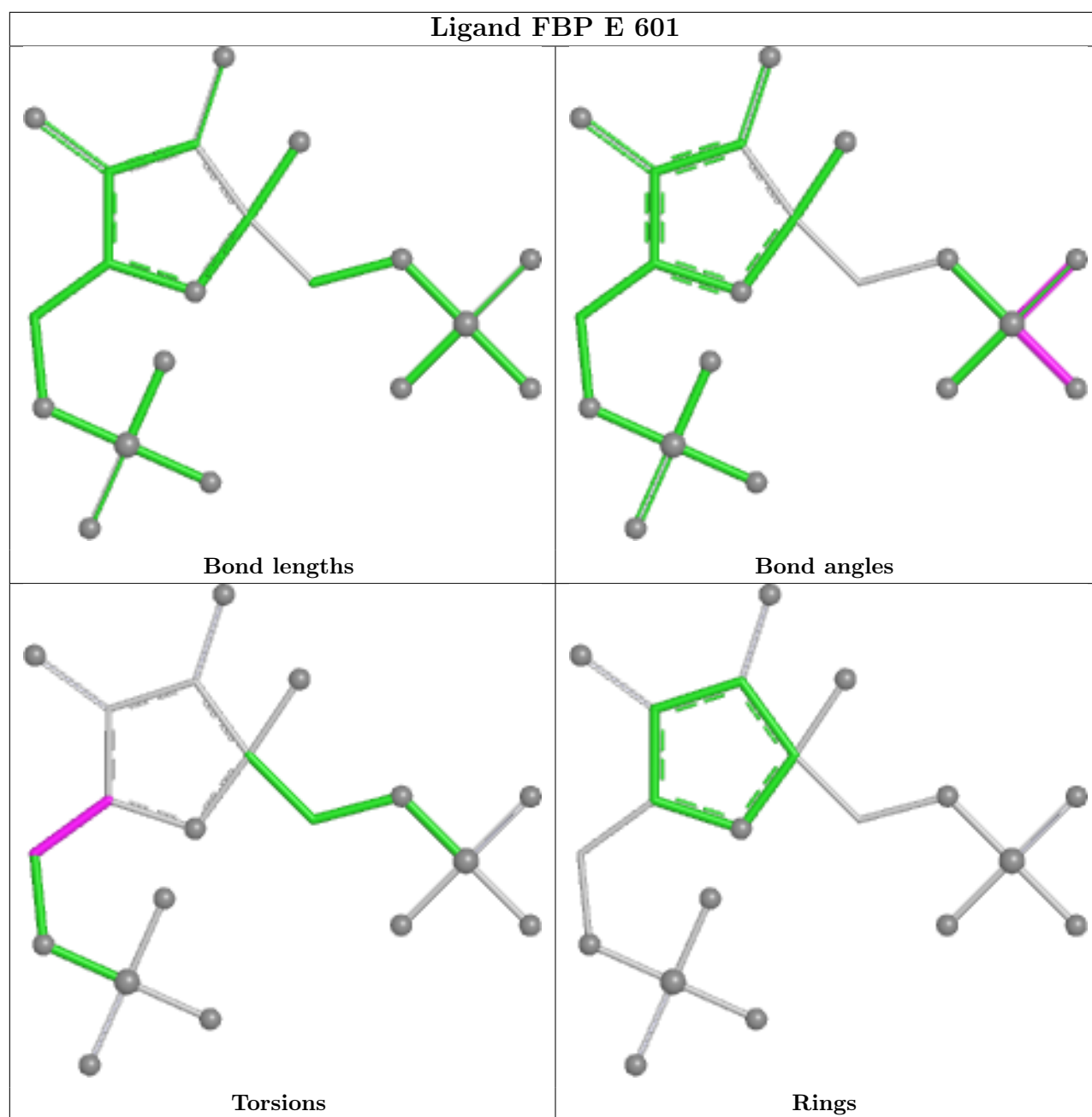


Ligand A1B77 H 602 (A)



