



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:32 AM UTC

PDB ID : 7FS8 / pdb_00007fs8
Title : Structure of liver pyruvate kinase in complex with allosteric modulator 21
Authors : Lulla, A.; Nilsson, O.; Brear, P.; Nain-Perez, A.; Grotli, M.; Hyvonen, M.
Deposited on : 2022-12-18
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

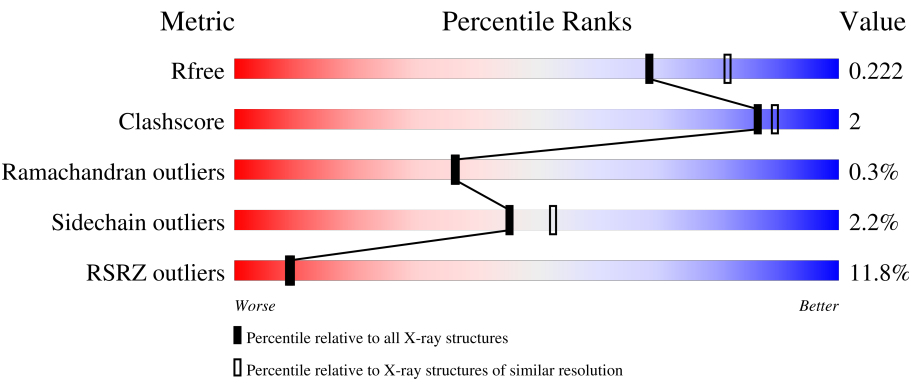
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	447	23% 88% 6% 6%
1	B	447	17% 91% 6% 6%
1	C	447	12% 87% 7% 5%
1	D	447	3% 90% 5% 5%
1	E	447	20% 87% 6% 6%

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Mol	Chain	Length	Quality of chain
1	F	447	
1	G	447	
1	H	447	

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
3	OXL	A	602	-	X	-	-
3	OXL	B	602	-	X	-	-
3	OXL	C	602	-	X	-	-
3	OXL	D	602	-	X	-	-
3	OXL	E	602	-	X	-	-
3	OXL	F	602	-	X	-	-
3	OXL	G	603	-	X	-	-
3	OXL	H	602	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 27860 atoms, of which 76 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 PKLR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	6	0
			3236	2034	585	597	20			
1	B	436	Total	C	N	O	S	0	4	0
			3329	2090	604	615	20			
1	C	425	Total	C	N	O	S	0	4	0
			3247	2040	585	603	19			
1	D	425	Total	C	N	O	S	0	5	0
			3244	2037	587	601	19			
1	E	419	Total	C	N	O	S	0	5	0
			3210	2018	579	593	20			
1	F	432	Total	C	N	O	S	0	7	0
			3321	2090	597	614	20			
1	G	421	Total	C	N	O	S	0	6	0
			3231	2031	581	600	19			
1	H	425	Total	C	N	O	S	0	4	0
			3251	2040	594	598	19			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P30613
A	0	SER	-	expression tag	UNP P30613
A	1	MET	-	expression tag	UNP P30613
A	2	GLU	-	expression tag	UNP P30613
A	12	ASP	SER	conflict	UNP P30613
A	130	GLY	-	linker	UNP P30613
A	131	SER	-	linker	UNP P30613
A	132	GLY	-	linker	UNP P30613
B	-1	GLY	-	expression tag	UNP P30613
B	0	SER	-	expression tag	UNP P30613
B	1	MET	-	expression tag	UNP P30613
B	2	GLU	-	expression tag	UNP P30613
B	12	ASP	SER	conflict	UNP P30613

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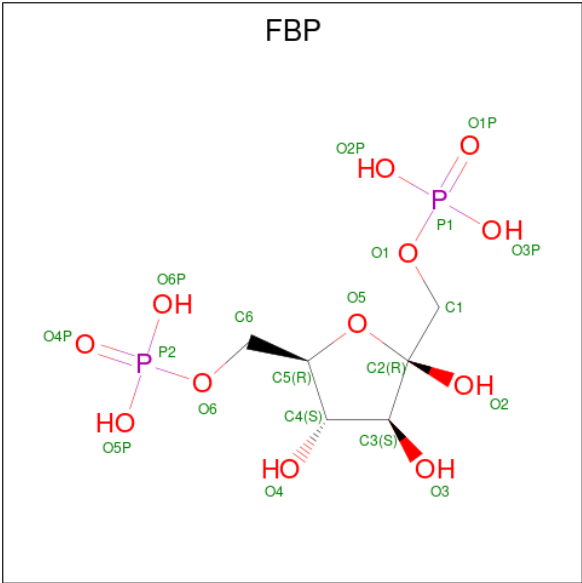
Chain	Residue	Modelled	Actual	Comment	Reference
B	130	GLY	-	linker	UNP P30613
B	131	SER	-	linker	UNP P30613
B	132	GLY	-	linker	UNP P30613
C	-1	GLY	-	expression tag	UNP P30613
C	0	SER	-	expression tag	UNP P30613
C	1	MET	-	expression tag	UNP P30613
C	2	GLU	-	expression tag	UNP P30613
C	12	ASP	SER	conflict	UNP P30613
C	130	GLY	-	linker	UNP P30613
C	131	SER	-	linker	UNP P30613
C	132	GLY	-	linker	UNP P30613
D	-1	GLY	-	expression tag	UNP P30613
D	0	SER	-	expression tag	UNP P30613
D	1	MET	-	expression tag	UNP P30613
D	2	GLU	-	expression tag	UNP P30613
D	12	ASP	SER	conflict	UNP P30613
D	130	GLY	-	linker	UNP P30613
D	131	SER	-	linker	UNP P30613
D	132	GLY	-	linker	UNP P30613
E	-1	GLY	-	expression tag	UNP P30613
E	0	SER	-	expression tag	UNP P30613
E	1	MET	-	expression tag	UNP P30613
E	2	GLU	-	expression tag	UNP P30613
E	12	ASP	SER	conflict	UNP P30613
E	228	GLY	-	linker	UNP P30613
E	229	SER	-	linker	UNP P30613
E	230	GLY	-	linker	UNP P30613
F	-1	GLY	-	expression tag	UNP P30613
F	0	SER	-	expression tag	UNP P30613
F	1	MET	-	expression tag	UNP P30613
F	2	GLU	-	expression tag	UNP P30613
F	12	ASP	SER	conflict	UNP P30613
F	228	GLY	-	linker	UNP P30613
F	229	SER	-	linker	UNP P30613
F	230	GLY	-	linker	UNP P30613
G	-1	GLY	-	expression tag	UNP P30613
G	0	SER	-	expression tag	UNP P30613
G	1	MET	-	expression tag	UNP P30613
G	2	GLU	-	expression tag	UNP P30613
G	12	ASP	SER	conflict	UNP P30613
G	130	GLY	-	linker	UNP P30613
G	131	SER	-	linker	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
G	132	GLY	-	linker	UNP P30613
H	-1	GLY	-	expression tag	UNP P30613
H	0	SER	-	expression tag	UNP P30613
H	1	MET	-	expression tag	UNP P30613
H	2	GLU	-	expression tag	UNP P30613
H	12	ASP	SER	conflict	UNP P30613
H	130	GLY	-	linker	UNP P30613
H	131	SER	-	linker	UNP P30613
H	132	GLY	-	linker	UNP P30613

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: C₆H₁₄O₁₂P₂).



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	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		
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		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	O	P	0	0
			20	6	12	2		
2	H	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	B	1	Total	C	O	0	0
			6	2	4		
3	C	1	Total	C	O	0	0
			6	2	4		
3	D	1	Total	C	O	0	0
			6	2	4		
3	E	1	Total	C	O	0	0
			6	2	4		
3	F	1	Total	C	O	0	0
			6	2	4		
3	G	1	Total	C	O	0	0
			6	2	4		
3	H	1	Total	C	O	0	0
			6	2	4		

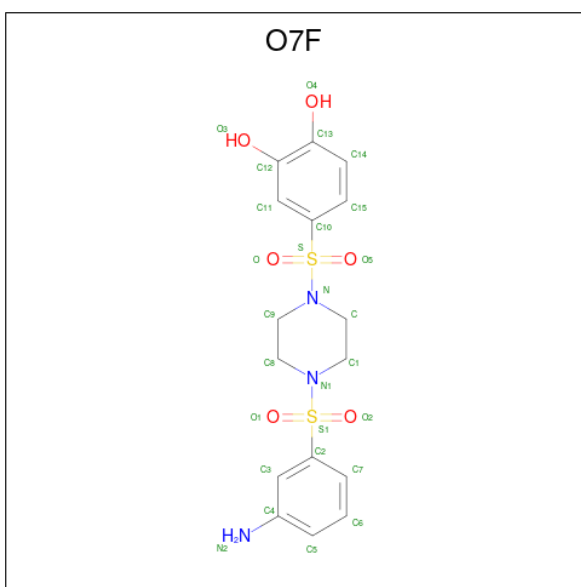
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 6 is 4-[4-(3-aminobenzene-1-sulfonyl)piperazine-1-sulfonyl]benzene-1,2-diol (CCD ID: O7F) (formula: C₁₆H₁₉N₃O₆S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total 46	C 16	H 19	N 3	O 6	S 2	19	0
6	B	1	Total 46	C 16	H 19	N 3	O 6	S 2	19	0
6	F	1	Total 46	C 16	H 19	N 3	O 6	S 2	19	0
6	G	1	Total 46	C 16	H 19	N 3	O 6	S 2	19	0

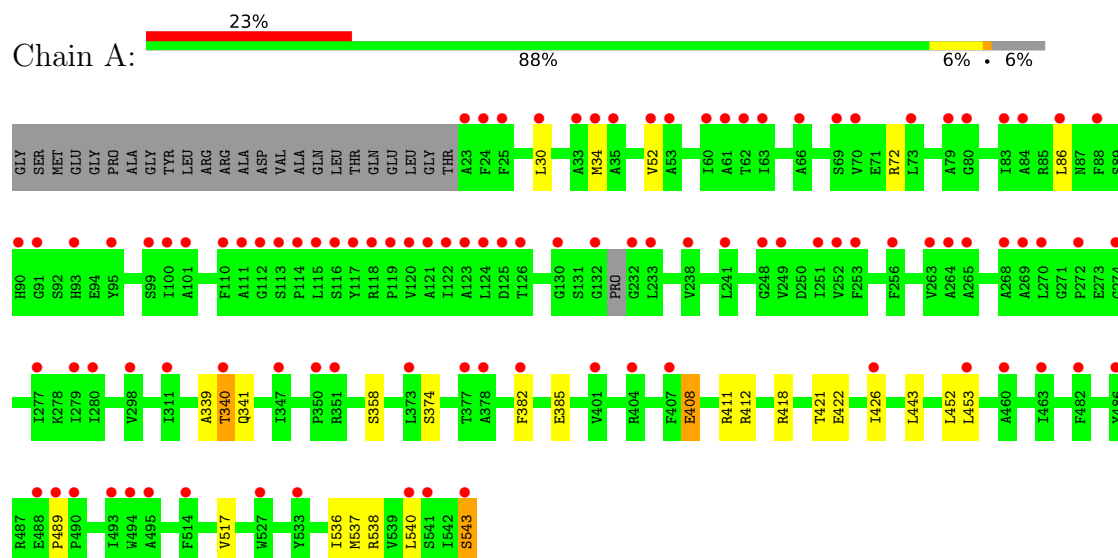
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	102	Total	O	0	0
			102	102		
7	B	114	Total	O	0	0
			114	114		
7	C	176	Total	O	0	0
			176	176		
7	D	229	Total	O	0	0
			229	229		
7	E	111	Total	O	0	0
			111	111		
7	F	165	Total	O	0	0
			165	165		
7	G	232	Total	O	0	0
			232	232		
7	H	254	Total	O	0	0
			254	254		

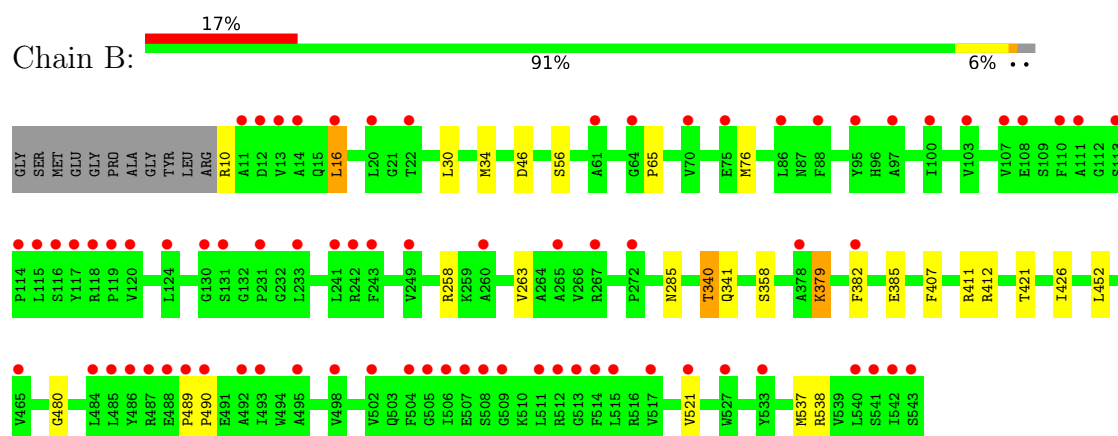
3 Residue-property plots [i](#)

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.

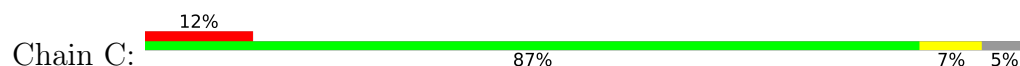
• Molecule 1: Pyruvate kinase PKLR

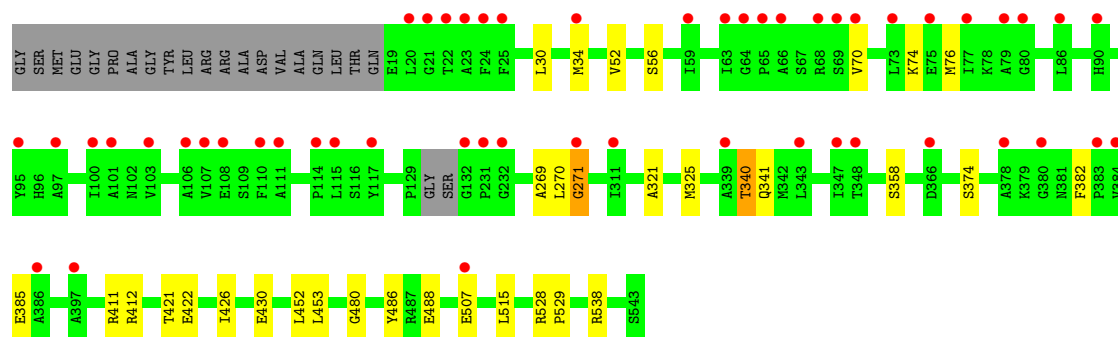


• Molecule 1: Pyruvate kinase PKLR

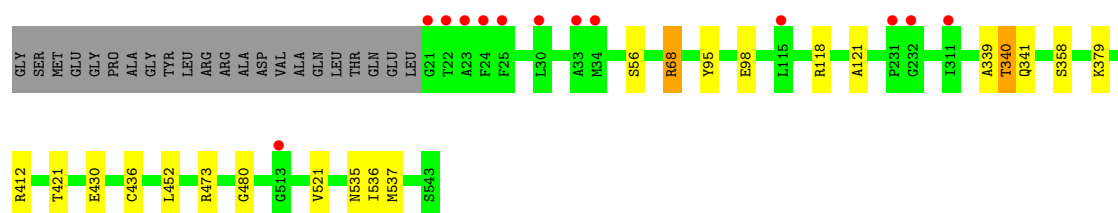


• Molecule 1: Pyruvate kinase PKLR

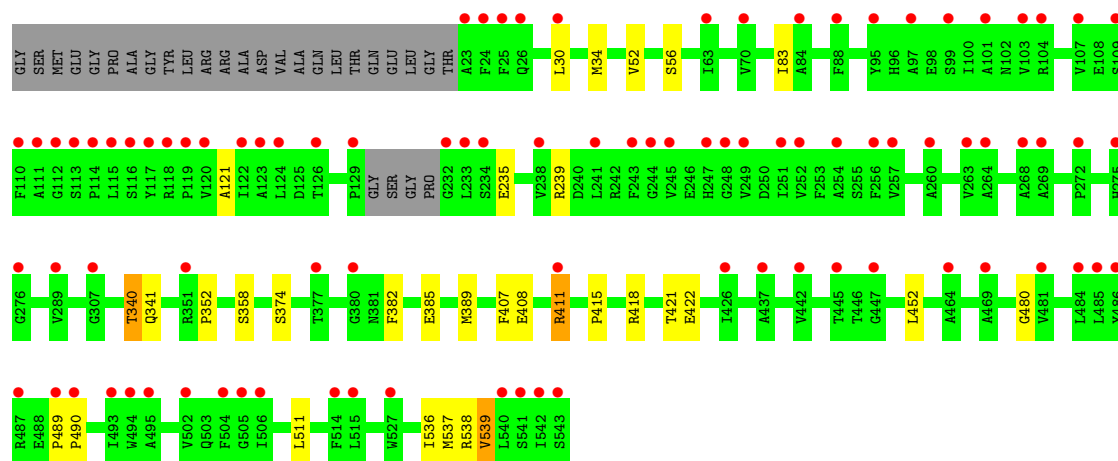
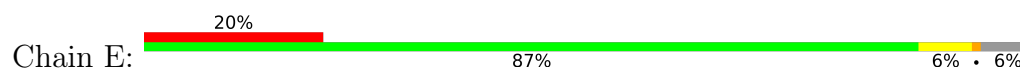




