



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:21 AM UTC

PDB ID : 7FRV / pdb_00007frv
Title : Structure of liver pyruvate kinase in complex with allosteric modulator 3
Authors : Lulla, A.; Nilsson, O.; Brear, P.; Nain-Perez, A.; Grotli, M.; Hyvonen, M.
Deposited on : 2022-12-18
Resolution : 2.00 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:

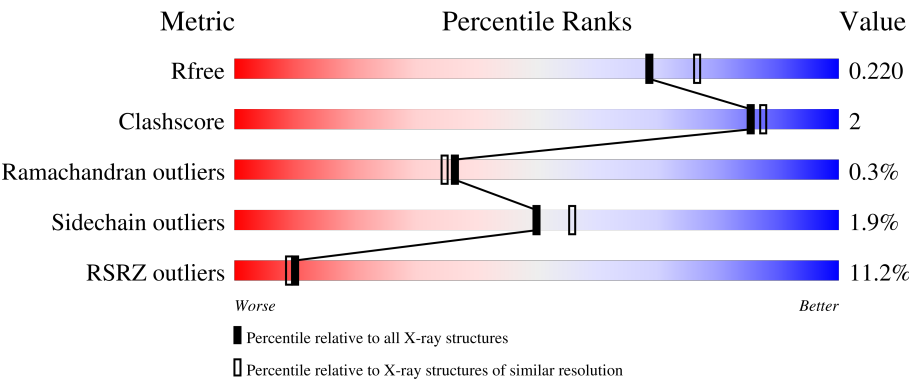
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	16% 87%7%6%
1	B	447	30% 91%6%•
1	C	447	7% 89%6%5%
1	D	447	2% 90%5%5%
1	E	447	14% 87%6%•6%

Continued on next page...

Continued from previous page...

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 28689 atoms, of which 80 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

Continued on next page...

Continued from previous page...

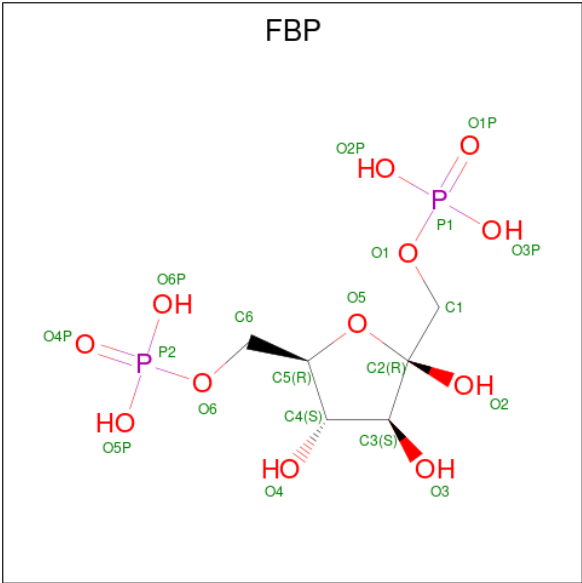
Chain	Residue	Modelled	Actual	Comment	Reference
B	130	GLY	-	linker	UNP P30613
B	131	SER	-	linker	UNP P30613
B	132	GLY	-	linker	UNP P30613
C	-1	GLY	-	expression tag	UNP P30613
C	0	SER	-	expression tag	UNP P30613
C	1	MET	-	expression tag	UNP P30613
C	2	GLU	-	expression tag	UNP P30613
C	12	ASP	SER	conflict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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

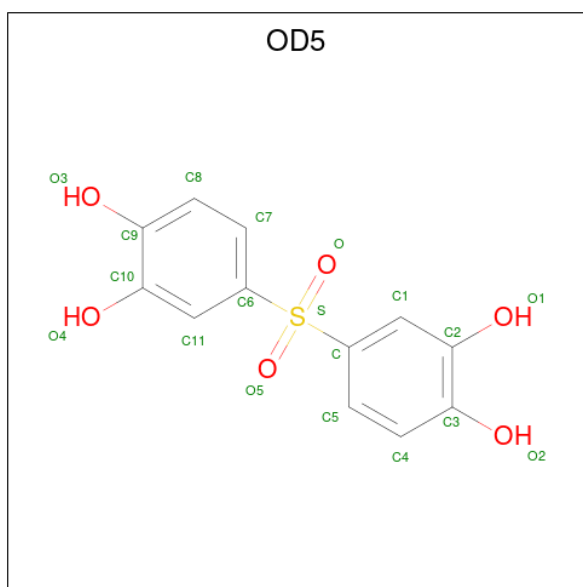
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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'-sulfonyldi(benzene-1,2-diol) (CCD ID: OD5) (formula: C₁₂H₁₀O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	O	S	20	1
			58	24	20	12	2		
6	D	1	Total	C	H	O	S	20	1
			58	24	20	12	2		
6	F	1	Total	C	H	O	S	20	1
			58	24	20	12	2		
6	G	1	Total	C	H	O	S	20	1
			58	24	20	12	2		

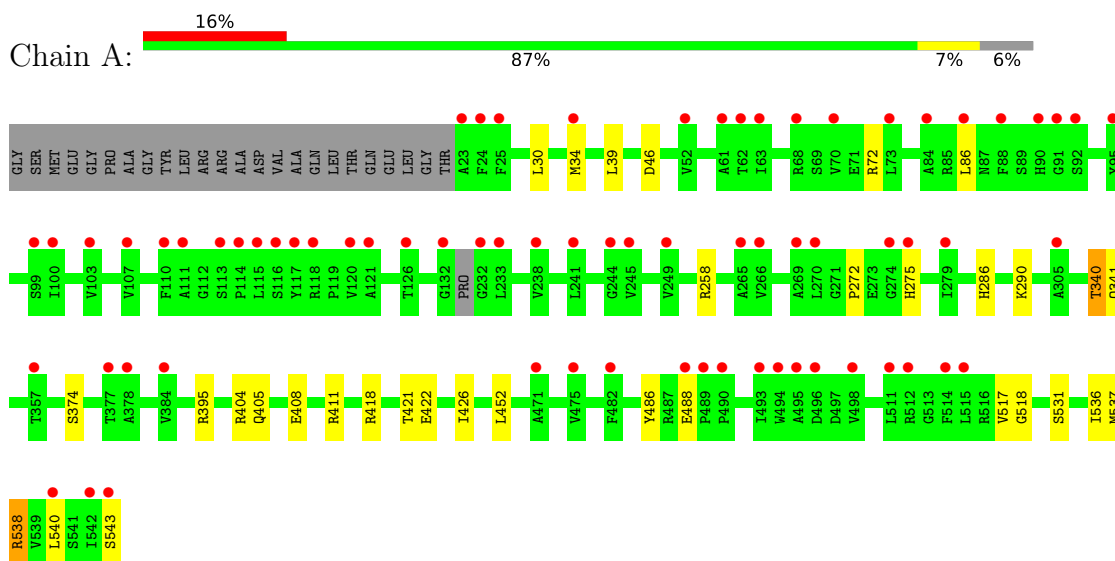
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	168	Total	O	0	0
			168	168		
7	B	156	Total	O	0	0
			156	156		
7	C	320	Total	O	0	0
			320	320		
7	D	321	Total	O	0	0
			321	321		
7	E	181	Total	O	0	0
			181	181		
7	F	280	Total	O	0	0
			280	280		
7	G	332	Total	O	0	0
			332	332		
7	H	398	Total	O	0	0
			398	398		

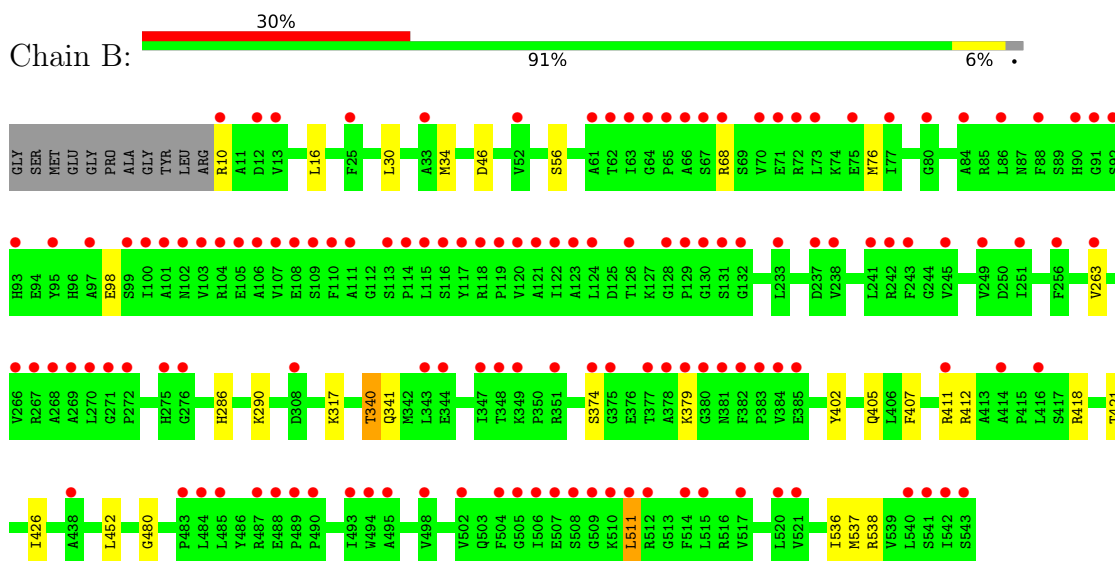
3 Residue-property plots [i](#)

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.

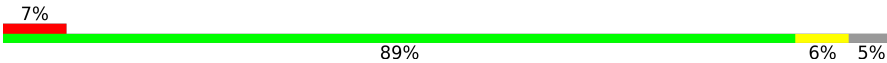
• Molecule 1: Pyruvate kinase PKLR

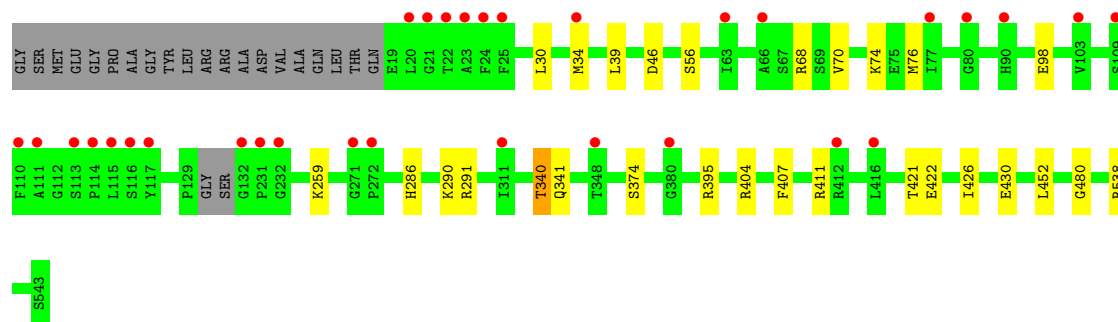


• Molecule 1: Pyruvate kinase PKLR

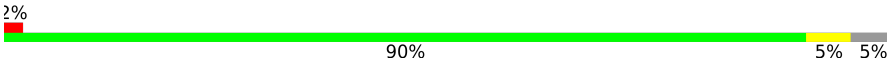


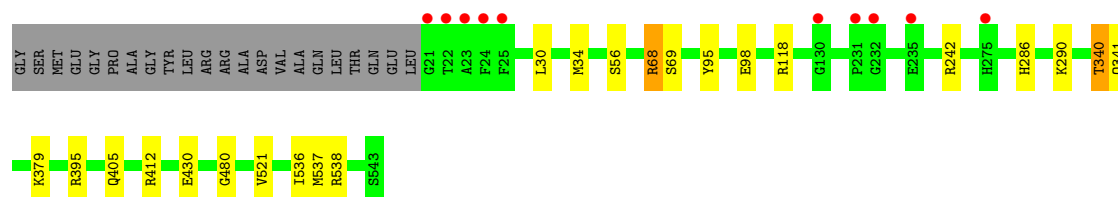
• Molecule 1: Pyruvate kinase PKLR

Chain C: 



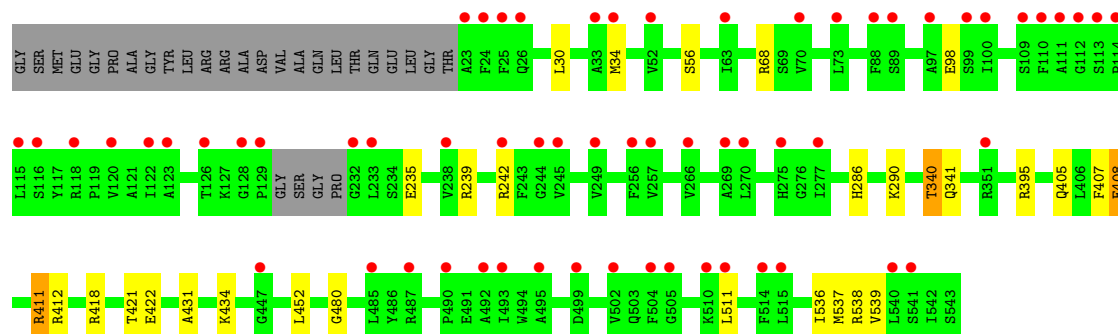
• Molecule 1: Pyruvate kinase PKLR

Chain D: 



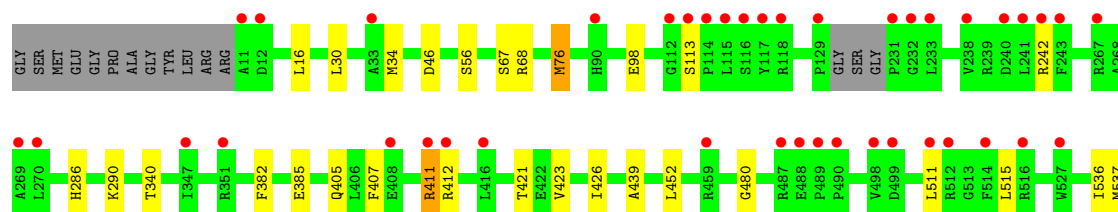
• Molecule 1: Pyruvate kinase PKLR

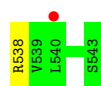
Chain E: 



