



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:44 AM UTC

PDB ID : 7FRW / pdb_00007frw
Title : Structure of liver pyruvate kinase in complex with allosteric modulator 4
Authors : Lulla, A.; Nilsson, O.; Brear, P.; Nain-Perez, A.; Grotli, M.; Hyvonen, M.
Deposited on : 2022-12-18
Resolution : 1.74 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:

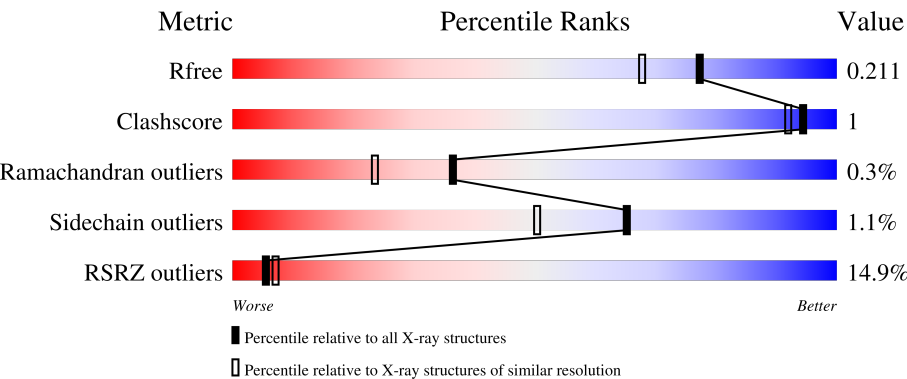
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.74 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	21% 90% 6%
1	B	447	38% 92% 5%
1	C	447	8% 91% 5%
1	D	447	5% 92% 5%
1	E	447	18% 90% 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	603	-	X	-	-
3	OXL	D	602	-	X	-	-
3	OXL	E	602	-	X	-	-
3	OXL	F	602	-	X	-	-
3	OXL	G	602	-	X	-	-
3	OXL	H	603	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 29252 atoms, of which 64 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	6	0
			3252	2042	590	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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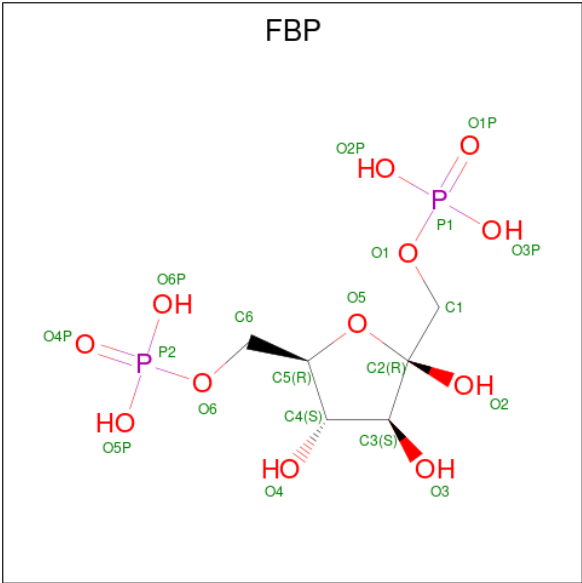
Chain	Residue	Modelled	Actual	Comment	Reference
B	130	GLY	-	linker	UNP P30613
B	131	SER	-	linker	UNP P30613
B	132	GLY	-	linker	UNP P30613
C	-1	GLY	-	expression tag	UNP P30613
C	0	SER	-	expression tag	UNP P30613
C	1	MET	-	expression tag	UNP P30613
C	2	GLU	-	expression tag	UNP P30613
C	12	ASP	SER	conflict	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		

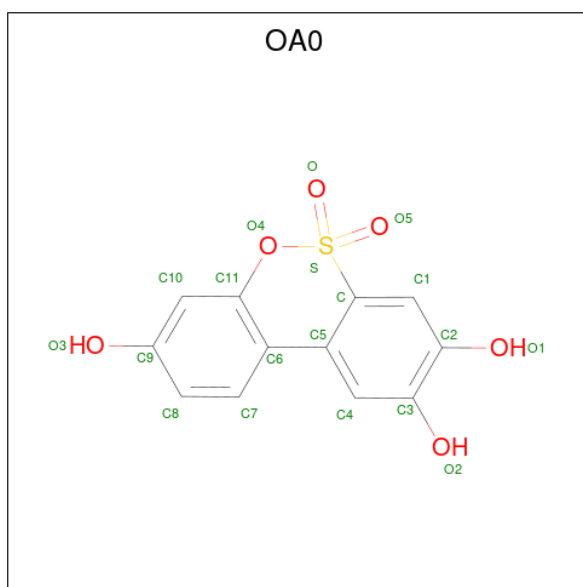
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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 (10aM)-3,8,9-trihydroxy-6H-6lambda 6 -dibenzo[c,e][1,2]oxathiine-6,6-dione (CCD ID: OA0) (formula: C₁₂H₈O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	O	S	8	0
			27	12	8	6	1		
6	B	1	Total	C	H	O	S	8	0
			27	12	8	6	1		
6	C	1	Total	C	H	O	S	8	0
			27	12	8	6	1		
6	D	1	Total	C	H	O	S	8	0
			27	12	8	6	1		
6	E	1	Total	C	H	O	S	8	0
			27	12	8	6	1		
6	F	1	Total	C	H	O	S	8	0
			27	12	8	6	1		
6	G	1	Total	C	H	O	S	8	0
			27	12	8	6	1		
6	H	1	Total	C	H	O	S	8	0
			27	12	8	6	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	233	Total	O	0	0
			233	233		
7	B	204	Total	O	0	0
			204	204		
7	C	355	Total	O	0	0
			355	355		
7	D	420	Total	O	0	0
			420	420		

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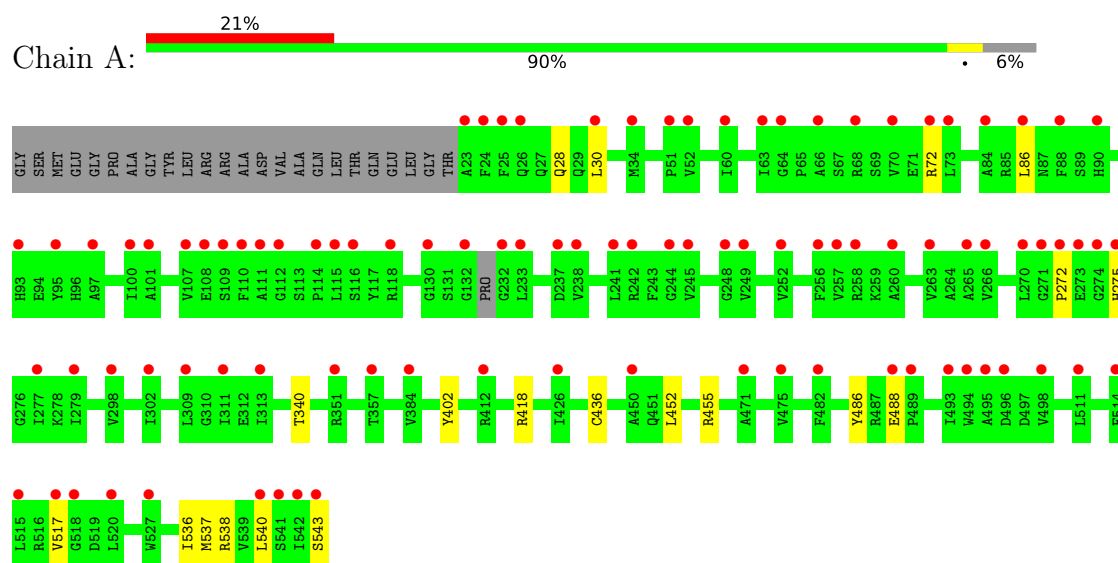
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	248	Total 248	O 248	0	0
7	F	374	Total 374	O 374	0	0
7	G	416	Total 416	O 416	0	0
7	H	485	Total 485	O 485	0	0

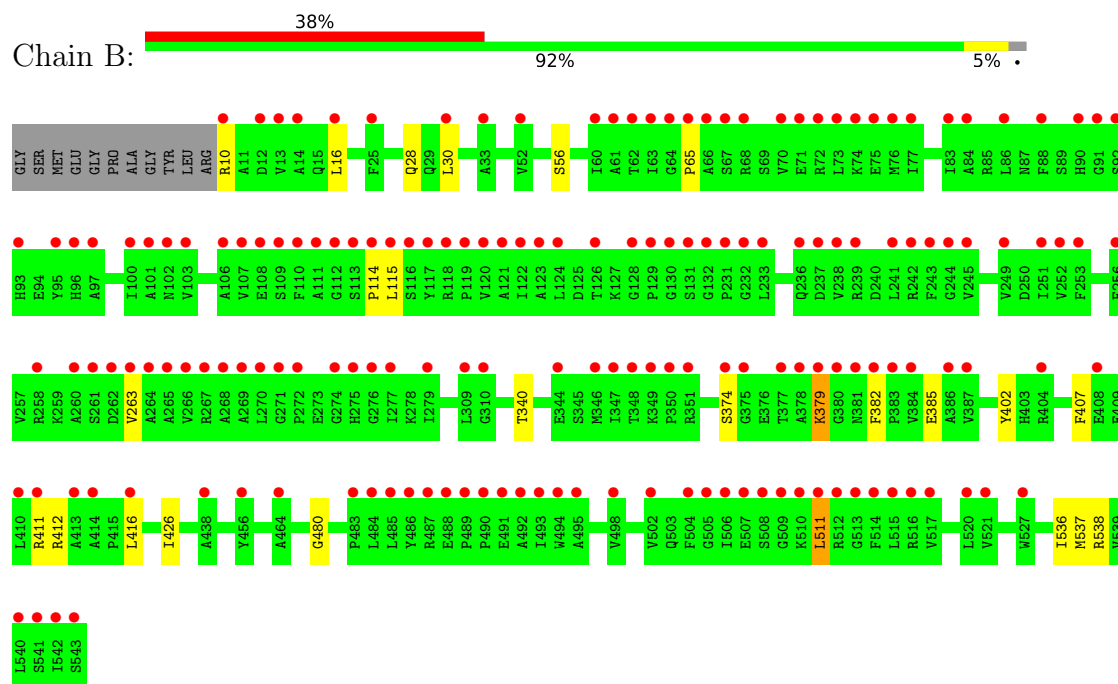
3 Residue-property plots [i](#)

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.

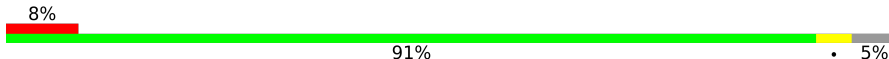
• Molecule 1: Pyruvate kinase PKLR

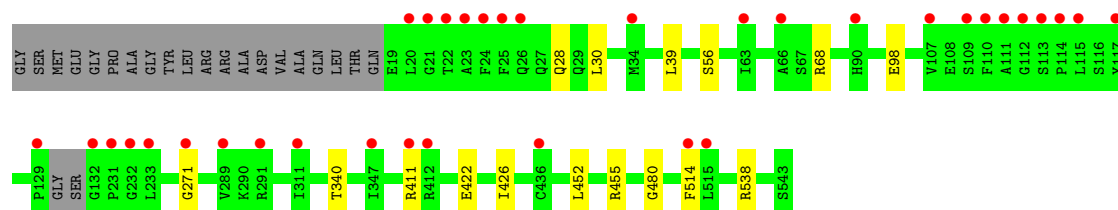


• Molecule 1: Pyruvate kinase PKLR

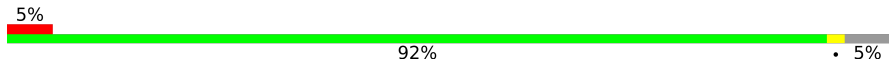


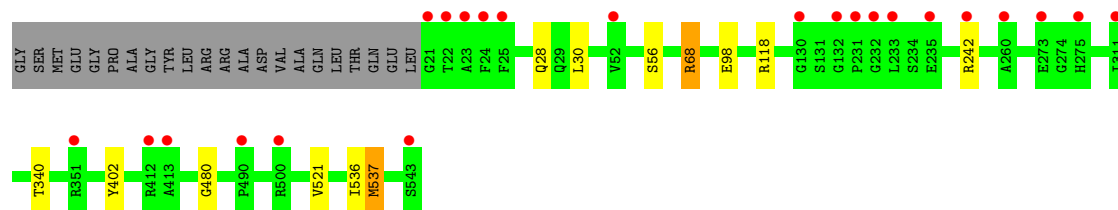
- Molecule 1: Pyruvate kinase PKLR

Chain C:  8% 91% 5%



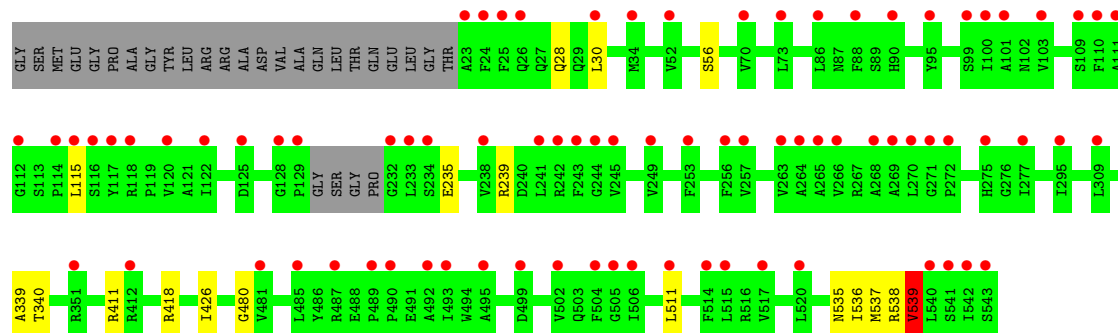
- Molecule 1: Pyruvate kinase PKLR

Chain D:  5% 92% 5%

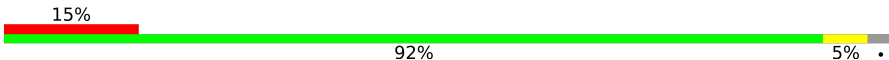


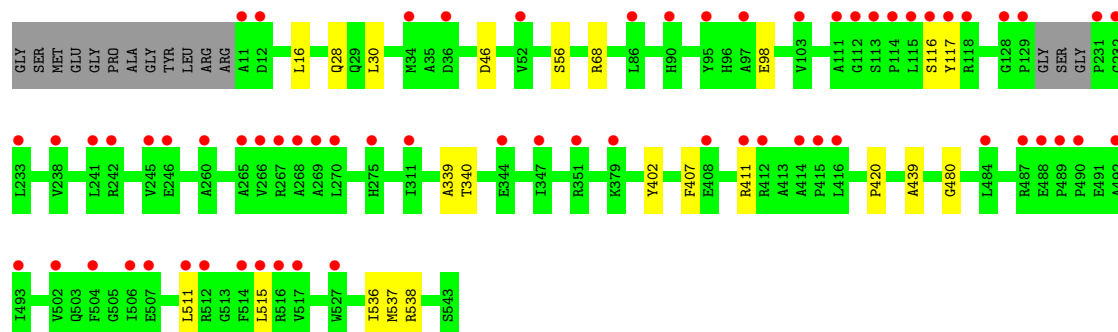
- Molecule 1: Pyruvate kinase PKLR

Chain E:  18% 90% 6%

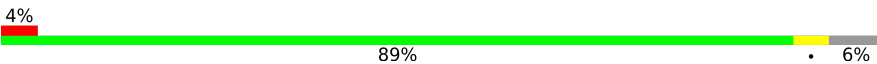


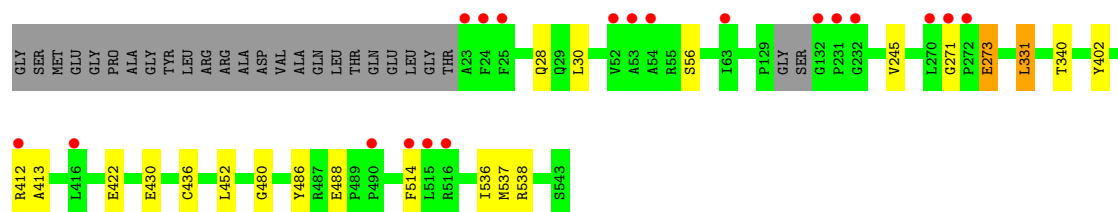
- Molecule 1: Pyruvate kinase PKLR

Chain F:  15% 92% 5%

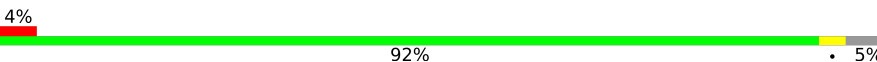


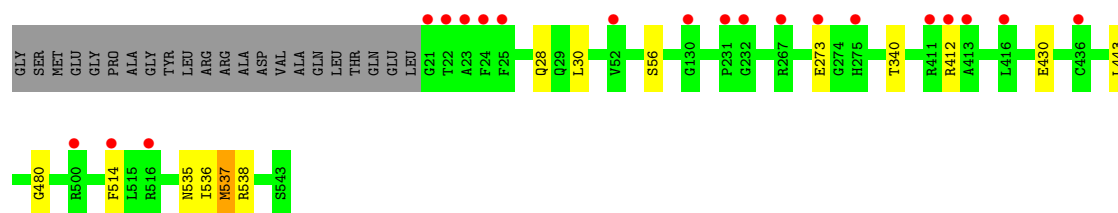
● Molecule 1: Pyruvate kinase PKLR

Chain G:  4% 89% 6%



● Molecule 1: Pyruvate kinase PKLR

Chain H:  4% 92% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	208.14Å 112.75Å 188.44Å 90.00° 91.41° 90.00°	Depositor
Resolution (Å)	104.04 – 1.74 104.04 – 1.74	Depositor EDS
% Data completeness (in resolution range)	72.1 (104.04-1.74) 72.1 (104.04-1.74)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.74Å)	Xtriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, R_{free}	0.202 , 0.220 0.194 , 0.211	Depositor DCC
R_{free} test set	16026 reflections (3.59%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.002 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	29252	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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 47.67 % 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 9.5948e-05. 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: OA0, K, FBP, OXL, 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	0.62	0/3307	0.95	0/4469
1	B	0.64	1/3396 (0.0%)	0.95	0/4592
1	C	0.67	0/3313	0.93	1/4479 (0.0%)
1	D	0.70	1/3326 (0.0%)	0.94	0/4497
1	E	0.61	0/3278	0.93	3/4430 (0.1%)
1	F	0.68	1/3396 (0.0%)	0.95	3/4591 (0.1%)
1	G	0.68	0/3303	0.93	1/4465 (0.0%)
1	H	0.73	0/3316	0.93	1/4483 (0.0%)
All	All	0.67	3/26635 (0.0%)	0.94	9/36006 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	116	SER	CA-C	6.61	1.60	1.52
1	B	374	SER	CA-C	6.00	1.55	1.52
1	D	537	MET	CA-C	5.18	1.58	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	514	PHE	CA-CB-CG	5.57	119.37	113.80
1	C	514	PHE	CA-CB-CG	5.44	119.24	113.80
1	E	539	VAL	N-CA-CB	5.42	117.55	111.21
1	F	339	ALA	CA-C-N	5.31	131.68	121.54
1	F	339	ALA	C-N-CA	5.31	131.68	121.54
1	H	514	PHE	CA-CB-CG	5.28	119.08	113.80
1	F	46	ASP	CA-CB-CG	5.16	117.76	112.60
1	E	339	ALA	CA-C-N	5.01	131.12	121.54
1	E	339	ALA	C-N-CA	5.01	131.12	121.54

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	11	0
1	B	3329	0	3394	13	1
1	C	3247	0	3299	10	0
1	D	3252	0	3310	6	0
1	E	3210	0	3270	10	0
1	F	3321	0	3393	11	0
1	G	3231	0	3284	13	0
1	H	3251	0	3306	9	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	19	8	0	2	0
6	B	19	8	0	1	0
6	C	19	8	0	0	0
6	D	19	8	0	1	0
6	E	19	8	0	0	0
6	F	19	8	0	1	0
6	G	19	8	0	1	0
6	H	19	8	0	0	0
7	A	233	0	0	0	0
7	B	204	0	0	1	0
7	C	355	0	0	1	0
7	D	420	0	0	0	0
7	E	248	0	0	0	0
7	F	374	0	0	0	0
7	G	416	0	0	0	0
7	H	485	0	0	0	0
All	All	29188	64	26635	69	1

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 1.