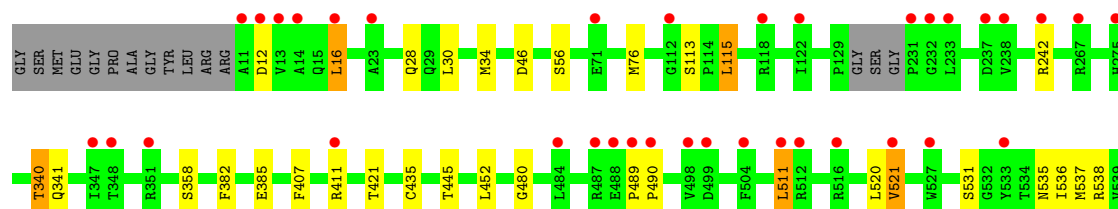
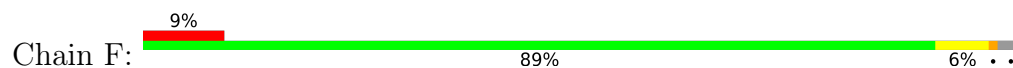
• Molecule 1: Pyruvate kinase PKLR



• Molecule 1: Pyruvate kinase PKLR

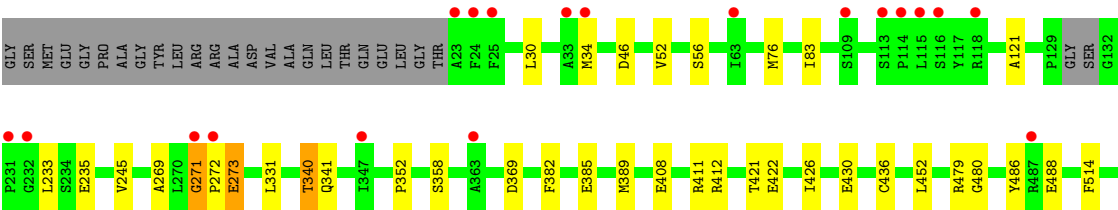
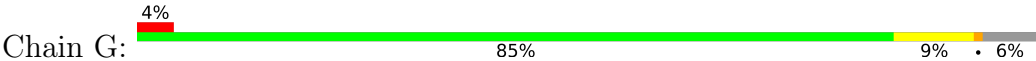


• Molecule 1: Pyruvate kinase PKLR

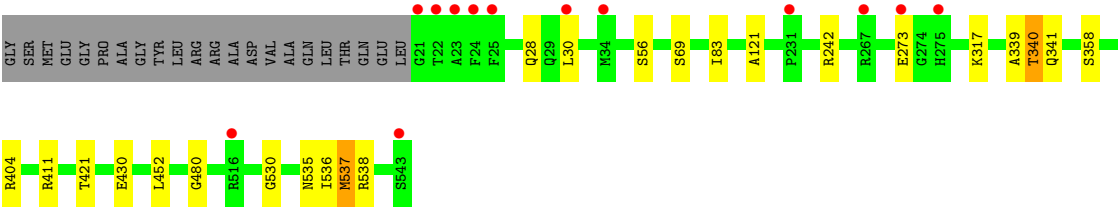
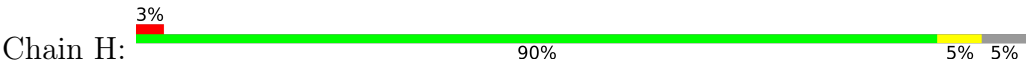




● Molecule 1: Pyruvate kinase PKLR



● Molecule 1: Pyruvate kinase PKLR



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	206.75Å 112.96Å 187.95Å 90.00° 92.36° 90.00°	Depositor
Resolution (Å)	187.79 – 2.10 187.79 – 2.10	Depositor EDS
% Data completeness (in resolution range)	68.2 (187.79-2.10) 68.2 (187.79-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, R_{free}	0.209 , 0.238 0.198 , 0.222	Depositor DCC
R_{free} test set	8588 reflections (3.41%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	27860	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.9570e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: OXL, O7F, K, FBP, MG

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	0.69	2/3307 (0.1%)	1.02	6/4469 (0.1%)
1	B	0.71	0/3396	1.00	1/4592 (0.0%)
1	C	0.73	1/3313 (0.0%)	1.02	5/4479 (0.1%)
1	D	0.80	0/3315	1.04	2/4483 (0.0%)
1	E	0.69	1/3278 (0.0%)	1.01	1/4430 (0.0%)
1	F	0.74	0/3396	1.02	1/4591 (0.0%)
1	G	0.78	0/3303	1.03	2/4465 (0.0%)
1	H	0.82	0/3316	1.04	4/4483 (0.1%)
All	All	0.74	4/26624 (0.0%)	1.02	22/35992 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	374	SER	CA-C	5.75	1.55	1.52
1	C	374	SER	CA-C	5.73	1.55	1.52
1	E	374	SER	CA-C	5.73	1.55	1.52
1	A	489	PRO	CA-C	5.40	1.54	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	422	GLU	CB-CG-CD	7.40	125.18	112.60
1	A	422	GLU	CB-CG-CD	7.13	124.72	112.60
1	G	514	PHE	CA-CB-CG	5.35	119.15	113.80
1	B	46	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	339	ALA	CA-C-N	5.25	131.56	121.54
1	A	339	ALA	C-N-CA	5.25	131.56	121.54
1	C	507	GLU	CB-CG-CD	5.22	121.47	112.60
1	D	339	ALA	CA-C-N	5.18	131.44	121.54
1	D	339	ALA	C-N-CA	5.18	131.44	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	46	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	489	PRO	N-CA-C	5.13	115.40	110.47
1	C	270	LEU	CA-C-N	5.11	129.89	121.87
1	C	270	LEU	C-N-CA	5.11	129.89	121.87
1	C	453	LEU	CA-C-N	5.10	127.12	120.28
1	C	453	LEU	C-N-CA	5.10	127.12	120.28
1	A	453	LEU	CA-C-N	5.10	127.12	120.28
1	A	453	LEU	C-N-CA	5.10	127.12	120.28
1	H	339	ALA	CA-C-N	5.07	131.23	121.54
1	H	339	ALA	C-N-CA	5.07	131.23	121.54
1	H	530	GLY	CA-C-N	5.03	128.83	120.94
1	H	530	GLY	C-N-CA	5.03	128.83	120.94
1	G	46	ASP	CA-CB-CG	5.01	117.61	112.60

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	3236	0	3299	9	0
1	B	3329	0	3394	15	0
1	C	3247	0	3299	18	0
1	D	3244	0	3297	10	0
1	E	3210	0	3270	16	0
1	F	3321	0	3393	21	0
1	G	3231	0	3284	27	0
1	H	3251	0	3306	14	0
2	A	20	0	10	0	0
2	B	20	0	10	0	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
2	E	20	0	10	0	0
2	F	20	0	10	0	0
2	G	20	0	10	0	0
2	H	20	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0
3	G	6	0	0	0	0
3	H	6	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	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	A	27	19	0	0	0
6	B	27	19	0	0	0
6	F	27	19	0	0	0
6	G	27	19	0	0	0
7	A	102	0	0	0	0
7	B	114	0	0	0	0
7	C	176	0	0	0	0
7	D	229	0	0	1	0
7	E	111	0	0	0	0
7	F	165	0	0	0	0
7	G	232	0	0	0	0
7	H	254	0	0	2	0
All	All	27784	76	26622	112	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (112) 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:C:411:ARG:HG3	1:C:426:ILE:HD11	1.49	0.93
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.54	0.89
1:C:528:ARG:NH2	1:G:233:LEU:O	2.09	0.85
1:C:422[A]:GLU:HG3	1:C:452:LEU:HD13	1.60	0.84
1:G:411:ARG:HD2	7:H:863:HOH:O	1.83	0.78
1:B:411:ARG:HG2	1:B:426:ILE:HD11	1.64	0.76
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.71	0.71
1:A:418[A]:ARG:HG3	1:B:16:LEU:HD11	1.75	0.67
1:G:56:SER:HB2	1:G:480:GLY:HA2	1.76	0.67
1:G:537:MET:HE3	1:H:537:MET:HG2	1.76	0.66
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.81	0.63
1:G:538:ARG:HG2	1:H:536:ILE:HG12	1.81	0.62
1:F:56:SER:HB2	1:F:480:GLY:HA2	1.82	0.62
1:H:56:SER:HB2	1:H:480:GLY:HA2	1.83	0.61
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.82	0.61
1:E:538:ARG:HG2	1:F:536:ILE:HG12	1.82	0.60
1:E:235:GLU:O	1:E:239:ARG:HD3	2.02	0.60
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.84	0.59
1:G:272:PRO:HD2	1:G:273:GLU:OE1	2.03	0.58
1:C:529:PRO:HG3	1:G:235:GLU:HG2	1.86	0.57
1:F:407:PHE:CE2	1:F:411:ARG:NH1	2.72	0.57
1:E:536:ILE:HG12	1:F:538:ARG:HG2	1.86	0.57
1:F:407:PHE:CD2	1:F:411:ARG:NH1	2.72	0.57
1:F:115:LEU:HD21	1:F:511:LEU:HD12	1.86	0.56
1:E:56:SER:HB2	1:E:480:GLY:HA2	1.87	0.56
1:G:408:GLU:HG3	1:G:411:ARG:HH22	1.70	0.55
1:G:486:TYR:CZ	1:G:488:GLU:HB2	2.43	0.54
1:G:408:GLU:HG3	1:G:411:ARG:NH2	2.22	0.54
1:E:539:VAL:HG13	1:F:535:ASN:HB2	1.90	0.54
1:G:340:THR:HG22	1:G:341:GLN:HG3	1.91	0.53
1:G:245:VAL:CG1	1:G:273:GLU:HG2	2.38	0.53
1:A:408:GLU:OE2	1:B:411:ARG:NH1	2.28	0.53
1:C:421:THR:HG22	1:C:452:LEU:HD12	1.88	0.53
1:B:407:PHE:CE2	1:B:411:ARG:HD2	2.45	0.52
1:F:521:VAL:HG12	1:F:540[B]:LEU:HB3	1.92	0.52
1:D:68:ARG:NH2	1:D:95:TYR:O	2.43	0.52
1:C:382:PHE:HB3	1:C:385:GLU:HB2	1.92	0.51
1:F:382:PHE:HB3	1:F:385:GLU:HB2	1.91	0.51
1:G:56:SER:HB2	1:G:480:GLY:CA	2.39	0.51
1:D:340:THR:HG22	1:D:341:GLN:HG3	1.92	0.51
1:B:382:PHE:HB3	1:B:385:GLU:HB2	1.94	0.50
1:E:382:PHE:HB3	1:E:385:GLU:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:THR:HG22	1:A:341:GLN:HG3	1.93	0.50
1:F:56:SER:HB2	1:F:480:GLY:CA	2.42	0.49
1:A:517:VAL:HG22	1:A:543:SER:HB2	1.95	0.49
1:B:56:SER:HB2	1:B:480:GLY:CA	2.43	0.49
1:A:382:PHE:HB3	1:A:385:GLU:HB2	1.93	0.49
1:E:340:THR:HG22	1:E:341:GLN:HG3	1.95	0.49
1:E:418:ARG:HG3	1:F:16:LEU:HD11	1.95	0.49
1:B:340:THR:HG22	1:B:341:GLN:HG3	1.95	0.49
1:C:340:THR:HG22	1:C:341:GLN:HG3	1.95	0.49
1:E:407:PHE:O	1:E:411:ARG:HB2	2.13	0.48
1:H:56:SER:HB2	1:H:480:GLY:CA	2.43	0.48
1:B:258:ARG:HD3	1:B:285:ASN:HD21	1.77	0.48
1:H:535:ASN:OD1	1:H:536:ILE:HG13	2.13	0.48
1:C:56:SER:HB2	1:C:480:GLY:CA	2.43	0.47
1:C:269:ALA:C	1:C:271:GLY:H	2.21	0.47
1:B:65:PRO:HG2	1:B:379:LYS:HG2	1.97	0.47
1:B:407:PHE:CZ	1:B:411:ARG:HD2	2.50	0.46
1:E:415:PRO:HB3	1:F:12:ASP:HA	1.97	0.46
1:F:421:THR:HG22	1:F:452:LEU:HD12	1.98	0.46
1:D:56:SER:HB2	1:D:480:GLY:CA	2.44	0.46
1:D:68:ARG:HH22	1:D:98:GLU:HB2	1.80	0.46
1:D:121:ALA:HA	1:D:473:ARG:HB3	1.98	0.46
1:G:411:ARG:HG2	1:G:426:ILE:HD11	1.97	0.45
1:H:340:THR:HG22	1:H:341:GLN:HG3	1.97	0.45
1:B:421:THR:HG22	1:B:452:LEU:HD12	1.98	0.45
1:C:486:TYR:CZ	1:C:488:GLU:HB2	2.50	0.45
1:F:340:THR:HG22	1:F:341:GLN:HG3	1.98	0.45
1:G:536:ILE:HG12	1:H:538[A]:ARG:HG2	1.97	0.45
1:F:521:VAL:HG12	1:F:540[A]:LEU:HB2	1.98	0.44
1:G:269:ALA:C	1:G:271:GLY:H	2.26	0.44
1:G:382:PHE:HB3	1:G:385:GLU:HB2	1.97	0.44
1:D:421:THR:HG22	1:D:452:LEU:HD12	2.00	0.44
1:C:411:ARG:CG	1:C:426:ILE:HD11	2.35	0.43
1:E:421:THR:HG22	1:E:452:LEU:HD12	1.99	0.43
1:A:421:THR:HG22	1:A:452:LEU:HD12	2.01	0.43
1:G:83:ILE:HG12	1:G:121:ALA:HB3	1.99	0.43
1:G:412:ARG:CZ	1:H:404:ARG:HD3	2.49	0.43
1:F:115:LEU:HD21	1:F:511:LEU:HB3	2.00	0.43
1:C:30:LEU:O	1:C:34:MET:HG2	2.19	0.42
1:G:411:ARG:CG	1:G:426:ILE:HD11	2.49	0.42
1:H:317:LYS:NZ	7:H:708:HOH:O	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:421:THR:HG22	1:H:452:LEU:HD12	2.02	0.42
1:E:56:SER:HB2	1:E:480:GLY:CA	2.48	0.42
1:A:30:LEU:O	1:A:34:MET:HG2	2.20	0.42
1:G:430[A]:GLU:OE1	1:H:430:GLU:OE1	2.37	0.42
1:A:411:ARG:HG3	1:A:426:ILE:HD11	2.02	0.42
1:C:321:ALA:O	1:C:325:MET:HG3	2.19	0.42
1:F:30:LEU:O	1:F:34:MET:HG2	2.20	0.42
1:G:30:LEU:O	1:G:34:MET:HG2	2.20	0.42
1:B:30:LEU:O	1:B:34:MET:HG2	2.20	0.42
1:G:352:PRO:HG3	1:G:389:MET:HG2	2.00	0.41
1:C:538:ARG:HG2	1:D:536:ILE:HG12	2.01	0.41
1:D:379:LYS:NZ	7:D:711:HOH:O	2.52	0.41
1:F:435:CYS:HB2	1:F:520:LEU:HD12	2.02	0.41
1:C:70:VAL:HG12	1:C:74:LYS:HE3	2.02	0.41
1:G:369:ASP:HA	1:G:479:ARG:HB2	2.02	0.41
1:E:83:ILE:HG12	1:E:121:ALA:HB3	2.03	0.41
1:F:28:GLN:HG3	1:F:30:LEU:HG	2.03	0.41
1:F:489:PRO:HA	1:F:490:PRO:HD3	1.99	0.41
1:E:352:PRO:HG3	1:E:389:MET:HG2	2.03	0.41
1:E:489:PRO:HA	1:E:490:PRO:HD3	1.98	0.41
1:H:28:GLN:HG3	1:H:30:LEU:HG	2.03	0.41
1:F:445:THR:HB	1:F:531:SER:OG	2.21	0.40
1:G:430[B]:GLU:OE2	1:H:430:GLU:OE1	2.39	0.40
1:B:489:PRO:HA	1:B:490:PRO:HD3	1.98	0.40
1:E:30:LEU:O	1:E:34:MET:HG3	2.22	0.40
1:C:528:ARG:NH1	1:C:529:PRO:O	2.54	0.40
1:C:430[A]:GLU:OE1	1:D:430[A]:GLU:OE1	2.39	0.40
1:G:421:THR:HG22	1:G:452:LEU:HD12	2.03	0.40
1:H:83:ILE:HG12	1:H:121:ALA:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	424/447 (95%)	419 (99%)	4 (1%)	1 (0%)	43	44
1	B	438/447 (98%)	431 (98%)	6 (1%)	1 (0%)	43	44
1	C	425/447 (95%)	416 (98%)	7 (2%)	2 (0%)	24	22
1	D	428/447 (96%)	422 (99%)	4 (1%)	2 (0%)	24	22
1	E	420/447 (94%)	416 (99%)	3 (1%)	1 (0%)	43	44
1	F	435/447 (97%)	429 (99%)	5 (1%)	1 (0%)	43	44
1	G	423/447 (95%)	414 (98%)	7 (2%)	2 (0%)	24	22
1	H	427/447 (96%)	422 (99%)	4 (1%)	1 (0%)	43	44
All	All	3420/3576 (96%)	3369 (98%)	40 (1%)	11 (0%)	36	36