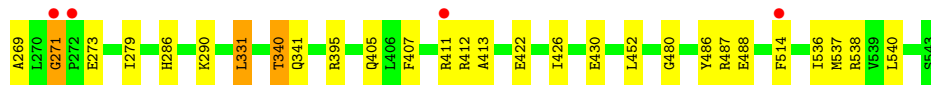
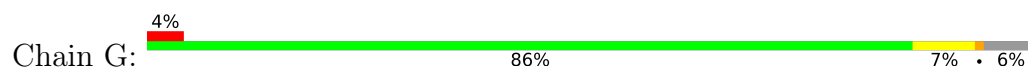
• Molecule 1: Pyruvate kinase PKLR

Chain F: 

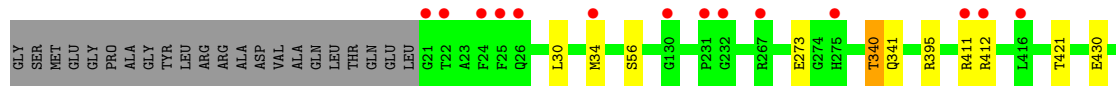
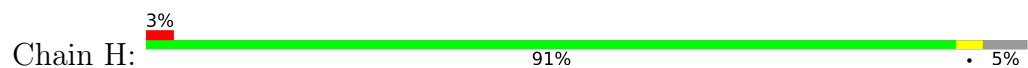




• Molecule 1: Pyruvate kinase PKLR



• 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	208.04Å 112.71Å 188.41Å 90.00° 91.59° 90.00°	Depositor
Resolution (Å)	188.34 – 2.00 188.34 – 2.00	Depositor EDS
% Data completeness (in resolution range)	83.5 (188.34-2.00) 83.5 (188.34-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, R_{free}	0.206 , 0.232 0.196 , 0.220	Depositor DCC
R_{free} test set	11907 reflections (4.09%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.9	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	28689	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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 60.78 % 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 1.4457e-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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, OXL, OD5, MG, FBP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.63	1/3307 (0.0%)	0.98	2/4469 (0.0%)
1	B	0.66	1/3396 (0.0%)	0.98	1/4592 (0.0%)
1	C	0.70	1/3313 (0.0%)	0.96	1/4479 (0.0%)
1	D	0.73	0/3326	0.98	0/4497
1	E	0.63	0/3278	0.97	1/4430 (0.0%)
1	F	0.70	0/3396	0.98	1/4591 (0.0%)
1	G	0.71	0/3303	0.97	1/4465 (0.0%)
1	H	0.76	1/3316 (0.0%)	0.98	0/4483
All	All	0.69	4/26635 (0.0%)	0.97	7/36006 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	374	SER	CA-C	6.66	1.55	1.52
1	C	374	SER	CA-C	5.53	1.55	1.52
1	H	537	MET	SD-CE	-5.25	1.66	1.79
1	A	374	SER	CA-C	5.08	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	422	GLU	CB-CG-CD	6.11	122.99	112.60
1	A	422	GLU	CB-CG-CD	5.62	122.16	112.60
1	G	514	PHE	CA-CB-CG	5.31	119.11	113.80
1	C	46	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	46	ASP	CA-CB-CG	5.16	117.76	112.60
1	B	46	ASP	CA-CB-CG	5.14	117.74	112.60
1	F	46	ASP	CA-CB-CG	5.00	117.60	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	17	0
1	B	3329	0	3394	17	1
1	C	3247	0	3299	19	0
1	D	3252	0	3310	13	0
1	E	3210	0	3270	16	0
1	F	3321	0	3393	20	0
1	G	3231	0	3284	23	0
1	H	3251	0	3306	12	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
5	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	38	20	0	3	0
6	D	38	20	0	3	0
6	F	38	20	0	1	0
6	G	38	20	0	2	0
7	A	168	0	0	0	0
7	B	156	0	0	2	0
7	C	320	0	0	1	0
7	D	321	0	0	0	0
7	E	181	0	0	3	0
7	F	280	0	0	1	0
7	G	332	0	0	0	0
7	H	398	0	0	0	0
All	All	28609	80	26635	117	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 2.

All (117) 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	0.92
1:B:411:ARG:HG3	1:B:426:ILE:HD11	1.58	0.85
7:E:701:HOH:O	1:F:423:VAL:HG13	1.80	0.82
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.63	0.81
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.63	0.81
1:G:538:ARG:HG2	1:H:536:ILE:HG12	1.63	0.80
1:C:422[A]:GLU:HG3	1:C:452:LEU:HD13	1.65	0.78
1:E:431:ALA:O	7:E:701:HOH:O	2.08	0.72
1:C:538:ARG:HG2	1:D:536:ILE:HG12	1.71	0.72
1:A:272:PRO:HA	1:A:275:HIS:NE2	2.04	0.72
1:E:434:LYS:HB3	7:E:701:HOH:O	1.92	0.69
1:A:418[A]:ARG:HG3	1:B:16:LEU:HD11	1.76	0.67
1:G:405:GLN:HB3	6:G:601[A]:OD5:O	1.95	0.67
1:C:538:ARG:HD3	7:C:737:HOH:O	1.96	0.66
1:E:538:ARG:HG2	1:F:536:ILE:HG12	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:536:ILE:HG12	1:F:538:ARG:HG2	1.78	0.64
1:G:537:MET:HE3	1:H:537:MET:HG2	1.80	0.63
1:F:407:PHE:CE2	1:F:411:ARG:NH1	2.67	0.62
1:A:408:GLU:OE2	1:B:411:ARG:NH2	2.35	0.60
1:A:272:PRO:HA	1:A:275:HIS:CE1	2.36	0.60
1:G:56:SER:HB2	1:G:480:GLY:HA2	1.84	0.59
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.85	0.59
1:H:56:SER:HB2	1:H:480:GLY:HA2	1.85	0.58
1:F:407:PHE:CD2	1:F:411:ARG:NH1	2.71	0.58
1:D:405:GLN:HB3	6:D:605[B]:OD5:O5	2.03	0.58
1:B:407:PHE:CD2	1:B:411:ARG:NH1	2.72	0.57
1:A:405:GLN:HB3	6:A:605[B]:OD5:O	2.05	0.56
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.87	0.56
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.88	0.56
1:B:405:GLN:HB3	6:D:605[A]:OD5:O5	2.07	0.55
1:D:68:ARG:NH2	1:D:95:TYR:O	2.39	0.55
1:F:56:SER:HB2	1:F:480:GLY:HA2	1.89	0.55
1:C:407:PHE:CD2	1:C:411:ARG:NH1	2.75	0.54
1:E:405:GLN:HB3	6:G:601[B]:OD5:O	2.07	0.53
1:E:235:GLU:O	1:E:239:ARG:HD3	2.08	0.53
1:F:411:ARG:HG2	1:F:426:ILE:HD11	1.90	0.53
1:E:56:SER:HB2	1:E:480:GLY:HA2	1.90	0.53
1:G:245:VAL:CG1	1:G:273:GLU:HG2	2.39	0.52
1:G:407:PHE:HD2	1:H:411:ARG:HH22	1.57	0.52
1:G:411:ARG:HG3	1:G:426:ILE:HD11	1.91	0.51
1:G:430[B]:GLU:OE2	1:H:430:GLU:OE1	2.28	0.51
1:A:411:ARG:HG3	1:A:426:ILE:HD11	1.94	0.49
1:F:411:ARG:CG	1:F:426:ILE:HD11	2.42	0.49
1:F:439:ALA:HB3	1:F:515:LEU:HD21	1.95	0.49
1:G:430[A]:GLU:OE1	1:H:430:GLU:OE1	2.29	0.49
1:F:405:GLN:HB3	6:F:605[A]:OD5:O	2.13	0.48
1:D:56:SER:HB2	1:D:480:GLY:CA	2.43	0.48
1:E:407:PHE:O	1:E:411:ARG:HB2	2.13	0.48
1:G:536:ILE:HG12	1:H:538[A]:ARG:HG2	1.96	0.48
1:H:56:SER:HB2	1:H:480:GLY:CA	2.44	0.48
1:A:517:VAL:HG13	1:A:543:SER:HB3	1.96	0.48
1:G:56:SER:HB2	1:G:480:GLY:CA	2.44	0.47
1:D:68:ARG:HH22	1:D:98:GLU:HB2	1.80	0.47
1:G:267:ARG:HG2	1:G:279:ILE:CD1	2.44	0.47
1:E:418:ARG:HD3	1:F:16:LEU:HD11	1.97	0.47
1:G:411:ARG:CG	1:G:426:ILE:HD11	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:340:THR:HG22	1:G:341:GLN:HG3	1.98	0.46
1:C:56:SER:HB2	1:C:480:GLY:CA	2.45	0.46
1:E:340:THR:HG22	1:E:341:GLN:HG3	1.97	0.46
1:B:340:THR:HG22	1:B:341:GLN:HG3	1.96	0.46
1:A:39:LEU:HB2	6:A:605[A]:OD5:O2	2.16	0.45
1:B:56:SER:HB2	1:B:480:GLY:CA	2.46	0.45
1:F:30:LEU:O	1:F:34:MET:HG2	2.16	0.45
1:A:30:LEU:O	1:A:34:MET:HG2	2.16	0.45
1:F:56:SER:HB2	1:F:480:GLY:CA	2.46	0.45
1:B:30:LEU:O	1:B:34:MET:HG2	2.17	0.45
1:C:286:HIS:CE1	1:C:290:LYS:HG3	2.52	0.45
1:D:340:THR:HG22	1:D:341:GLN:HG3	2.00	0.44
1:A:518:GLY:O	1:B:418:ARG:NH2	2.48	0.44
1:F:286:HIS:CE1	1:F:290:LYS:HG3	2.52	0.44
1:F:67:SER:HB2	1:F:76[B]:MET:SD	2.58	0.44
1:B:317:LYS:NZ	7:B:704:HOH:O	2.41	0.44
1:E:408:GLU:CD	1:F:411:ARG:HH21	2.26	0.44
1:F:68:ARG:NH2	1:F:98:GLU:HB3	2.33	0.44
1:G:286:HIS:CE1	1:G:290:LYS:HG3	2.53	0.44
1:B:286:HIS:CE1	1:B:290:LYS:HG3	2.53	0.43
1:C:30:LEU:O	1:C:34:MET:HG2	2.18	0.43
1:C:430[B]:GLU:OE2	1:D:430[B]:GLU:OE1	2.36	0.43
1:F:113:SER:HB3	7:F:735:HOH:O	2.18	0.43
1:G:411:ARG:HH21	1:H:411:ARG:NH2	2.16	0.43
1:C:259:LYS:HB3	1:C:291:ARG:HH11	1.84	0.43
1:G:269:ALA:C	1:G:271:GLY:H	2.26	0.43
1:C:68:ARG:NH2	1:C:98:GLU:HB3	2.34	0.43
1:C:404:ARG:HD3	1:D:412:ARG:NH2	2.33	0.43
1:D:68:ARG:NH2	1:D:98:GLU:HB2	2.34	0.43
1:C:340:THR:HG22	1:C:341:GLN:HG3	2.00	0.43
1:D:286:HIS:CE1	1:D:290:LYS:HG3	2.54	0.43
1:G:331:LEU:HD21	1:G:413:ALA:HB1	2.01	0.43
1:C:430[A]:GLU:OE1	1:D:430[A]:GLU:OE1	2.37	0.43
1:B:421:THR:HG22	1:B:452:LEU:HD12	2.01	0.42
1:E:68:ARG:NH2	1:E:98:GLU:HB3	2.33	0.42
1:G:486:TYR:CZ	1:G:488:GLU:HB2	2.54	0.42
1:G:30:LEU:O	1:G:34:MET:HG2	2.19	0.42
1:A:340:THR:HG22	1:A:341:GLN:HG3	2.00	0.42
1:A:404:ARG:HD3	7:B:803:HOH:O	2.18	0.42
1:A:421:THR:HG22	1:A:452:LEU:HD12	2.02	0.42
1:A:538:ARG:HG3	1:B:536:ILE:HG12	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:SER:HB2	1:E:480:GLY:CA	2.48	0.42
1:F:382:PHE:HB3	1:F:385:GLU:HB2	2.01	0.42
1:E:286:HIS:CE1	1:E:290:LYS:HG3	2.55	0.42
1:H:421:THR:HG22	1:H:452:LEU:HD12	2.02	0.42
1:B:68:ARG:NH2	1:B:98:GLU:HB3	2.34	0.42
1:F:421:THR:HG22	1:F:452:LEU:HD12	2.02	0.42
1:E:30:LEU:O	1:E:34:MET:HG3	2.20	0.41
6:A:605[B]:OD5:O1	1:C:39:LEU:HB2	2.21	0.41
1:C:70:VAL:HG12	1:C:74:LYS:HE3	2.03	0.41
1:C:259:LYS:CB	1:C:291:ARG:HH11	2.34	0.41
1:G:267:ARG:HG2	1:G:279:ILE:HD12	2.03	0.41
1:H:30:LEU:O	1:H:34:MET:HG2	2.20	0.41
1:A:286:HIS:CE1	1:A:290:LYS:HG3	2.55	0.41
1:H:340:THR:HG22	1:H:341:GLN:HG3	2.03	0.41
1:E:421:THR:HG22	1:E:452:LEU:HD12	2.02	0.40
1:D:30:LEU:O	1:D:34:MET:HG3	2.21	0.40
1:G:68:ARG:NH2	1:G:98[B]:GLU:HB3	2.35	0.40
1:B:402:TYR:HB3	6:D:605[A]:OD5:O	2.21	0.40
1:C:421:THR:HG22	1:C:452:LEU:HD12	2.02	0.40
1:A:486:TYR:CZ	1:A:488[B]:GLU:HB2	2.57	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]	2.09	0.11