All (69) 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:538:ARG:HG2	1:D:536:ILE:HG12	1.59	0.84
1:C:411:ARG:HG3	1:C:426:ILE:HD11	1.63	0.80
1:G:538:ARG:HG2	1:H:536:ILE:HG12	1.64	0.79
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.65	0.77
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.70	0.72
1:A:418[A]:ARG:HG3	1:B:16:LEU:HD11	1.72	0.70
1:E:538:ARG:HG2	1:F:536:ILE:HG12	1.74	0.69
1:C:422[A]:GLU:HG3	1:C:452:LEU:HD13	1.74	0.69
1:B:411:ARG:HG2	1:B:426:ILE:HD11	1.73	0.69
1:C:538:ARG:HD3	7:C:795:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:PRO:HA	7:B:706:HOH:O	1.94	0.67
1:E:536:ILE:HG12	1:F:538:ARG:HG2	1.79	0.65
1:F:407:PHE:CE2	1:F:411:ARG:NH1	2.67	0.63
1:E:411:ARG:HG3	1:E:426:ILE:HD11	1.82	0.61
1:G:331:LEU:HD21	1:G:413:ALA:HB1	1.84	0.59
1:A:272:PRO:HA	1:A:275:HIS:NE2	2.20	0.57
6:A:605:OA0:O3	1:C:39:LEU:HB2	2.04	0.57
1:G:56:SER:HB2	1:G:480:GLY:HA2	1.86	0.57
1:E:418:ARG:HD3	1:F:16:LEU:HD11	1.86	0.56
1:H:56:SER:HB2	1:H:480:GLY:HA2	1.87	0.56
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.91	0.53
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.91	0.53
1:G:537:MET:HE3	1:H:537:MET:HG2	1.91	0.52
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.91	0.52
1:G:536:ILE:HG12	1:H:538[A]:ARG:HG2	1.93	0.51
1:E:56:SER:HB2	1:E:480:GLY:HA2	1.91	0.51
1:F:56:SER:HB2	1:F:480:GLY:HA2	1.93	0.50
1:G:430[B]:GLU:OE2	1:H:430:GLU:OE1	2.30	0.49
1:F:28:GLN:HG3	1:F:30:LEU:HG	1.96	0.48
1:E:235:GLU:O	1:E:239:ARG:HD3	2.14	0.48
1:E:539:VAL:HG22	1:F:420:PRO:HB3	1.95	0.48
1:H:56:SER:HB2	1:H:480:GLY:CA	2.44	0.47
1:G:245:VAL:CG1	1:G:273:GLU:HG2	2.45	0.47
1:G:430[A]:GLU:OE1	1:H:430:GLU:OE1	2.32	0.47
1:G:56:SER:HB2	1:G:480:GLY:CA	2.45	0.46
1:B:56:SER:HB2	1:B:480:GLY:CA	2.46	0.46
1:E:28:GLN:HG3	1:E:30:LEU:HG	1.98	0.46
1:B:28:GLN:HG3	1:B:30:LEU:HG	1.97	0.45
1:F:439:ALA:HB3	1:F:515:LEU:HD21	1.98	0.45
1:A:28:GLN:HG3	1:A:30:LEU:HG	1.98	0.45
1:D:56:SER:HB2	1:D:480:GLY:CA	2.46	0.45
1:H:28:GLN:HG3	1:H:30:LEU:HG	1.99	0.45
1:A:517:VAL:HG13	1:A:543:SER:HB3	1.99	0.45
1:D:68:ARG:NH2	1:D:98:GLU:HB2	2.31	0.44
1:E:535:ASN:OD1	1:E:536:ILE:HG13	2.17	0.44
1:C:56:SER:HB2	1:C:480:GLY:CA	2.46	0.44
1:D:28:GLN:HG3	1:D:30:LEU:HG	2.00	0.44
1:B:407:PHE:CZ	1:B:411:ARG:HD2	2.53	0.44
1:C:28:GLN:HG3	1:C:30:LEU:HG	2.00	0.44
1:B:65:PRO:HG2	1:B:379:LYS:HG2	2.00	0.43
1:F:56:SER:HB2	1:F:480:GLY:CA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:535:ASN:OD1	1:H:536:ILE:HG13	2.17	0.43
1:A:402:TYR:HB3	6:A:605:OA0:O5	2.18	0.43
1:G:28:GLN:HG3	1:G:30:LEU:HG	1.99	0.43
1:G:486:TYR:CZ	1:G:488:GLU:HB2	2.53	0.43
1:B:402:TYR:HB3	6:B:605:OA0:O	2.19	0.42
1:A:486:TYR:CZ	1:A:488[B]:GLU:HB2	2.55	0.42
1:E:56:SER:HB2	1:E:480:GLY:CA	2.48	0.42
1:F:402:TYR:HB3	6:F:605:OA0:O	2.18	0.42
1:B:382:PHE:HB3	1:B:385:GLU:HB2	2.02	0.41
1:A:272:PRO:HA	1:A:275:HIS:CE1	2.54	0.41
1:C:452:LEU:O	1:C:455:ARG:HG2	2.20	0.41
1:G:402:TYR:HB3	6:G:605:OA0:O	2.20	0.41
1:A:436:CYS:SG	1:B:416:LEU:HD13	2.61	0.41
1:A:538:ARG:HG3	1:B:536:ILE:HG12	2.03	0.41
1:D:402:TYR:HB3	6:D:605:OA0:O	2.20	0.41
1:C:68:ARG:NH2	1:C:98:GLU:HB3	2.36	0.41
1:A:452:LEU:O	1:A:455:ARG:HG2	2.21	0.40
1:F:68:ARG:NH2	1:F:98:GLU:HB3	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:LEU:O	1:B:511:LEU:O[2_555]	2.06	0.14

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	424/447 (95%)	419 (99%)	4 (1%)	1 (0%)	43 29
1	B	438/447 (98%)	433 (99%)	4 (1%)	1 (0%)	43 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	425/447 (95%)	418 (98%)	5 (1%)	2 (0%)	24	12
1	D	429/447 (96%)	425 (99%)	3 (1%)	1 (0%)	43	29
1	E	420/447 (94%)	415 (99%)	4 (1%)	1 (0%)	43	29
1	F	435/447 (97%)	428 (98%)	5 (1%)	2 (0%)	24	12
1	G	423/447 (95%)	413 (98%)	8 (2%)	2 (0%)	24	12
1	H	427/447 (96%)	423 (99%)	3 (1%)	1 (0%)	43	29
All	All	3421/3576 (96%)	3374 (99%)	36 (1%)	11 (0%)	36	23

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	117	TYR
1	G	271	GLY
1	A	340	THR
1	B	340	THR
1	C	271	GLY
1	C	340	THR
1	D	340	THR
1	E	340	THR
1	F	340	THR
1	G	340	THR
1	H	340	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	340/352 (97%)	335 (98%)	5 (2%)	57	38
1	B	349/352 (99%)	341 (98%)	8 (2%)	44	20
1	C	341/352 (97%)	341 (100%)	0	100	100
1	D	342/352 (97%)	336 (98%)	6 (2%)	51	30
1	E	338/352 (96%)	333 (98%)	5 (2%)	57	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	350/352 (99%)	347 (99%)	3 (1%)	70	59
1	G	340/352 (97%)	336 (99%)	4 (1%)	63	47
1	H	340/352 (97%)	336 (99%)	4 (1%)	63	47
All	All	2740/2816 (97%)	2705 (99%)	35 (1%)	65	43

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ARG
1	A	86	LEU
1	A	537[A]	MET
1	A	537[B]	MET
1	A	540	LEU
1	B	10	ARG
1	B	115	LEU
1	B	263	VAL
1	B	379	LYS
1	B	412	ARG
1	B	511	LEU
1	B	537[A]	MET
1	B	537[B]	MET
1	D	68	ARG
1	D	118	ARG
1	D	242[A]	ARG
1	D	242[B]	ARG
1	D	521	VAL
1	D	537	MET
1	E	115	LEU
1	E	511	LEU
1	E	537[A]	MET
1	E	537[B]	MET
1	E	539	VAL
1	F	511	LEU
1	F	537[A]	MET
1	F	537[B]	MET
1	G	273	GLU
1	G	331	LEU
1	G	412	ARG
1	G	436	CYS
1	H	273	GLU
1	H	412	ARG

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Mol	Chain	Res	Type
1	H	443	LEU
1	H	537	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	405	GLN
1	B	405	GLN
1	C	405	GLN
1	D	405	GLN
1	E	405	GLN
1	F	405	GLN
1	G	405	GLN
1	H	405	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 16 are monoatomic - leaving 24 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
2	FBP	F	601	-	18,20,20	0.48	0	21,32,32	0.50	0
2	FBP	C	602	-	18,20,20	0.57	0	21,32,32	0.70	0
6	OA0	C	601	-	21,21,21	0.32	0	32,33,33	1.73	7 (21%)
3	OXL	G	602	4	5,5,5	2.22	2 (40%)	6,6,6	2.06	2 (33%)
6	OA0	H	601	-	21,21,21	0.32	0	32,33,33	1.66	6 (18%)
2	FBP	H	602	-	18,20,20	0.88	1 (5%)	21,32,32	0.59	0
2	FBP	A	601	-	18,20,20	0.47	0	21,32,32	0.58	0
3	OXL	E	602	4	5,5,5	2.30	2 (40%)	6,6,6	2.10	2 (33%)
3	OXL	A	602	4	5,5,5	2.21	2 (40%)	6,6,6	1.84	2 (33%)
6	OA0	E	605	-	21,21,21	0.32	0	32,33,33	1.68	6 (18%)
6	OA0	A	605	-	21,21,21	0.30	0	32,33,33	1.88	7 (21%)
3	OXL	F	602	4	5,5,5	3.23	5 (100%)	6,6,6	2.34	2 (33%)
3	OXL	B	602	4	5,5,5	2.34	3 (60%)	6,6,6	2.02	2 (33%)
2	FBP	E	601	-	18,20,20	0.53	0	21,32,32	0.72	1 (4%)
3	OXL	C	603	4	5,5,5	2.11	2 (40%)	6,6,6	1.90	2 (33%)
2	FBP	G	601	-	18,20,20	0.54	0	21,32,32	0.79	0
6	OA0	F	605	-	21,21,21	0.32	0	32,33,33	1.71	6 (18%)
3	OXL	D	602	4	5,5,5	2.63	3 (60%)	6,6,6	1.81	2 (33%)
6	OA0	G	605	-	21,21,21	0.30	0	32,33,33	1.68	6 (18%)
2	FBP	B	601	-	18,20,20	0.79	1 (5%)	21,32,32	0.83	1 (4%)
2	FBP	D	601	-	18,20,20	0.59	0	21,32,32	0.80	1 (4%)
3	OXL	H	603	4	5,5,5	2.45	3 (60%)	6,6,6	1.95	2 (33%)
6	OA0	D	605	-	21,21,21	0.34	0	32,33,33	1.66	6 (18%)
6	OA0	B	605	-	21,21,21	0.30	0	32,33,33	1.69	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
2	FBP	C	602	-	-	2/13/32/32	0/1/1/1
6	OA0	C	601	-	-	-	0/2/3/3
3	OXL	G	602	4	-	4/4/4/4	-
6	OA0	H	601	-	-	-	0/2/3/3
2	FBP	H	602	-	-	2/13/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
3	OXL	E	602	4	-	4/4/4/4	-
3	OXL	A	602	4	-	4/4/4/4	-
6	OA0	E	605	-	-	-	0/2/3/3
6	OA0	A	605	-	-	-	0/2/3/3
3	OXL	F	602	4	-	4/4/4/4	-
3	OXL	B	602	4	-	4/4/4/4	-
2	FBP	E	601	-	-	2/13/32/32	0/1/1/1
3	OXL	C	603	4	-	4/4/4/4	-
2	FBP	G	601	-	-	2/13/32/32	0/1/1/1
6	OA0	F	605	-	-	-	0/2/3/3
3	OXL	D	602	4	-	4/4/4/4	-
6	OA0	G	605	-	-	-	0/2/3/3
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
3	OXL	H	603	4	-	4/4/4/4	-
6	OA0	D	605	-	-	-	0/2/3/3
6	OA0	B	605	-	-	-	0/2/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	602	OXL	O2-C2	4.09	1.32	1.22
3	E	602	OXL	O1-C1	3.99	1.32	1.22
3	B	602	OXL	O2-C2	3.86	1.32	1.22
3	A	602	OXL	O2-C2	3.78	1.31	1.22
3	D	602	OXL	C2-C1	3.50	1.60	1.54
3	D	602	OXL	O2-C2	3.50	1.31	1.22
3	G	602	OXL	O1-C1	3.43	1.31	1.22
3	H	603	OXL	C2-C1	3.35	1.60	1.54
3	C	603	OXL	O1-C1	3.25	1.30	1.22
3	F	602	OXL	C2-C1	3.20	1.60	1.54
3	F	602	OXL	O1-C1	3.20	1.30	1.22
3	F	602	OXL	O3-C1	-3.13	1.22	1.30
3	G	602	OXL	O3-C1	-3.12	1.22	1.30
3	H	603	OXL	O2-C2	2.98	1.29	1.22
3	D	602	OXL	O4-C2	-2.92	1.22	1.30
3	H	603	OXL	O4-C2	-2.83	1.22	1.30
3	C	603	OXL	O3-C1	-2.81	1.22	1.30
3	A	602	OXL	O4-C2	-2.64	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	OXL	O3-C1	-2.62	1.23	1.30
3	B	602	OXL	O4-C2	-2.61	1.23	1.30
3	B	602	OXL	C2-C1	2.37	1.58	1.54
3	F	602	OXL	O4-C2	-2.25	1.24	1.30
2	H	602	FBP	P2-O5P	-2.05	1.47	1.54
2	B	601	FBP	P2-O5P	-2.03	1.47	1.54

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	605	OA0	O5-S-O	5.82	123.62	114.97
6	C	601	OA0	O5-S-O	5.78	123.56	114.97
6	G	605	OA0	O5-S-O	5.78	123.55	114.97
6	H	601	OA0	O5-S-O	5.72	123.47	114.97
6	D	605	OA0	O5-S-O	5.61	123.31	114.97
6	A	605	OA0	C11-O4-S	5.50	126.93	116.34
6	B	605	OA0	O5-S-O	5.23	122.74	114.97
6	E	605	OA0	O5-S-O	5.14	122.60	114.97
6	A	605	OA0	O4-C11-C6	4.74	123.82	119.90
6	A	605	OA0	O5-S-O	4.39	121.49	114.97
6	E	605	OA0	C11-O4-S	3.96	123.96	116.34
3	H	603	OXL	O4-C2-C1	3.91	120.41	112.83
6	C	601	OA0	C11-O4-S	3.85	123.74	116.34
6	B	605	OA0	C11-O4-S	3.83	123.71	116.34
3	F	602	OXL	O4-C2-C1	3.81	120.23	112.83
6	G	605	OA0	C11-O4-S	3.75	123.55	116.34
3	E	602	OXL	O3-C1-C2	3.75	120.10	112.83
3	C	603	OXL	O3-C1-C2	3.73	120.06	112.83
6	B	605	OA0	O4-C11-C6	3.70	122.96	119.90
6	H	601	OA0	C11-O4-S	3.66	123.38	116.34
3	B	602	OXL	O4-C2-C1	3.63	119.87	112.83
3	F	602	OXL	O3-C1-C2	3.61	119.83	112.83
6	F	605	OA0	C11-O4-S	3.60	123.27	116.34
6	D	605	OA0	C11-O4-S	3.58	123.22	116.34
3	G	602	OXL	O3-C1-C2	3.53	119.69	112.83
6	F	605	OA0	O4-C11-C6	3.47	122.77	119.90
3	A	602	OXL	O4-C2-C1	3.46	119.54	112.83
6	B	605	OA0	O5-S-C	3.43	111.64	106.62
6	C	601	OA0	O4-C11-C6	3.41	122.72	119.90
3	D	602	OXL	O4-C2-C1	3.32	119.26	112.83
6	E	605	OA0	O4-C11-C6	3.31	122.64	119.90
6	D	605	OA0	O4-C11-C6	3.29	122.62	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	601	OA0	O4-C11-C6	3.22	122.56	119.90
6	G	605	OA0	O5-S-C	3.15	111.23	106.62
6	D	605	OA0	O5-S-C	3.10	111.17	106.62
6	F	605	OA0	O5-S-C	3.08	111.13	106.62
6	G	605	OA0	O4-C11-C6	3.06	122.43	119.90
6	E	605	OA0	O4-S-C	-3.00	99.85	105.39
6	G	605	OA0	O4-S-C	-3.00	99.86	105.39
6	E	605	OA0	O5-S-C	2.99	111.01	106.62
3	G	602	OXL	O4-C2-C1	2.98	118.61	112.83
6	H	601	OA0	O5-S-C	2.95	110.95	106.62
6	C	601	OA0	O5-S-C	2.92	110.90	106.62
6	F	605	OA0	O4-S-C	-2.92	100.00	105.39
6	C	601	OA0	O4-S-C	-2.91	100.02	105.39
6	A	605	OA0	O5-S-C	2.88	110.84	106.62
3	E	602	OXL	O4-C2-C1	2.84	118.34	112.83
6	A	605	OA0	C5-C-S	2.81	124.50	118.49
6	B	605	OA0	O4-S-C	-2.78	100.25	105.39
3	B	602	OXL	O3-C1-C2	2.77	118.20	112.83
6	H	601	OA0	O4-S-C	-2.69	100.42	105.39
6	D	605	OA0	O4-S-C	-2.67	100.47	105.39
6	A	605	OA0	O-S-C	2.67	110.53	106.62
6	A	605	OA0	C1-C-S	-2.66	114.40	118.90
3	D	602	OXL	O3-C1-C2	2.55	117.78	112.83
2	E	601	FBP	O3P-P1-O2P	2.43	116.89	107.80
2	D	601	FBP	O5P-P2-O6	2.35	112.80	106.67
3	A	602	OXL	O3-C1-C2	2.33	117.36	112.83
2	B	601	FBP	O3P-P1-O2P	2.33	116.53	107.80
6	B	605	OA0	C5-C-S	2.23	123.26	118.49
6	C	601	OA0	C5-C-S	2.20	123.19	118.49
3	C	603	OXL	O4-C2-C1	2.12	116.93	112.83
6	G	605	OA0	C5-C-S	2.11	123.00	118.49
6	E	605	OA0	C5-C-S	2.09	122.95	118.49
6	F	605	OA0	C5-C-S	2.06	122.89	118.49
3	H	603	OXL	O3-C1-C2	2.05	116.81	112.83
6	D	605	OA0	C5-C-S	2.03	122.83	118.49
6	H	601	OA0	C5-C-S	2.03	122.83	118.49
6	C	601	OA0	C1-C-S	-2.02	115.48	118.90
6	B	605	OA0	C1-C-S	-2.02	115.49	118.90