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	271	GLY
1	D	535	ASN
1	A	340	THR
1	B	340	THR
1	C	340	THR
1	D	340	THR
1	E	340	THR
1	F	340	THR
1	G	340	THR
1	H	340	THR
1	C	271	GLY

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	340/352 (97%)	328 (96%)	12 (4%)	32	35
1	B	349/352 (99%)	338 (97%)	11 (3%)	34	38
1	C	341/352 (97%)	335 (98%)	6 (2%)	51	60
1	D	341/352 (97%)	334 (98%)	7 (2%)	47	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	338/352 (96%)	330 (98%)	8 (2%)	43	49
1	F	350/352 (99%)	339 (97%)	11 (3%)	35	39
1	G	340/352 (97%)	333 (98%)	7 (2%)	47	54
1	H	340/352 (97%)	334 (98%)	6 (2%)	51	60
All	All	2739/2816 (97%)	2671 (98%)	68 (2%)	45	48

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	72	ARG
1	A	86	LEU
1	A	358	SER
1	A	408	GLU
1	A	412	ARG
1	A	443	LEU
1	A	537[A]	MET
1	A	537[B]	MET
1	A	538	ARG
1	A	540	LEU
1	A	543	SER
1	B	10	ARG
1	B	16	LEU
1	B	76[A]	MET
1	B	76[B]	MET
1	B	263	VAL
1	B	358	SER
1	B	379	LYS
1	B	412	ARG
1	B	521	VAL
1	B	537[A]	MET
1	B	537[B]	MET
1	C	52	VAL
1	C	76[A]	MET
1	C	76[B]	MET
1	C	358	SER
1	C	412	ARG
1	C	515	LEU
1	D	68	ARG
1	D	118	ARG
1	D	358	SER

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Mol	Chain	Res	Type
1	D	412	ARG
1	D	436	CYS
1	D	521	VAL
1	D	537	MET
1	E	52	VAL
1	E	358	SER
1	E	408	GLU
1	E	411	ARG
1	E	511	LEU
1	E	537[A]	MET
1	E	537[B]	MET
1	E	539	VAL
1	F	16	LEU
1	F	76[A]	MET
1	F	76[B]	MET
1	F	113	SER
1	F	115	LEU
1	F	242	ARG
1	F	358	SER
1	F	511	LEU
1	F	521	VAL
1	F	537[A]	MET
1	F	537[B]	MET
1	G	52	VAL
1	G	76[A]	MET
1	G	76[B]	MET
1	G	273	GLU
1	G	331	LEU
1	G	358	SER
1	G	436	CYS
1	H	69	SER
1	H	242	ARG
1	H	273	GLU
1	H	358	SER
1	H	411	ARG
1	H	537	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	B	90	HIS

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Mol	Chain	Res	Type
1	B	390	GLN
1	C	90	HIS
1	C	275	HIS
1	D	90	HIS
1	E	90	HIS
1	F	90	HIS
1	F	390	GLN
1	F	405	GLN
1	G	90	HIS
1	G	390	GLN
1	H	90	HIS
1	H	405	GLN
1	H	535	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 36 ligands modelled in this entry, 16 are monoatomic - leaving 20 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	OXL	H	602	4	5,5,5	1.99	3 (60%)	6,6,6	1.93	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OXL	E	602	4	5,5,5	2.34	2 (40%)	6,6,6	1.74	2 (33%)
2	FBP	A	601	-	18,20,20	0.61	0	21,32,32	0.74	0
2	FBP	G	602	-	18,20,20	0.66	0	21,32,32	0.97	2 (9%)
6	O7F	B	605	-	29,29,29	0.53	1 (3%)	43,44,44	0.39	0
2	FBP	E	601	-	18,20,20	0.48	0	21,32,32	0.81	1 (4%)
6	O7F	A	605	-	29,29,29	0.45	0	43,44,44	0.63	0
3	OXL	F	602	4	5,5,5	3.05	5 (100%)	6,6,6	2.99	3 (50%)
6	O7F	F	605	-	29,29,29	0.56	0	43,44,44	0.75	0
2	FBP	B	601	-	18,20,20	0.56	0	21,32,32	0.89	1 (4%)
3	OXL	C	602	4	5,5,5	1.99	2 (40%)	6,6,6	1.90	2 (33%)
2	FBP	D	601	-	18,20,20	0.78	0	21,32,32	1.15	2 (9%)
3	OXL	D	602	4	5,5,5	2.38	3 (60%)	6,6,6	2.57	3 (50%)
3	OXL	B	602	4	5,5,5	2.15	2 (40%)	6,6,6	2.02	2 (33%)
2	FBP	F	601	-	18,20,20	0.34	0	21,32,32	0.74	0
6	O7F	G	601	-	29,29,29	0.48	0	43,44,44	0.59	0
3	OXL	A	602	4	5,5,5	2.02	2 (40%)	6,6,6	2.15	3 (50%)
3	OXL	G	603	4	5,5,5	2.16	2 (40%)	6,6,6	2.46	4 (66%)
2	FBP	H	601	-	18,20,20	1.03	3 (16%)	21,32,32	0.89	1 (4%)
2	FBP	C	601	-	18,20,20	0.95	1 (5%)	21,32,32	0.95	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	OXL	H	602	4	-	4/4/4/4	-
3	OXL	E	602	4	-	4/4/4/4	-
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
2	FBP	G	602	-	-	2/13/32/32	0/1/1/1
6	O7F	B	605	-	-	12/24/34/34	0/3/3/3
2	FBP	E	601	-	-	4/13/32/32	0/1/1/1
6	O7F	A	605	-	-	1/24/34/34	0/3/3/3
3	OXL	F	602	4	-	4/4/4/4	-
6	O7F	F	605	-	-	0/24/34/34	0/3/3/3
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
3	OXL	C	602	4	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
3	OXL	D	602	4	-	4/4/4/4	-
3	OXL	B	602	4	-	4/4/4/4	-
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
6	O7F	G	601	-	-	0/24/34/34	0/3/3/3
3	OXL	A	602	4	-	4/4/4/4	-
3	OXL	G	603	4	-	4/4/4/4	-
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	OXL	O1-C1	4.34	1.33	1.22
3	B	602	OXL	O2-C2	3.94	1.32	1.22
3	F	602	OXL	O2-C2	3.90	1.32	1.22
3	C	602	OXL	O1-C1	3.56	1.31	1.22
3	A	602	OXL	O2-C2	3.53	1.31	1.22
3	G	603	OXL	O1-C1	3.42	1.31	1.22
3	D	602	OXL	O2-C2	3.40	1.31	1.22
3	F	602	OXL	O3-C1	-3.40	1.21	1.30
2	C	601	FBP	P1-O3P	-3.38	1.42	1.54
3	F	602	OXL	O1-C1	3.19	1.30	1.22
3	G	603	OXL	O3-C1	-3.10	1.22	1.30
3	D	602	OXL	O4-C2	-2.86	1.22	1.30
3	H	602	OXL	O2-C2	2.79	1.29	1.22
3	D	602	OXL	C2-C1	2.63	1.59	1.54
3	A	602	OXL	O4-C2	-2.61	1.23	1.30
3	B	602	OXL	O4-C2	-2.60	1.23	1.30
3	C	602	OXL	O3-C1	-2.59	1.23	1.30
3	H	602	OXL	O4-C2	-2.53	1.23	1.30
3	E	602	OXL	O3-C1	-2.50	1.23	1.30
3	F	602	OXL	C2-C1	2.20	1.58	1.54
3	F	602	OXL	O4-C2	-2.18	1.24	1.30
2	H	601	FBP	P1-O1	-2.18	1.53	1.60
3	H	602	OXL	C2-C1	2.17	1.58	1.54
2	H	601	FBP	P2-O5P	-2.14	1.46	1.54
2	H	601	FBP	P1-O3P	-2.13	1.46	1.54
6	B	605	O7F	S1-N1	2.00	1.66	1.63

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	602	OXL	O4-C2-C1	4.71	121.96	112.83
3	F	602	OXL	O3-C1-C2	4.25	121.08	112.83
3	H	602	OXL	O4-C2-C1	4.04	120.67	112.83
3	A	602	OXL	O4-C2-C1	4.03	120.65	112.83
3	D	602	OXL	O4-C2-C1	3.98	120.55	112.83
3	D	602	OXL	O3-C1-C2	3.92	120.43	112.83
3	G	603	OXL	O3-C1-C2	3.79	120.19	112.83
3	C	602	OXL	O3-C1-C2	3.62	119.86	112.83
2	D	601	FBP	O5P-P2-O6	3.62	116.11	106.67
3	G	603	OXL	O4-C2-C1	3.50	119.62	112.83
3	B	602	OXL	O4-C2-C1	3.39	119.40	112.83
3	E	602	OXL	O3-C1-C2	3.10	118.85	112.83
3	F	602	OXL	O2-C2-C1	-3.06	114.26	120.63
3	B	602	OXL	O3-C1-C2	2.93	118.52	112.83
2	B	601	FBP	O3P-P1-O2P	2.48	117.09	107.80
3	E	602	OXL	O4-C2-C1	2.41	117.50	112.83
3	A	602	OXL	O3-C1-C2	2.40	117.49	112.83
2	C	601	FBP	O6-P2-O4P	2.37	112.84	106.44
2	G	602	FBP	O3P-P1-O2P	2.33	116.53	107.80
3	A	602	OXL	O2-C2-C1	-2.28	115.89	120.63
2	H	601	FBP	O2P-P1-O1	2.26	112.57	106.67
3	G	603	OXL	O2-C2-C1	-2.24	115.96	120.63
3	D	602	OXL	O1-C1-C2	-2.17	116.10	120.63
3	H	602	OXL	O2-C2-C1	-2.16	116.13	120.63
3	G	603	OXL	O1-C1-C2	-2.14	116.17	120.63
2	E	601	FBP	O3P-P1-O2P	2.11	115.71	107.80
3	C	602	OXL	O4-C2-C1	2.08	116.86	112.83
2	D	601	FBP	O6-P2-O4P	-2.07	100.83	106.44
2	G	602	FBP	O6P-P2-O6	2.07	112.07	106.67

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	605	O7F	C1-N1-S1-O2
6	B	605	O7F	C9-N-S-O5
6	B	605	O7F	C8-N1-S1-O1
6	B	605	O7F	C8-N1-S1-O2
6	B	605	O7F	C1-N1-S1-O1
6	B	605	O7F	C1-N1-S1-C2
6	B	605	O7F	C9-N-S-C10
6	B	605	O7F	C8-N1-S1-C2
2	A	601	FBP	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	B	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6
2	E	601	FBP	C4-C5-C6-O6
2	F	601	FBP	C4-C5-C6-O6
2	G	602	FBP	C4-C5-C6-O6
2	H	601	FBP	C4-C5-C6-O6
2	B	601	FBP	O5-C5-C6-O6
6	B	605	O7F	C9-N-S-O
2	A	601	FBP	O5-C5-C6-O6
2	C	601	FBP	O5-C5-C6-O6
2	D	601	FBP	C4-C5-C6-O6
2	F	601	FBP	O5-C5-C6-O6
2	E	601	FBP	O5-C5-C6-O6
2	H	601	FBP	O5-C5-C6-O6
6	B	605	O7F	C-N-S-O
6	B	605	O7F	C-N-S-O5
2	G	602	FBP	O5-C5-C6-O6
2	D	601	FBP	O5-C5-C6-O6
3	A	602	OXL	O3-C1-C2-O4
3	B	602	OXL	O3-C1-C2-O4
3	C	602	OXL	O3-C1-C2-O4
3	D	602	OXL	O3-C1-C2-O4
3	F	602	OXL	O3-C1-C2-O4
3	G	603	OXL	O3-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O4
3	A	602	OXL	O1-C1-C2-O2
3	B	602	OXL	O1-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O2
3	F	602	OXL	O1-C1-C2-O2
3	G	603	OXL	O1-C1-C2-O2
3	H	602	OXL	O3-C1-C2-O4
3	C	602	OXL	O1-C1-C2-O2
3	E	602	OXL	O1-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O2
2	E	601	FBP	C1-O1-P1-O1P
2	E	601	FBP	C6-O6-P2-O4P
6	B	605	O7F	C-N-S-C10
3	A	602	OXL	O1-C1-C2-O4
3	D	602	OXL	O1-C1-C2-O4
3	F	602	OXL	O3-C1-C2-O2
3	A	602	OXL	O3-C1-C2-O2
3	B	602	OXL	O1-C1-C2-O4