Ligand A1B77 F 601 (B)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	519/550 (94%)	-1.30	0 100 100	20, 39, 123, 146	0
1	B	505/550 (91%)	-1.41	0 100 100	15, 40, 93, 119	1 (0%)
1	C	521/550 (94%)	-1.40	0 100 100	24, 49, 73, 90	0
1	D	502/550 (91%)	-1.28	0 100 100	23, 48, 107, 134	0
1	E	504/550 (91%)	-1.37	0 100 100	15, 40, 97, 120	1 (0%)
1	F	520/550 (94%)	-1.31	0 100 100	20, 39, 125, 148	0
1	G	503/550 (91%)	-1.28	0 100 100	24, 47, 110, 128	0
1	H	521/550 (94%)	-1.41	0 100 100	16, 49, 71, 87	0
All	All	4095/4400 (93%)	-1.35	0 100 100	15, 44, 106, 148	2 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

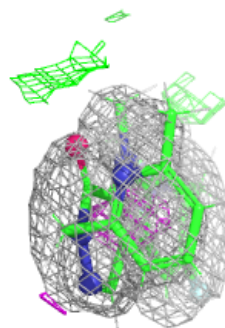
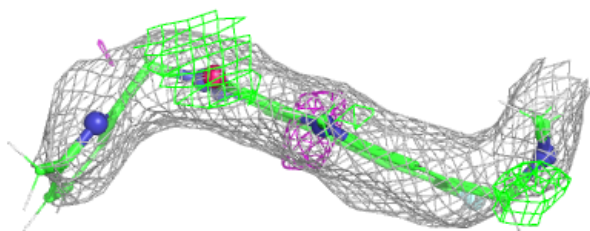
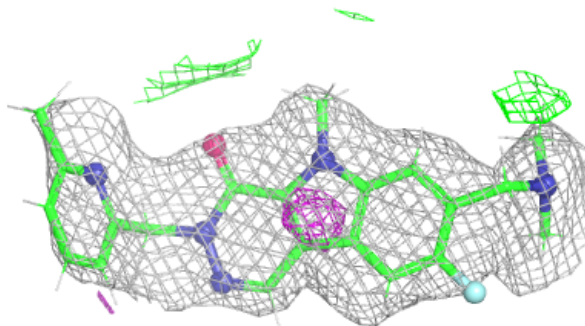
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	A	603	4/4	0.98	0.06	53,53,53,53	0
4	EDO	C	603	4/4	0.98	0.09	68,68,68,68	0
5	MG	B	604	1/1	0.98	0.07	65,65,65,65	0
5	MG	G	602	1/1	0.98	0.05	61,61,61,61	0
6	A1B77	B	601[A]	28/28	0.98	0.05	25,27,29,29	50
6	A1B77	B	601[B]	28/28	0.98	0.05	24,27,30,30	50
3	OXL	H	601	6/6	0.99	0.04	56,56,56,56	0
2	FBP	A	601	20/20	0.99	0.04	53,66,74,74	0
4	EDO	B	603	4/4	0.99	0.03	41,41,41,41	0
2	FBP	E	601	20/20	0.99	0.03	27,31,36,36	0
4	EDO	E	602	4/4	0.99	0.04	40,41,41,41	0
4	EDO	G	601	4/4	0.99	0.04	48,48,48,48	0
4	EDO	H	603	4/4	0.99	0.05	55,55,55,55	0
5	MG	A	604	1/1	0.99	0.03	38,38,38,38	0
2	FBP	F	602	20/20	0.99	0.04	60,72,79,79	0
5	MG	C	604	1/1	0.99	0.02	47,47,47,47	0
5	MG	D	601	1/1	0.99	0.06	61,61,61,61	0
5	MG	E	603	1/1	0.99	0.07	54,54,54,54	0
5	MG	F	604	1/1	0.99	0.03	40,40,40,40	0
3	OXL	A	602	6/6	0.99	0.03	43,44,45,45	0
5	MG	H	604	1/1	0.99	0.02	49,49,49,49	0
3	OXL	C	601	6/6	0.99	0.03	53,54,54,54	0
3	OXL	F	603	6/6	0.99	0.03	43,44,45,46	0
6	A1B77	C	602[A]	28/28	0.99	0.05	28,30,33,33	50
6	A1B77	C	602[B]	28/28	0.99	0.05	28,30,32,32	50
6	A1B77	F	601[A]	28/28	0.99	0.04	20,22,25,25	50
6	A1B77	F	601[B]	28/28	0.99	0.04	41,42,43,43	50
6	A1B77	H	602[A]	28/28	0.99	0.04	28,30,33,33	50
6	A1B77	H	602[B]	28/28	0.99	0.04	33,36,38,38	50
7	PO4	D	602	5/5	0.99	0.03	62,62,62,63	0
7	PO4	G	603	5/5	0.99	0.03	60,60,61,61	0
2	FBP	B	602	20/20	1.00	0.03	28,32,37,38	0
7	PO4	C	605	5/5	1.00	0.02	51,51,52,52	0
7	PO4	H	605	5/5	1.00	0.03	45,45,46,46	0