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 42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	438/447 (98%)	433 (99%)	4 (1%)	1 (0%)	43	42
1	C	425/447 (95%)	418 (98%)	6 (1%)	1 (0%)	43	42
1	D	429/447 (96%)	425 (99%)	3 (1%)	1 (0%)	43	42
1	E	420/447 (94%)	416 (99%)	3 (1%)	1 (0%)	43	42
1	F	435/447 (97%)	431 (99%)	3 (1%)	1 (0%)	43	42
1	G	423/447 (95%)	414 (98%)	7 (2%)	2 (0%)	24	21
1	H	427/447 (96%)	423 (99%)	3 (1%)	1 (0%)	43	42
All	All	3421/3576 (96%)	3379 (99%)	33 (1%)	9 (0%)	36	35

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	271	GLY
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

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%)	331 (97%)	9 (3%)	40	44
1	B	349/352 (99%)	340 (97%)	9 (3%)	40	44
1	C	341/352 (97%)	338 (99%)	3 (1%)	70	78
1	D	342/352 (97%)	332 (97%)	10 (3%)	37	40
1	E	338/352 (96%)	329 (97%)	9 (3%)	39	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	350/352 (99%)	342 (98%)	8 (2%)	44	49
1	G	340/352 (97%)	333 (98%)	7 (2%)	47	52
1	H	340/352 (97%)	335 (98%)	5 (2%)	57	64
All	All	2740/2816 (97%)	2680 (98%)	60 (2%)	50	50

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ARG
1	A	86	LEU
1	A	258	ARG
1	A	395	ARG
1	A	531	SER
1	A	537[A]	MET
1	A	537[B]	MET
1	A	538	ARG
1	A	540	LEU
1	B	10	ARG
1	B	76[A]	MET
1	B	76[B]	MET
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	C	76[A]	MET
1	C	76[B]	MET
1	C	395	ARG
1	D	68	ARG
1	D	69	SER
1	D	118	ARG
1	D	242[A]	ARG
1	D	242[B]	ARG
1	D	379	LYS
1	D	395	ARG
1	D	521	VAL
1	D	537	MET
1	D	538	ARG
1	E	242	ARG
1	E	395	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	408	GLU
1	E	411	ARG
1	E	412	ARG
1	E	511	LEU
1	E	537[A]	MET
1	E	537[B]	MET
1	E	539	VAL
1	F	76[A]	MET
1	F	76[B]	MET
1	F	242	ARG
1	F	411	ARG
1	F	412	ARG
1	F	511	LEU
1	F	537[A]	MET
1	F	537[B]	MET
1	G	76[A]	MET
1	G	76[B]	MET
1	G	331	LEU
1	G	395	ARG
1	G	412	ARG
1	G	487	ARG
1	G	540	LEU
1	H	273	GLU
1	H	395	ARG
1	H	412	ARG
1	H	443	LEU
1	H	537	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	405	GLN
1	B	405	GLN
1	C	275	HIS
1	C	405	GLN
1	D	405	GLN
1	E	405	GLN
1	F	405	GLN
1	G	275	HIS
1	G	405	GLN
1	H	405	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	E	601	-	18,20,20	0.53	0	21,32,32	0.79	1 (4%)
6	OD5	F	605[A]	-	20,20,20	0.18	0	28,30,30	0.36	0
3	OXL	G	603	4	5,5,5	2.32	3 (60%)	6,6,6	1.82	2 (33%)
2	FBP	C	601	-	18,20,20	0.63	0	21,32,32	0.86	1 (4%)
2	FBP	G	602	-	18,20,20	0.50	0	21,32,32	0.81	0
3	OXL	D	602	4	5,5,5	2.88	3 (60%)	6,6,6	1.83	2 (33%)
6	OD5	D	605[B]	-	20,20,20	0.19	0	28,30,30	0.42	0
2	FBP	D	601	-	18,20,20	0.55	0	21,32,32	0.90	1 (4%)
2	FBP	F	601	-	18,20,20	0.35	0	21,32,32	0.65	0
6	OD5	D	605[A]	-	20,20,20	0.21	0	28,30,30	0.45	0
2	FBP	H	601	-	18,20,20	0.87	1 (5%)	21,32,32	0.76	1 (4%)
3	OXL	B	602	4	5,5,5	2.29	2 (40%)	6,6,6	1.45	2 (33%)
6	OD5	G	601[B]	-	20,20,20	0.16	0	28,30,30	0.48	0
3	OXL	E	602	4	5,5,5	2.35	3 (60%)	6,6,6	2.13	2 (33%)
3	OXL	A	602	4	5,5,5	2.20	2 (40%)	6,6,6	2.02	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	OD5	G	601[A]	-	20,20,20	0.15	0	28,30,30	0.37	0
2	FBP	A	601	-	18,20,20	0.45	0	21,32,32	0.61	0
2	FBP	B	601	-	18,20,20	0.78	1 (5%)	21,32,32	0.89	1 (4%)
3	OXL	H	602	4	5,5,5	2.47	3 (60%)	6,6,6	2.10	2 (33%)
6	OD5	A	605[B]	-	20,20,20	0.18	0	28,30,30	0.38	0
3	OXL	F	602	4	5,5,5	3.35	5 (100%)	6,6,6	2.32	2 (33%)
3	OXL	C	602	4	5,5,5	2.13	2 (40%)	6,6,6	1.79	1 (16%)
6	OD5	A	605[A]	-	20,20,20	0.22	0	28,30,30	0.38	0
6	OD5	F	605[B]	-	20,20,20	0.15	0	28,30,30	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	E	601	-	-	2/13/32/32	0/1/1/1
6	OD5	F	605[A]	-	-	0/12/12/12	0/2/2/2
3	OXL	G	603	4	-	4/4/4/4	-
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
2	FBP	G	602	-	-	2/13/32/32	0/1/1/1
3	OXL	D	602	4	-	4/4/4/4	-
6	OD5	D	605[B]	-	-	0/12/12/12	0/2/2/2
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
6	OD5	D	605[A]	-	-	0/12/12/12	0/2/2/2
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1
3	OXL	B	602	4	-	4/4/4/4	-
6	OD5	G	601[B]	-	-	0/12/12/12	0/2/2/2
3	OXL	E	602	4	-	4/4/4/4	-
3	OXL	A	602	4	-	4/4/4/4	-
6	OD5	G	601[A]	-	-	0/12/12/12	0/2/2/2
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
3	OXL	H	602	4	-	4/4/4/4	-
6	OD5	A	605[B]	-	-	0/12/12/12	0/2/2/2
3	OXL	F	602	4	-	4/4/4/4	-
3	OXL	C	602	4	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OD5	A	605[A]	-	-	0/12/12/12	0/2/2/2
6	OD5	F	605[B]	-	-	0/12/12/12	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	602	OXL	O2-C2	4.12	1.32	1.22
3	D	602	OXL	C2-C1	4.10	1.61	1.54
3	E	602	OXL	O1-C1	3.96	1.32	1.22
3	B	602	OXL	O2-C2	3.93	1.32	1.22
3	A	602	OXL	O2-C2	3.78	1.31	1.22
3	D	602	OXL	O2-C2	3.68	1.31	1.22
3	F	602	OXL	C2-C1	3.46	1.60	1.54
3	C	602	OXL	O1-C1	3.44	1.31	1.22
3	F	602	OXL	O3-C1	-3.37	1.21	1.30
3	F	602	OXL	O1-C1	3.33	1.30	1.22
3	G	603	OXL	O1-C1	3.29	1.30	1.22
3	G	603	OXL	O3-C1	-3.09	1.22	1.30
3	D	602	OXL	O4-C2	-3.08	1.22	1.30
3	H	602	OXL	O2-C2	3.07	1.30	1.22
3	H	602	OXL	C2-C1	3.04	1.59	1.54
3	H	602	OXL	O4-C2	-3.01	1.22	1.30
3	B	602	OXL	O4-C2	-2.80	1.22	1.30
3	C	602	OXL	O3-C1	-2.79	1.23	1.30
3	E	602	OXL	O3-C1	-2.69	1.23	1.30
3	A	602	OXL	O4-C2	-2.48	1.23	1.30
2	B	601	FBP	P2-O5P	-2.37	1.46	1.54
3	G	603	OXL	C2-C1	2.36	1.58	1.54
3	E	602	OXL	C2-C1	2.14	1.58	1.54
3	F	602	OXL	O4-C2	-2.14	1.24	1.30
2	H	601	FBP	P1-O1	-2.12	1.53	1.60

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	602	OXL	O4-C2-C1	4.06	120.71	112.83
3	F	602	OXL	O4-C2-C1	3.93	120.46	112.83
3	A	602	OXL	O4-C2-C1	3.69	120.00	112.83
3	E	602	OXL	O3-C1-C2	3.64	119.89	112.83
3	C	602	OXL	O3-C1-C2	3.52	119.65	112.83
3	G	603	OXL	O3-C1-C2	3.47	119.55	112.83
3	F	602	OXL	O3-C1-C2	3.39	119.41	112.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	OXL	O4-C2-C1	3.26	119.15	112.83
3	E	602	OXL	O4-C2-C1	3.12	118.89	112.83
2	D	601	FBP	O5P-P2-O6	2.89	114.20	106.67
3	B	602	OXL	O4-C2-C1	2.71	118.09	112.83
3	D	602	OXL	O3-C1-C2	2.70	118.06	112.83
2	E	601	FBP	O3P-P1-O2P	2.68	117.84	107.80
2	B	601	FBP	O3P-P1-O2P	2.60	117.55	107.80
3	A	602	OXL	O3-C1-C2	2.59	117.85	112.83
2	C	601	FBP	O6-P2-O4P	2.48	113.13	106.44
3	G	603	OXL	O4-C2-C1	2.34	117.37	112.83
2	H	601	FBP	O5P-P2-O6	2.33	112.75	106.67
3	H	602	OXL	O3-C1-C2	2.33	117.34	112.83
3	B	602	OXL	O3-C1-C2	2.03	116.77	112.83

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	B	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6
2	D	601	FBP	C4-C5-C6-O6
2	E	601	FBP	C4-C5-C6-O6
2	F	601	FBP	C4-C5-C6-O6
2	H	601	FBP	C4-C5-C6-O6
2	G	602	FBP	C4-C5-C6-O6
2	A	601	FBP	O5-C5-C6-O6
2	B	601	FBP	O5-C5-C6-O6
2	C	601	FBP	O5-C5-C6-O6
2	D	601	FBP	O5-C5-C6-O6
2	E	601	FBP	O5-C5-C6-O6
2	F	601	FBP	O5-C5-C6-O6
2	H	601	FBP	O5-C5-C6-O6
2	G	602	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	603	OXL	O3-C1-C2-O4
3	H	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

Continued on next page...

Continued from previous page...

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

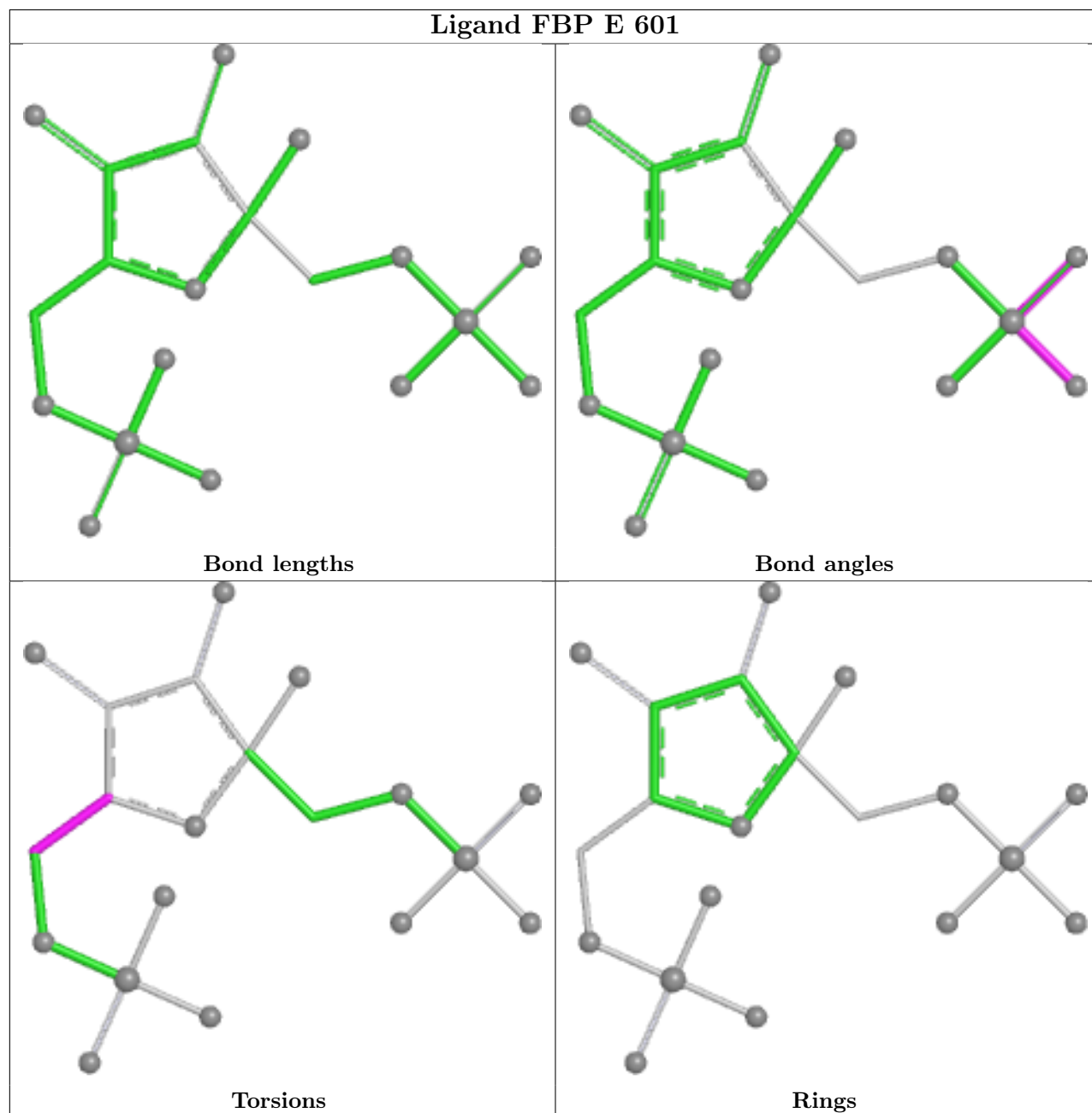
There are no ring outliers.