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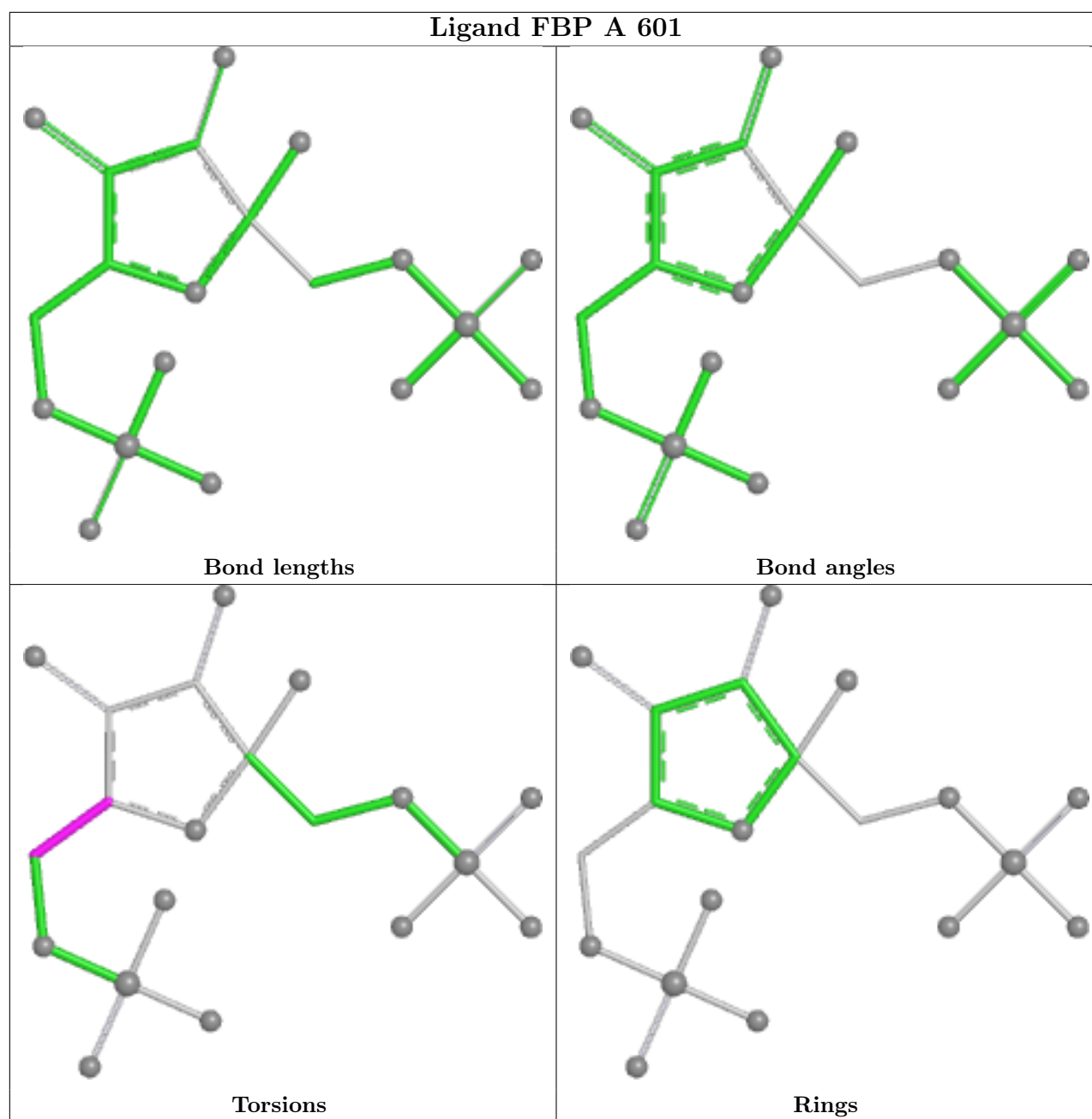
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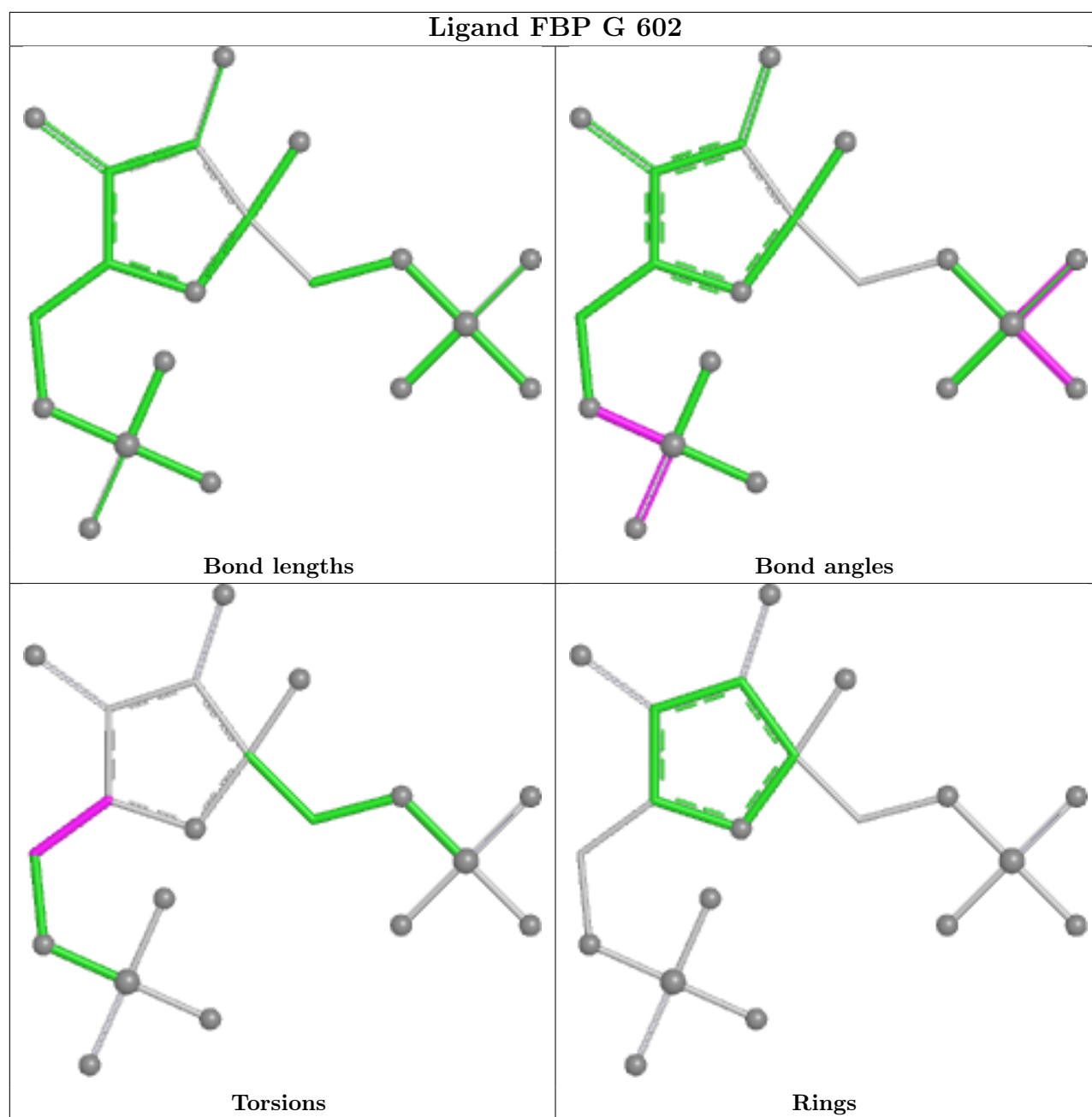
Mol	Chain	Res	Type	Atoms
3	B	602	OXL	O3-C1-C2-O2
3	C	602	OXL	O1-C1-C2-O4
3	C	602	OXL	O3-C1-C2-O2
3	D	602	OXL	O3-C1-C2-O2
3	F	602	OXL	O1-C1-C2-O4
3	G	603	OXL	O1-C1-C2-O4
3	G	603	OXL	O3-C1-C2-O2
3	E	602	OXL	O1-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O4
3	H	602	OXL	O3-C1-C2-O2
6	A	605	O7F	C-N-S-O

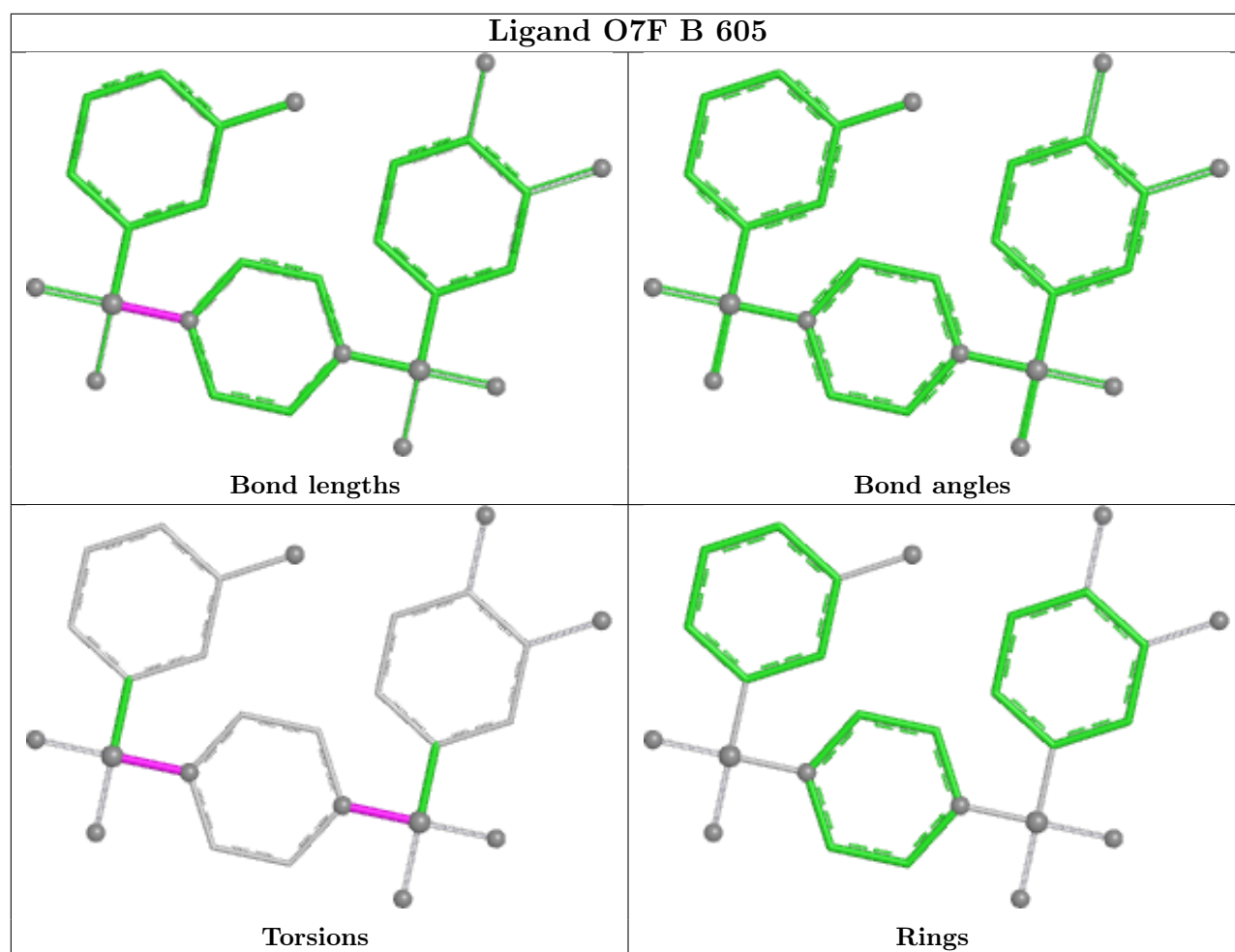
There are no ring outliers.

No monomer is involved in short contacts.

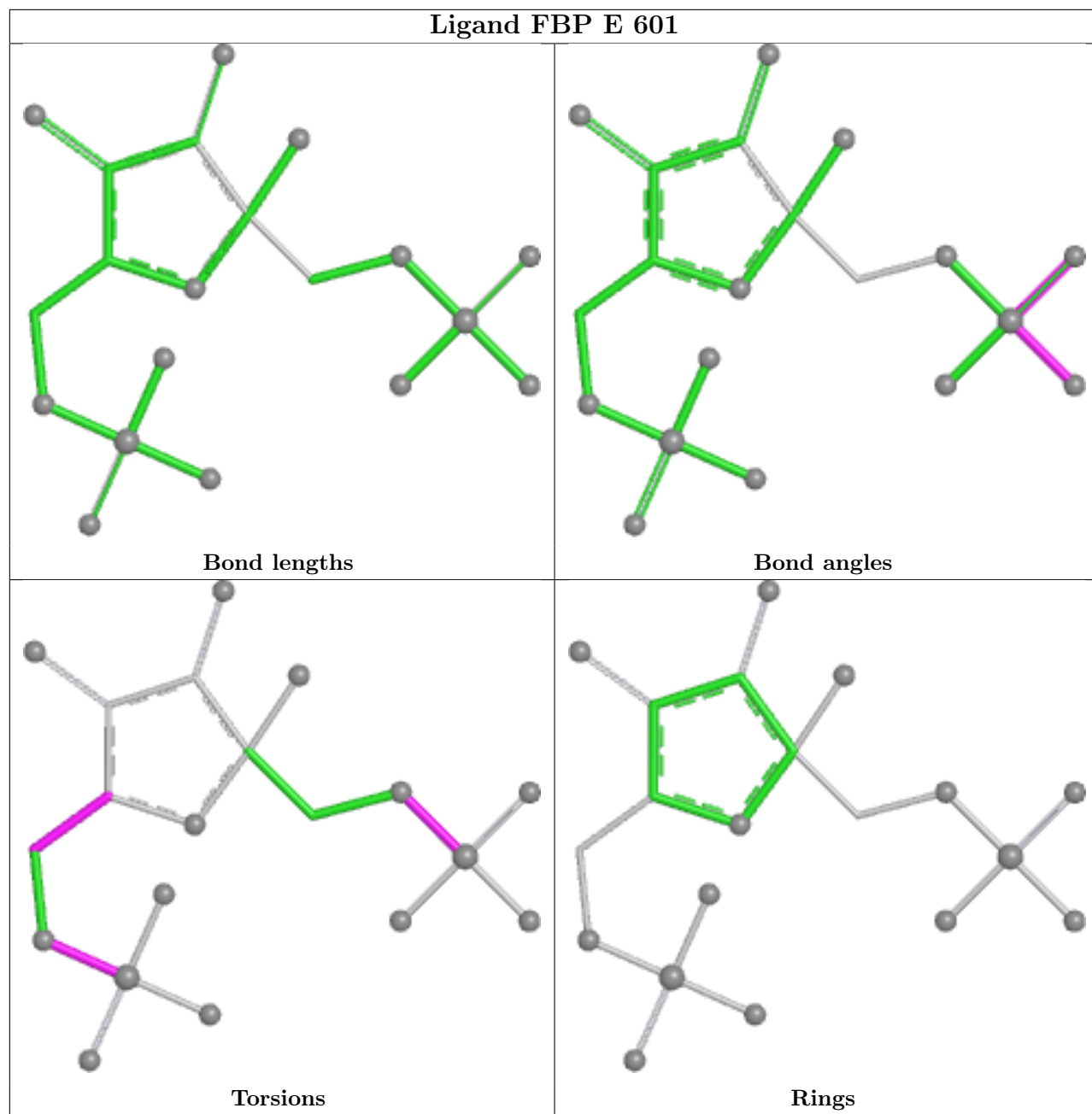
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