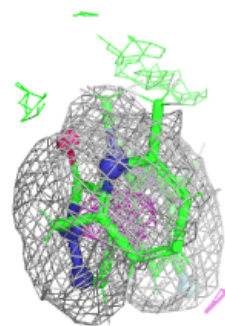
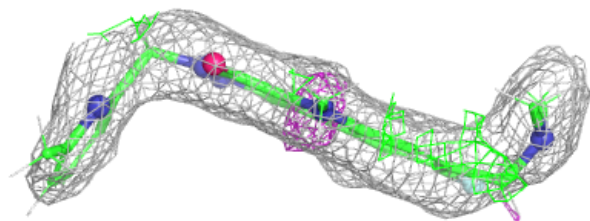
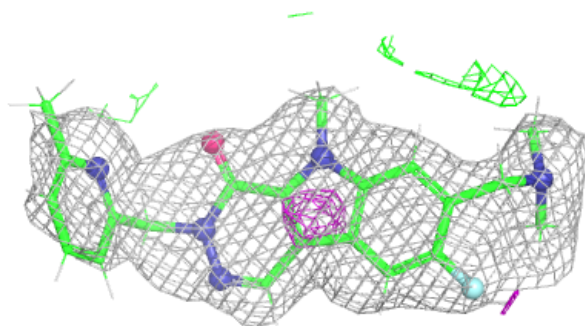
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1B77 B 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)

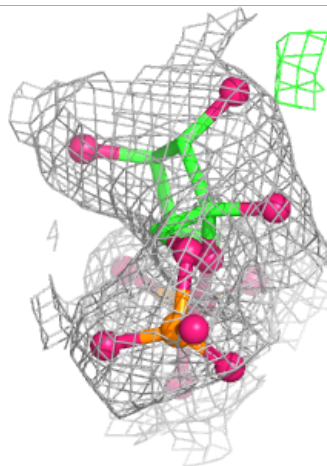
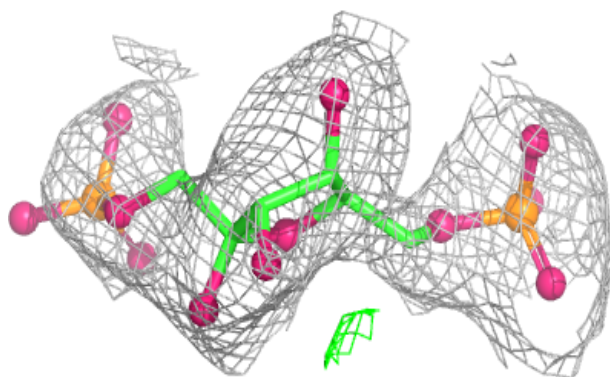
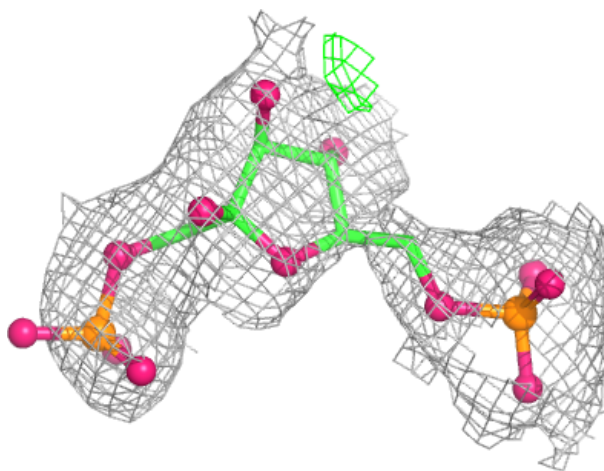
**Electron density around A1B77 B 601 (B):**