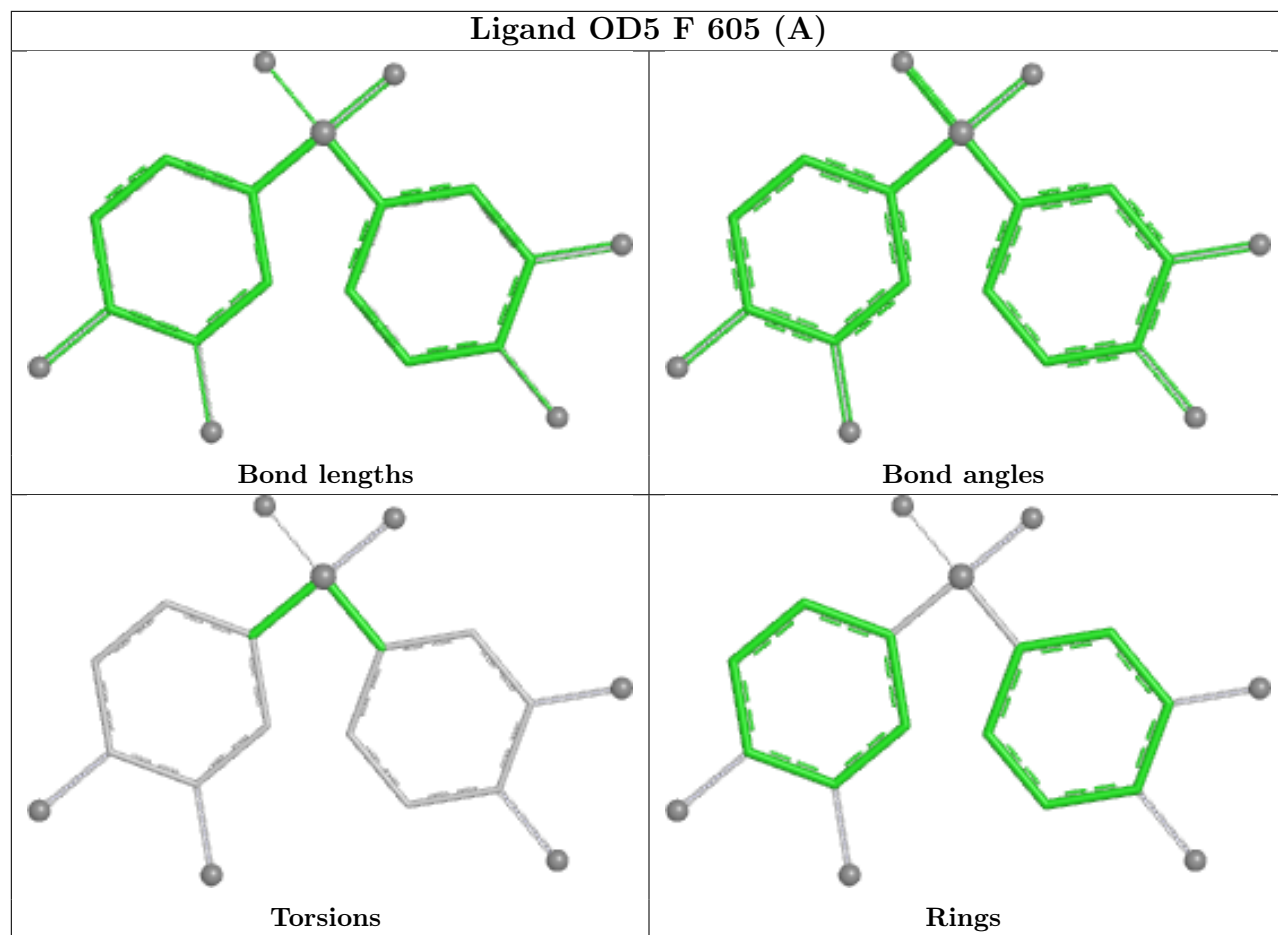
7 monomers are involved in 9 short contacts:

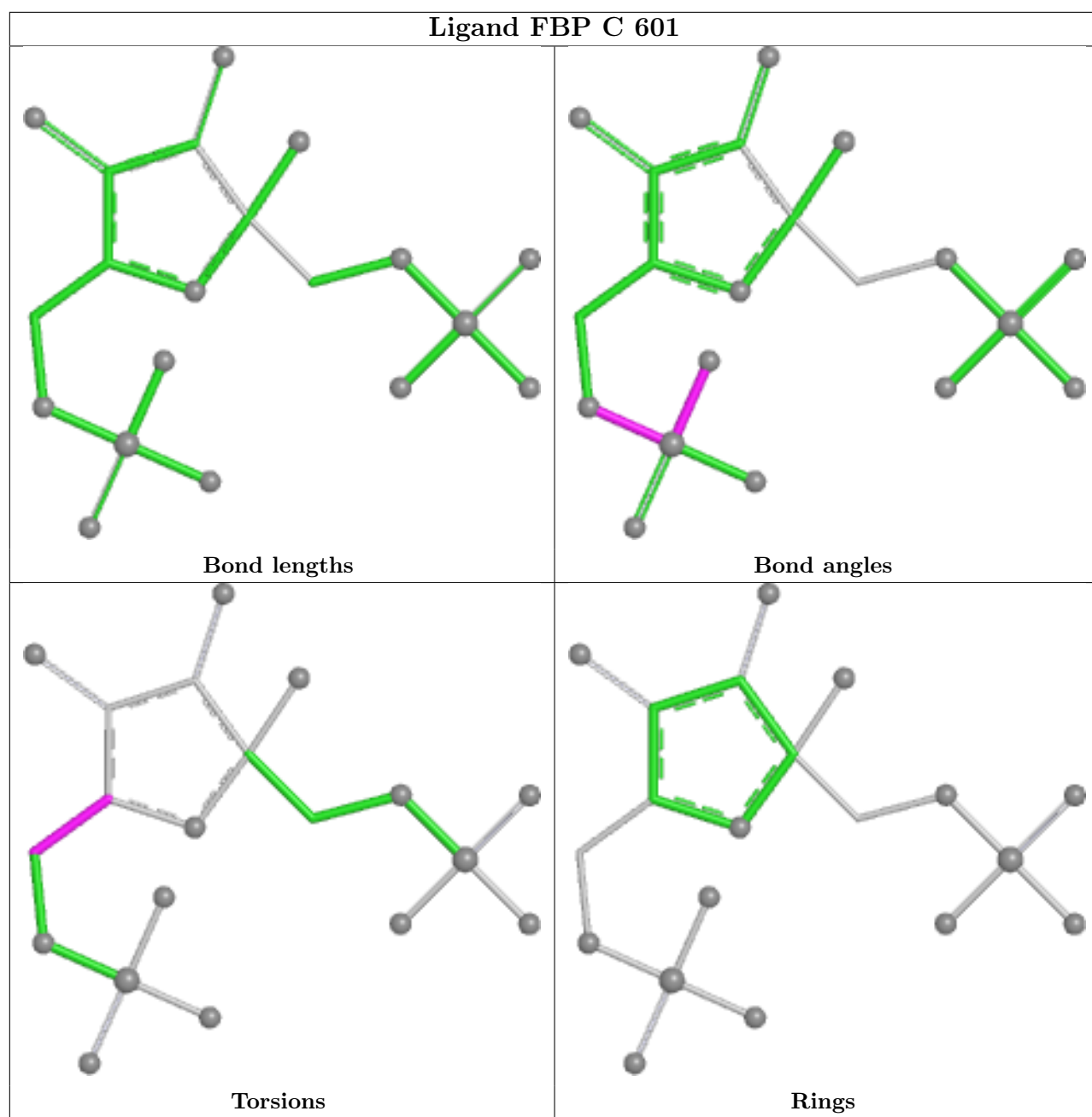
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	605[A]	OD5	1	0
6	D	605[B]	OD5	1	0
6	D	605[A]	OD5	2	0
6	G	601[B]	OD5	1	0
6	G	601[A]	OD5	1	0
6	A	605[B]	OD5	2	0
6	A	605[A]	OD5	1	0

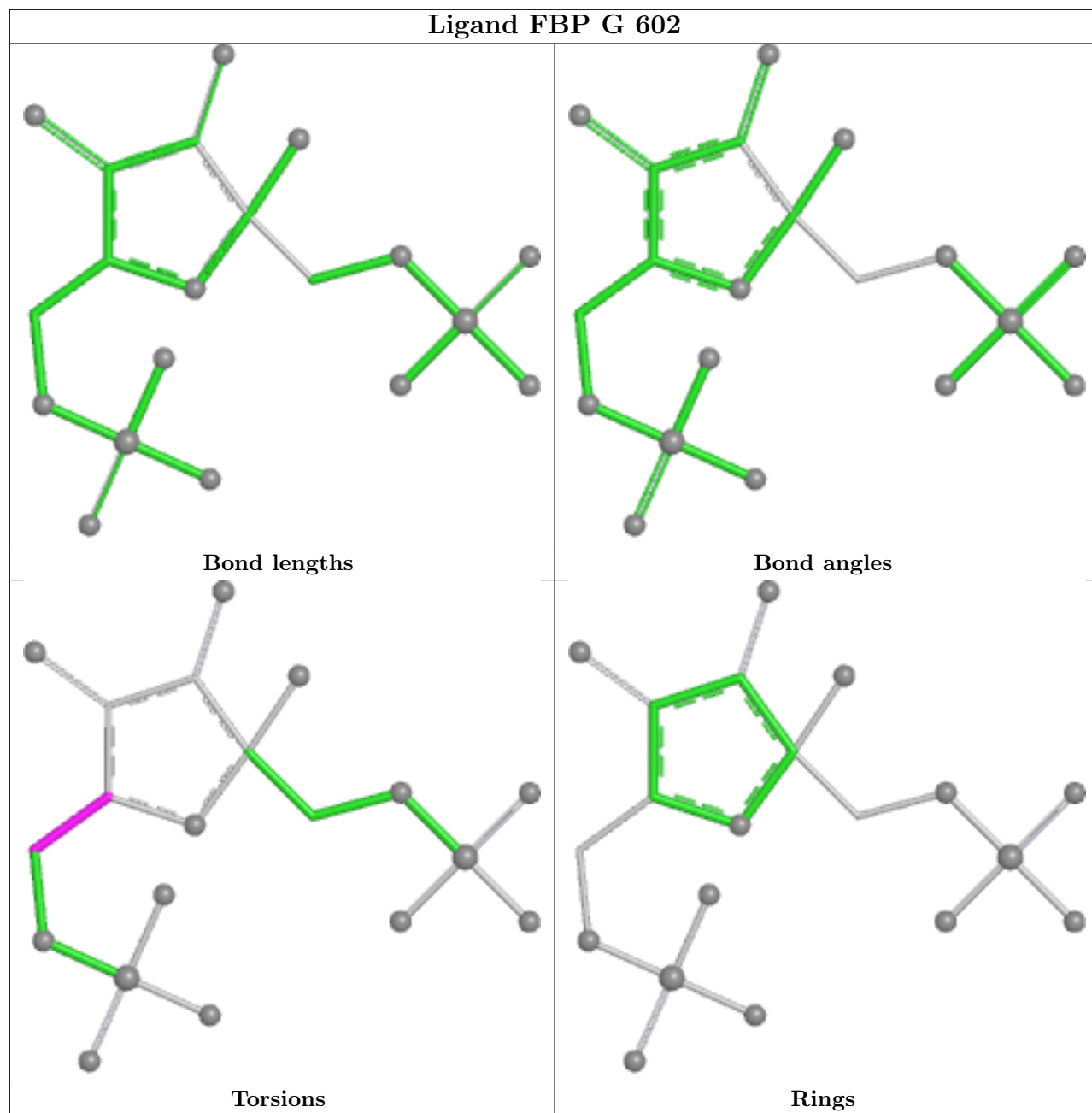
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