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FBP	C4-C5-C6-O6
2	C	602	FBP	C4-C5-C6-O6
2	E	601	FBP	C4-C5-C6-O6
2	G	601	FBP	C4-C5-C6-O6
2	B	601	FBP	C4-C5-C6-O6
2	D	601	FBP	C4-C5-C6-O6
2	F	601	FBP	C4-C5-C6-O6
2	H	602	FBP	C4-C5-C6-O6
2	A	601	FBP	O5-C5-C6-O6
2	B	601	FBP	O5-C5-C6-O6
2	C	602	FBP	O5-C5-C6-O6
2	D	601	FBP	O5-C5-C6-O6
2	E	601	FBP	O5-C5-C6-O6
2	G	601	FBP	O5-C5-C6-O6
2	H	602	FBP	O5-C5-C6-O6
2	F	601	FBP	O5-C5-C6-O6
3	A	602	OXL	O3-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O4
3	F	602	OXL	O3-C1-C2-O4
3	G	602	OXL	O3-C1-C2-O4
3	C	603	OXL	O3-C1-C2-O4
3	D	602	OXL	O3-C1-C2-O4
3	H	603	OXL	O3-C1-C2-O4
3	A	602	OXL	O1-C1-C2-O2
3	G	602	OXL	O1-C1-C2-O2
3	B	602	OXL	O3-C1-C2-O4
3	B	602	OXL	O1-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O2
3	E	602	OXL	O1-C1-C2-O2
3	F	602	OXL	O1-C1-C2-O2
3	H	603	OXL	O1-C1-C2-O2
3	C	603	OXL	O1-C1-C2-O2
3	H	603	OXL	O1-C1-C2-O4
3	A	602	OXL	O1-C1-C2-O4
3	A	602	OXL	O3-C1-C2-O2
3	B	602	OXL	O1-C1-C2-O4
3	E	602	OXL	O1-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O2
3	F	602	OXL	O3-C1-C2-O2
3	G	602	OXL	O1-C1-C2-O4
3	G	602	OXL	O3-C1-C2-O2
3	B	602	OXL	O3-C1-C2-O2
3	C	603	OXL	O1-C1-C2-O4

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Mol	Chain	Res	Type	Atoms
3	C	603	OXL	O3-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O4
3	F	602	OXL	O1-C1-C2-O4
3	D	602	OXL	O3-C1-C2-O2
3	H	603	OXL	O3-C1-C2-O2

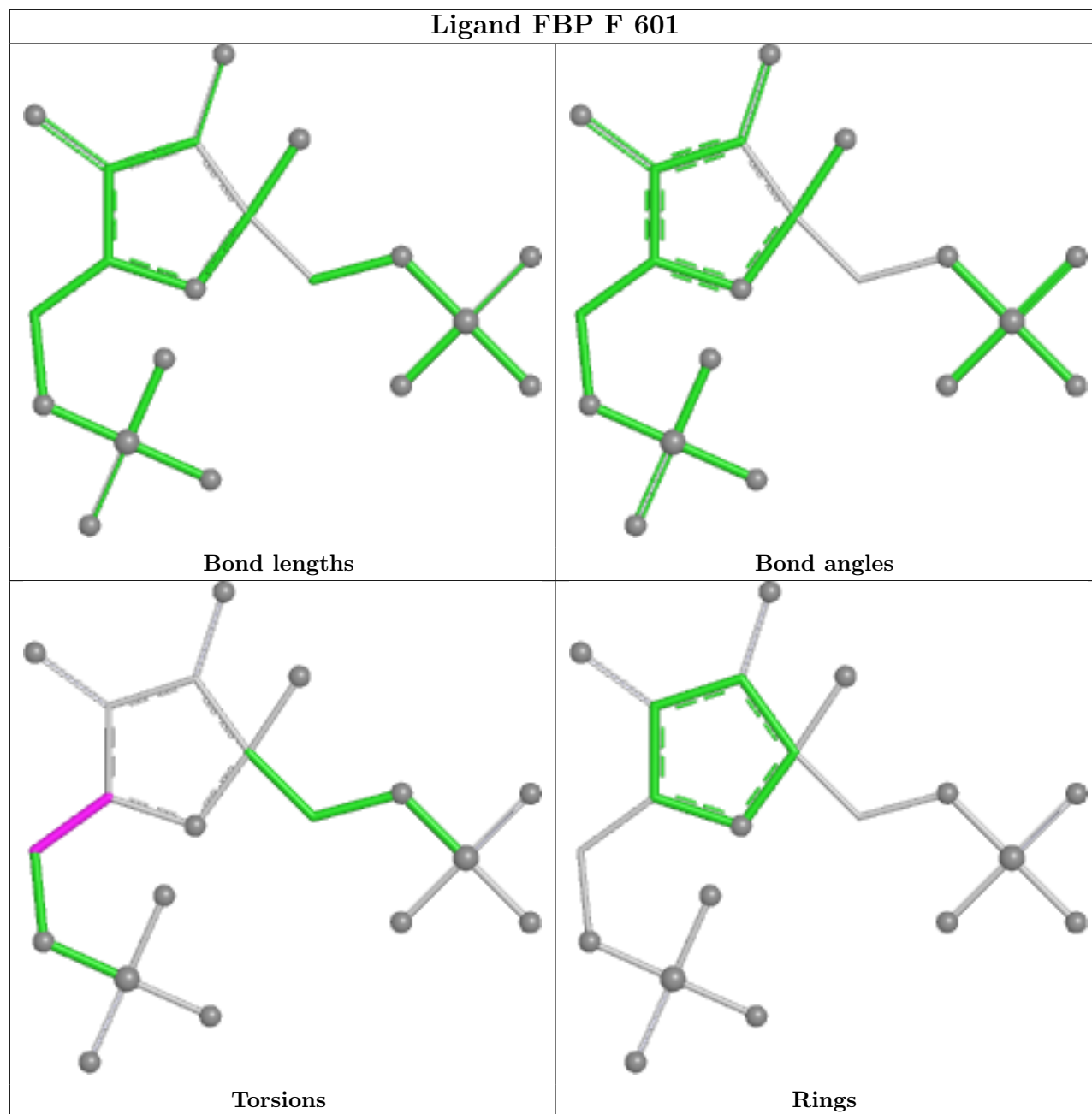
There are no ring outliers.

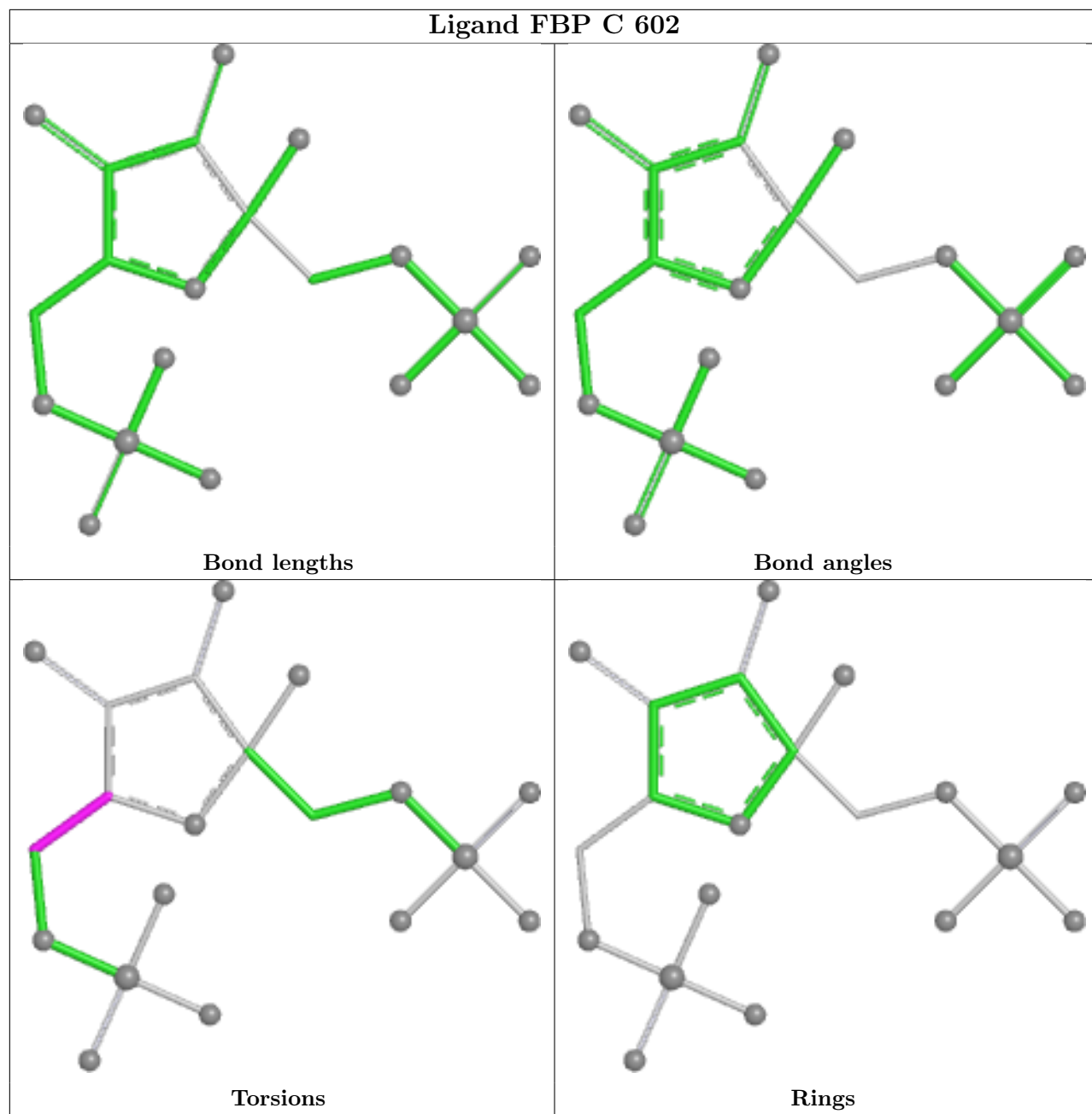
5 monomers are involved in 6 short contacts:

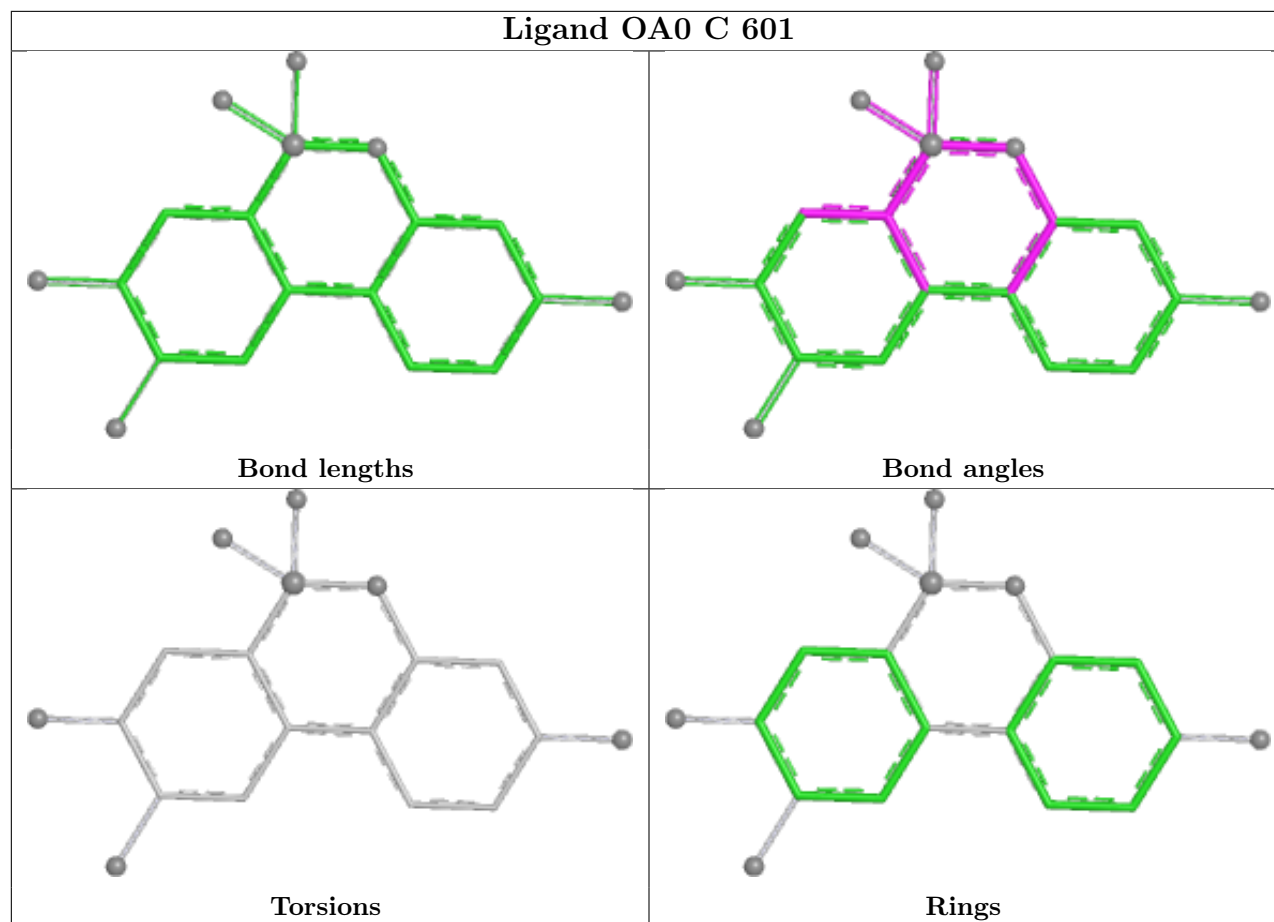
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	605	OA0	2	0
6	F	605	OA0	1	0
6	G	605	OA0	1	0
6	D	605	OA0	1	0
6	B	605	OA0	1	0

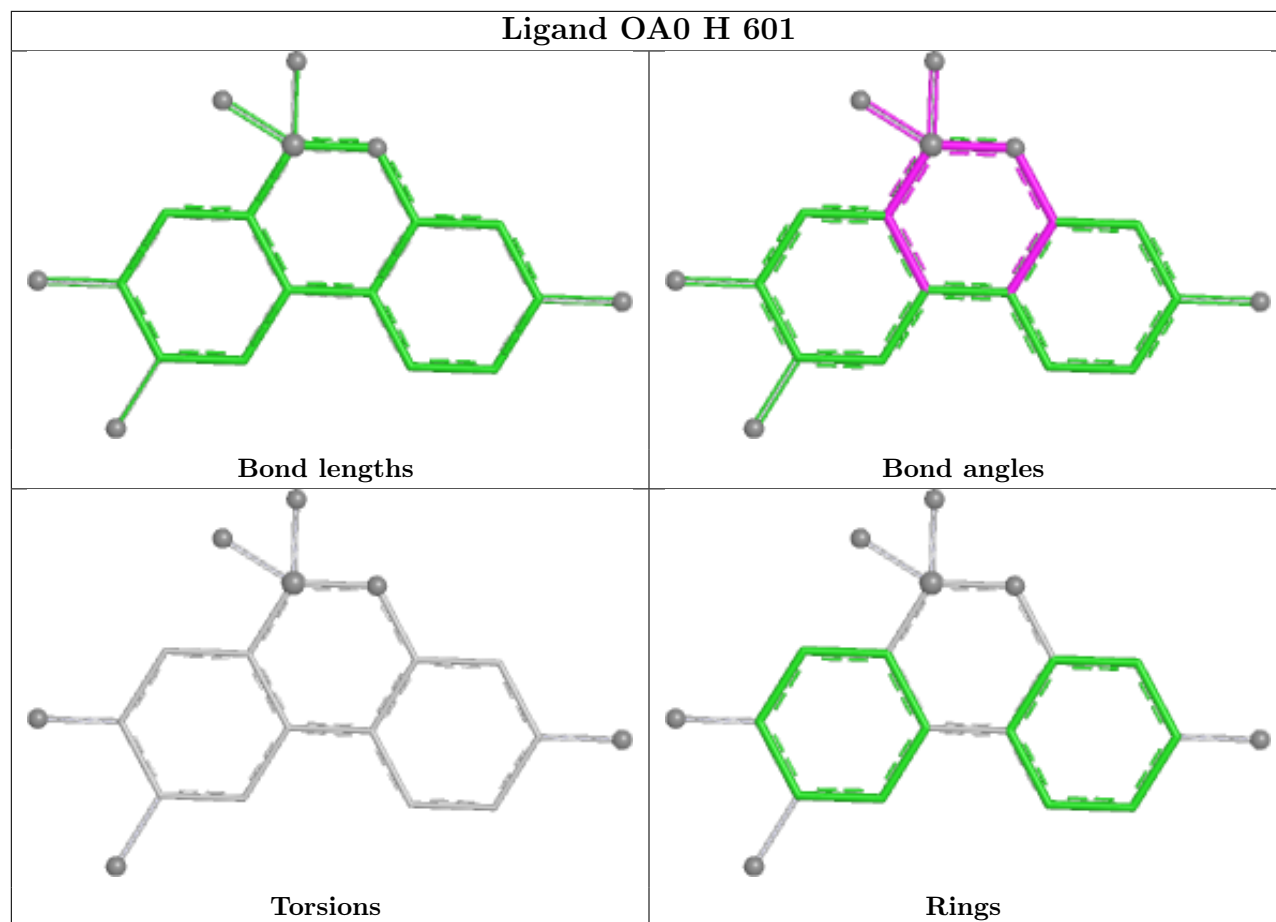
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