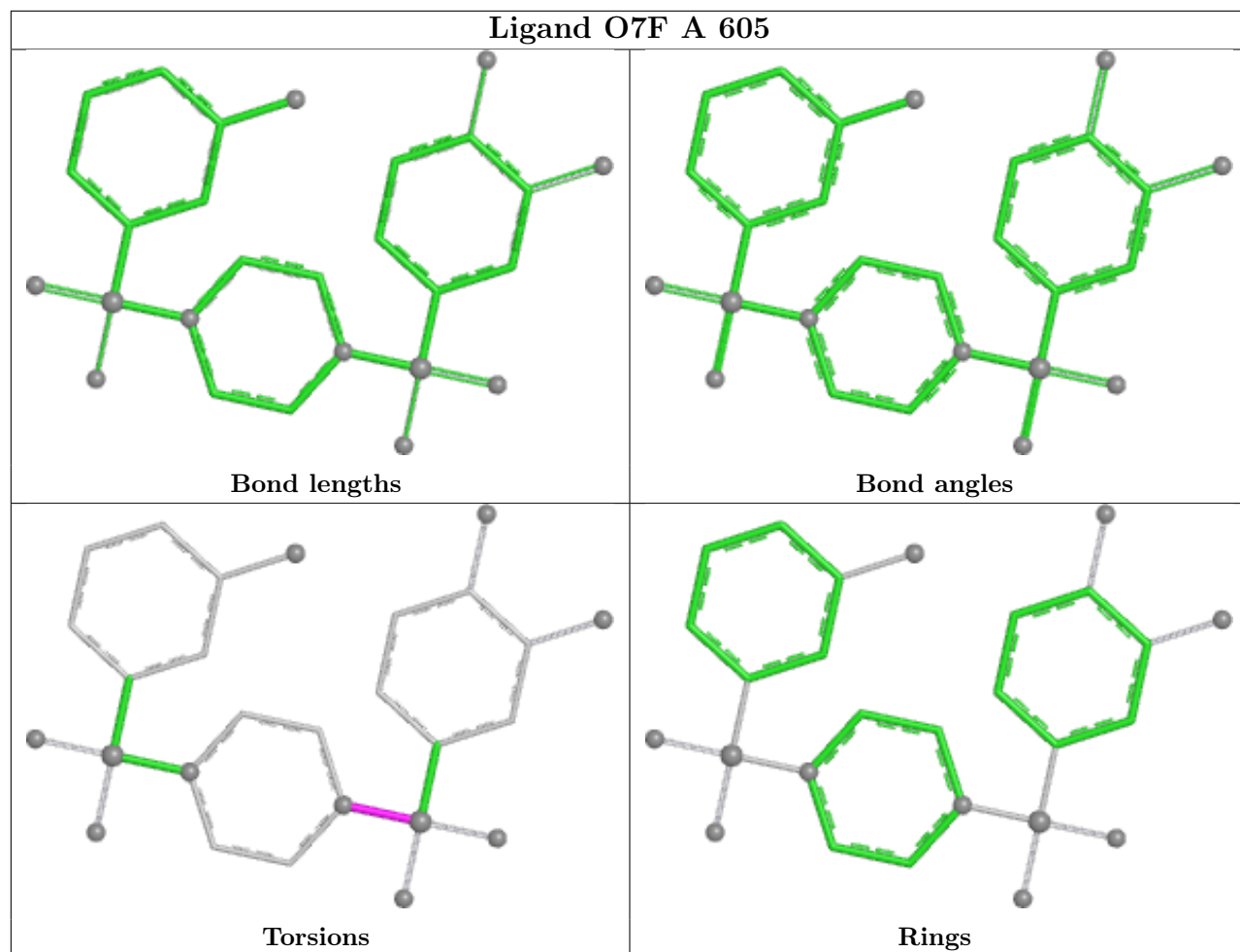




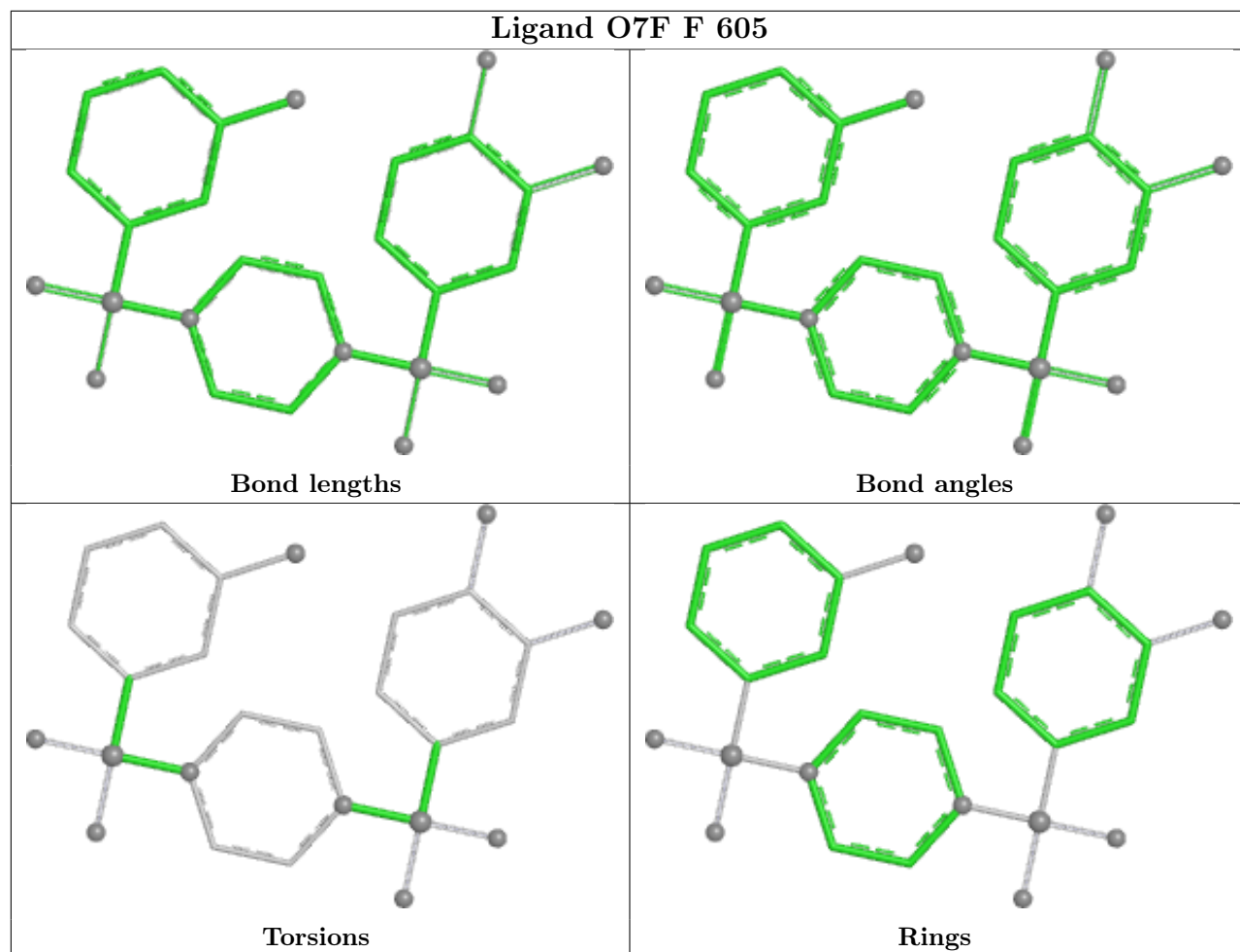
Ligand FBP E 601



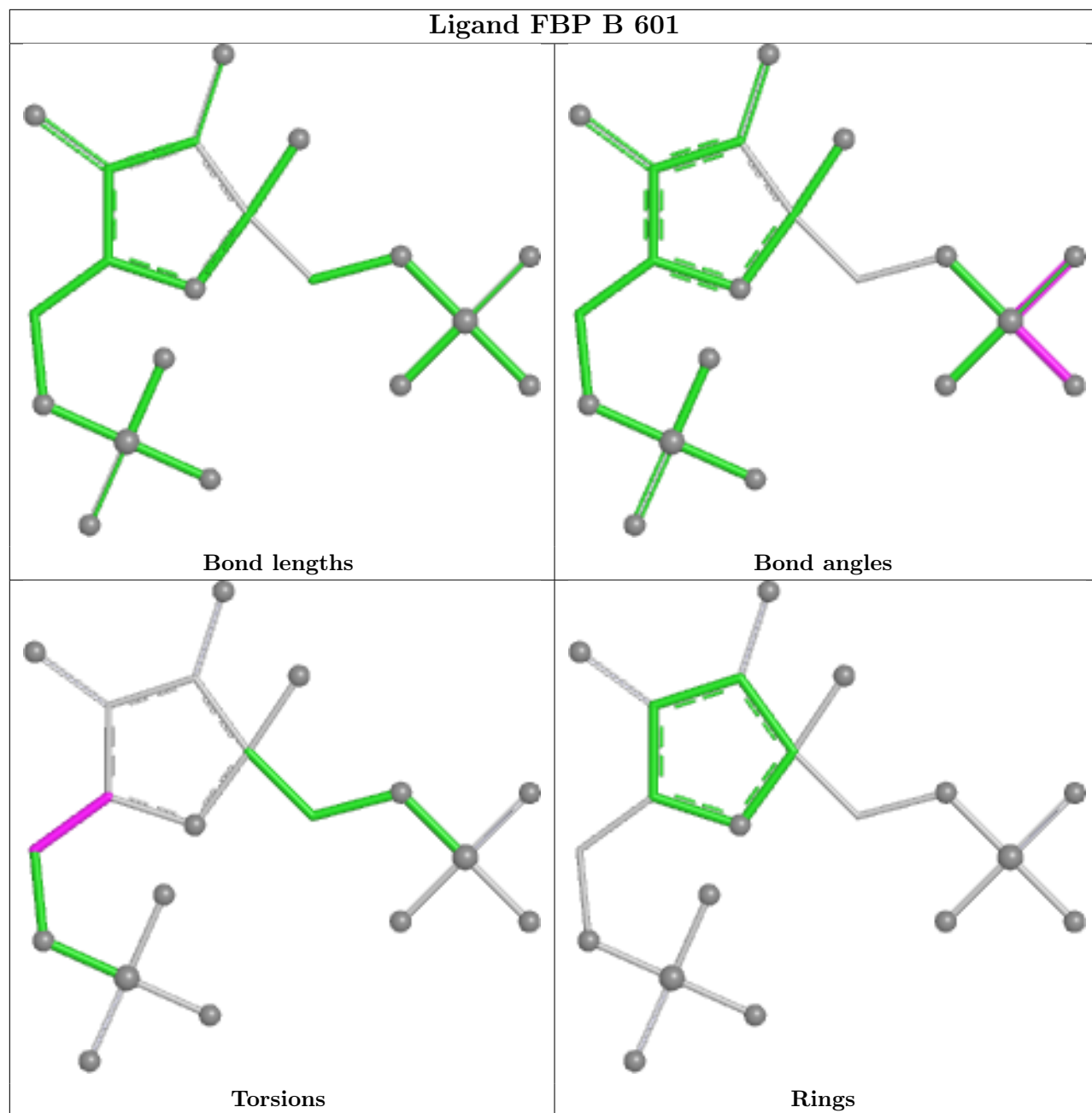
Ligand O7F A 605

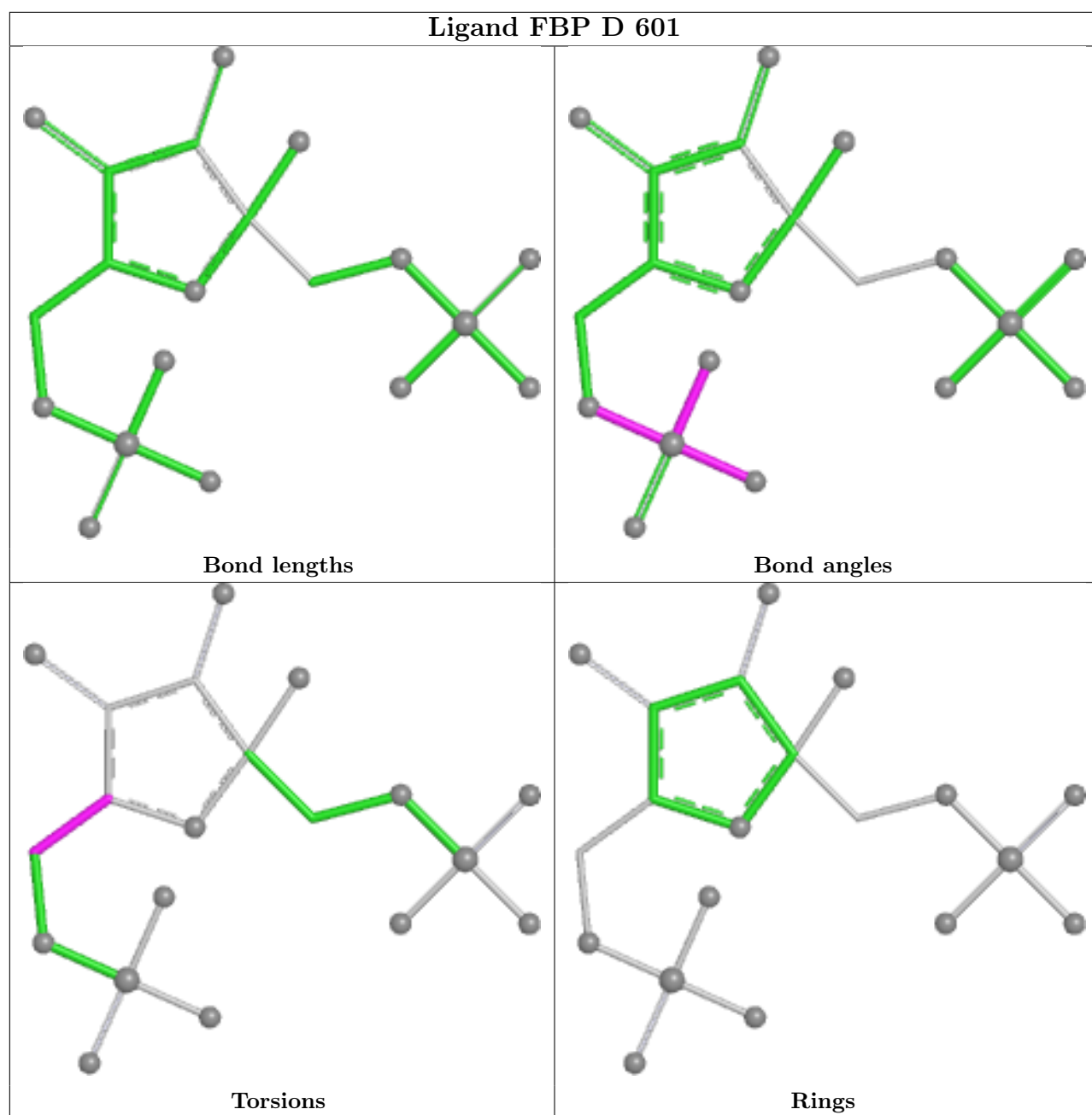


Ligand O7F F 605

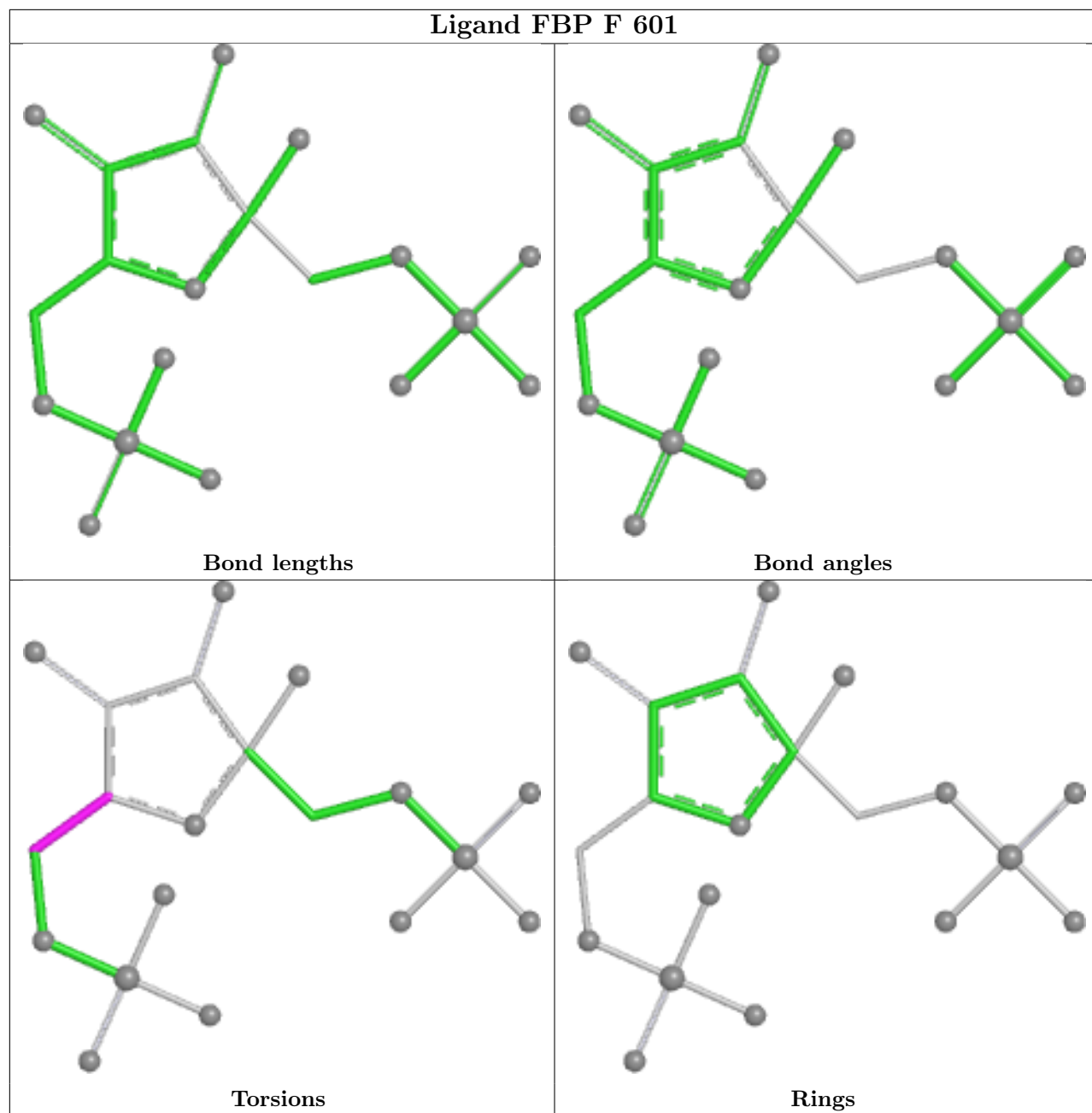


Ligand FBP B 601

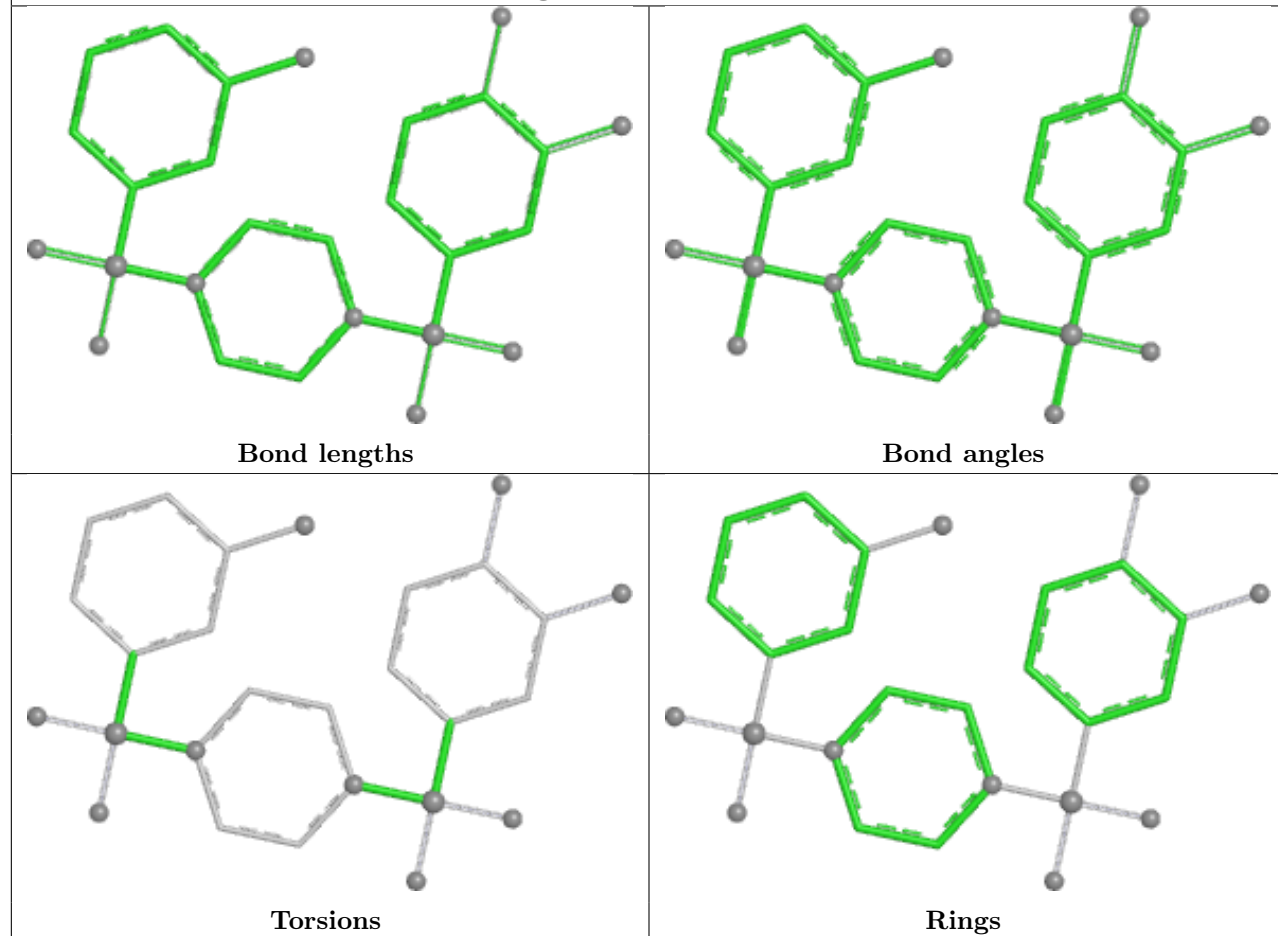


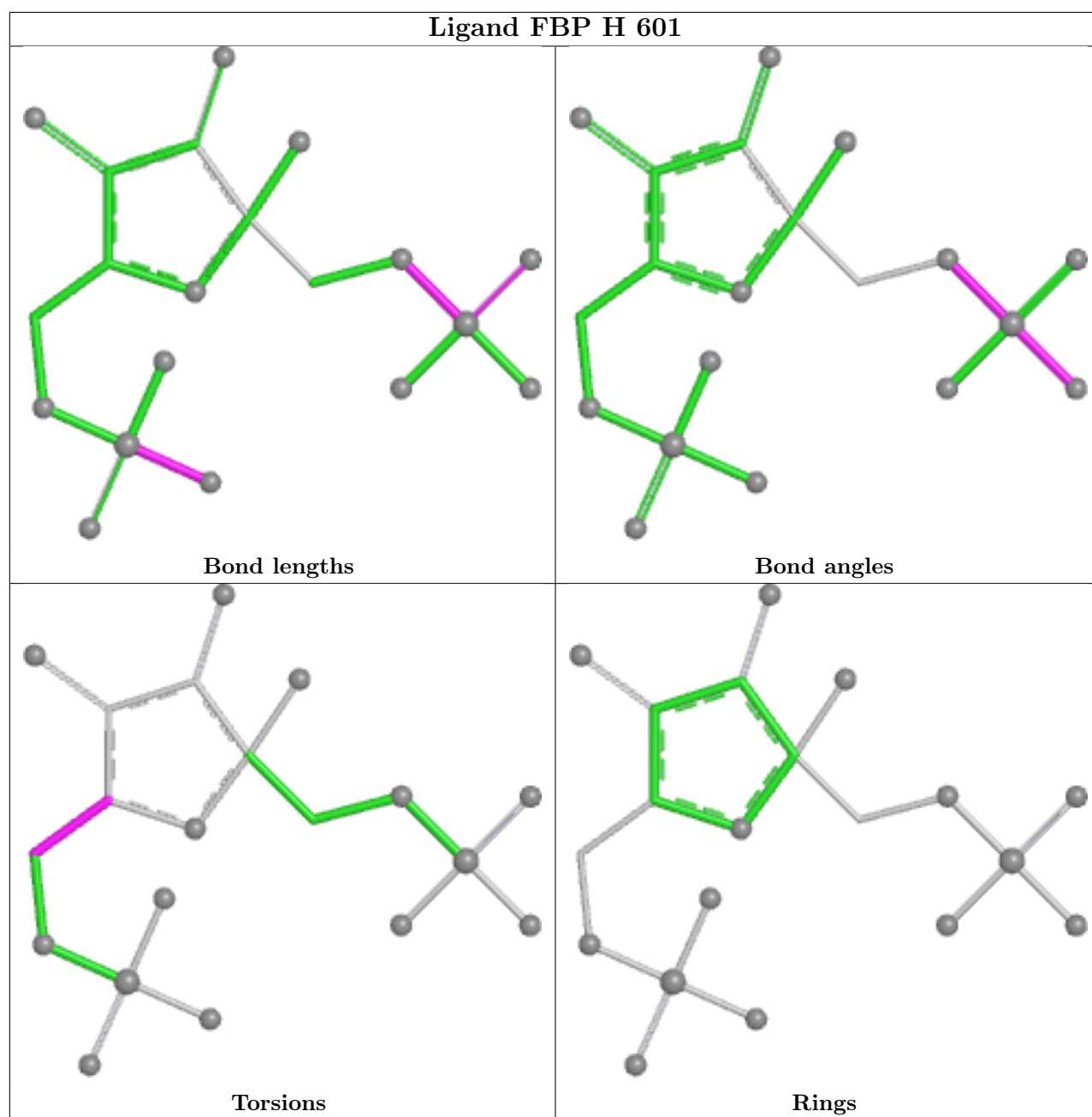


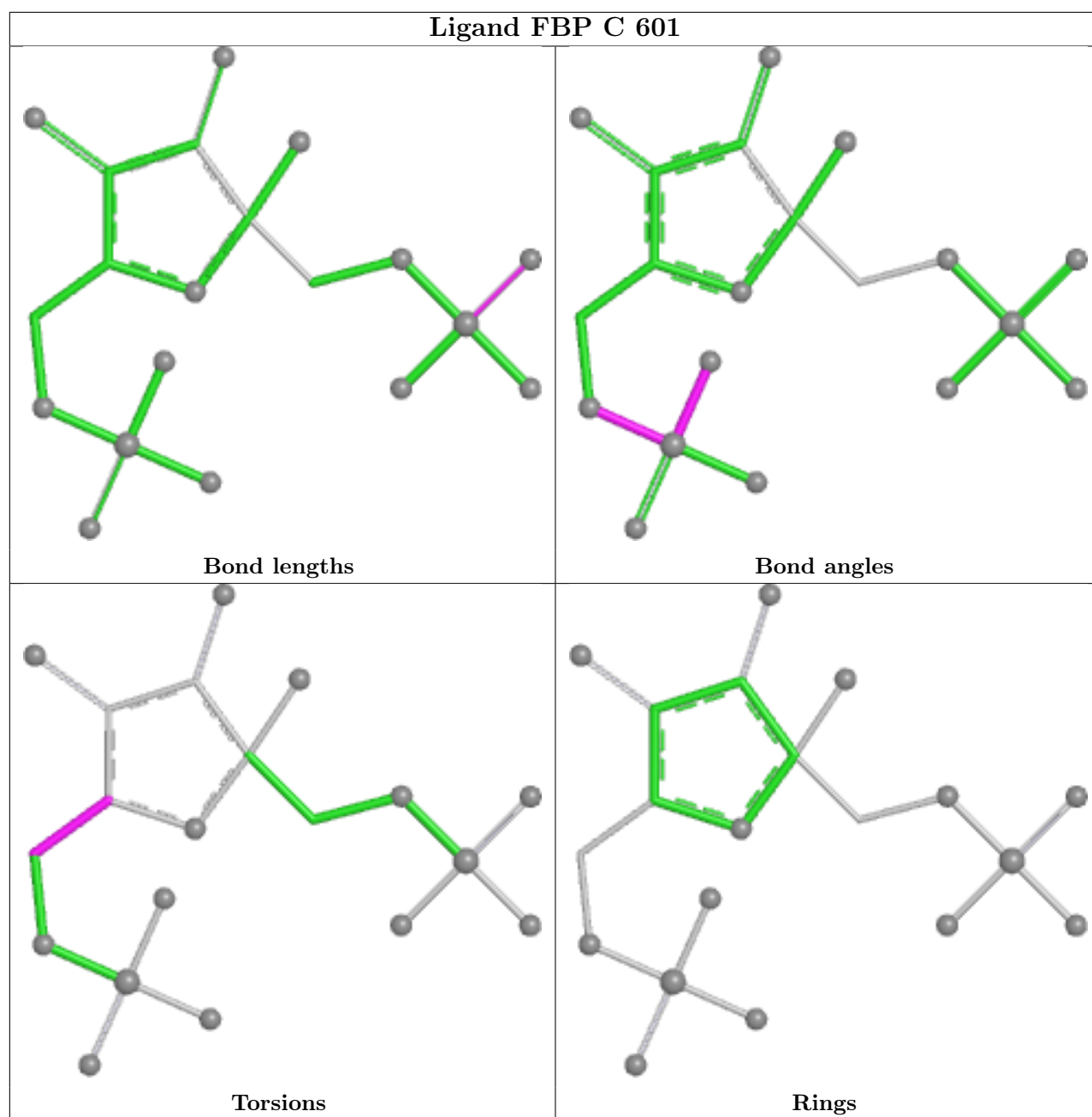
Ligand FBP F 601



Ligand O7F G 601







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	422/447 (94%)	1.45	101 (23%) 2 2	36, 70, 104, 120	6 (1%)
1	B	436/447 (97%)	1.16	76 (17%) 4 4	34, 60, 98, 108	4 (0%)
1	C	425/447 (95%)	0.85	52 (12%) 8 8	27, 54, 81, 124	4 (0%)
1	D	425/447 (95%)	0.18	13 (3%) 51 54	20, 41, 69, 122	5 (1%)
1	E	419/447 (93%)	1.35	91 (21%) 2 2	31, 66, 101, 118	5 (1%)
1	F	432/447 (96%)	0.73	38 (8%) 15 16	33, 53, 80, 102	7 (1%)
1	G	421/447 (94%)	0.39	19 (4%) 38 40	25, 46, 69, 99	7 (1%)
1	H	425/447 (95%)	0.04	13 (3%) 51 54	20, 39, 64, 114	4 (0%)
All	All	3405/3576 (95%)	0.77	403 (11%) 9 9	20, 54, 93, 124	42 (1%)