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



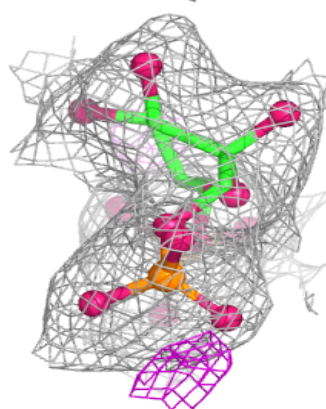
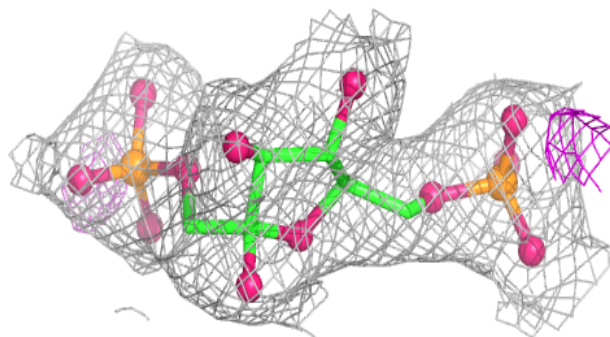
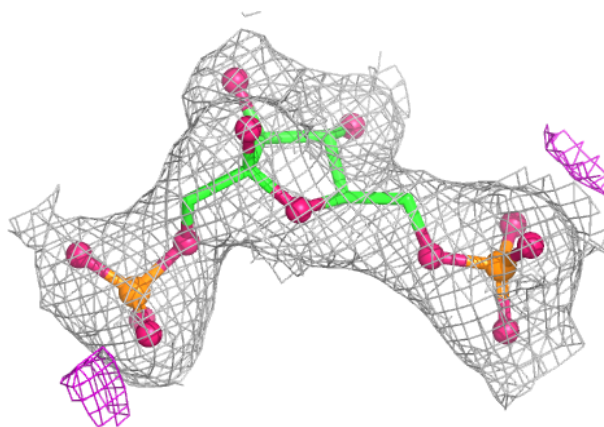
Electron density around FBP A 601:

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



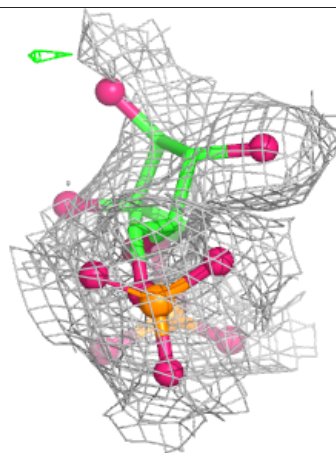
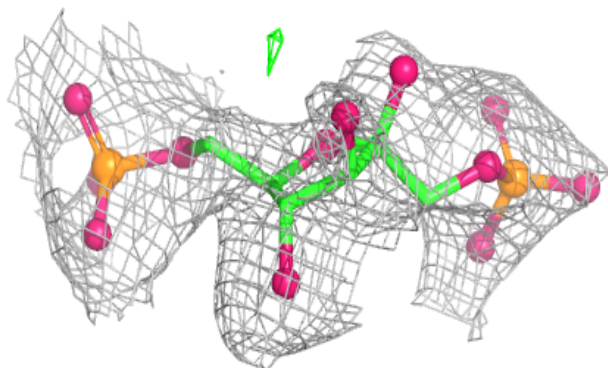
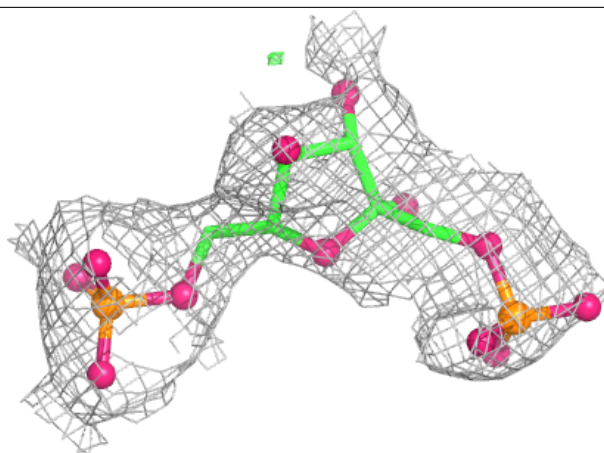
Electron density around FBP E 601:

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

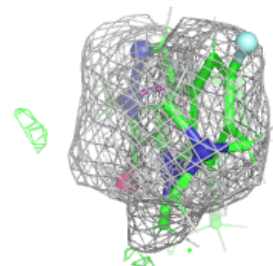
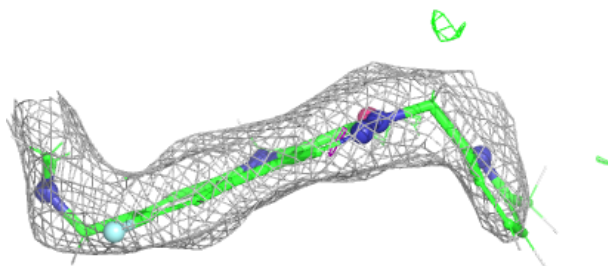
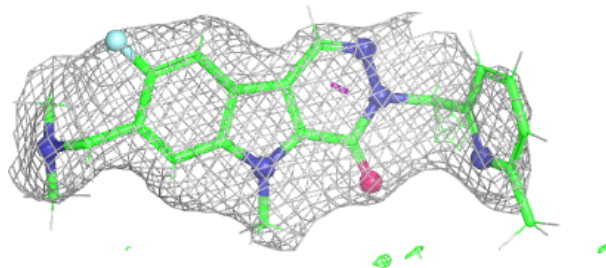


Electron density around FBP F 602:

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

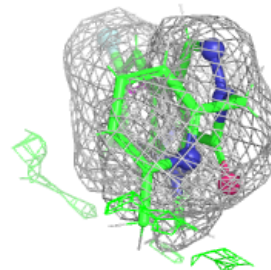
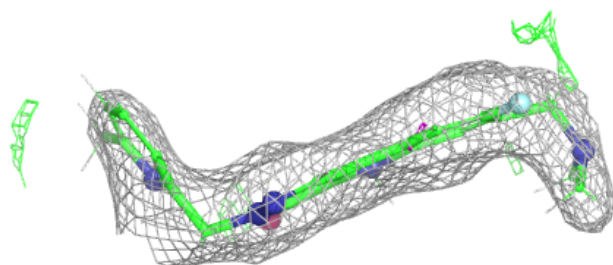
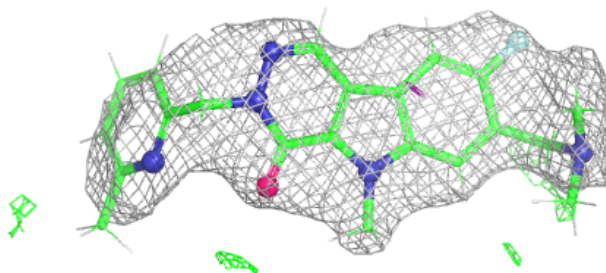
**Electron density around A1B77 C 602 (A):**