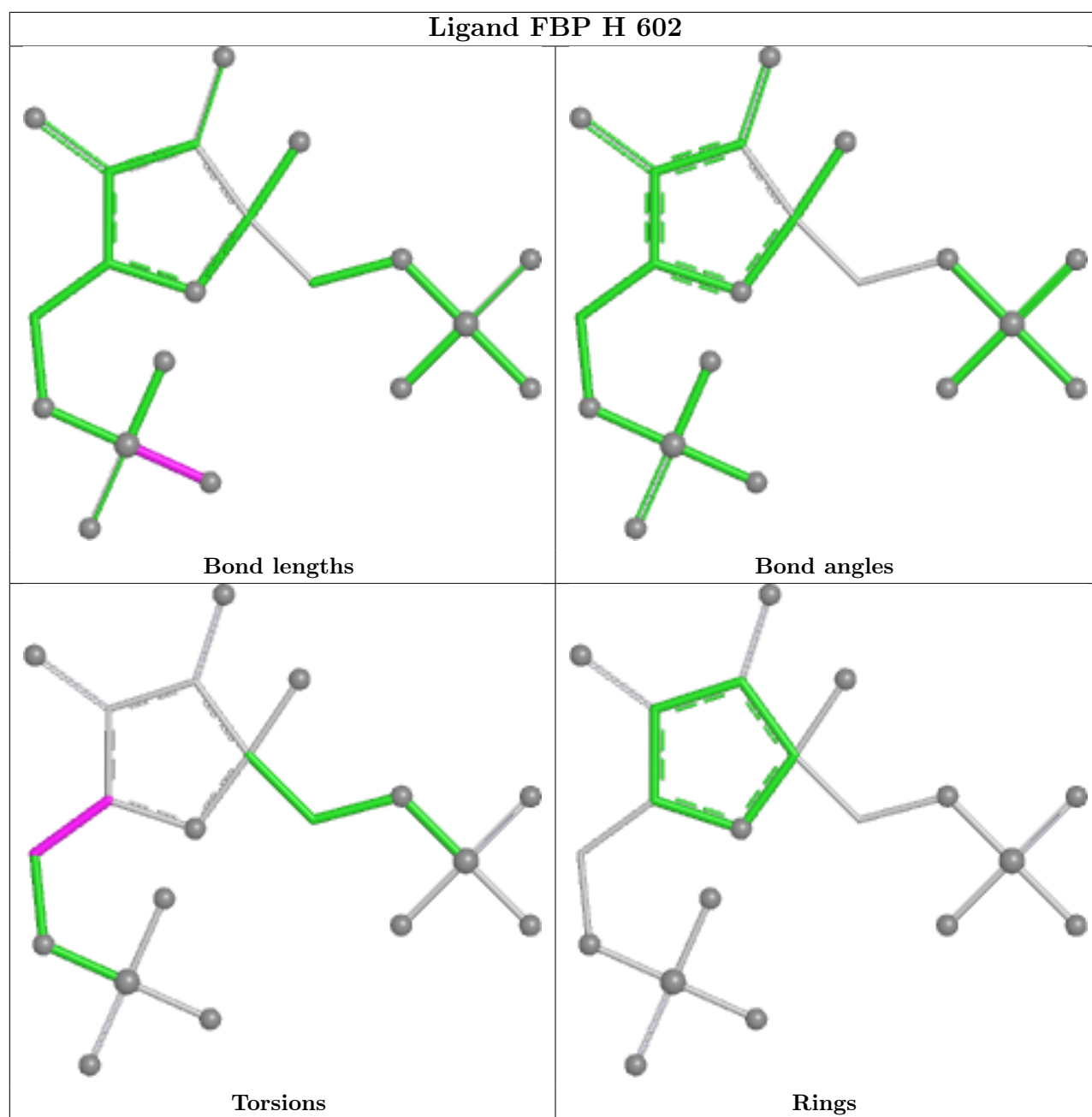
Ligand FBP F 601

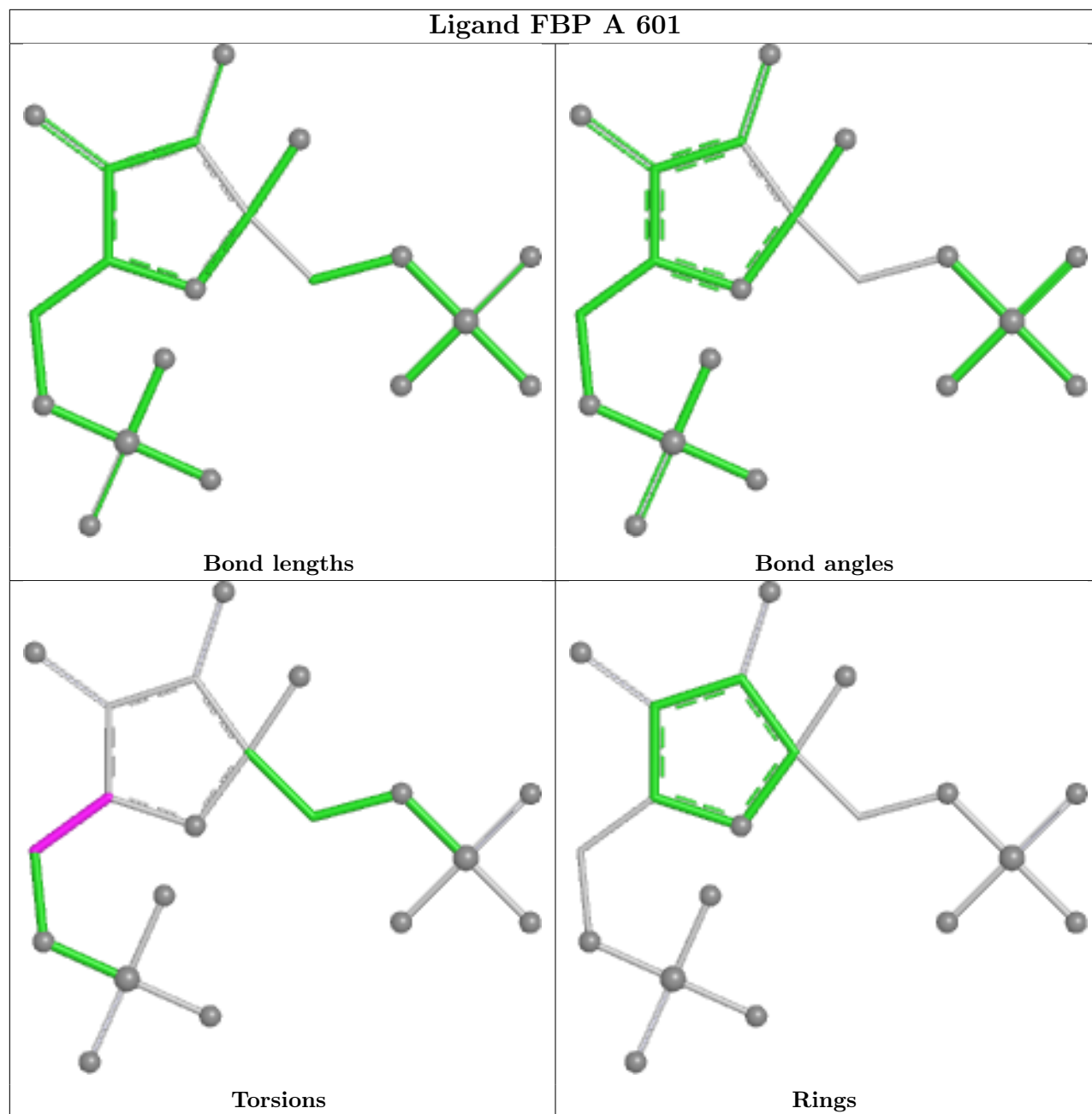




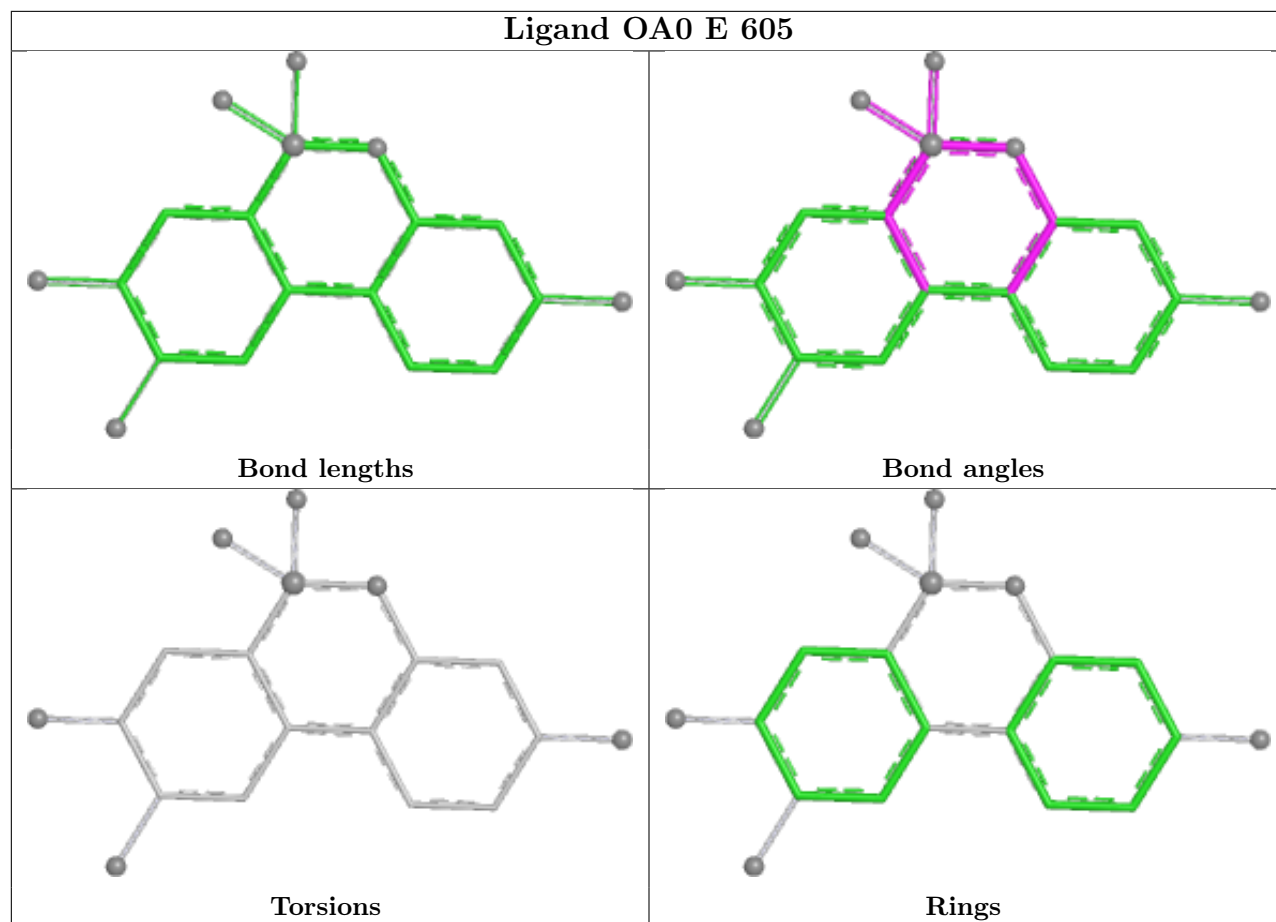


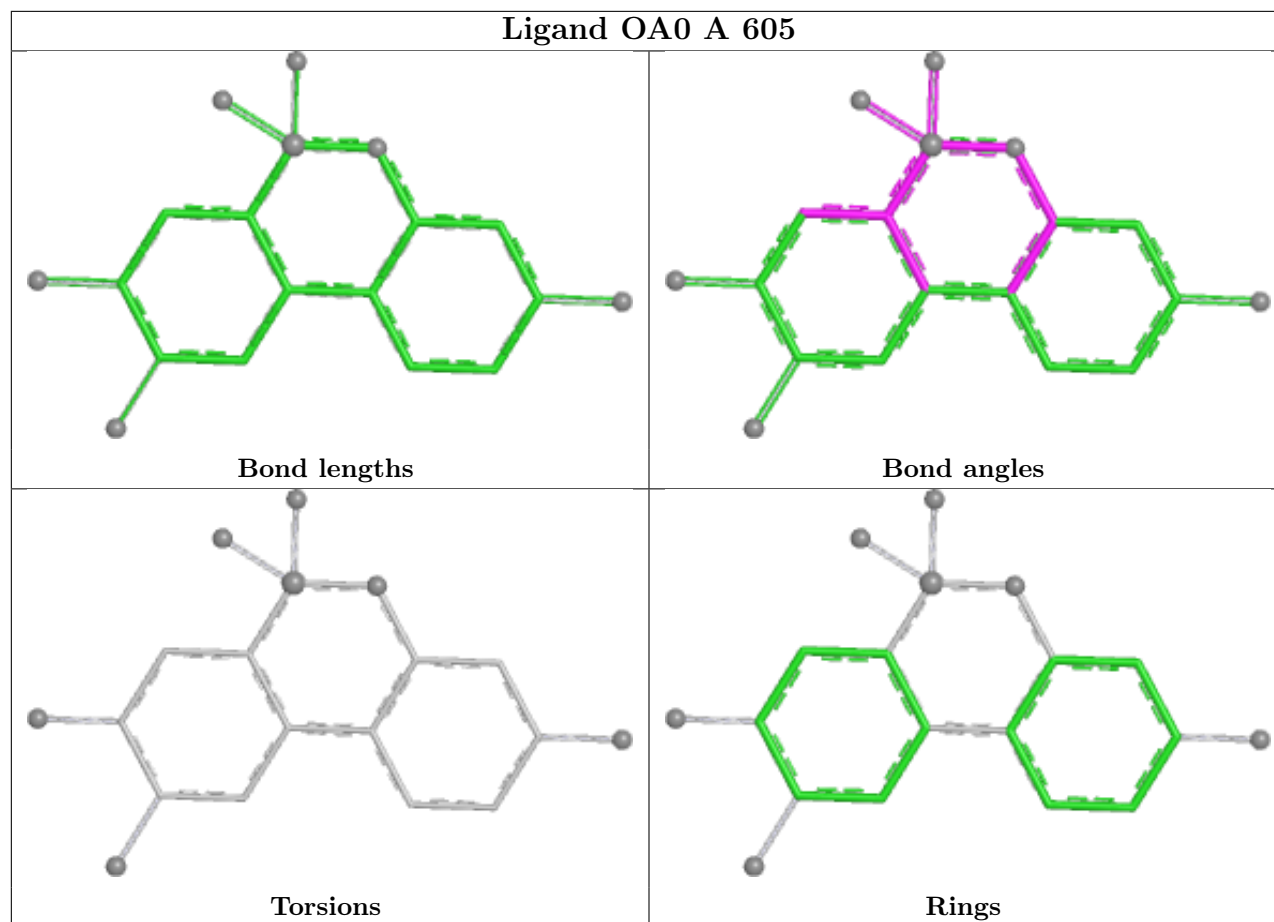




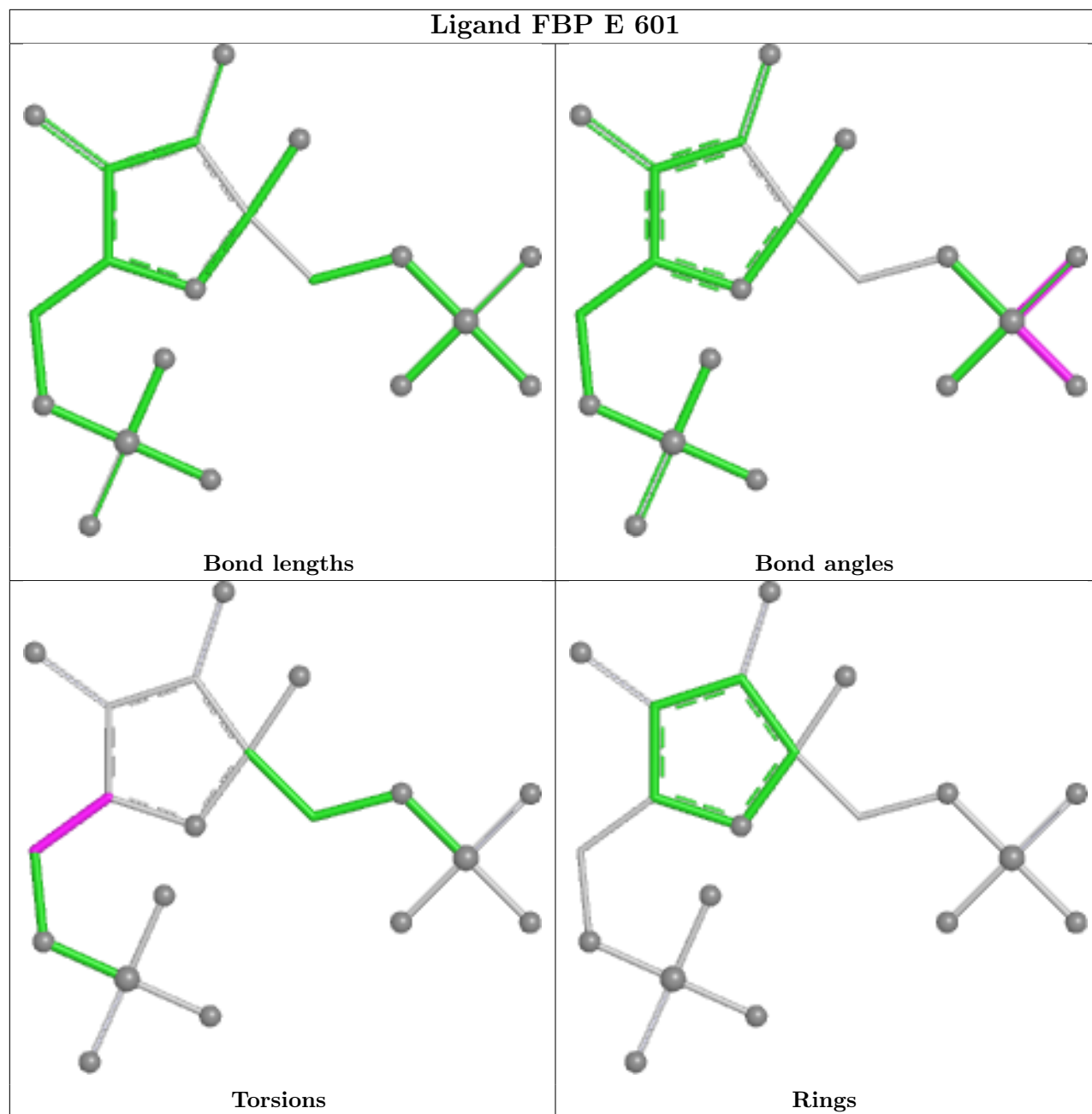


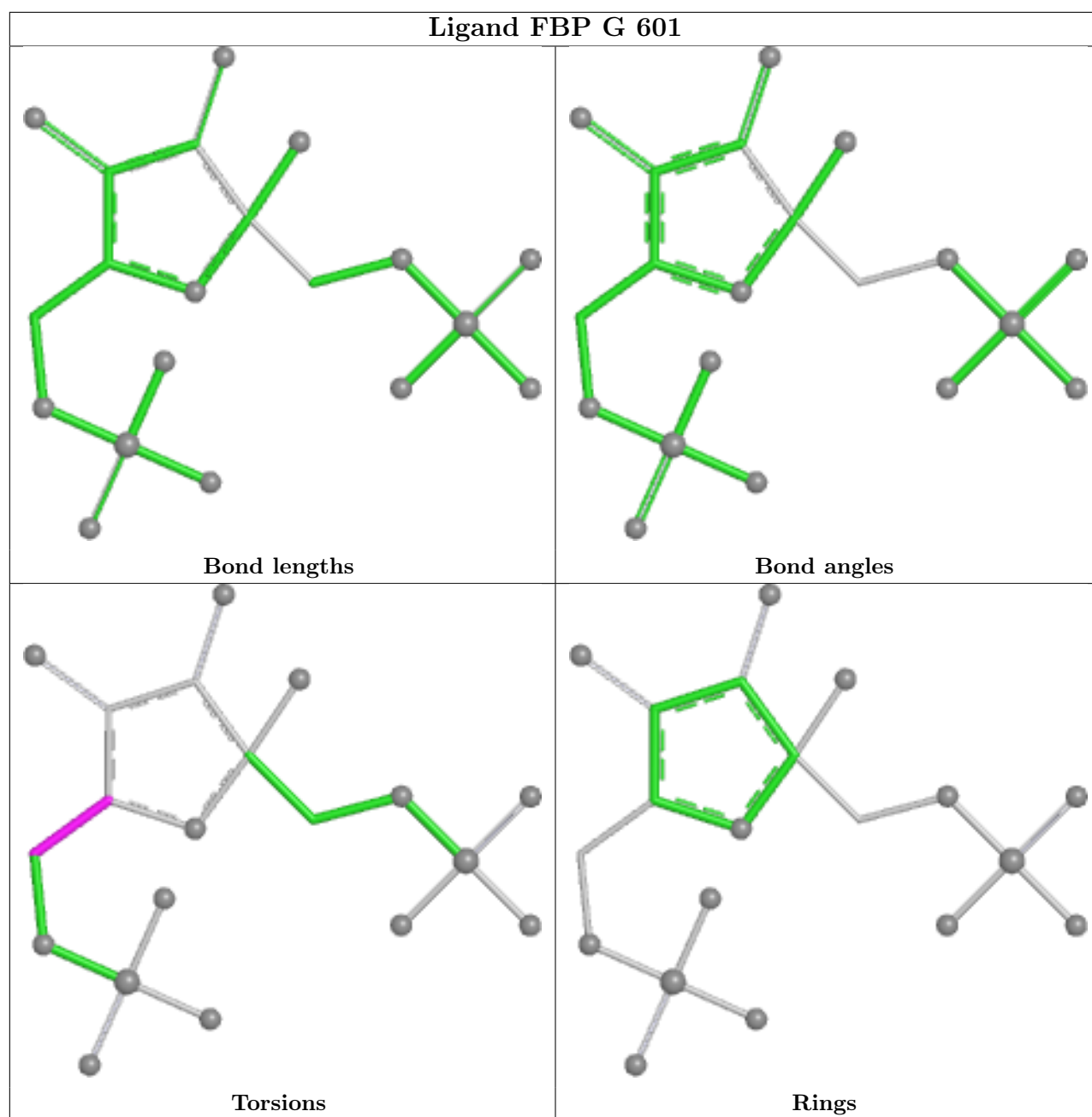
Ligand OA0 E 605

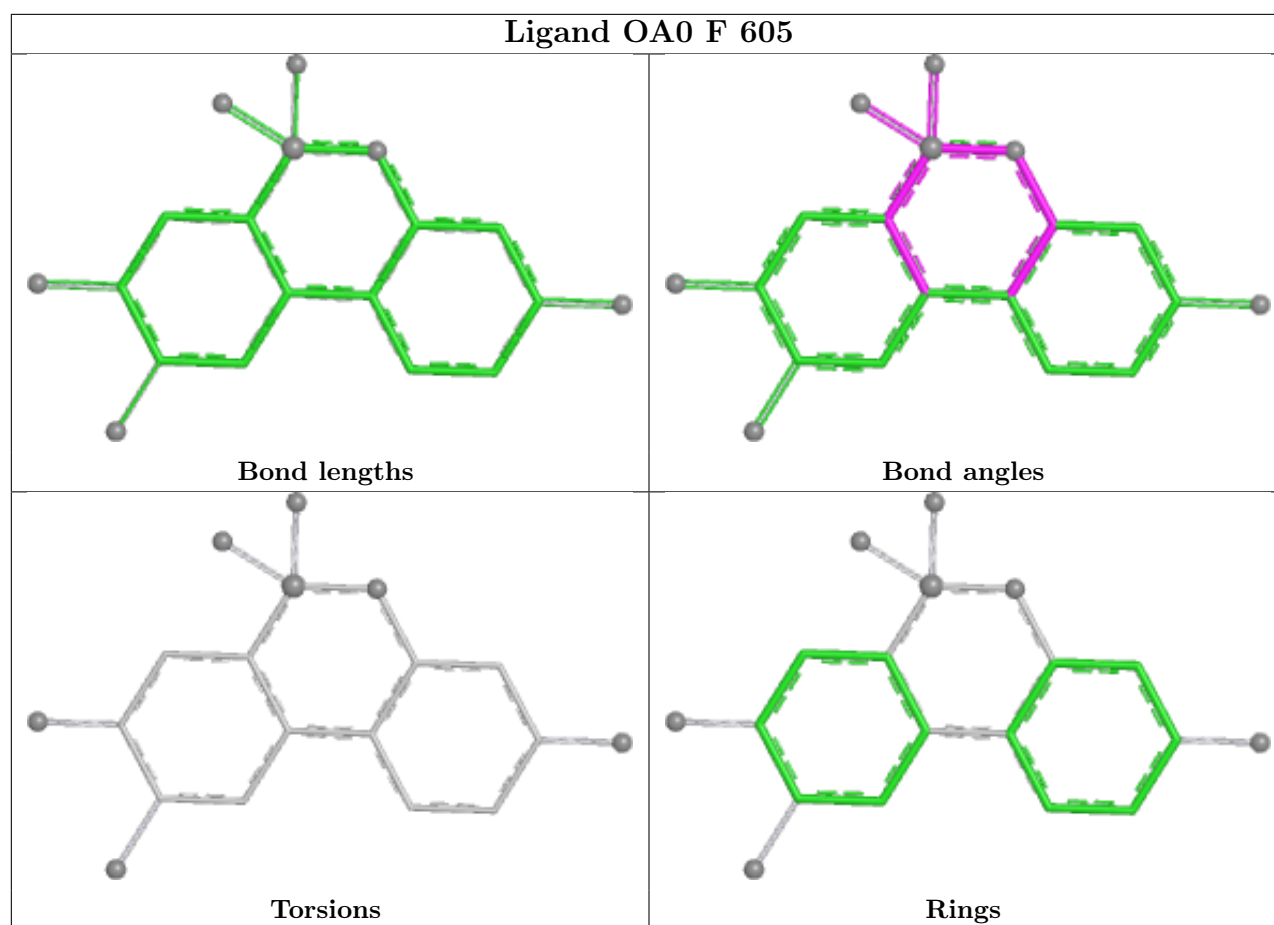


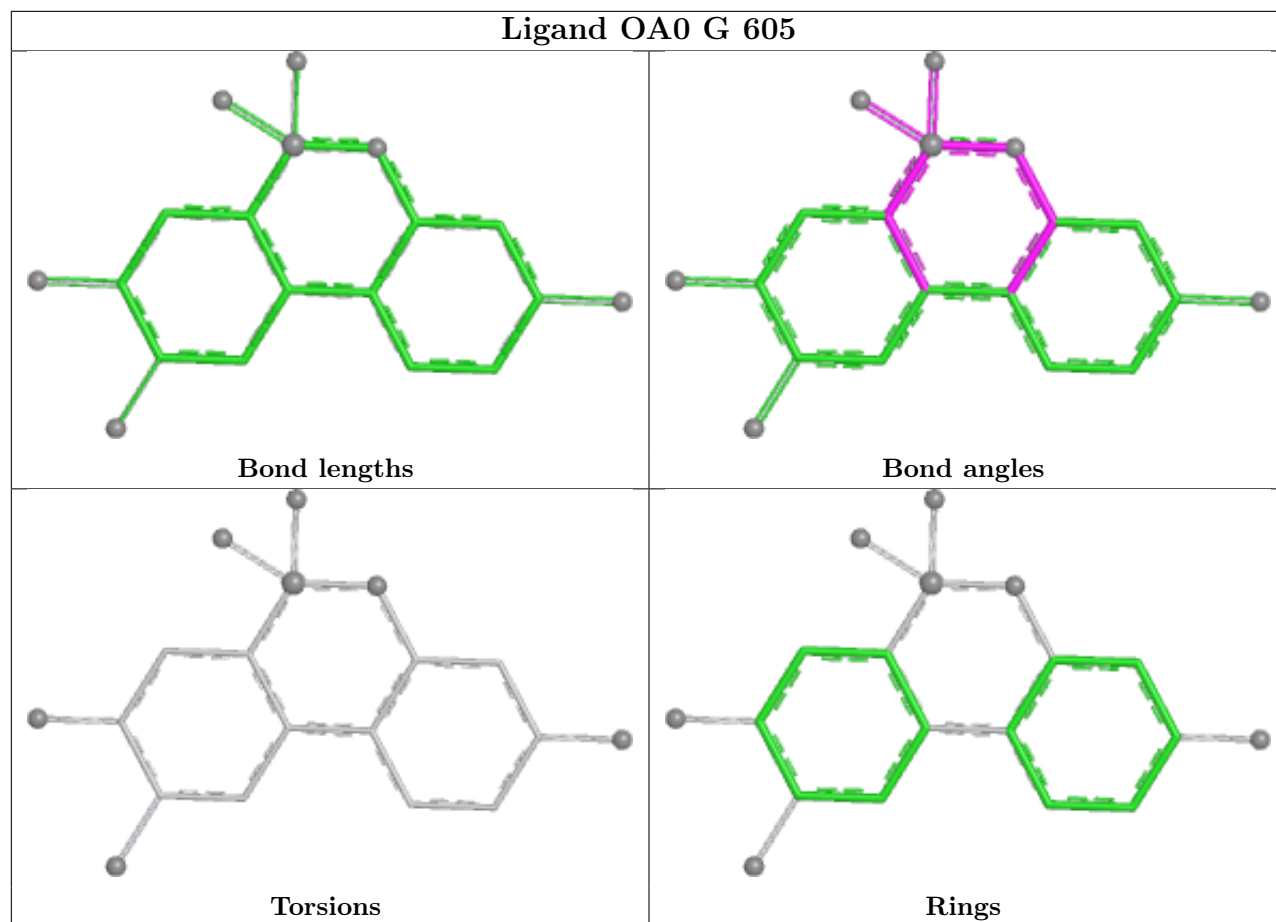


Ligand FBP E 601

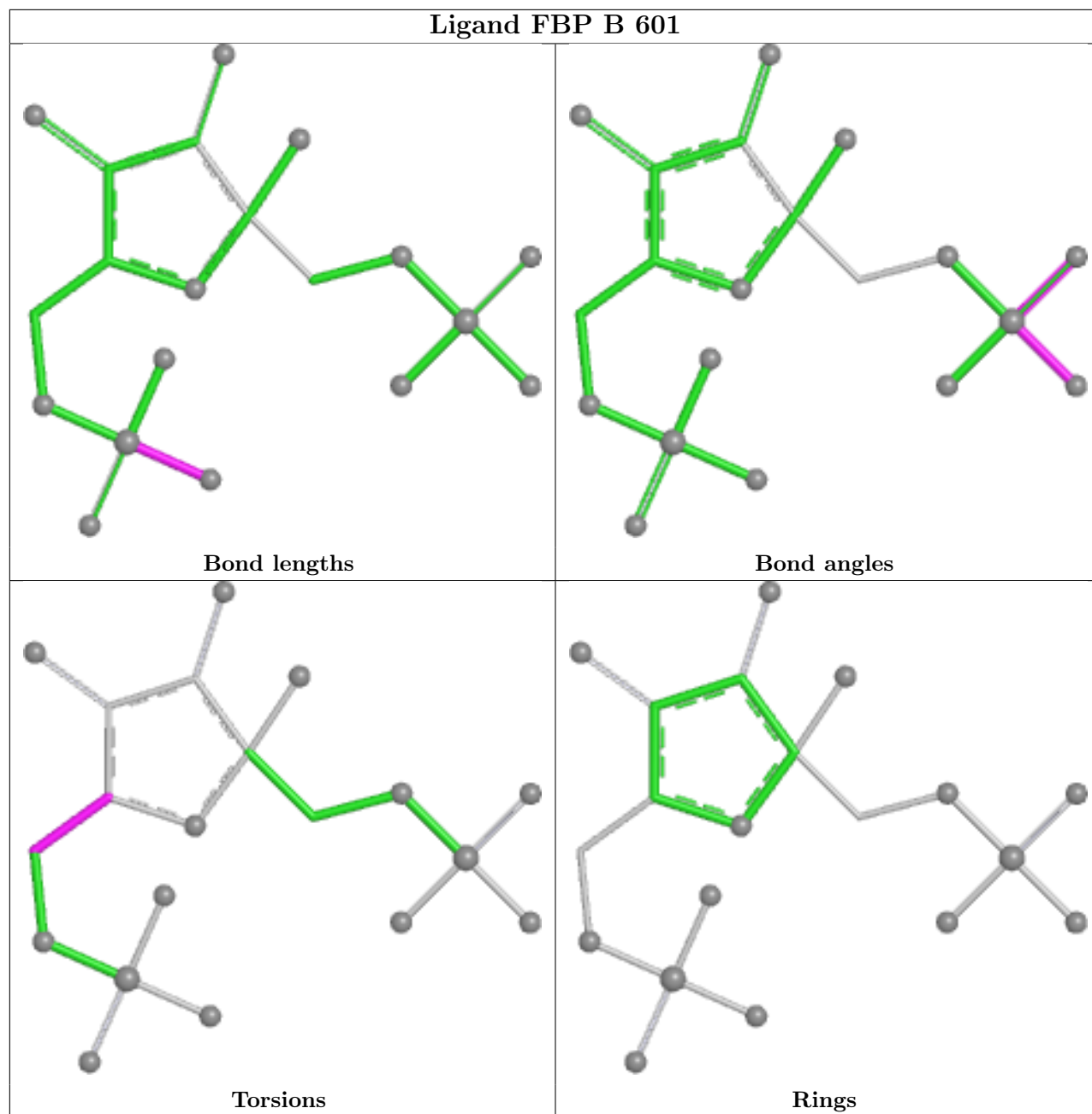




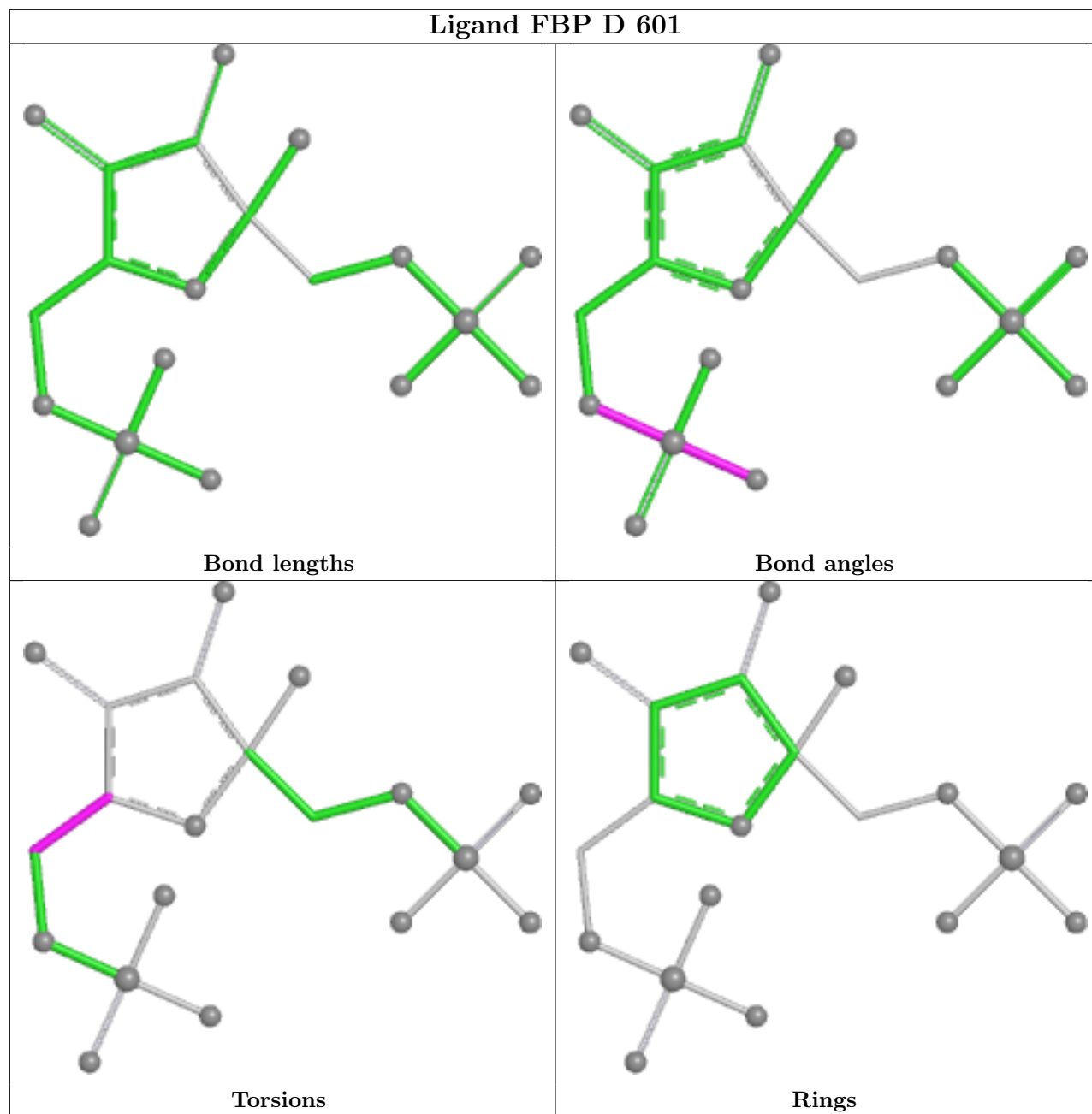


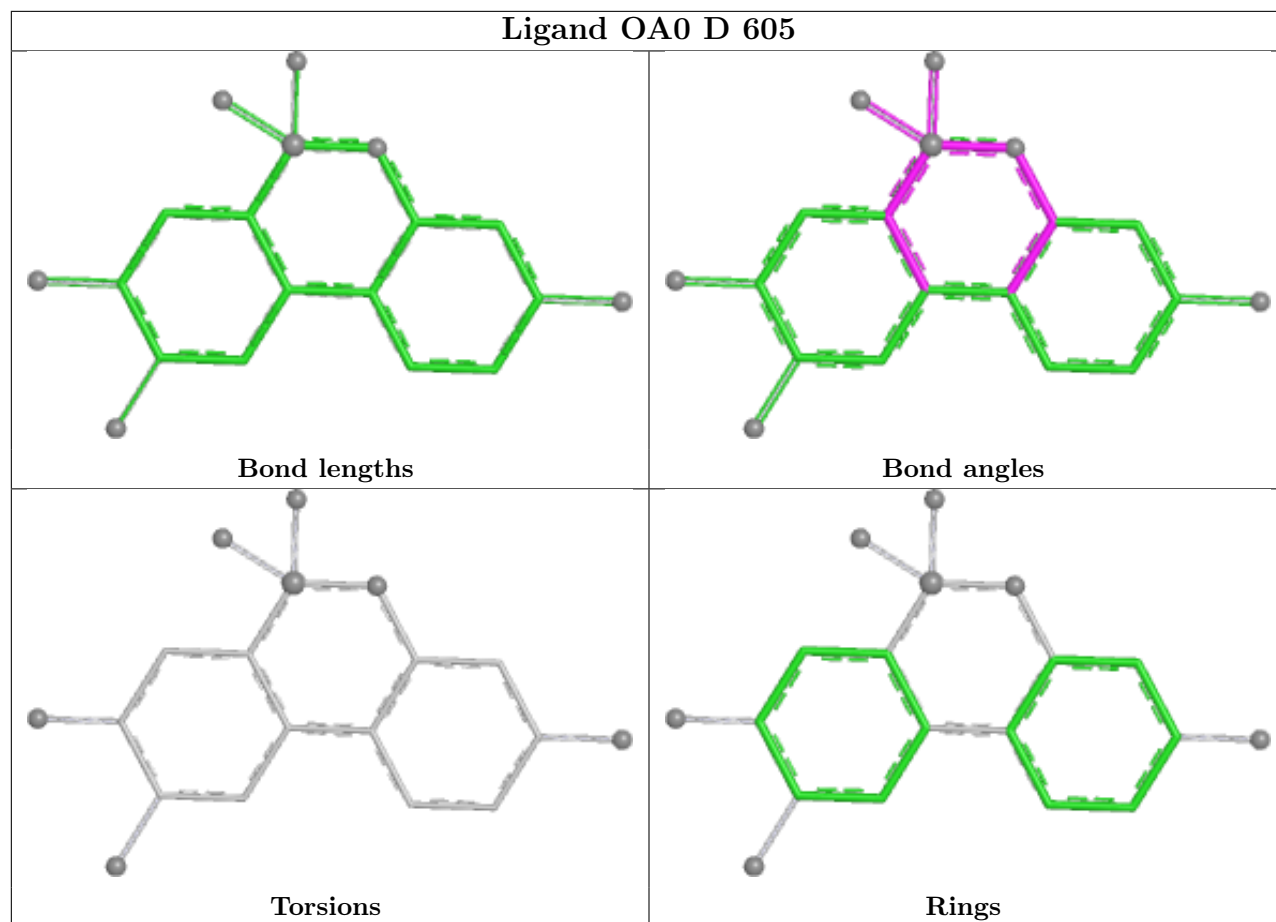


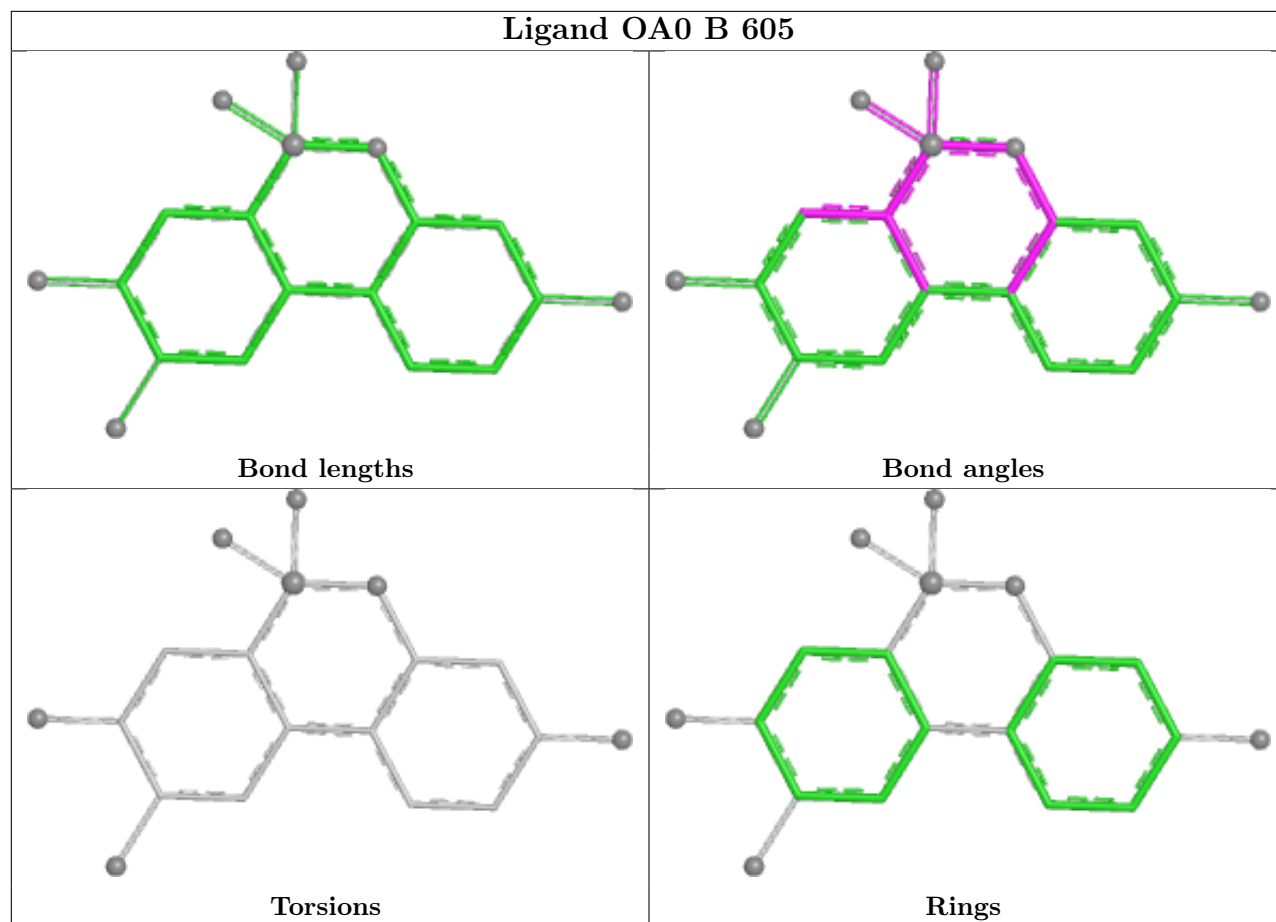
Ligand FBP B 601



Ligand FBP D 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%)	1.36	95 (22%) 2 3	24, 48, 73, 87	6 (1%)
1	B	436/447 (97%)	1.78	169 (38%) 1 1	23, 47, 77, 91	4 (0%)
1	C	425/447 (95%)	0.63	35 (8%) 17 23	22, 36, 55, 87	4 (0%)
1	D	425/447 (95%)	0.33	23 (5%) 31 38	16, 31, 53, 79	6 (1%)
1	E	419/447 (93%)	1.18	81 (19%) 3 3	22, 45, 72, 87	5 (1%)
1	F	432/447 (96%)	0.88	65 (15%) 5 7	22, 36, 62, 76	7 (1%)
1	G	421/447 (94%)	0.38	19 (4%) 38 47	19, 32, 47, 64	7 (1%)
1	H	425/447 (95%)	0.12	20 (4%) 36 44	14, 27, 49, 65	4 (0%)
All	All	3405/3576 (95%)	0.83	507 (14%) 5 7	14, 38, 68, 91	43 (1%)

All (507) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	115	LEU	10.5
1	F	115	LEU	9.3
1	B	511	LEU	9.1
1	F	114	PRO	7.7
1	A	25	PHE	7.7
1	F	116	SER	7.3
1	G	271	GLY	7.1
1	H	21	GLY	6.9
1	F	511	LEU	6.8
1	G	25	PHE	6.6
1	E	23	ALA	6.3
1	C	271	GLY	6.2
1	B	117	TYR	5.9
1	D	21	GLY	5.9
1	D	25	PHE	5.9
1	C	232	GLY	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	116	SER	5.8
1	E	25	PHE	5.8
1	B	348	THR	5.6
1	A	238	VAL	5.5
1	B	118	ARG	5.3
1	B	489	PRO	5.3
1	H	25	PHE	5.2
1	B	347	ILE	5.2
1	C	231	PRO	5.1
1	E	129	PRO	5.1
1	A	543	SER	5.0
1	B	114	PRO	4.9
1	D	24	PHE	4.9
1	B	378	ALA	4.8
1	B	267[A]	ARG	4.7
1	B	238	VAL	4.7
1	B	490	PRO	4.6
1	B	88	PHE	4.5
1	C	20	LEU	4.5
1	B	270	LEU	4.5
1	G	23	ALA	4.5
1	A	132	GLY	4.5
1	B	416	LEU	4.5
1	C	132	GLY	4.4
1	F	231	PRO	4.4
1	B	382	PHE	4.4
1	E	115	LEU	4.4
1	B	123	ALA	4.4
1	H	411	ARG	4.4
1	B	73	LEU	4.4
1	A	23	ALA	4.4
1	C	25	PHE	4.4
1	B	379	LYS	4.4
1	F	233	LEU	4.3
1	G	52	VAL	4.3
1	B	268	ALA	4.2
1	B	504	PHE	4.2
1	B	266	VAL	4.2
1	B	251	ILE	4.2
1	B	506	ILE	4.2
1	F	267[A]	ARG	4.2
1	A	514	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	232	GLY	4.2
1	B	86	LEU	4.1
1	B	233	LEU	4.1
1	A	24	PHE	4.1
1	A	70	VAL	4.1
1	B	120	VAL	4.1
1	B	106	ALA	4.0
1	B	132	GLY	4.0
1	F	489	PRO	4.0
1	B	241	LEU	4.0
1	B	484	LEU	4.0
1	C	111	ALA	4.0
1	G	132	GLY	4.0
1	E	490	PRO	4.0
1	B	66	ALA	4.0
1	D	22	THR	3.9
1	B	517	VAL	3.9
1	B	128	GLY	3.9
1	F	512	ARG	3.9
1	E	514	PHE	3.9
1	B	384	VAL	3.8
1	B	543	SER	3.8
1	B	509	GLY	3.8
1	G	232	GLY	3.8
1	F	117	TYR	3.8
1	H	231	PRO	3.8
1	F	516	ARG	3.8
1	B	107	VAL	3.8
1	B	414	ALA	3.8
1	D	23	ALA	3.8
1	B	95	TYR	3.8
1	B	512	ARG	3.8
1	A	241	LEU	3.8
1	B	97	ALA	3.8
1	B	508	SER	3.7
1	E	511	LEU	3.7
1	E	114	PRO	3.7
1	E	269	ALA	3.7
1	E	275	HIS	3.7
1	A	111	ALA	3.7
1	E	256	PHE	3.7
1	C	22	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	100	ILE	3.6
1	H	22	THR	3.6
1	A	232	GLY	3.6
1	F	517	VAL	3.6
1	F	112	GLY	3.6
1	G	231	PRO	3.5
1	C	21	GLY	3.5
1	B	249	VAL	3.5
1	A	114	PRO	3.5
1	F	129	PRO	3.5
1	B	271	GLY	3.5
1	A	63	ILE	3.5
1	D	275[A]	HIS	3.5
1	A	73	LEU	3.5
1	A	511	LEU	3.5
1	B	498	VAL	3.5
1	G	272	PRO	3.5
1	B	70	VAL	3.5
1	B	263	VAL	3.5
1	F	514	PHE	3.4
1	E	270	LEU	3.4
1	B	103	VAL	3.4
1	B	494	TRP	3.4
1	A	233	LEU	3.4
1	B	260	ALA	3.4
1	E	493	ILE	3.4
1	E	233	LEU	3.4
1	B	231	PRO	3.4
1	B	67	SER	3.4
1	A	95	TYR	3.3
1	A	488[A]	GLU	3.3
1	B	91	GLY	3.3
1	B	380	GLY	3.3
1	B	377	THR	3.3
1	E	70	VAL	3.3
1	B	495	ALA	3.3
1	C	23	ALA	3.3
1	C	412	ARG	3.3
1	H	516	ARG	3.3
1	B	493	ILE	3.3
1	B	272	PRO	3.3
1	A	541	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	485	LEU	3.3
1	H	514	PHE	3.3
1	B	502	VAL	3.3
1	B	344	GLU	3.2
1	B	93	HIS	3.2
1	B	119	PRO	3.2
1	B	383	PRO	3.2