All (403) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	511	LEU	7.7
1	B	115	LEU	7.6
1	E	115	LEU	6.4
1	D	25	PHE	6.3
1	E	238	VAL	5.8
1	C	20	LEU	5.8
1	A	25	PHE	5.4
1	E	114	PRO	5.4
1	H	21	GLY	5.1
1	F	231	PRO	5.1
1	H	25	PHE	5.0
1	E	120	VAL	5.0
1	A	132	GLY	4.9
1	B	517	VAL	4.8
1	A	115	LEU	4.8
1	A	238	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	129	PRO	4.7
1	A	63	ILE	4.7
1	E	25	PHE	4.6
1	G	271	GLY	4.5
1	C	22	THR	4.5
1	G	24	PHE	4.4
1	A	232	GLY	4.4
1	E	244	GLY	4.3
1	G	25	PHE	4.3
1	A	482	PHE	4.3
1	C	66	ALA	4.3
1	E	23	ALA	4.3
1	E	502	VAL	4.3
1	B	116	SER	4.3
1	B	543	SER	4.3
1	A	24	PHE	4.2
1	E	116	SER	4.1
1	C	117	TYR	4.1
1	B	11	ALA	4.0
1	D	22	THR	4.0
1	F	512	ARG	4.0
1	A	30	LEU	4.0
1	B	267[A]	ARG	4.0
1	F	484	LEU	3.9
1	G	116	SER	3.9
1	B	527	TRP	3.9
1	B	114	PRO	3.9
1	B	490	PRO	3.9
1	D	24	PHE	3.9
1	D	21	GLY	3.9
1	B	13	VAL	3.9
1	E	249	VAL	3.9
1	A	378	ALA	3.9
1	A	241	LEU	3.8
1	H	24	PHE	3.8
1	A	95	TYR	3.8
1	A	34	MET	3.8
1	E	122	ILE	3.8
1	F	267[A]	ARG	3.8
1	C	80	GLY	3.8
1	E	232	GLY	3.8
1	C	397	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	23	ALA	3.7
1	C	114	PRO	3.7
1	A	249	VAL	3.7
1	C	21	GLY	3.7
1	E	495	ALA	3.7
1	E	119	PRO	3.7
1	E	112	GLY	3.7
1	B	493	ILE	3.7
1	H	22	THR	3.7
1	E	245	VAL	3.6
1	B	117	TYR	3.6
1	B	504	PHE	3.6
1	E	489	PRO	3.5
1	H	23	ALA	3.5
1	A	124	LEU	3.5
1	B	506	ILE	3.5
1	E	447	GLY	3.5
1	A	84	ALA	3.5
1	A	495	ALA	3.5
1	C	231	PRO	3.5
1	E	24	PHE	3.5
1	E	264	ALA	3.5
1	B	512	ARG	3.5
1	A	120	VAL	3.5
1	E	248	GLY	3.4
1	A	79	ALA	3.4
1	F	11	ALA	3.4
1	E	124	LEU	3.4
1	A	116	SER	3.3
1	C	65	PRO	3.3
1	C	63	ILE	3.3
1	C	311	ILE	3.3
1	B	485	LEU	3.3
1	E	442	VAL	3.3
1	E	110	PHE	3.3
1	B	502	VAL	3.3
1	A	100	ILE	3.3
1	E	493	ILE	3.2
1	A	73	LEU	3.2
1	E	257	VAL	3.2
1	A	277	ILE	3.2
1	C	77	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	533	TYR	3.2
1	C	25	PHE	3.2
1	A	114	PRO	3.2
1	A	122	ILE	3.2
1	B	542	ILE	3.2
1	B	118	ARG	3.2
1	E	126	THR	3.2
1	E	527	TRP	3.1
1	B	540[A]	LEU	3.1
1	B	130	GLY	3.1
1	A	23	ALA	3.1
1	B	110	PHE	3.1
1	F	12	ASP	3.1
1	B	495	ALA	3.1
1	B	508	SER	3.1
1	E	99	SER	3.1
1	A	112	GLY	3.1
1	C	386	ALA	3.1
1	C	103	VAL	3.1
1	C	115	LEU	3.1
1	F	233	LEU	3.1
1	C	34	MET	3.1
1	E	113	SER	3.1
1	E	464	ALA	3.0
1	F	13	VAL	3.0
1	A	117	TYR	3.0
1	A	488[A]	GLU	3.0
1	G	23	ALA	3.0
1	A	233	LEU	3.0
1	A	270	LEU	3.0
1	E	540	LEU	3.0
1	F	498	VAL	3.0
1	C	380	GLY	3.0
1	A	543	SER	3.0
1	E	485	LEU	3.0
1	F	348	THR	3.0
1	F	489	PRO	3.0
1	E	254	ALA	2.9
1	B	515	LEU	2.9
1	A	263	VAL	2.9
1	B	107	VAL	2.9
1	C	232	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	350	PRO	2.9
1	A	490	PRO	2.9
1	G	114	PRO	2.9
1	H	516	ARG	2.9
1	A	494	TRP	2.9
1	B	507	GLU	2.9
1	E	111	ALA	2.9
1	E	123	ALA	2.9
1	E	260	ALA	2.9
1	C	75	GLU	2.9
1	A	61	ALA	2.9
1	E	118	ARG	2.9
1	C	111	ALA	2.9
1	A	527	TRP	2.9
1	F	527	TRP	2.9
1	E	30	LEU	2.8
1	A	119	PRO	2.8
1	G	113	SER	2.8
1	E	117	TYR	2.8
1	A	351	ARG	2.8
1	B	378	ALA	2.8
1	C	23	ALA	2.8
1	C	271	GLY	2.8
1	A	52	VAL	2.8
1	A	279	ILE	2.8
1	F	490	PRO	2.8
1	E	514	PHE	2.8
1	F	511	LEU	2.8
1	E	541[A]	SER	2.8
1	C	132	GLY	2.8
1	D	30	LEU	2.8
1	A	489	PRO	2.8
1	E	490	PRO	2.8
1	F	347	ILE	2.8
1	G	63	ILE	2.8
1	B	113	SER	2.7
1	E	234	SER	2.7
1	A	514	PHE	2.7
1	B	88	PHE	2.7
1	B	514	PHE	2.7
1	A	123	ALA	2.7
1	C	339	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	486	TYR	2.7
1	B	97	ALA	2.7
1	E	484	LEU	2.7
1	B	249	VAL	2.7
1	B	521	VAL	2.7
1	C	70	VAL	2.7
1	E	275	HIS	2.7
1	G	34	MET	2.7
1	F	351	ARG	2.7
1	A	269	ALA	2.7
1	E	269	ALA	2.7
1	B	484	LEU	2.7
1	E	233	LEU	2.7
1	E	97	ALA	2.6
1	B	124	LEU	2.6
1	B	95	TYR	2.6
1	A	256	PHE	2.6
1	B	241	LEU	2.6
1	F	543	SER	2.6
1	F	516	ARG	2.6
1	A	70	VAL	2.6
1	A	274	GLY	2.6
1	E	26	GLN	2.6
1	E	437	ALA	2.6
1	B	86	LEU	2.6
1	F	540[A]	LEU	2.6
1	G	272	PRO	2.6
1	C	24	PHE	2.6
1	E	88	PHE	2.6
1	E	256	PHE	2.6
1	E	487	ARG	2.6
1	H	543	SER	2.6
1	B	100	ILE	2.6
1	C	107	VAL	2.6
1	F	238	VAL	2.6
1	B	513	GLY	2.6
1	C	101	ALA	2.6
1	E	104	ARG	2.6
1	A	86	LEU	2.6
1	A	99	SER	2.6
1	F	16	LEU	2.6
1	B	70	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	426	ILE	2.5
1	E	505	GLY	2.5
1	H	34	MET	2.5
1	C	366	ASP	2.5
1	H	231	PRO	2.5
1	G	115	LEU	2.5
1	A	407	PHE	2.5
1	B	243	PHE	2.5
1	E	243	PHE	2.5
1	E	63	ILE	2.5
1	E	70	VAL	2.5
1	E	289	VAL	2.5
1	A	265	ALA	2.5
1	B	231	PRO	2.5
1	E	469	ALA	2.5
1	B	233	LEU	2.5
1	A	80	GLY	2.5
1	E	251	ILE	2.5
1	A	62	THR	2.5
1	A	66	ALA	2.5
1	A	264	ALA	2.5
1	A	382	PHE	2.5
1	C	110	PHE	2.5
1	F	112	GLY	2.5
1	C	384	VAL	2.4
1	E	103	VAL	2.4
1	B	12	ASP	2.4
1	C	378	ALA	2.4
1	A	88	PHE	2.4
1	B	64	GLY	2.4
1	C	59	ILE	2.4
1	A	33	ALA	2.4
1	B	14	ALA	2.4
1	C	79	ALA	2.4
1	E	84	ALA	2.4
1	E	268	ALA	2.4
1	G	487	ARG	2.4
1	A	540	LEU	2.4
1	C	86	LEU	2.4
1	A	130	GLY	2.4
1	B	509	GLY	2.4
1	C	100	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	487	ARG	2.4
1	B	119	PRO	2.4
1	A	111	ALA	2.4
1	B	505	GLY	2.4
1	C	64	GLY	2.4
1	E	307	GLY	2.4
1	A	493	ILE	2.4
1	E	351	ARG	2.4
1	A	541	SER	2.4
1	B	489	PRO	2.4
1	G	118	ARG	2.3
1	A	60	ILE	2.3
1	A	113	SER	2.3
1	A	347	ILE	2.3
1	G	109	SER	2.3
1	C	106	ALA	2.3
1	E	101	ALA	2.3
1	F	499	ASP	2.3
1	A	253	PHE	2.3
1	A	280	ILE	2.3
1	A	426	ILE	2.3
1	E	506	ILE	2.3
1	E	542	ILE	2.3
1	F	275	HIS	2.3
1	A	252	VAL	2.3
1	H	273	GLU	2.3
1	C	383	PRO	2.3
1	E	272	PRO	2.3
1	F	14	ALA	2.3
1	D	232	GLY	2.3
1	E	241	LEU	2.3
1	E	494	TRP	2.3
1	A	118	ARG	2.3
1	B	487	ARG	2.3
1	F	118	ARG	2.3
1	F	232	GLY	2.3
1	B	131	SER	2.3
1	B	120	VAL	2.3
1	E	445	THR	2.3
1	A	53	ALA	2.3
1	B	16	LEU	2.3
1	D	115	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	95	TYR	2.3
1	E	95	TYR	2.3
1	E	247	HIS	2.2
1	A	125	ASP	2.2
1	A	91	GLY	2.2
1	A	248	GLY	2.2
1	D	33	ALA	2.2
1	B	108	GLU	2.2
1	A	90	HIS	2.2
1	F	411	ARG	2.2
1	F	504	PHE	2.2
1	A	251	ILE	2.2
1	B	22	THR	2.2
1	B	498	VAL	2.2
1	G	231	PRO	2.2
1	E	276	GLY	2.2
1	G	232	GLY	2.2
1	B	488	GLU	2.2
1	A	453	LEU	2.2
1	E	486	TYR	2.2
1	A	69	SER	2.2
1	A	311	ILE	2.2
1	B	272	PRO	2.2
1	A	298	VAL	2.2
1	B	465	VAL	2.2
1	E	107	VAL	2.2
1	C	507	GLU	2.2
1	F	488	GLU	2.2
1	A	460	ALA	2.2
1	G	33	ALA	2.2
1	C	343	LEU	2.2
1	B	541	SER	2.2
1	F	242	ARG	2.2
1	H	267[A]	ARG	2.2
1	A	272	PRO	2.1
1	A	377	THR	2.2
1	A	110	PHE	2.1
1	C	108	GLU	2.1
1	B	103	VAL	2.1
1	A	93	HIS	2.1
1	A	121	ALA	2.1
1	B	111	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	265	ALA	2.1
1	D	231	PRO	2.1
1	A	83	ILE	2.1
1	D	311	ILE	2.1
1	E	252	VAL	2.1
1	F	521	VAL	2.1
1	A	404	ARG	2.1
1	A	101	ALA	2.1
1	B	61	ALA	2.1
1	B	260	ALA	2.1
1	H	30	LEU	2.1
1	D	34	MET	2.1
1	B	75	GLU	2.1
1	F	71	GLU	2.1
1	A	486	TYR	2.1
1	B	533	TYR	2.1
1	C	68	ARG	2.1
1	F	122	ILE	2.1
1	G	347	ILE	2.1
1	E	481	VAL	2.1
1	E	515	LEU	2.1
1	F	237	ASP	2.1
1	A	126	THR	2.1
1	A	533	TYR	2.1
1	C	90	HIS	2.1
1	C	348	THR	2.1
1	A	463	ILE	2.1
1	C	347	ILE	2.1
1	E	504	PHE	2.1
1	A	35	ALA	2.1
1	A	268	ALA	2.1
1	C	69	SER	2.1
1	E	109	SER	2.1
1	E	543	SER	2.1
1	F	23	ALA	2.1
1	G	363	ALA	2.1
1	B	20	LEU	2.0
1	C	73	LEU	2.0
1	B	242	ARG	2.0
1	E	411	ARG	2.0
1	H	275[A]	HIS	2.0
1	E	377	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	401	VAL	2.0
1	B	382	PHE	2.0
1	E	263	VAL	2.0
1	B	492	ALA	2.0
1	C	97	ALA	2.0
1	A	373	LEU	2.0
1	A	340	THR	2.0
1	D	513	GLY	2.0
1	E	380	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	K	E	604	1/1	0.74	0.22	135,135,135,135	0
3	OXL	E	602	6/6	0.77	0.14	84,85,85,85	0
3	OXL	D	602	6/6	0.88	0.14	58,58,59,59	0
6	O7F	A	605	27/27	0.89	0.15	64,70,73,74	19
5	K	C	604	1/1	0.90	0.15	80,80,80,80	0
2	FBP	E	601	20/20	0.90	0.11	61,65,69,69	0
3	OXL	C	602	6/6	0.90	0.12	78,78,79,79	0
6	O7F	G	601	27/27	0.90	0.14	65,67,68,70	19
3	OXL	A	602	6/6	0.91	0.10	83,84,84,84	0
6	O7F	F	605	27/27	0.91	0.14	55,57,58,59	19
3	OXL	F	602	6/6	0.91	0.11	68,69,70,70	0
5	K	A	604	1/1	0.92	0.14	102,102,102,102	0
3	OXL	B	602	6/6	0.92	0.09	65,66,67,67	0
3	OXL	H	602	6/6	0.92	0.10	48,49,50,50	0

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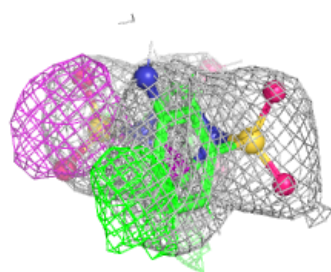
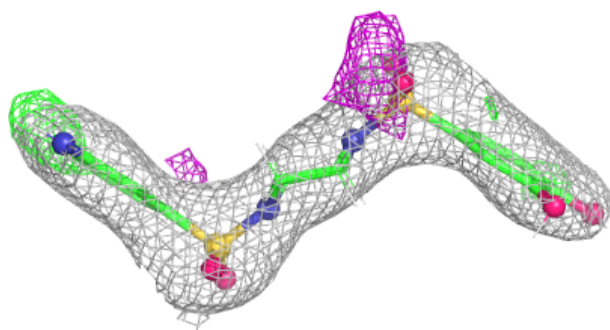
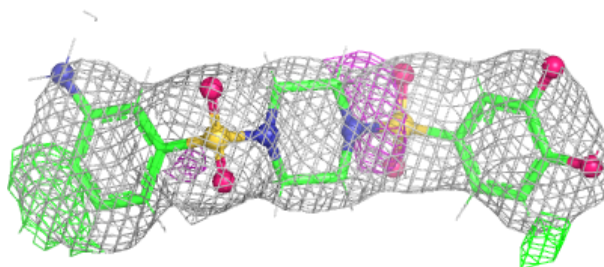
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	K	F	604	1/1	0.93	0.09	85,85,85,85	0
2	FBP	A	601	20/20	0.93	0.09	63,65,67,67	0
3	OXL	G	603	6/6	0.94	0.09	62,62,63,63	0
5	K	G	605	1/1	0.94	0.10	79,79,79,79	0
5	K	B	604	1/1	0.94	0.08	96,96,96,96	0
6	O7F	B	605	27/27	0.94	0.12	58,59,60,61	19
2	FBP	B	601	20/20	0.94	0.09	60,61,64,65	0
4	MG	D	603	1/1	0.94	0.17	31,31,31,31	0
2	FBP	F	601	20/20	0.95	0.07	53,59,62,63	0
4	MG	A	603	1/1	0.96	0.12	55,55,55,55	0
4	MG	E	603	1/1	0.97	0.08	48,48,48,48	0
4	MG	F	603	1/1	0.97	0.09	35,35,35,35	0
4	MG	B	603	1/1	0.97	0.11	39,39,39,39	0
2	FBP	C	601	20/20	0.98	0.05	36,38,42,42	0
2	FBP	D	601	20/20	0.98	0.04	32,33,36,37	0
5	K	H	604	1/1	0.98	0.15	58,58,58,58	0
4	MG	C	603	1/1	0.98	0.11	38,38,38,38	0
2	FBP	G	602	20/20	0.98	0.05	34,35,41,42	0
5	K	D	604	1/1	0.98	0.07	63,63,63,63	0
2	FBP	H	601	20/20	0.98	0.05	29,31,34,34	0
4	MG	G	604	1/1	1.00	0.05	25,25,25,25	0
4	MG	H	603	1/1	1.00	0.07	24,24,24,24	0

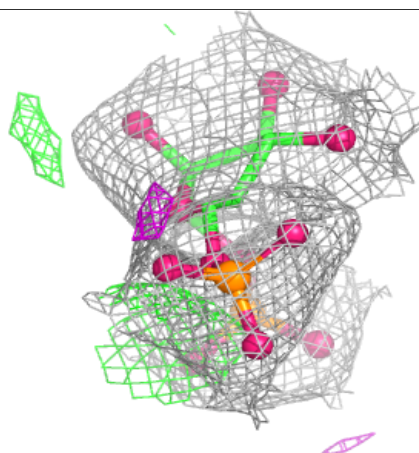
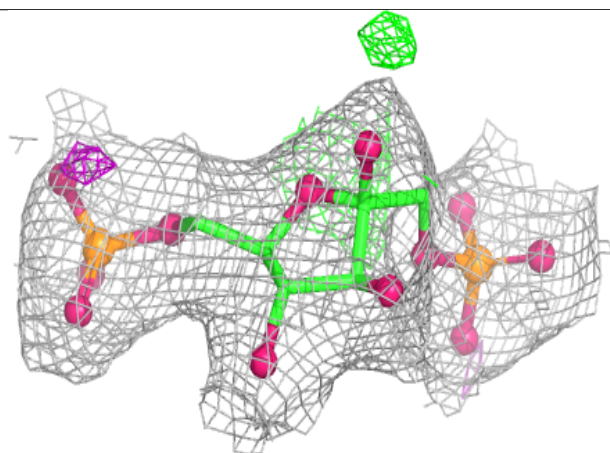
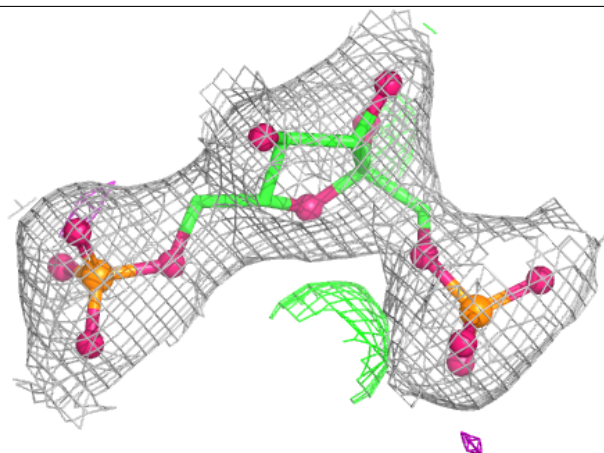
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around O7F A 605:

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

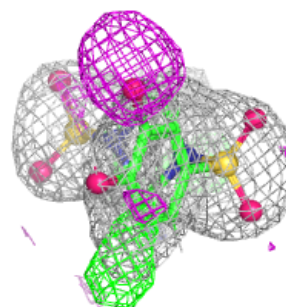
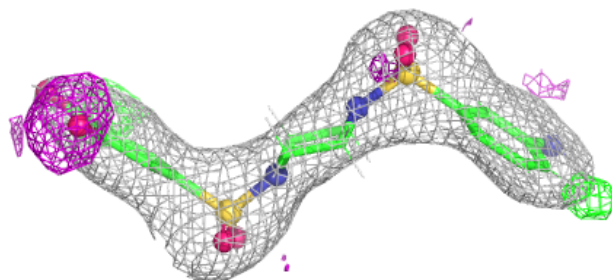
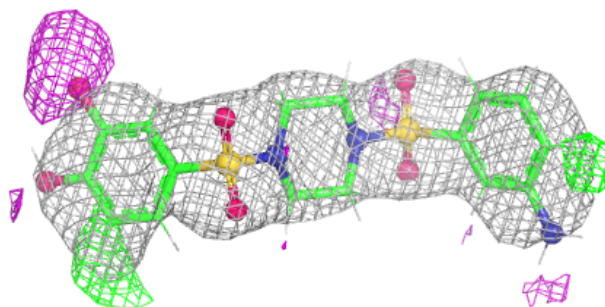
**Electron density around FBP E 601:**