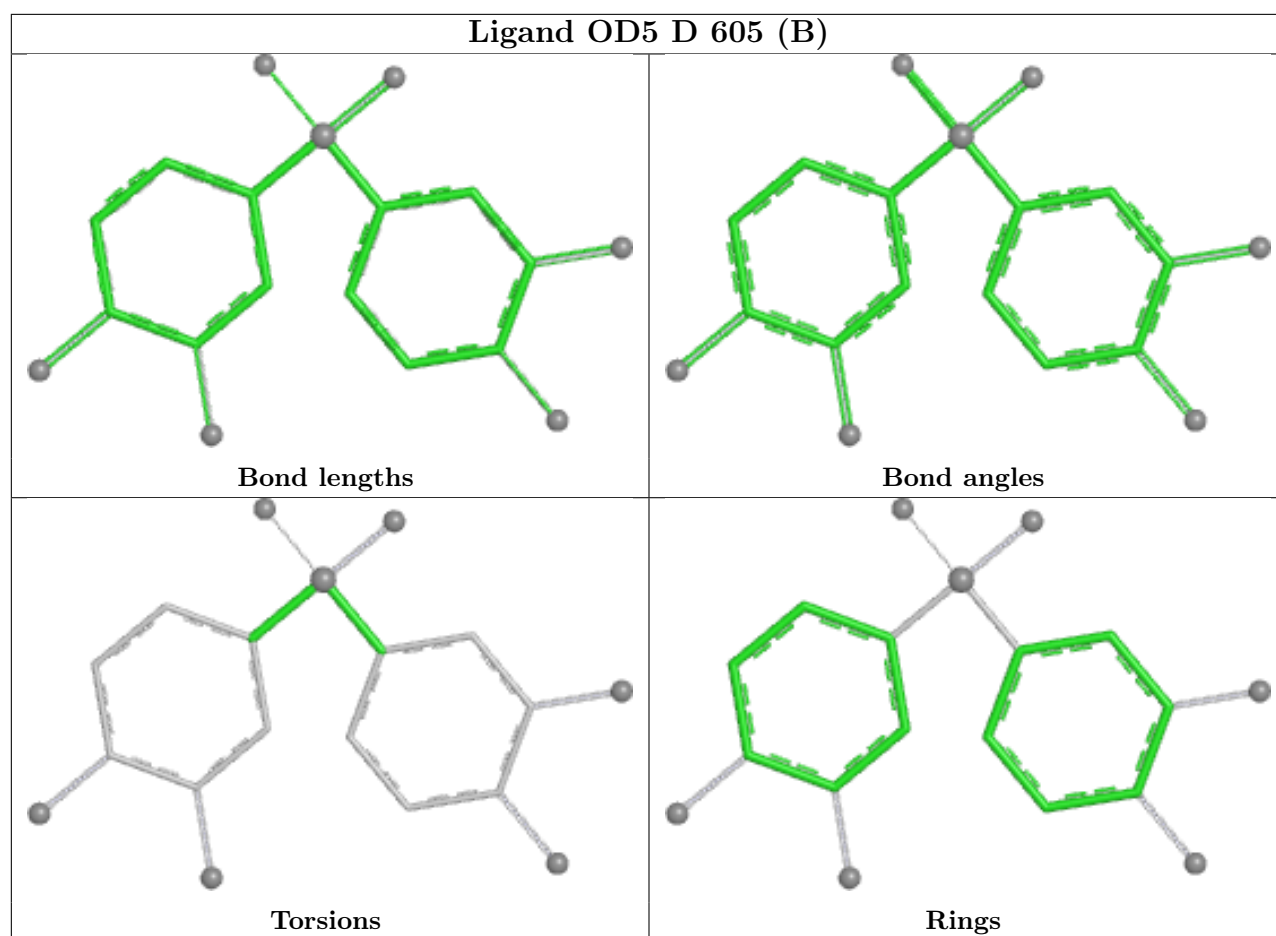
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