1	C	114	PRO	3.2
1	A	118	ARG	3.2
1	B	514	PHE	3.2
1	B	269	ALA	3.2
1	B	64	GLY	3.2
1	B	375	GLY	3.2
1	G	24	PHE	3.2
1	B	111	ALA	3.2
1	B	52	VAL	3.2
1	B	245	VAL	3.2
1	B	279	ILE	3.2
1	B	374	SER	3.2
1	H	24	PHE	3.2
1	A	498	VAL	3.2
1	E	238	VAL	3.2
1	B	349	LYS	3.1
1	A	270	LEU	3.1
1	B	540[A]	LEU	3.1
1	A	249	VAL	3.1
1	E	26	GLN	3.1
1	D	231	PRO	3.1
1	B	92	SER	3.1
1	B	113	SER	3.1
1	F	12	ASP	3.1
1	A	115	LEU	3.1
1	A	84	ALA	3.1
1	B	62	THR	3.1
1	E	110	PHE	3.1
1	E	249	VAL	3.0
1	A	30	LEU	3.0
1	A	279	ILE	3.0
1	B	515	LEU	3.0
1	B	256	PHE	3.0
1	F	490	PRO	3.0
1	F	488	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	311	ILE	3.0
1	A	495	ALA	3.0
1	F	270	LEU	3.0
1	F	416	LEU	3.0
1	G	412	ARG	3.0
1	E	112	GLY	3.0
1	B	252	VAL	3.0
1	B	61	ALA	3.0
1	F	90	HIS	3.0
1	A	426	ILE	3.0
1	C	233	LEU	3.0
1	B	130	GLY	3.0
1	E	100	ILE	2.9
1	H	232	GLY	2.9
1	B	65	PRO	2.9
1	B	72	ARG	2.9
1	E	109	SER	2.9
1	A	515	LEU	2.9
1	F	484	LEU	2.9
1	F	493	ILE	2.9
1	H	130	GLY	2.9
1	B	411	ARG	2.9
1	A	237	ASP	2.9
1	B	510	LYS	2.9
1	A	88	PHE	2.9
1	A	263	VAL	2.9
1	E	266	VAL	2.9
1	F	245	VAL	2.9
1	E	264	ALA	2.9
1	F	11	ALA	2.9
1	B	10	ARG	2.9
1	B	516	ARG	2.9
1	E	540	LEU	2.9
1	A	493	ILE	2.9
1	B	542	ILE	2.9
1	B	109	SER	2.9
1	E	90	HIS	2.9
1	E	351	ARG	2.8
1	F	351	ARG	2.8
1	F	238	VAL	2.8
1	H	52	VAL	2.8
1	A	34	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	271	GLY	2.8
1	C	115	LEU	2.8
1	D	242[A]	ARG	2.8
1	F	507	GLU	2.8
1	A	110	PHE	2.8
1	C	34	MET	2.8
1	C	110	PHE	2.8
1	B	505	GLY	2.8
1	B	521	VAL	2.8
1	F	52	VAL	2.8
1	E	241	LEU	2.8
1	B	63	ILE	2.8
1	E	118	ARG	2.8
1	F	411	ARG	2.8
1	B	507	GLU	2.8
1	H	273	GLU	2.8
1	E	505	GLY	2.8
1	B	101	ALA	2.8
1	B	110	PHE	2.8
1	C	24	PHE	2.8
1	F	242	ARG	2.8
1	B	71	GLU	2.8
1	E	117	TYR	2.8
1	A	542	ILE	2.8
1	A	496	ASP	2.8
1	B	237	ASP	2.8
1	B	513	GLY	2.8
1	E	116	SER	2.8
1	F	487	ARG	2.7
1	E	24	PHE	2.7
1	E	504	PHE	2.7
1	A	245	VAL	2.7
1	A	90	HIS	2.7
1	B	242	ARG	2.7
1	B	258	ARG	2.7
1	F	492	ALA	2.7
1	D	52	VAL	2.7
1	E	234	SER	2.7
1	E	277	ILE	2.7
1	F	379	LYS	2.7
1	B	84	ALA	2.7
1	B	413	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	66	ALA	2.7
1	G	54	ALA	2.7
1	E	88	PHE	2.7
1	A	275	HIS	2.7
1	B	108	GLU	2.7
1	A	86	LEU	2.7
1	A	540	LEU	2.7
1	B	124	LEU	2.7
1	B	126	THR	2.7
1	E	30	LEU	2.7
1	F	506	ILE	2.7
1	E	268	ALA	2.7
1	E	487	ARG	2.6
1	A	489	PRO	2.6
1	E	272	PRO	2.6
1	E	541[A]	SER	2.6
1	E	95	TYR	2.6
1	H	275[A]	HIS	2.6
1	A	64	GLY	2.6
1	E	128	GLY	2.6
1	B	351	ARG	2.6
1	E	515	LEU	2.6
1	A	52	VAL	2.6
1	A	107	VAL	2.6
1	A	475	VAL	2.6
1	B	77	ILE	2.6
1	A	471	ALA	2.6
1	B	33	ALA	2.6
1	E	543	SER	2.6
1	A	351	ARG	2.6
1	B	90	HIS	2.6
1	B	410	LEU	2.6
1	C	90	HIS	2.6
1	E	485	LEU	2.6
1	E	245	VAL	2.6
1	B	386	ALA	2.6
1	A	412	ARG	2.6
1	B	274	GLY	2.5
1	G	514	PHE	2.5
1	E	120	VAL	2.5
1	E	502	VAL	2.5
1	A	271	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	112	GLY	2.5
1	E	242	ARG	2.5
1	B	243	PHE	2.5
1	C	117	TYR	2.5
1	A	100	ILE	2.5
1	A	101	ALA	2.5
1	B	264	ALA	2.5
1	E	265	ALA	2.5
1	E	295	ILE	2.5
1	F	414	ALA	2.5
1	A	112	GLY	2.5
1	A	273	GLU	2.5
1	B	75	GLU	2.5
1	C	113	SER	2.5
1	A	494	TRP	2.5
1	B	381	ASN	2.5
1	B	12	ASP	2.5
1	B	25	PHE	2.5
1	B	350	PRO	2.5
1	E	111	ALA	2.5
1	E	489	PRO	2.5
1	B	112	GLY	2.5
1	A	277	ILE	2.5
1	B	122	ILE	2.5
1	F	103	VAL	2.5
1	A	68	ARG	2.5
1	F	412	ARG	2.5
1	C	109	SER	2.5
1	B	236	GLN	2.4
1	B	16	LEU	2.4
1	F	415	PRO	2.4
1	A	298	VAL	2.4
1	C	347	ILE	2.4
1	E	481	VAL	2.4
1	C	411	ARG	2.4
1	B	76[A]	MET	2.4
1	A	256	PHE	2.4
1	A	66	ALA	2.4
1	B	265	ALA	2.4
1	B	102	ASN	2.4
1	A	257	VAL	2.4
1	E	263	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	262	ASP	2.4
1	E	125	ASP	2.4
1	E	34	MET	2.4
1	A	130	GLY	2.4
1	A	26	GLN	2.4
1	A	260	ALA	2.4
1	E	243	PHE	2.4
1	A	108	GLU	2.4
1	D	235	GLU	2.4
1	B	239	ARG	2.4
1	H	412	ARG	2.4
1	C	63	ILE	2.4
1	F	347	ILE	2.4
1	A	517	VAL	2.4
1	B	131	SER	2.3
1	B	129	PRO	2.3
1	D	273	GLU	2.3
1	A	242	ARG	2.3
1	F	265	ALA	2.3
1	G	515	LEU	2.3
1	E	103	VAL	2.3
1	A	116	SER	2.3