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

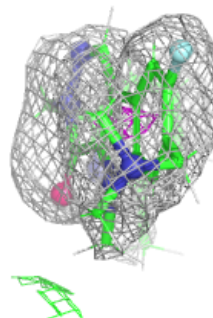
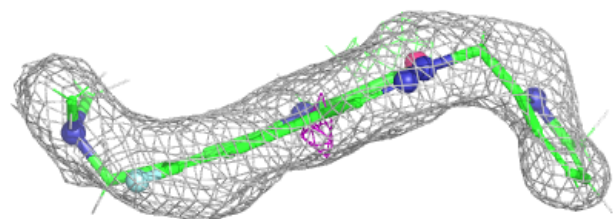
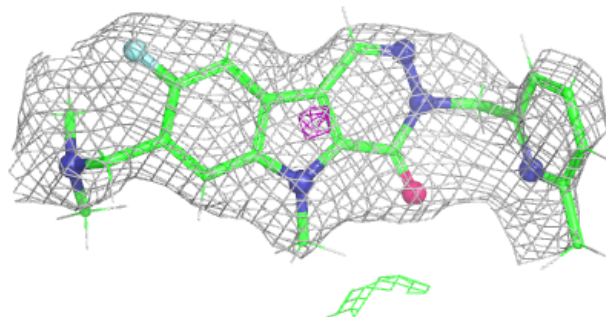


Electron density around A1B77 C 602 (B):

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

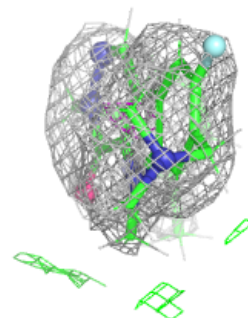
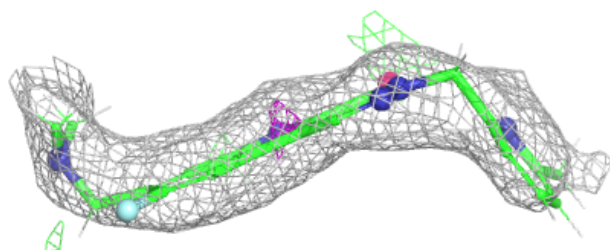
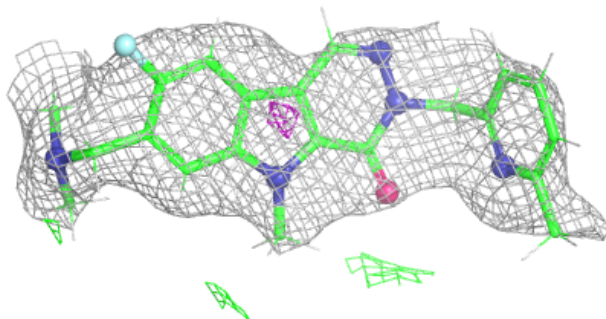
**Electron density around A1B77 F 601 (A):**

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

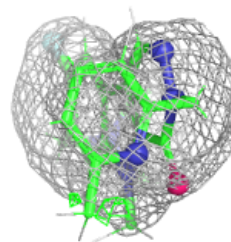
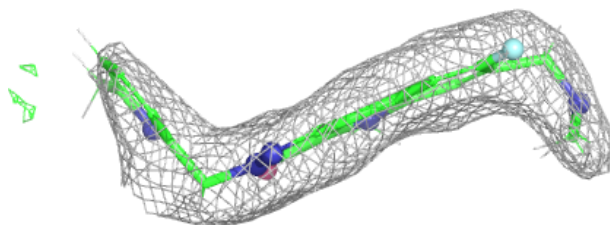
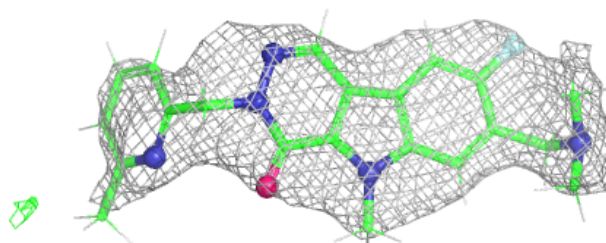