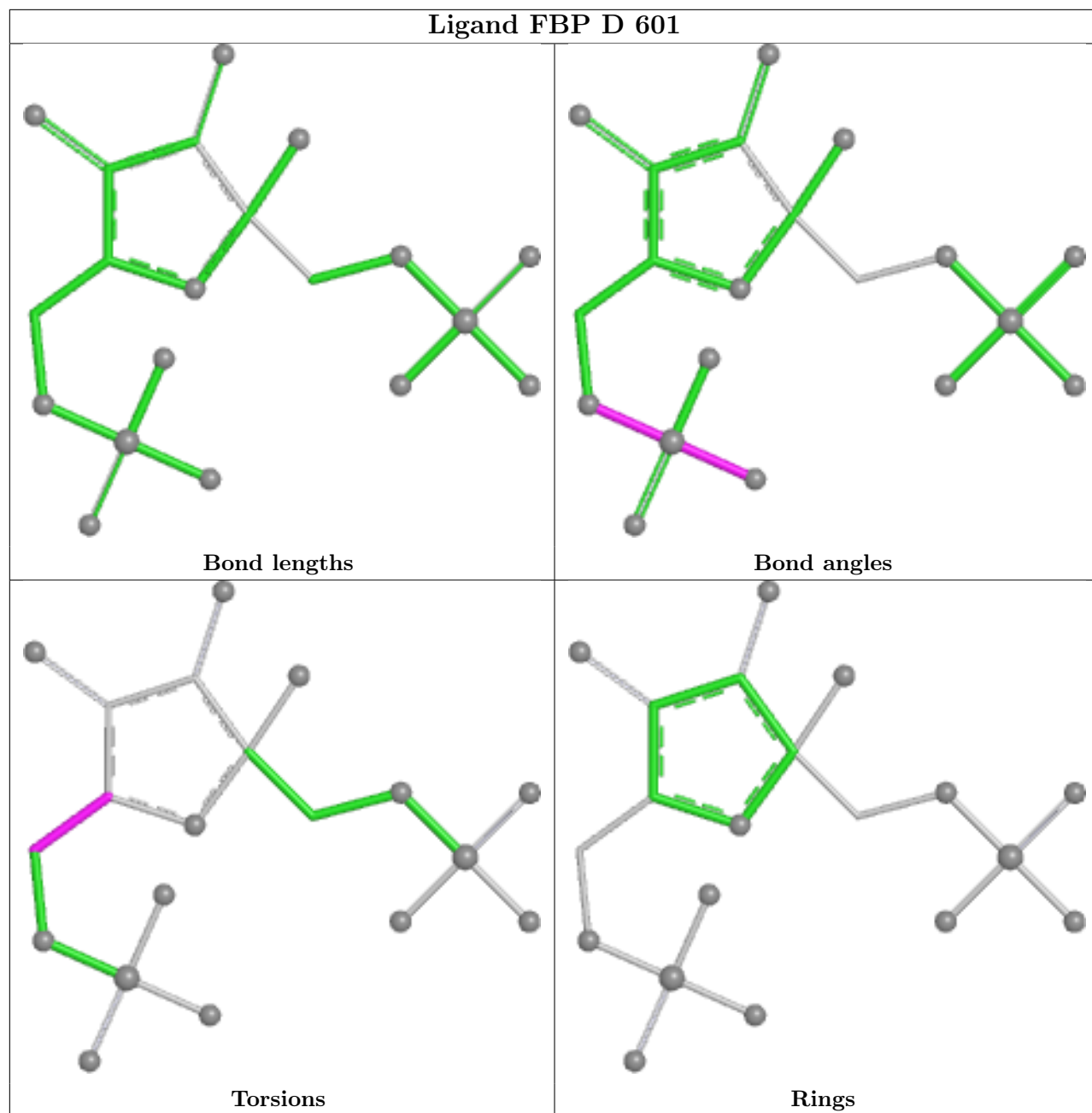




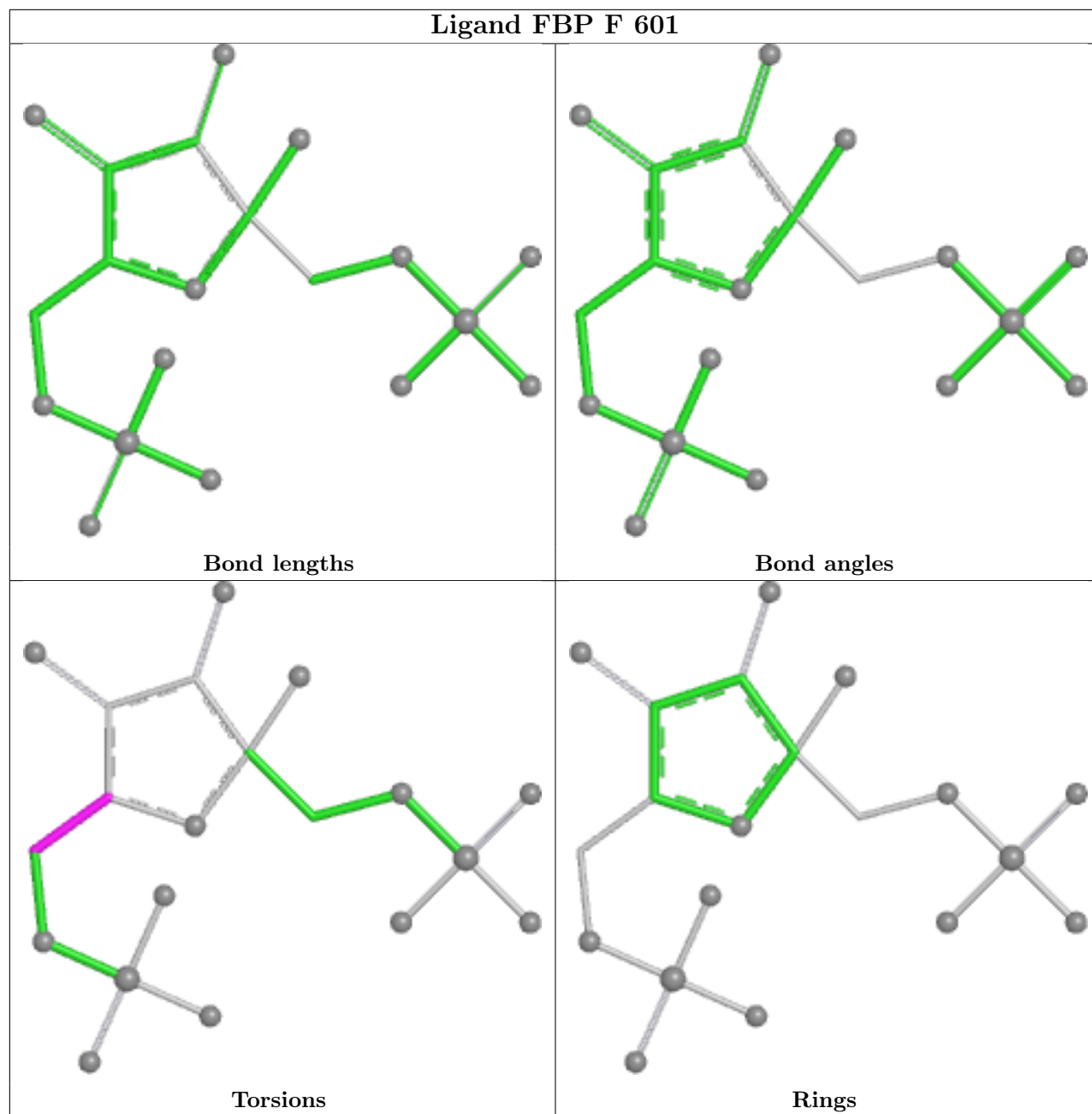


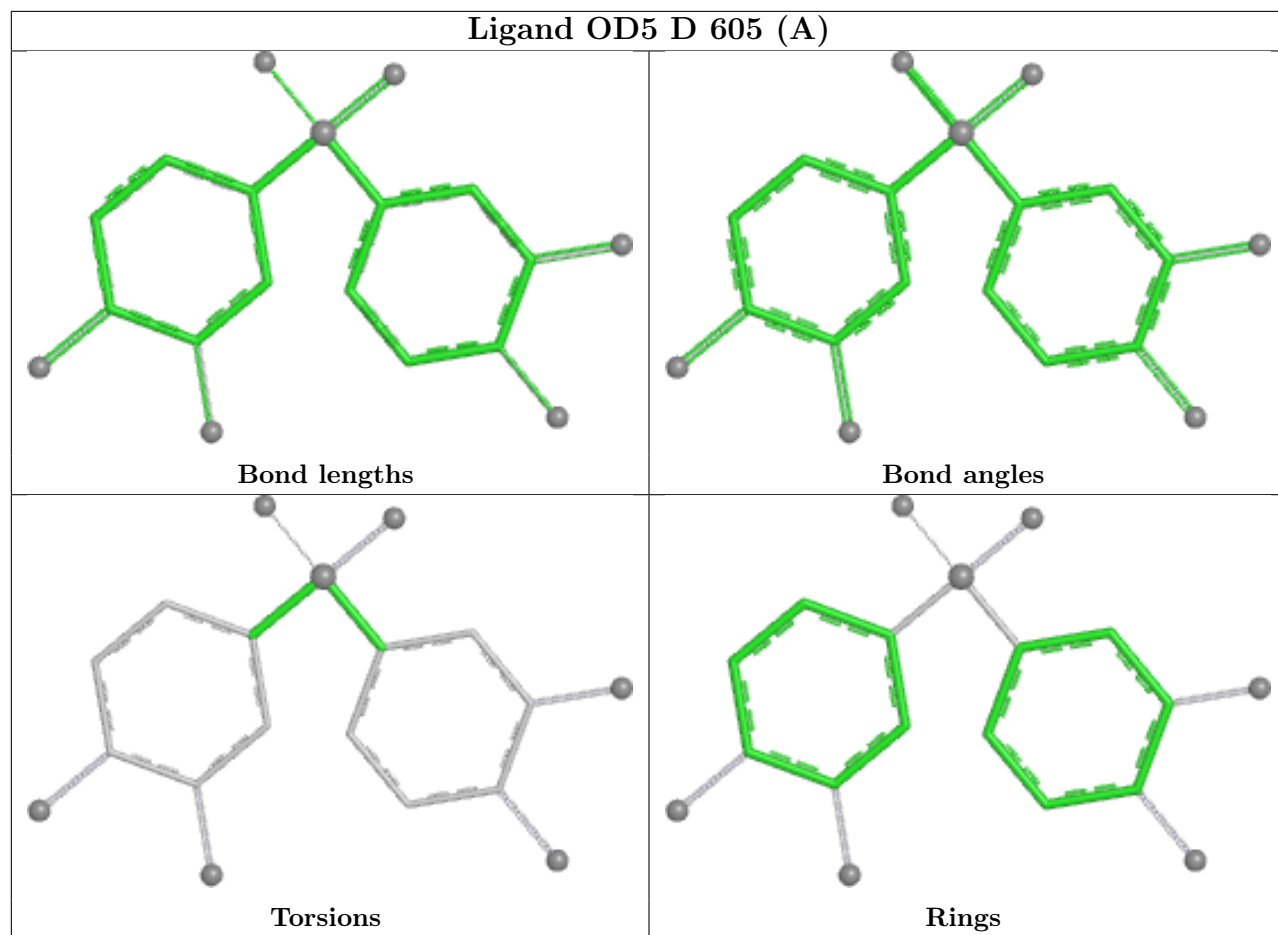


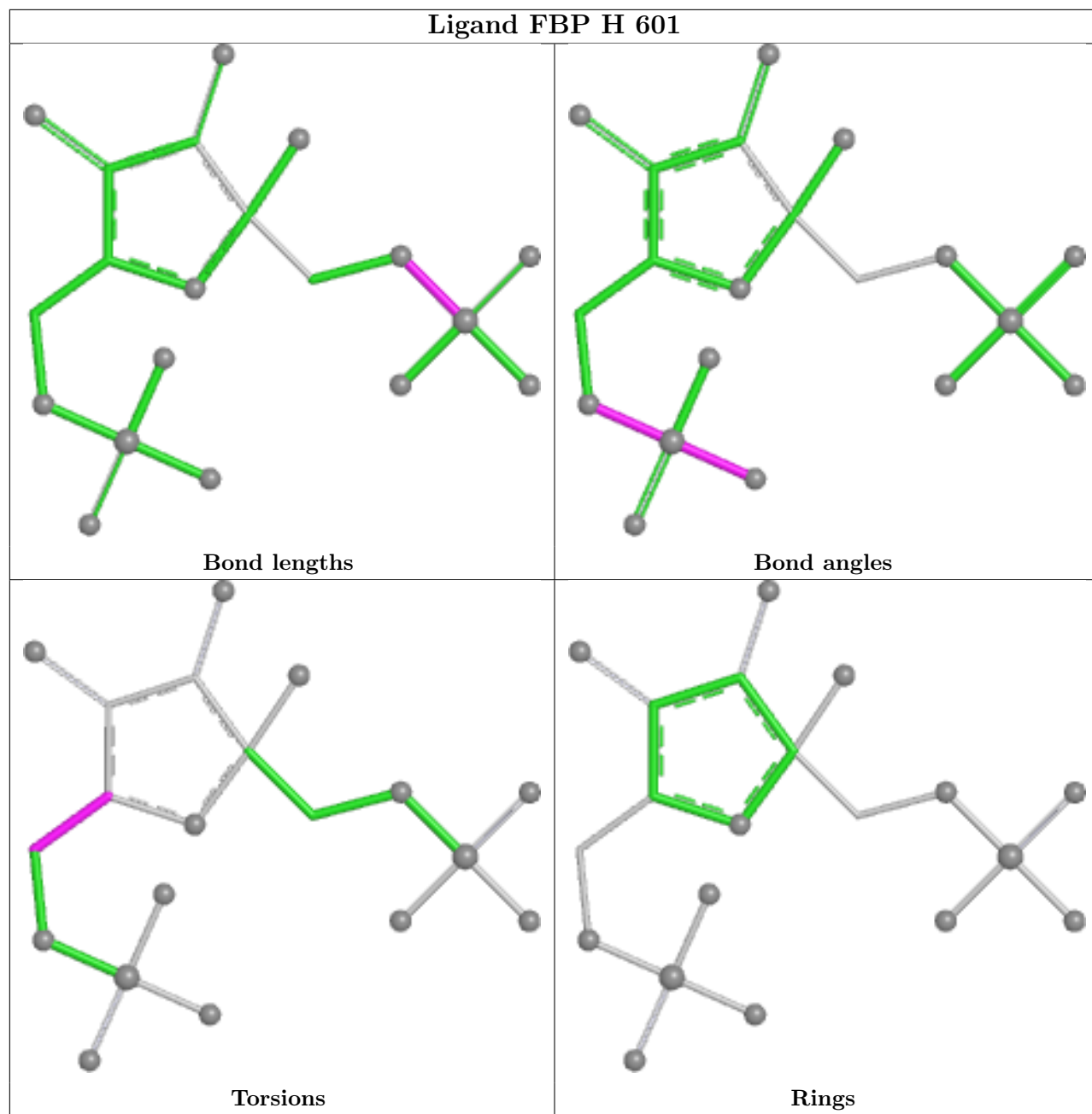




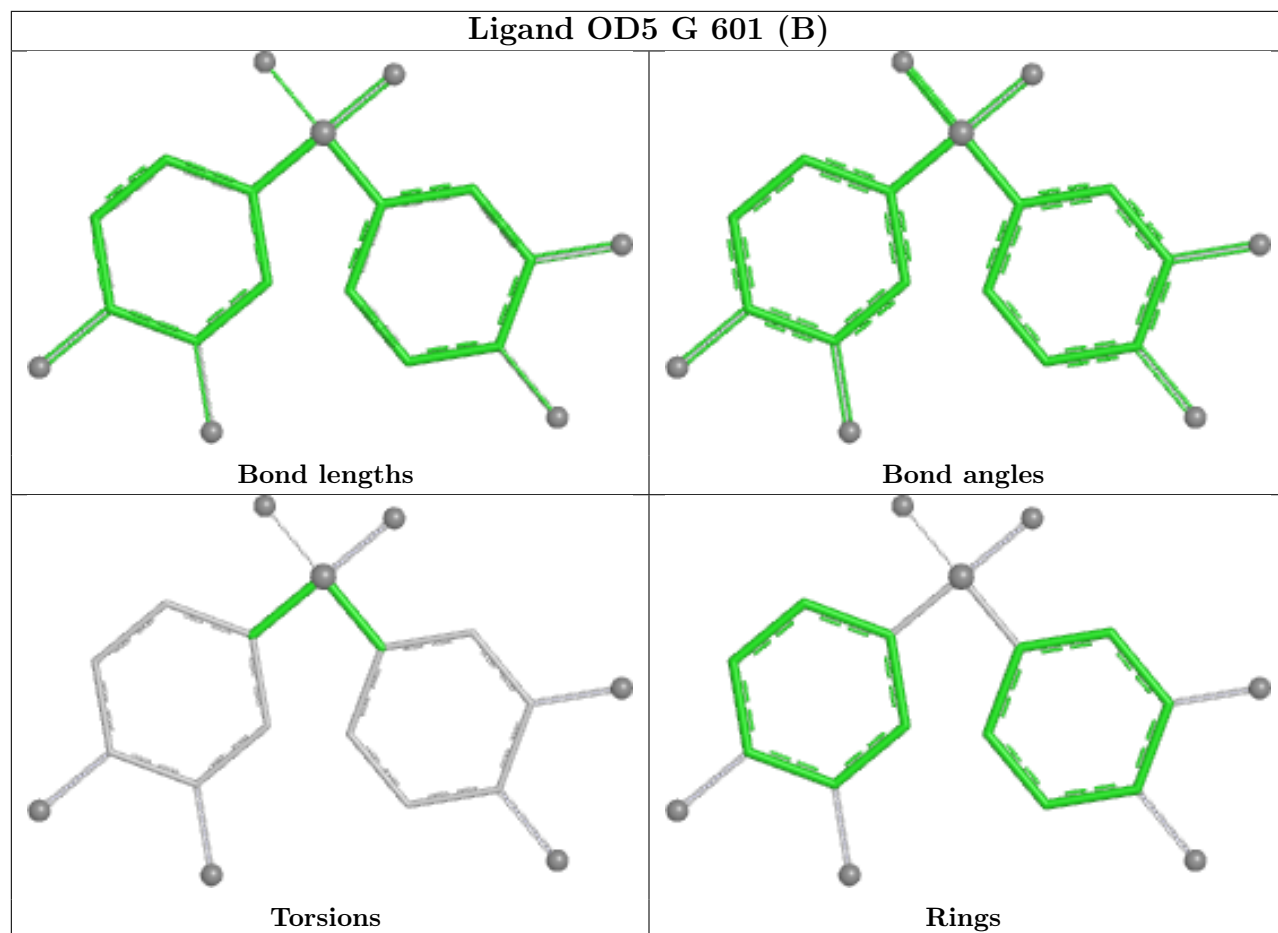
Ligand FBP F 601

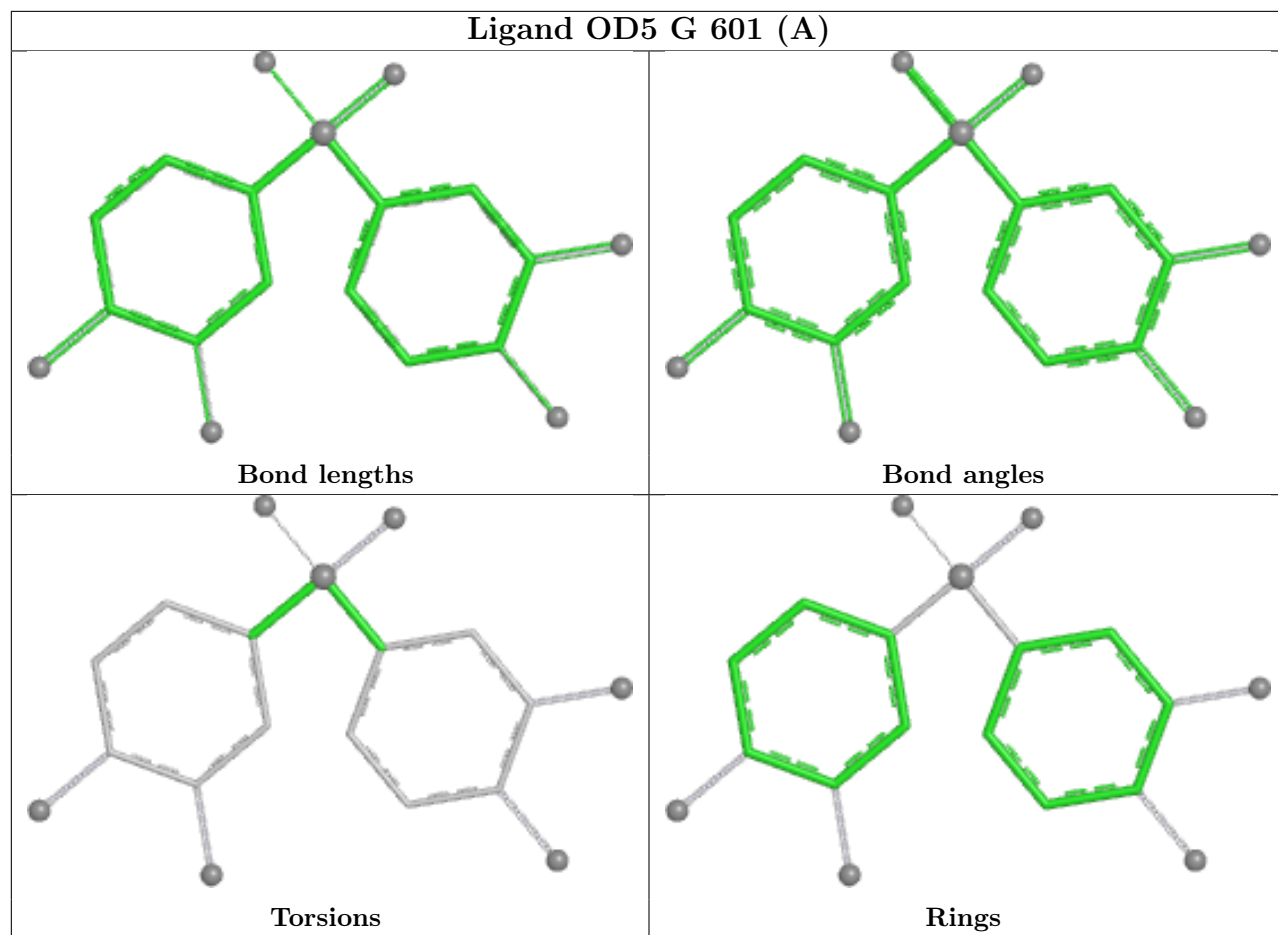




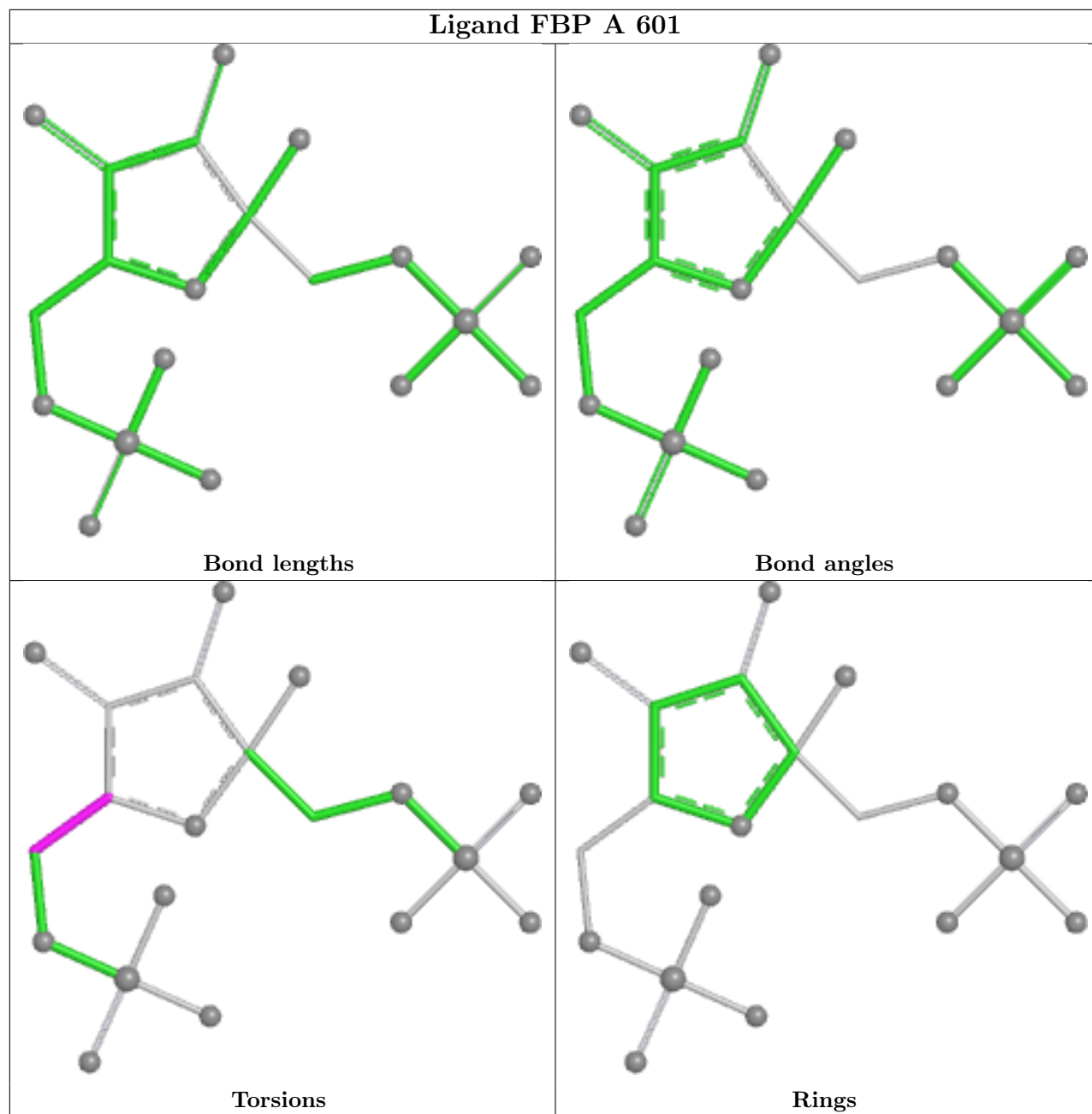


Ligand OD5 G 601 (B)