1	B	244	GLY	2.3
1	D	132	GLY	2.3
1	B	488	GLU	2.3
1	F	118	ARG	2.3
1	E	499	ASP	2.3
1	C	129	PRO	2.3
1	H	23	ALA	2.3
1	F	515	LEU	2.3
1	H	416	LEU	2.3
1	B	275	HIS	2.3
1	E	253	PHE	2.3
1	B	277	ILE	2.3
1	A	109	SER	2.3
1	B	408	GLU	2.3
1	E	542	ILE	2.3
1	A	258	ARG	2.3
1	E	52	VAL	2.3
1	A	274	GLY	2.3
1	B	310	GLY	2.3
1	A	51	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	490	PRO	2.3
1	B	121	ALA	2.3
1	B	492	ALA	2.3
1	H	413	ALA	2.3
1	F	86	LEU	2.3
1	G	416	LEU	2.3
1	B	487	ARG	2.3
1	D	500	ARG	2.3
1	C	311	ILE	2.3
1	D	130	GLY	2.3
1	F	266	VAL	2.3
1	C	291	ARG	2.2
1	B	253	PHE	2.2
1	D	232	GLY	2.2
1	F	128	GLY	2.2
1	E	122	ILE	2.2
1	E	506	ILE	2.2
1	F	275	HIS	2.2
1	A	266	VAL	2.2
1	A	384	VAL	2.2
1	F	527	TRP	2.2
1	F	269	ALA	2.2
1	A	309	LEU	2.2
1	B	30	LEU	2.2
1	B	309	LEU	2.2
1	F	34	MET	2.2
1	F	232	GLY	2.2
1	F	344	GLU	2.2
1	F	504	PHE	2.2
1	B	68	ARG	2.2
1	B	486	TYR	2.2
1	H	500	ARG	2.2
1	D	543	SER	2.2
1	E	99	SER	2.2
1	B	14	ALA	2.2
1	B	346	MET	2.2
1	C	26	GLN	2.2
1	A	248	GLY	2.2
1	A	518	GLY	2.2
1	E	86	LEU	2.2
1	A	72	ARG	2.2
1	A	93	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	412	ARG	2.2
1	B	83	ILE	2.2
1	D	311	ILE	2.2
1	B	261	SER	2.2
1	B	387	VAL	2.1
1	B	491	GLU	2.1
1	A	97	ALA	2.1
1	B	438	ALA	2.1
1	D	260	ALA	2.1
1	E	101	ALA	2.1
1	F	111	ALA	2.1
1	B	404	ARG	2.1
1	B	96	HIS	2.1
1	E	520	LEU	2.1
1	F	241	LEU	2.1
1	G	270	LEU	2.1
1	B	541	SER	2.1
1	D	490	PRO	2.1
1	A	313	ILE	2.1
1	H	267[A]	ARG	2.1
1	A	252	VAL	2.1
1	B	464	ALA	2.1
1	D	413	ALA	2.1
1	E	492	ALA	2.1
1	F	260	ALA	2.1
1	B	276	GLY	2.1
1	B	74	LYS	2.1
1	E	309	LEU	2.1
1	A	527	TRP	2.1
1	B	527	TRP	2.1
1	F	36	ASP	2.1
1	F	113	SER	2.1
1	A	357	THR	2.1
1	B	483	PRO	2.1
1	G	516	ARG	2.1
1	A	60	ILE	2.1
1	A	302	ILE	2.1
1	B	456	TYR	2.1
1	A	244	GLY	2.1
1	A	265	ALA	2.1
1	A	450	ALA	2.1
1	E	495	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	97	ALA	2.1
1	C	436	CYS	2.1
1	H	436	CYS	2.1
1	A	520	LEU	2.1
1	B	520	LEU	2.1
1	C	515	LEU	2.1
1	A	272	PRO	2.1
1	A	482	PHE	2.1
1	B	60	ILE	2.1
1	F	95	TYR	2.1
1	F	311	ILE	2.1
1	G	63	ILE	2.1
1	E	244	GLY	2.0
1	F	246	GLU	2.0
1	F	408	GLU	2.0
1	C	107	VAL	2.0
1	C	289	VAL	2.0
1	D	351	ARG	2.0
1	F	502	VAL	2.0
1	D	233	LEU	2.0
1	E	73	LEU	2.0
1	B	232	GLY	2.0
1	C	514	PHE	2.0
1	E	412	ARG	2.0
1	F	268	ALA	2.0
1	G	53	ALA	2.0
1	B	13	VAL	2.0
1	E	257	VAL	2.0
1	E	517	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	OA0	G	605	19/19	0.70	0.23	72,72,74,74	8
6	OA0	H	601	19/19	0.73	0.21	60,61,63,63	8
6	OA0	A	605	19/19	0.74	0.26	99,100,100,100	8
6	OA0	C	601	19/19	0.74	0.21	64,65,67,67	8
6	OA0	D	605	19/19	0.75	0.24	86,87,87,88	8
4	MG	A	603	1/1	0.78	0.10	74,74,74,74	0
6	OA0	F	605	19/19	0.78	0.22	76,77,78,79	8
3	OXL	F	602	6/6	0.80	0.16	52,53,54,54	0
3	OXL	E	602	6/6	0.80	0.19	77,77,77,78	0
3	OXL	C	603	6/6	0.81	0.18	69,69,70,70	0
3	OXL	G	602	6/6	0.81	0.15	50,50,51,51	0
3	OXL	H	603	6/6	0.81	0.15	40,41,43,44	0
3	OXL	D	602	6/6	0.81	0.15	51,52,53,53	0
3	OXL	A	602	6/6	0.81	0.14	74,74,75,75	0
6	OA0	E	605	19/19	0.82	0.22	86,87,87,88	8
3	OXL	B	602	6/6	0.82	0.16	63,64,65,65	0
6	OA0	B	605	19/19	0.83	0.16	58,59,60,61	8
4	MG	C	604	1/1	0.88	0.07	55,55,55,55	0
4	MG	E	603	1/1	0.91	0.07	63,63,63,63	0
4	MG	H	604	1/1	0.91	0.06	42,42,42,42	0
5	K	F	604	1/1	0.92	0.13	67,67,67,67	0
5	K	A	604	1/1	0.93	0.13	77,77,77,77	0
4	MG	F	603	1/1	0.93	0.06	49,49,49,49	0
5	K	B	604	1/1	0.94	0.12	77,77,77,77	0
5	K	E	604	1/1	0.94	0.19	75,75,75,75	0
2	FBP	B	601	20/20	0.94	0.09	41,42,48,48	0
5	K	G	604	1/1	0.94	0.12	49,49,49,49	0
2	FBP	A	601	20/20	0.95	0.08	39,41,43,43	0
5	K	C	605	1/1	0.96	0.15	49,49,49,49	0
2	FBP	F	601	20/20	0.96	0.08	34,38,42,43	0
2	FBP	E	601	20/20	0.96	0.07	38,39,41,41	0
4	MG	B	603	1/1	0.97	0.06	60,60,60,60	0
2	FBP	H	602	20/20	0.98	0.05	20,22,23,24	0
2	FBP	G	601	20/20	0.98	0.04	24,26,27,28	0
4	MG	D	603	1/1	0.98	0.07	43,43,43,43	0
5	K	H	605	1/1	0.98	0.06	44,44,44,44	0
2	FBP	D	601	20/20	0.99	0.04	24,25,27,28	0