Electron density around A1B77 F 601 (B):

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

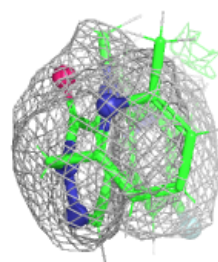
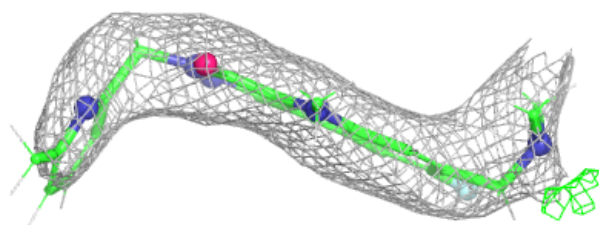
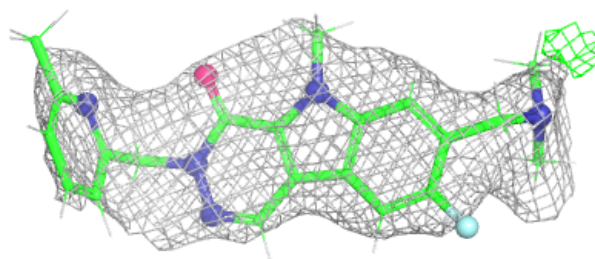
**Electron density around A1B77 H 602 (A):**

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

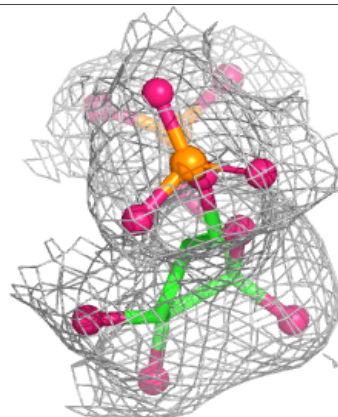
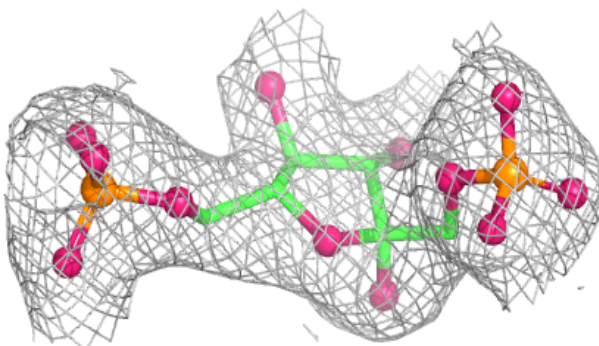
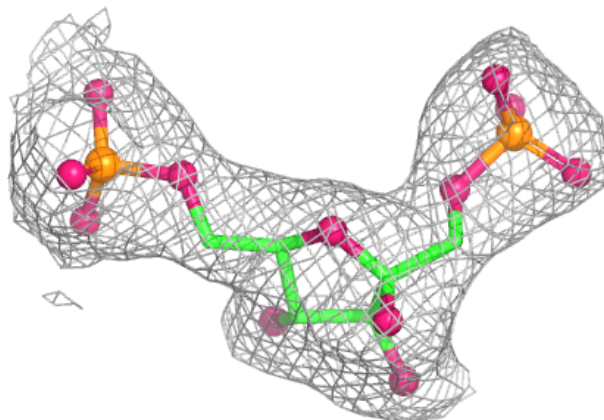


Electron density around A1B77 H 602 (B):

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

**Electron density around FBP B 602:**

$2mF_o-DF_c$ (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.