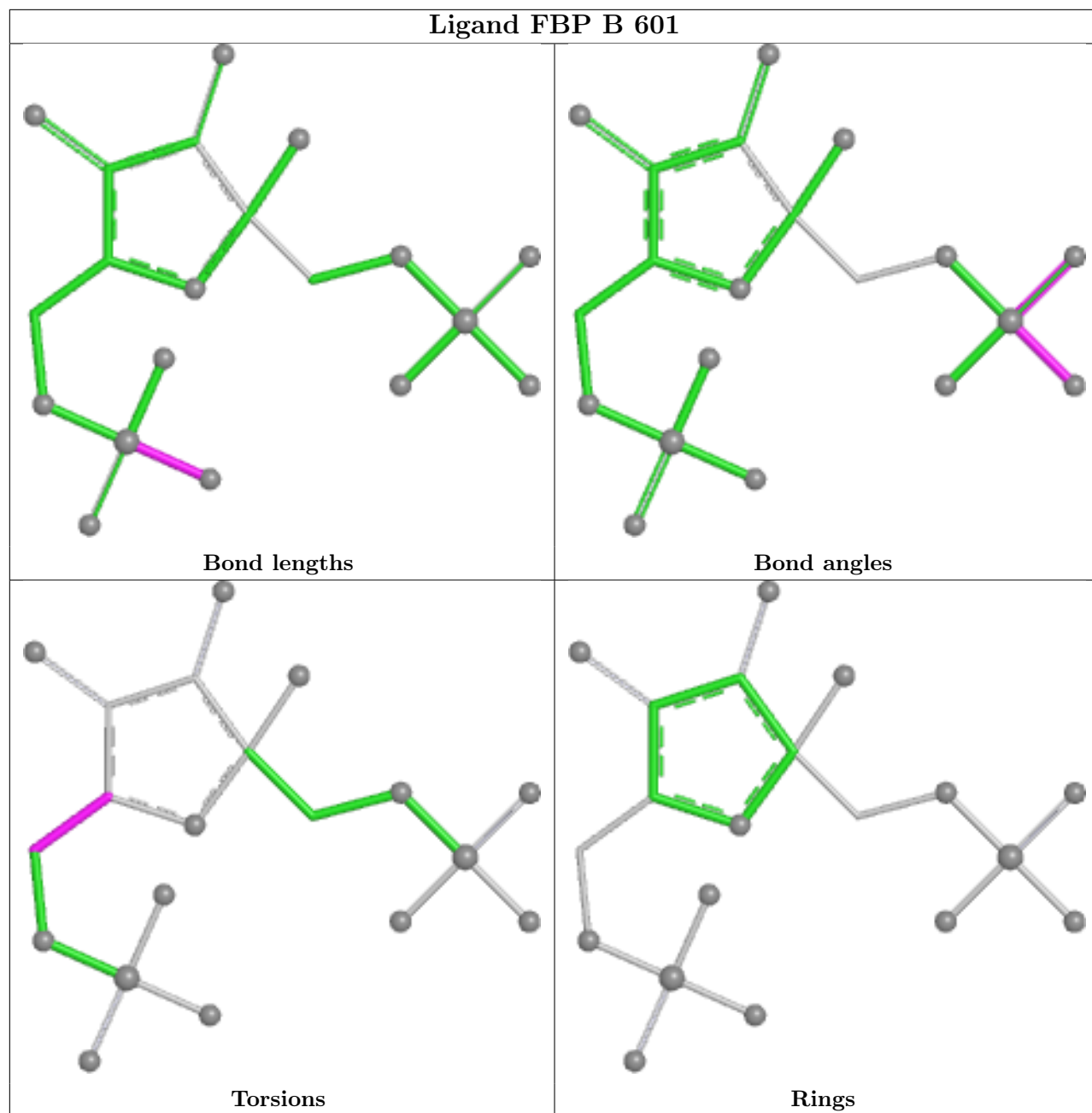


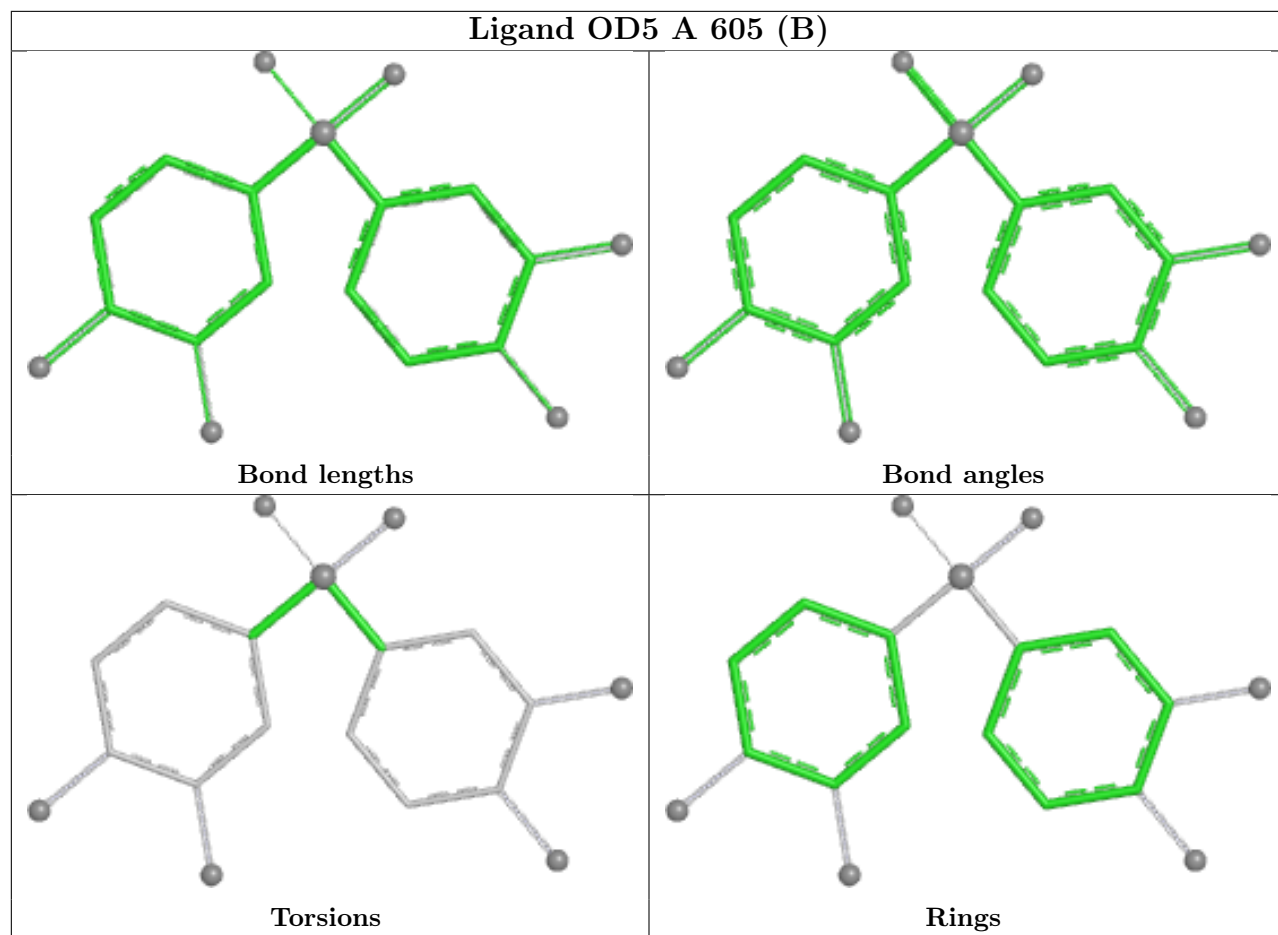


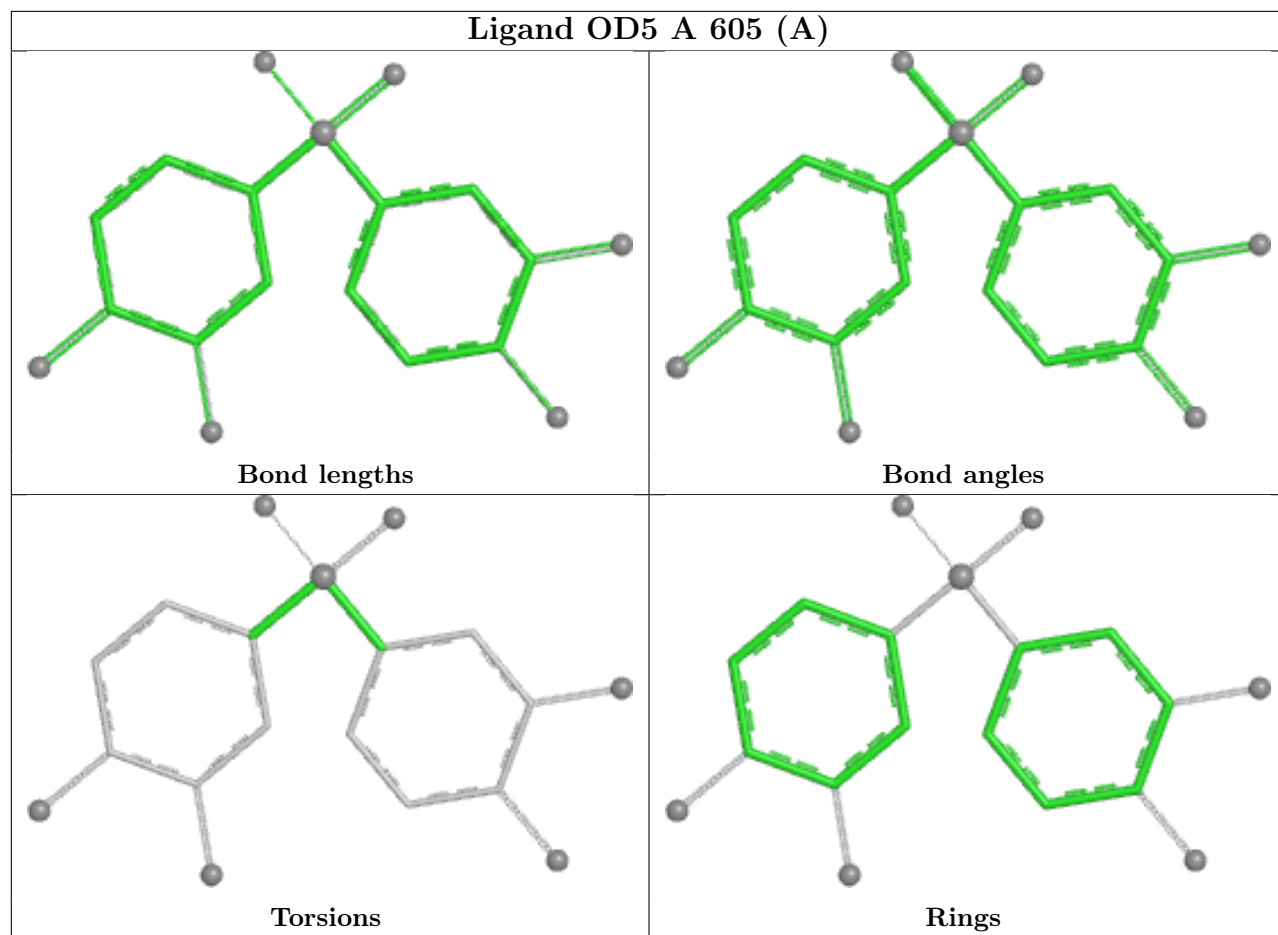
Ligand FBP A 601

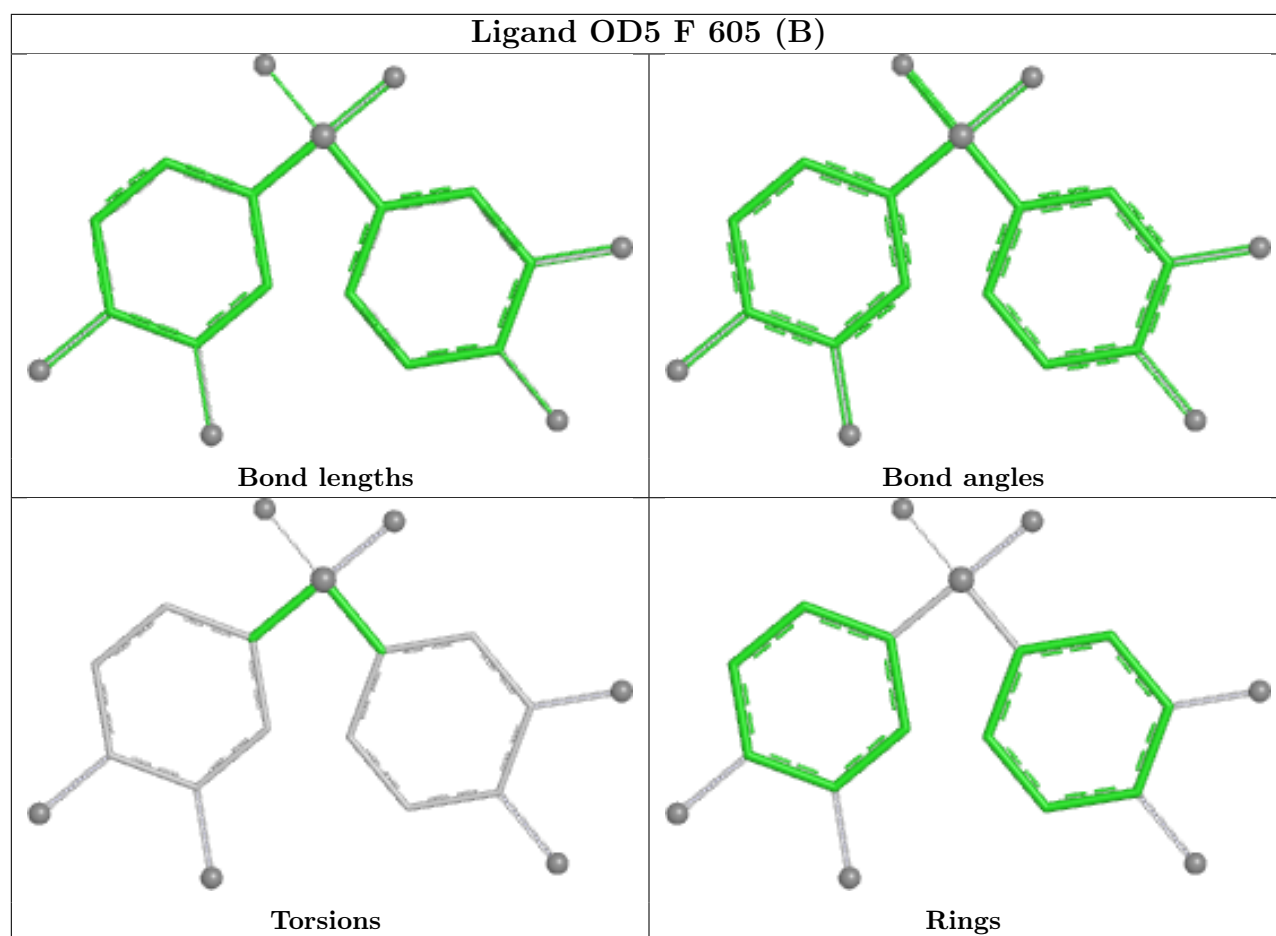


Ligand FBP B 601









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%)	1.19	71 (16%) 4 4	28, 54, 83, 97	6 (1%)
1	B	436/447 (97%)	1.36	133 (30%) 1 1	27, 53, 88, 100	4 (0%)
1	C	425/447 (95%)	0.44	31 (7%) 21 19	23, 40, 63, 99	4 (0%)
1	D	425/447 (95%)	0.01	10 (2%) 59 59	16, 33, 55, 84	6 (1%)
1	E	419/447 (93%)	0.97	62 (14%) 5 5	23, 51, 81, 94	5 (1%)
1	F	432/447 (96%)	0.61	42 (9%) 13 12	25, 41, 69, 84	7 (1%)
1	G	421/447 (94%)	0.23	16 (3%) 44 43	21, 37, 53, 72	7 (1%)
1	H	425/447 (95%)	-0.13	15 (3%) 47 46	15, 30, 53, 80	4 (0%)
All	All	3405/3576 (95%)	0.59	380 (11%) 10 9	15, 43, 77, 100	43 (1%)

All (380) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	115	LEU	7.9
1	F	116	SER	6.8
1	B	115	LEU	6.7
1	B	511	LEU	6.4
1	H	21	GLY	5.7
1	G	271	GLY	5.5
1	E	23	ALA	5.3
1	A	543	SER	5.2
1	E	114	PRO	5.1
1	G	25	PHE	5.1
1	A	132	GLY	5.1
1	B	116	SER	5.0
1	F	511	LEU	5.0
1	B	378	ALA	5.0
1	C	271	GLY	4.8
1	A	232	GLY	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	238	VAL	4.6
1	B	348	THR	4.6
1	B	114	PRO	4.6
1	D	21	GLY	4.5
1	C	231	PRO	4.5
1	C	20	LEU	4.4
1	B	379	LYS	4.4
1	D	25	PHE	4.3
1	H	25	PHE	4.3
1	B	267[A]	ARG	4.3
1	A	115	LEU	4.3
1	C	22	THR	4.3
1	A	25	PHE	4.2
1	F	117	TYR	4.2
1	B	73	LEU	4.2
1	B	117	TYR	4.1
1	B	241	LEU	4.1
1	C	232	GLY	4.1
1	E	115	LEU	4.0
1	B	382	PHE	4.0
1	B	506	ILE	4.0
1	A	34	MET	4.0
1	B	490	PRO	3.9
1	E	129	PRO	3.9
1	A	114	PRO	3.9
1	F	112	GLY	3.9
1	B	66	ALA	3.9
1	C	111	ALA	3.9
1	B	489	PRO	3.9
1	B	110	PHE	3.8
1	H	411	ARG	3.8
1	F	114	PRO	3.8
1	B	118	ARG	3.8
1	E	249	VAL	3.7
1	A	241	LEU	3.7
1	B	91	GLY	3.7
1	B	383	PRO	3.7
1	B	502	VAL	3.7
1	C	66	ALA	3.7
1	B	484	LEU	3.6
1	F	231	PRO	3.6
1	F	267[A]	ARG	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	67	SER	3.6
1	B	13	VAL	3.6
1	A	514	PHE	3.6
1	B	504	PHE	3.6
1	B	414	ALA	3.6
1	B	106	ALA	3.5
1	E	232	GLY	3.5
1	A	63	ILE	3.5
1	D	130	GLY	3.5
1	C	25	PHE	3.5
1	C	132	GLY	3.5
1	A	496	ASP	3.5
1	A	23	ALA	3.4
1	B	102	ASN	3.4
1	E	490	PRO	3.4
1	D	24	PHE	3.4
1	D	22	THR	3.4
1	B	384	VAL	3.4
1	B	237	ASP	3.4
1	E	233	LEU	3.4
1	F	487	ARG	3.3
1	A	70	VAL	3.3
1	B	416	LEU	3.3
1	F	489	PRO	3.3
1	B	238	VAL	3.3
1	B	495	ALA	3.3
1	B	485	LEU	3.3
1	F	516	ARG	3.2
1	B	270	LEU	3.2
1	B	120	VAL	3.2
1	E	238	VAL	3.2
1	B	493	ILE	3.2
1	A	118	ARG	3.1
1	B	103	VAL	3.1
1	B	380	GLY	3.1
1	G	132	GLY	3.1
1	B	88	PHE	3.1
1	E	25	PHE	3.1
1	G	23	ALA	3.1
1	G	231	PRO	3.0
1	B	123	ALA	3.0
1	B	70	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	249	VAL	3.0
1	B	64	GLY	3.0
1	A	378	ALA	3.0
1	A	249	VAL	3.0
1	F	233	LEU	3.0
1	B	542	ILE	3.0
1	A	233	LEU	3.0
1	B	86	LEU	3.0
1	E	485	LEU	3.0
1	E	511	LEU	3.0
1	B	251	ILE	3.0
1	C	117	TYR	3.0
1	B	33	ALA	2.9
1	E	257	VAL	2.9
1	E	275	HIS	2.9
1	A	489	PRO	2.9
1	A	24	PHE	2.9
1	B	543	SER	2.9
1	A	61	ALA	2.9
1	A	471	ALA	2.9
1	B	107	VAL	2.9
1	H	22	THR	2.9
1	B	124	LEU	2.9
1	B	233	LEU	2.9
1	E	70	VAL	2.9
1	F	129	PRO	2.9
1	E	110	PHE	2.9
1	G	24	PHE	2.9
1	B	128	GLY	2.9
1	A	270	LEU	2.8
1	E	351	ARG	2.8
1	B	517	VAL	2.8
1	F	347	ILE	2.8
1	B	95	TYR	2.8
1	C	21	GLY	2.8
1	E	112	GLY	2.8
1	A	73	LEU	2.8
1	F	238	VAL	2.8
1	G	52	VAL	2.8
1	F	490	PRO	2.8