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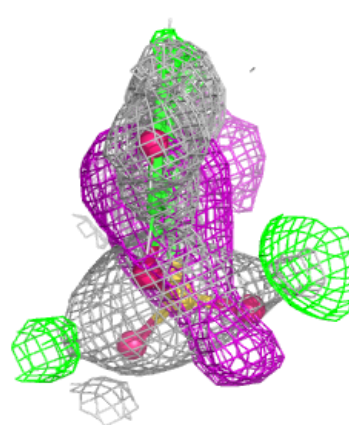
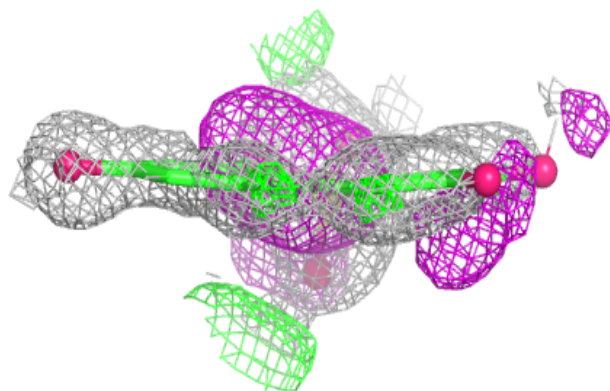
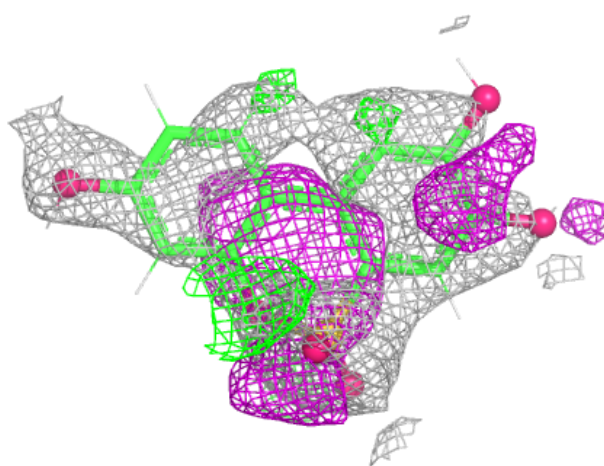
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	G	603	1/1	0.99	0.03	40,40,40,40	0
2	FBP	C	602	20/20	0.99	0.04	27,29,30,31	0
5	K	D	604	1/1	0.99	0.08	43,43,43,43	0

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.

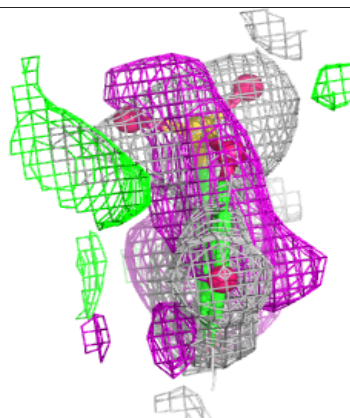
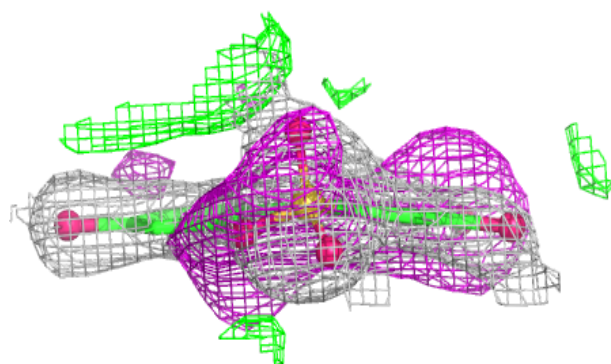
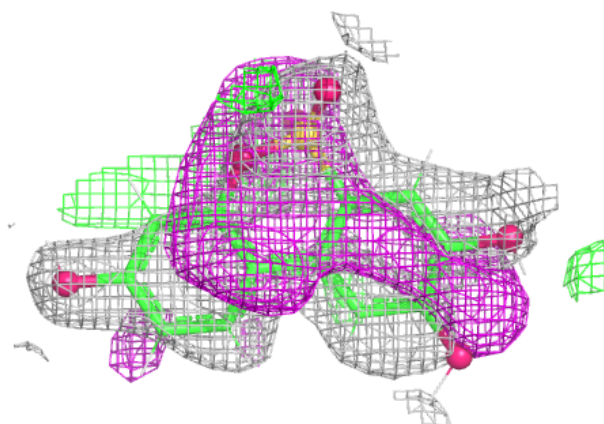
Electron density around OA0 G 605:

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



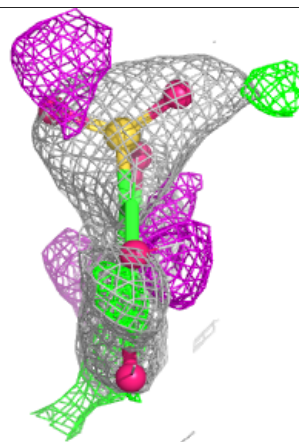
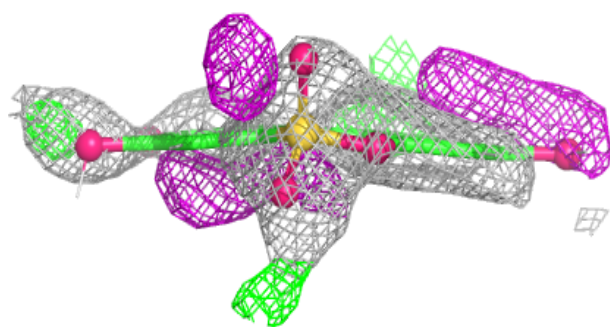
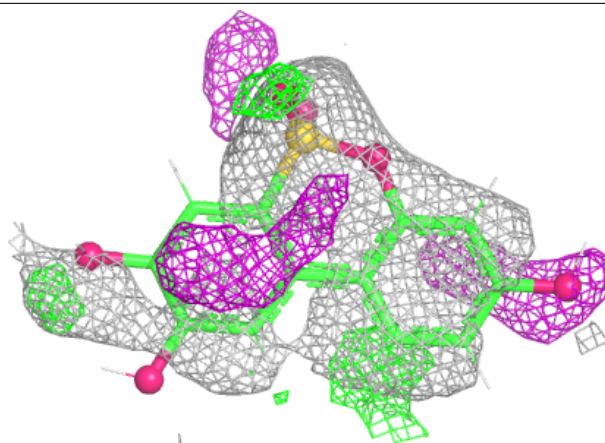
Electron density around OA0 H 601:

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



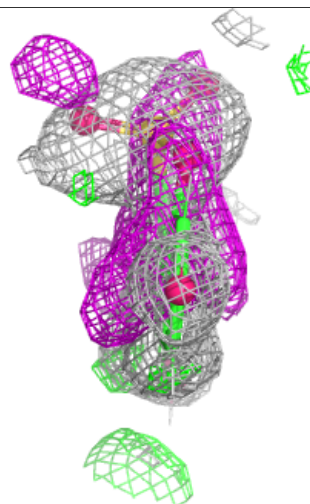
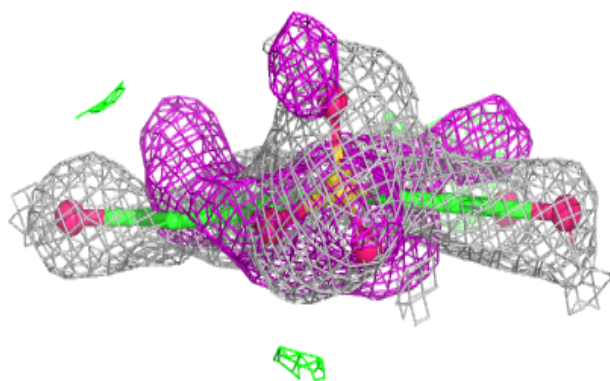
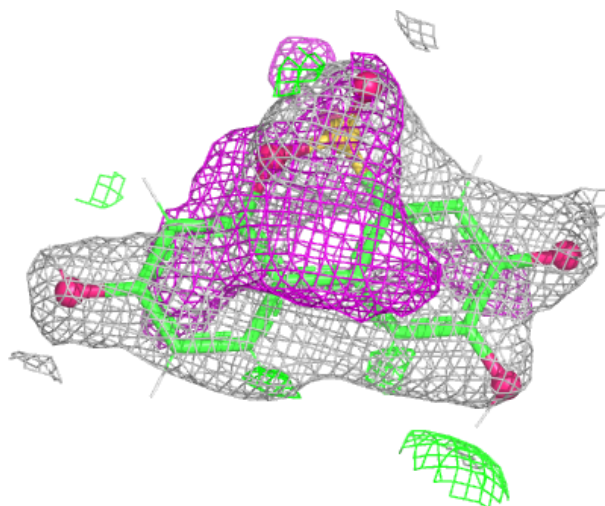
Electron density around OA0 A 605:

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



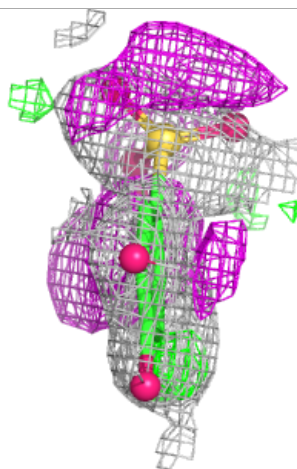
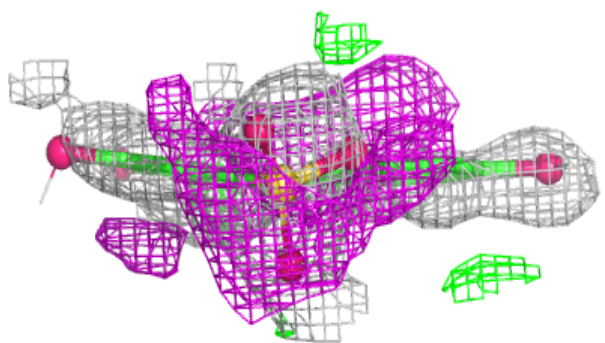
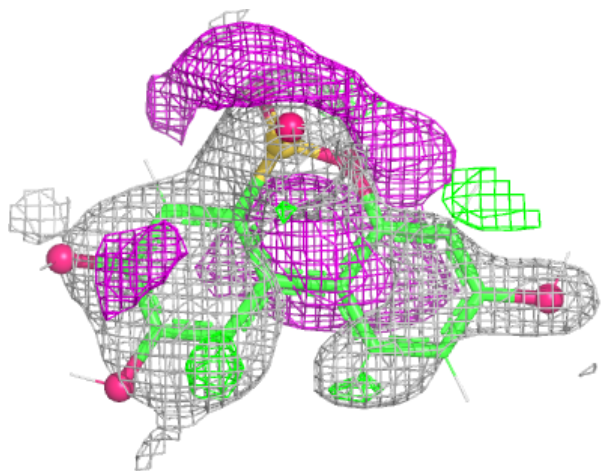
Electron density around OA0 C 601:

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



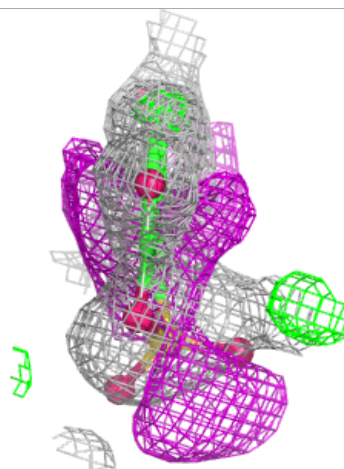
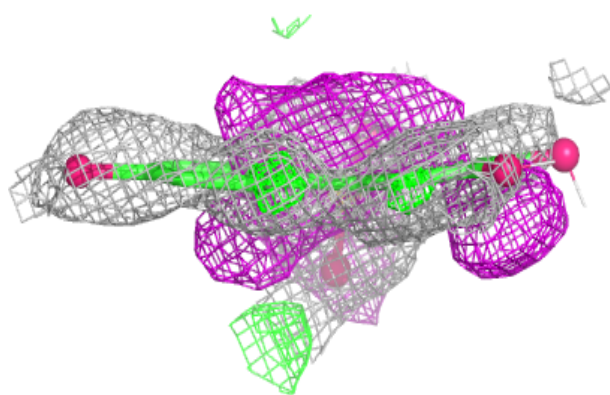
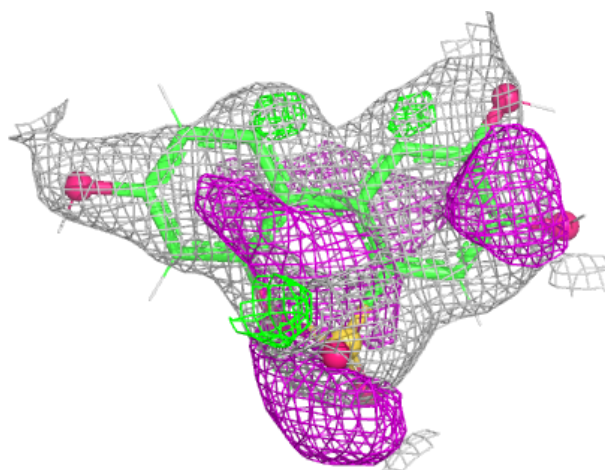
Electron density around OA0 D 605:

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



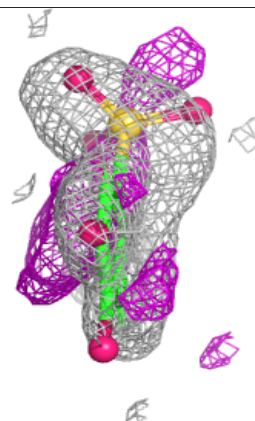
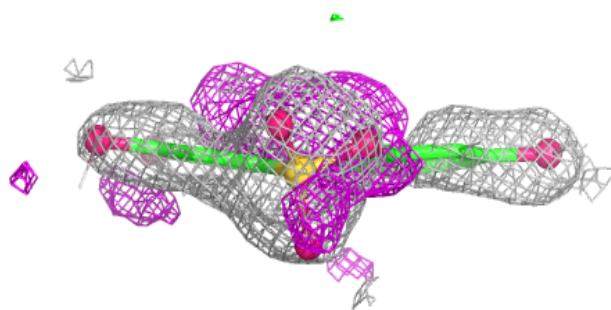
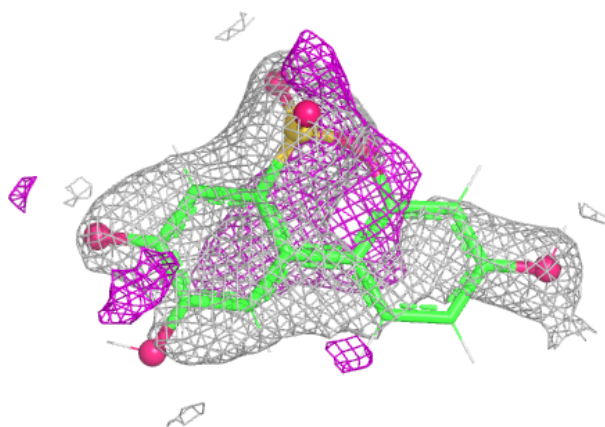
Electron density around OA0 F 605:

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



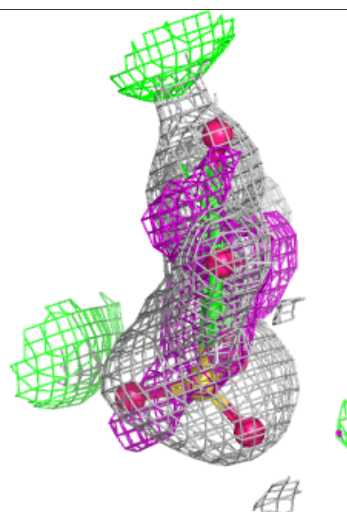
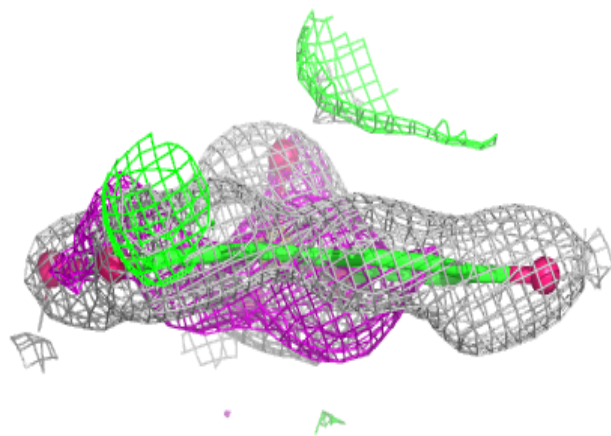
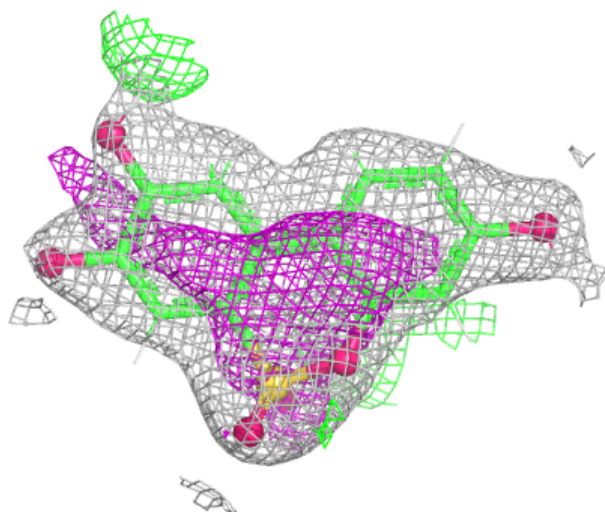
Electron density around OA0 E 605:

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



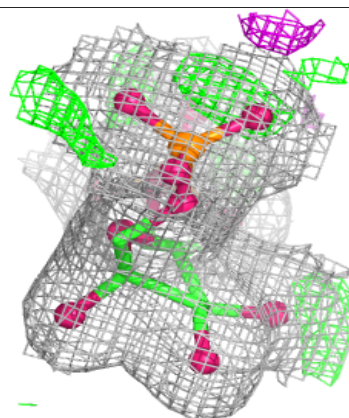
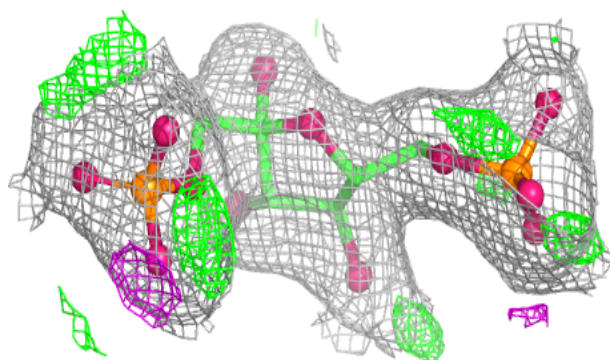
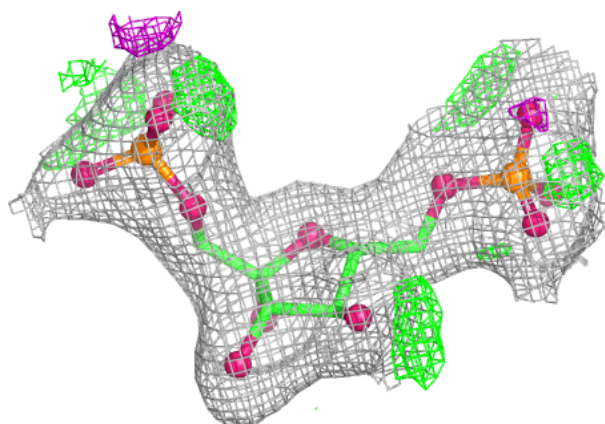
Electron density around OA0 B 605:

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

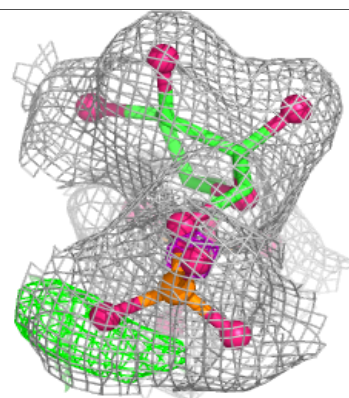
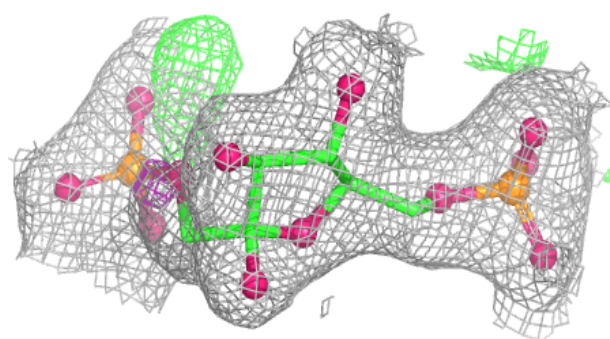
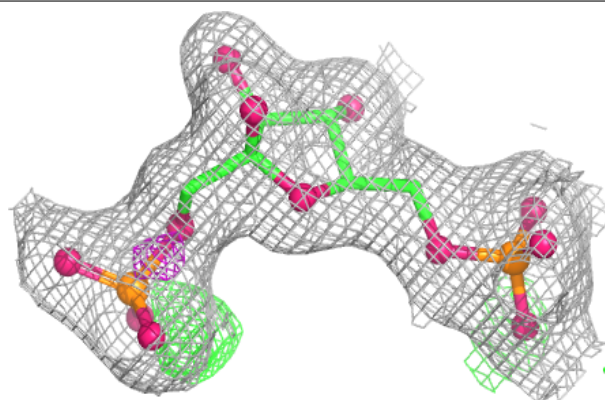


Electron density around FBP B 601:

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

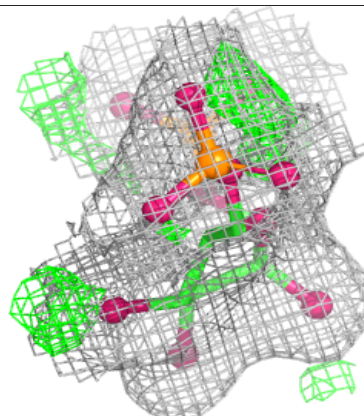
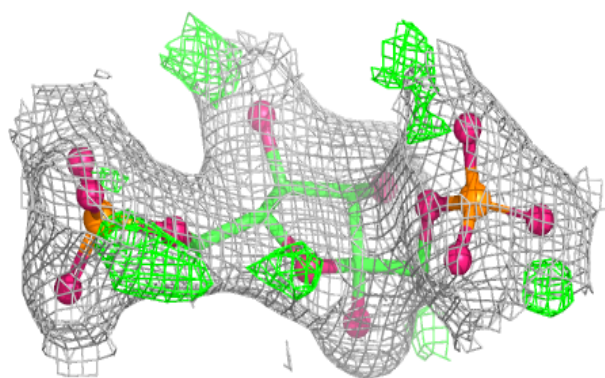
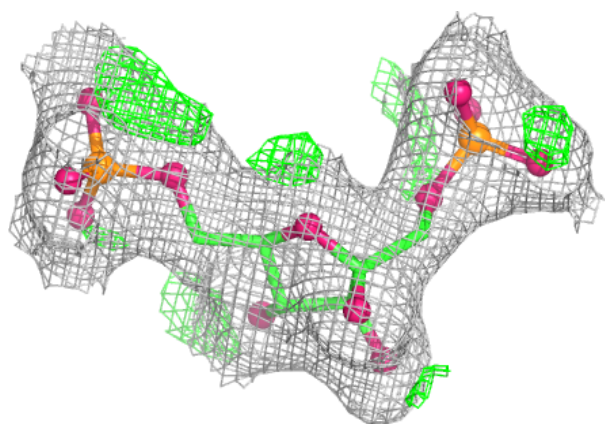
**Electron density around FBP A 601:**

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

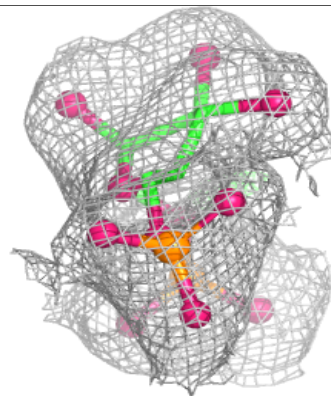
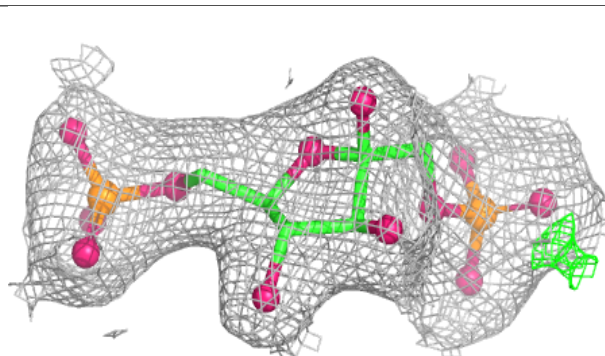
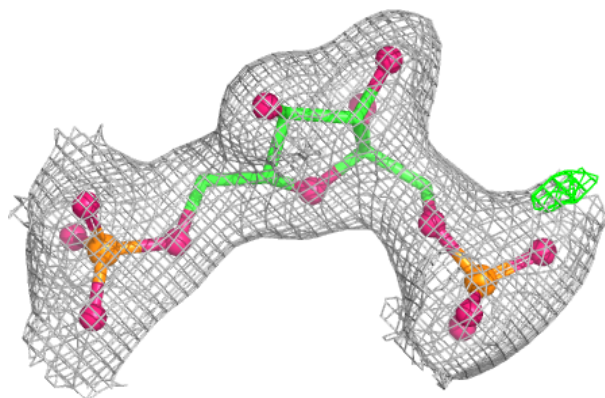


Electron density around FBP F 601:

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

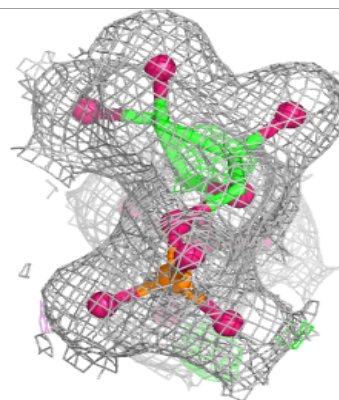
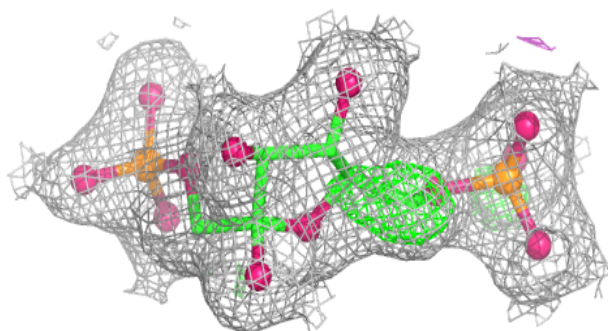
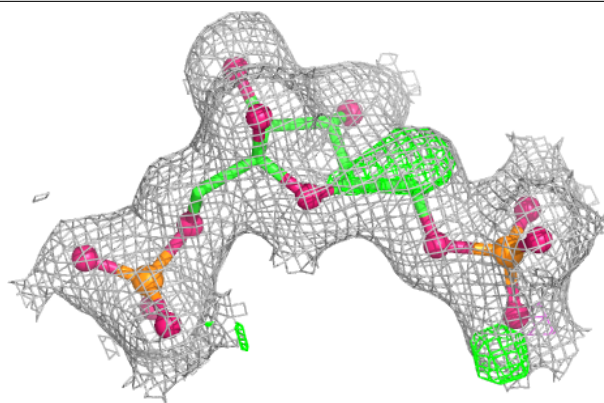
**Electron density around FBP E 601:**

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

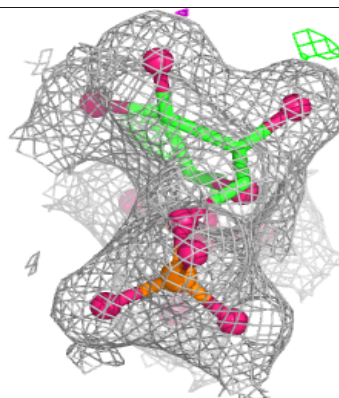
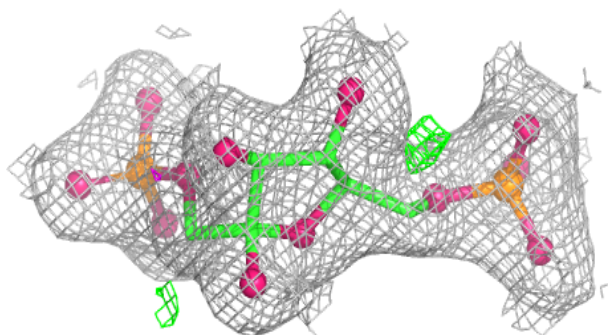
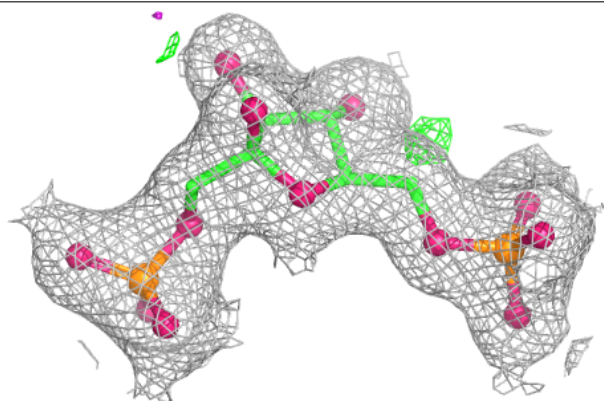


Electron density around FBP H 602:

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

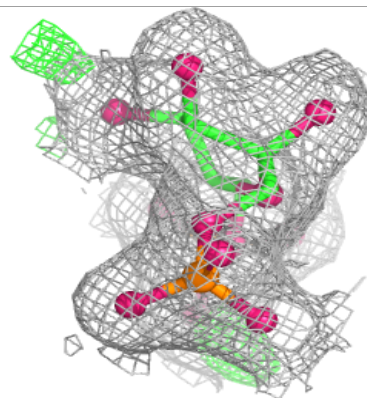
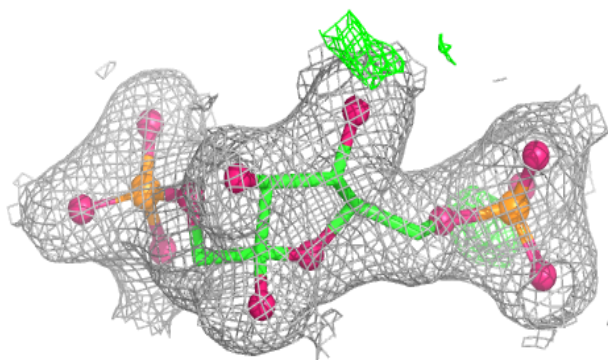
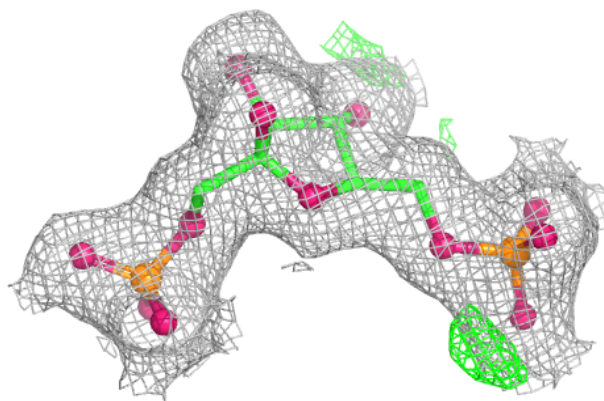
**Electron density around FBP G 601:**

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

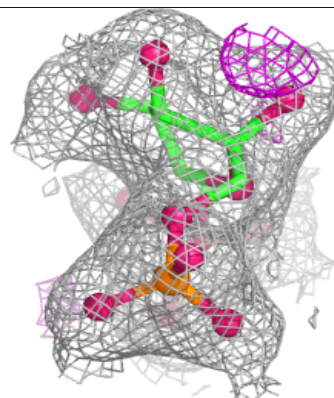
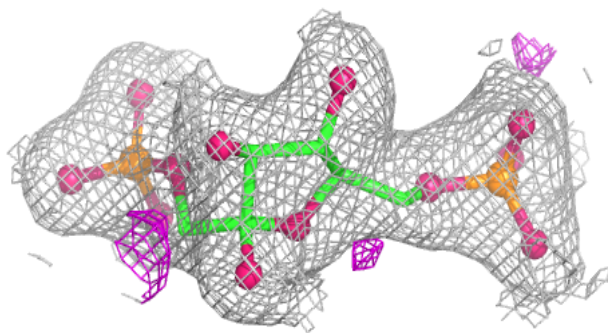
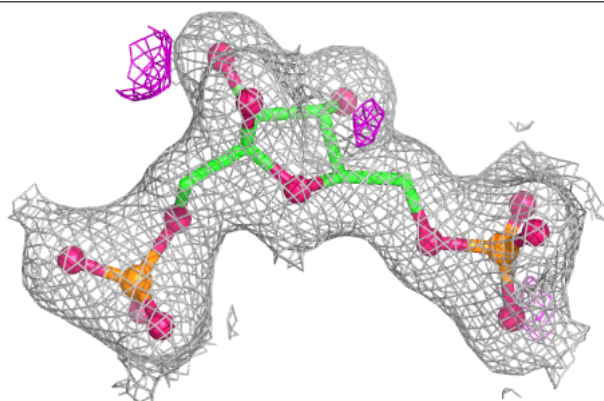


Electron density around FBP D 601:

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

**Electron density around FBP C 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.