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

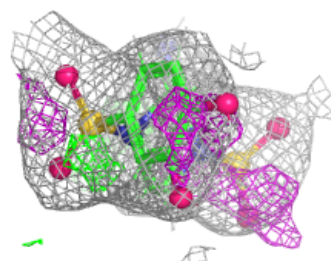
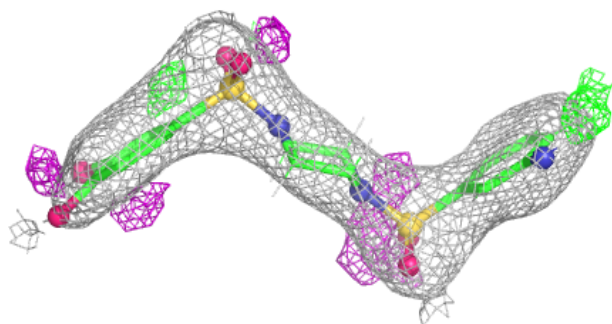
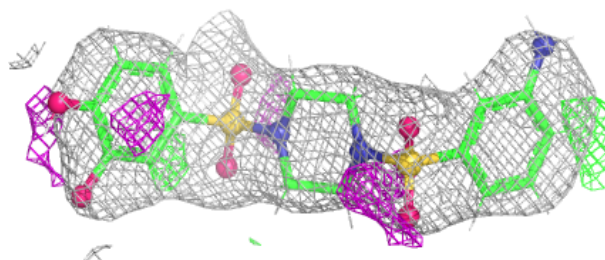


Electron density around O7F G 601:

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

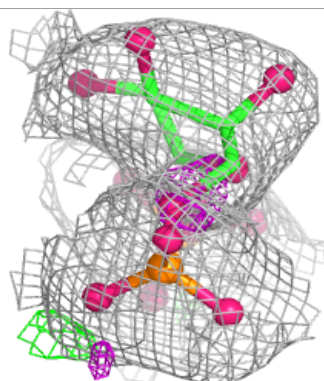
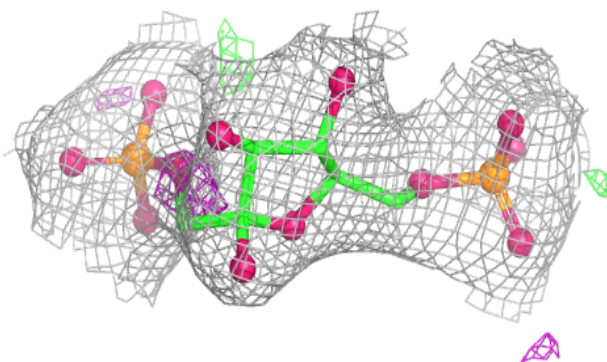
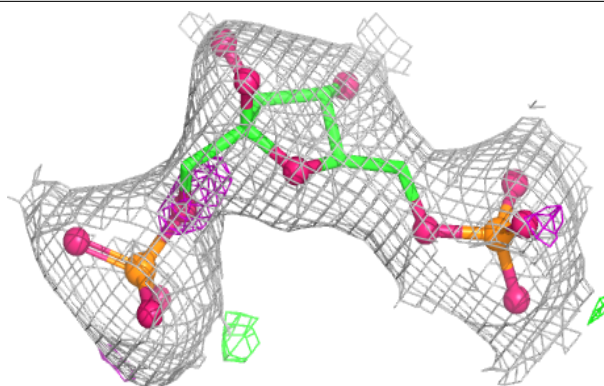
**Electron density around O7F F 605:**

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

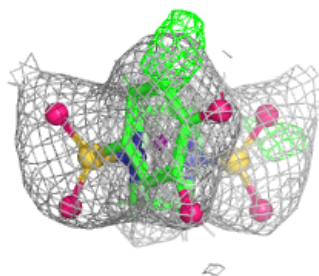
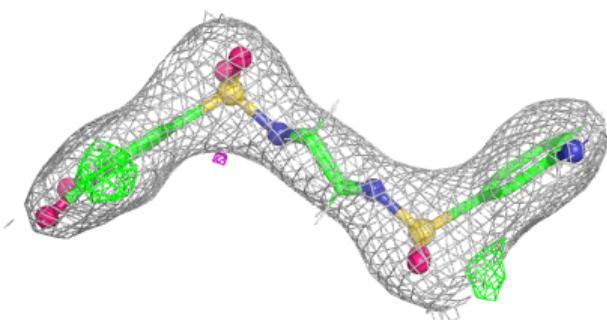
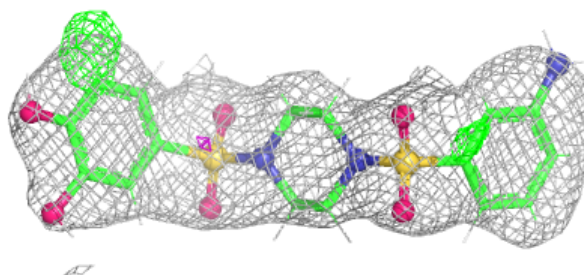


Electron density around FBP A 601:

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

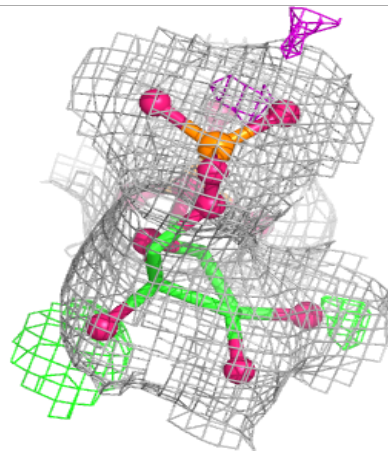
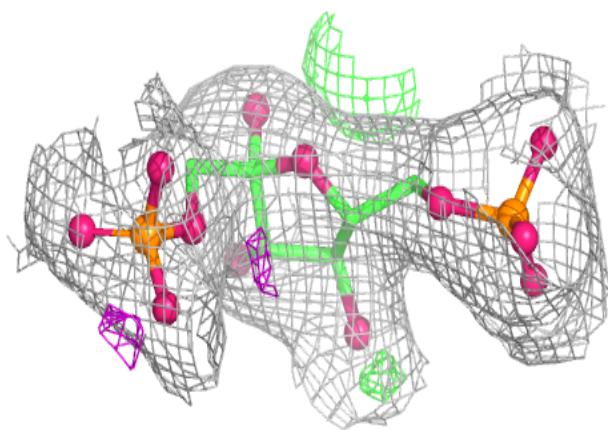
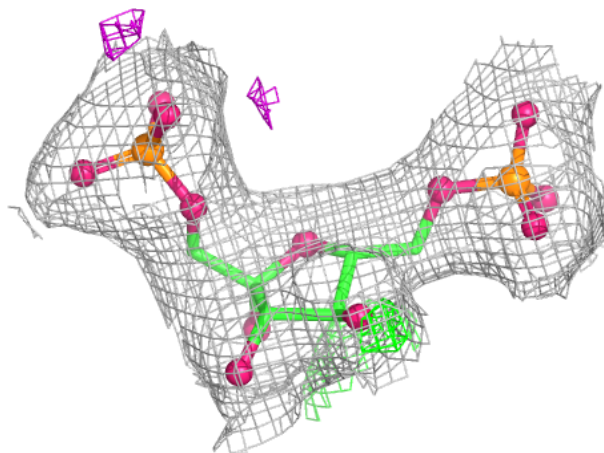
**Electron density around O7F B 605:**

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



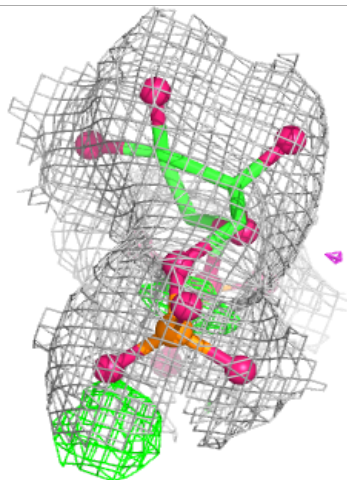
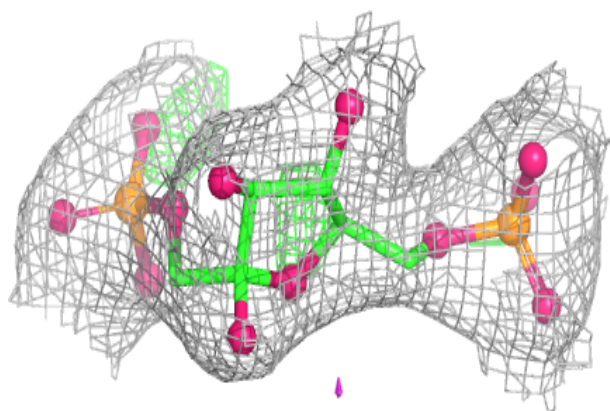
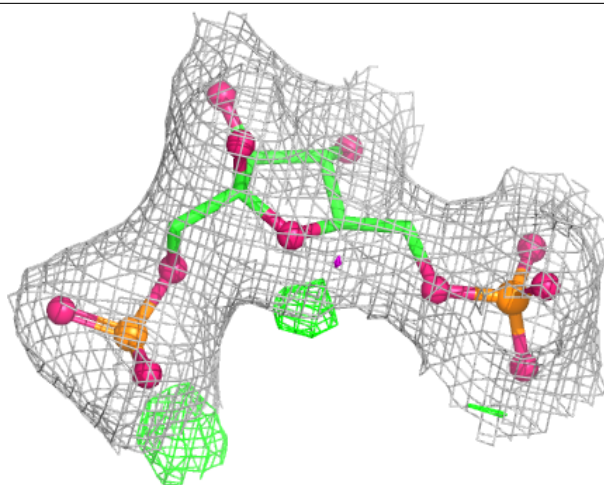
Electron density around FBP B 601:

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



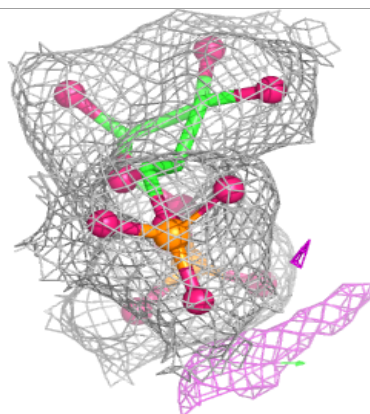
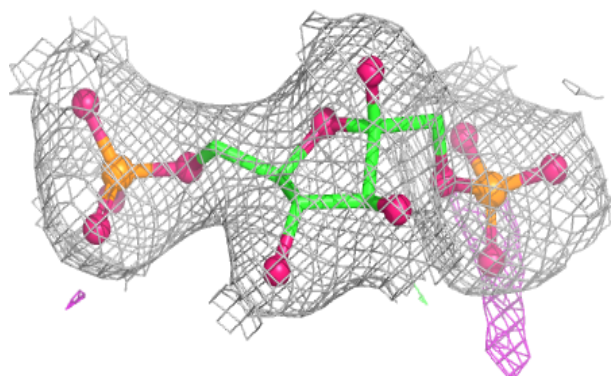
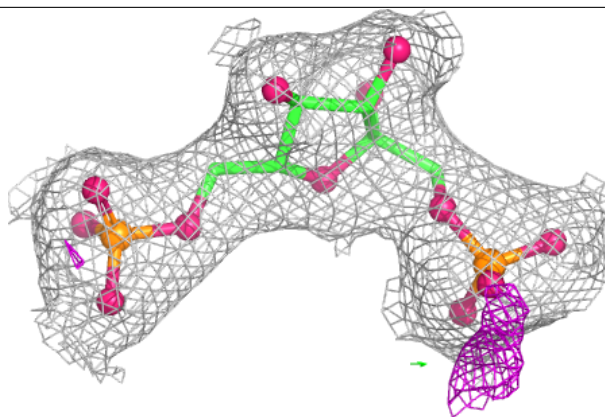
Electron density around FBP F 601:

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

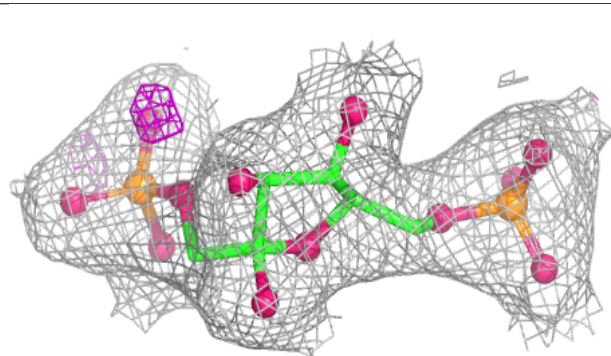
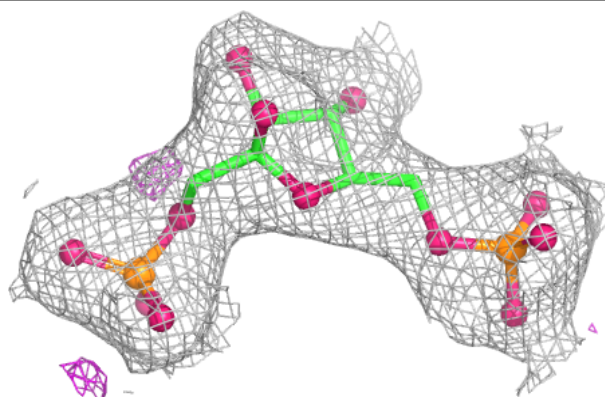


Electron density around FBP C 601:

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

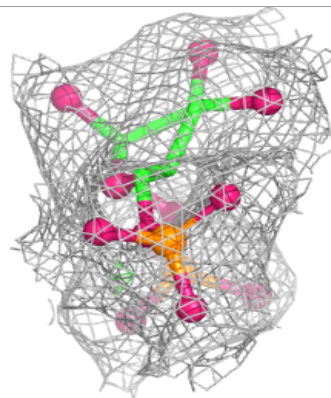
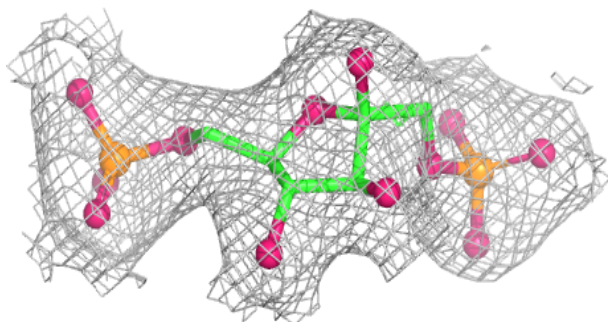
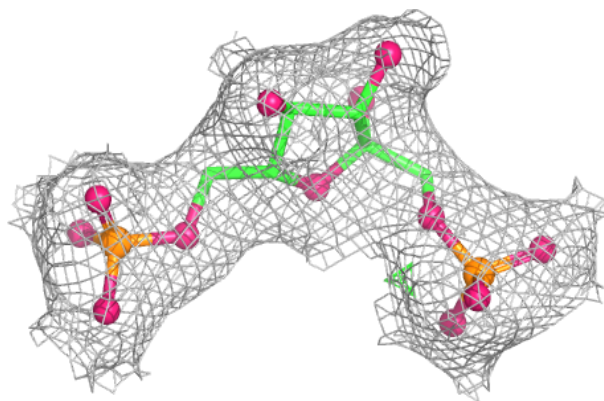
**Electron density around FBP D 601:**

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

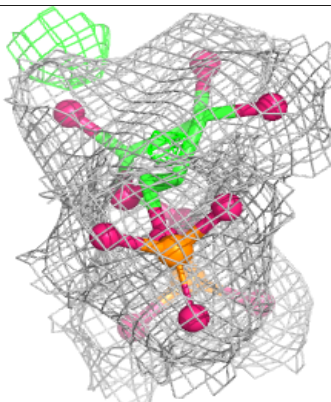
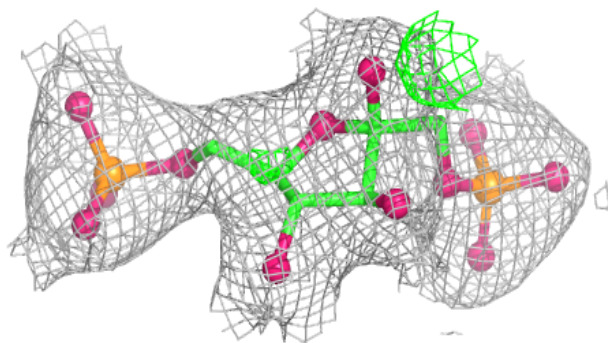
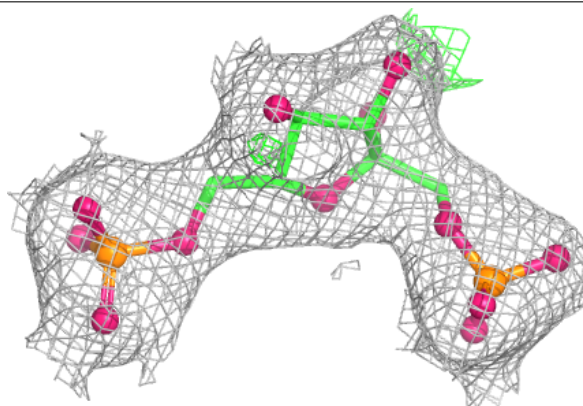


Electron density around FBP G 602:

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

**Electron density around FBP H 601:**

$2mF_o-DF_c$ (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.