1	B	92	SER	2.8
1	A	88	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	507	GLU	2.8
1	E	116	SER	2.8
1	B	90	HIS	2.8
1	F	488	GLU	2.8
1	A	540	LEU	2.8
1	B	498	VAL	2.8
1	A	100	ILE	2.8
1	B	494	TRP	2.8
1	D	275[A]	HIS	2.7
1	B	130	GLY	2.7
1	E	244	GLY	2.7
1	A	493	ILE	2.7
1	E	256	PHE	2.7
1	E	269	ALA	2.7
1	A	62	THR	2.7
1	F	416	LEU	2.7
1	B	245	VAL	2.7
1	B	347	ILE	2.7
1	B	512	ARG	2.7
1	B	377	THR	2.7
1	B	108	GLU	2.7
1	E	277	ILE	2.7
1	A	495	ALA	2.6
1	F	270	LEU	2.6
1	H	231	PRO	2.6
1	B	100	ILE	2.6
1	B	68	ARG	2.6
1	H	267[A]	ARG	2.6
1	A	86	LEU	2.6
1	B	119	PRO	2.6
1	H	24	PHE	2.6
1	B	72	ARG	2.6
1	E	493	ILE	2.6
1	A	111	ALA	2.6
1	C	23	ALA	2.6
1	A	113	SER	2.6
1	B	113	SER	2.6
1	A	488[A]	GLU	2.6
1	B	271	GLY	2.6
1	G	232	GLY	2.6
1	C	90	HIS	2.6
1	A	377	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	272	PRO	2.6
1	F	459	ARG	2.6
1	A	494	TRP	2.6
1	B	374	SER	2.6
1	B	256	PHE	2.5
1	E	266	VAL	2.5
1	A	84	ALA	2.5
1	A	305	ALA	2.5
1	E	89	SER	2.5
1	C	34	MET	2.5
1	A	107	VAL	2.5
1	H	275[A]	HIS	2.5
1	E	540	LEU	2.5
1	C	110	PHE	2.5
1	F	351	ARG	2.5
1	A	269	ALA	2.5
1	C	114	PRO	2.5
1	D	23	ALA	2.5
1	E	495	ALA	2.5
1	F	33	ALA	2.5
1	B	540[A]	LEU	2.5
1	H	34	MET	2.5
1	A	542	ILE	2.5
1	C	77	ILE	2.5
1	E	63	ILE	2.5
1	B	344	GLU	2.4
1	B	65	PRO	2.4
1	A	121	ALA	2.4
1	E	492	ALA	2.4
1	A	511	LEU	2.4
1	H	516	ARG	2.4
1	E	24	PHE	2.4
1	F	514	PHE	2.4
1	B	266	VAL	2.4
1	A	95	TYR	2.4
1	G	34	MET	2.4
1	B	97	ALA	2.4
1	B	351	ARG	2.4
1	H	412	ARG	2.4
1	B	12	ASP	2.4
1	B	541	SER	2.4
1	E	541[A]	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	488	GLU	2.4
1	E	514	PHE	2.4
1	E	245	VAL	2.4
1	F	113	SER	2.4
1	B	62	THR	2.4
1	E	126	THR	2.4
1	E	515	LEU	2.3
1	F	241	LEU	2.3
1	B	10	ARG	2.3
1	C	412	ARG	2.3
1	F	242	ARG	2.3
1	F	512	ARG	2.3
1	B	52	VAL	2.3
1	B	508	SER	2.3
1	B	61	ALA	2.3
1	B	84	ALA	2.3
1	B	375	GLY	2.3
1	B	242	ARG	2.3
1	E	510	LYS	2.3
1	B	109	SER	2.3
1	E	99	SER	2.3
1	A	475	VAL	2.3
1	D	231	PRO	2.3
1	E	97	ALA	2.3
1	E	111	ALA	2.3
1	G	33	ALA	2.3
1	A	512	ARG	2.3
1	B	308	ASP	2.3
1	B	487	ARG	2.3
1	C	80	GLY	2.3
1	E	447	GLY	2.3
1	A	116	SER	2.3
1	F	90	HIS	2.3
1	A	482	PHE	2.3
1	B	243	PHE	2.3
1	B	63	ILE	2.3
1	C	311	ILE	2.3
1	E	122	ILE	2.3
1	A	498	VAL	2.3
1	E	120	VAL	2.3
1	B	129	PRO	2.3
1	B	101	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	527	TRP	2.3
1	B	93	HIS	2.2
1	C	116	SER	2.2
1	E	109	SER	2.2
1	E	100	ILE	2.2
1	G	63	ILE	2.2
1	A	357	THR	2.2
1	B	272	PRO	2.2
1	B	483	PRO	2.2
1	G	272	PRO	2.2
1	B	132	GLY	2.2
1	B	509	GLY	2.2
1	E	33	ALA	2.2
1	E	34	MET	2.2
1	B	515	LEU	2.2
1	F	540[A]	LEU	2.2
1	A	90	HIS	2.2
1	H	26	GLN	2.2
1	B	411	ARG	2.2
1	E	504	PHE	2.2
1	F	411	ARG	2.2
1	B	381	ASN	2.2
1	E	502	VAL	2.2
1	H	130	GLY	2.2
1	H	232	GLY	2.2
1	B	269	ALA	2.2
1	E	270	LEU	2.2
1	A	99	SER	2.2
1	E	487	ARG	2.2
1	A	279	ILE	2.2
1	A	52	VAL	2.2
1	A	266	VAL	2.2
1	B	263	VAL	2.2
1	C	103	VAL	2.2
1	A	244	GLY	2.2
1	B	71	GLU	2.2
1	B	75	GLU	2.2
1	B	276	GLY	2.2
1	B	385	GLU	2.2
1	E	123	ALA	2.2
1	F	269	ALA	2.2
1	B	275	HIS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	515	LEU	2.2
1	H	416	LEU	2.2
1	A	92	SER	2.2
1	A	490	PRO	2.1
1	A	110	PHE	2.1
1	A	384	VAL	2.1
1	F	498	VAL	2.1
1	B	80	GLY	2.1
1	B	505	GLY	2.1
1	E	128	GLY	2.1
1	B	268	ALA	2.1
1	F	11	ALA	2.1
1	B	104	ARG	2.1
1	C	416	LEU	2.1
1	E	73	LEU	2.1
1	E	118	ARG	2.1
1	E	113	SER	2.1
1	B	126	THR	2.1
1	B	514	PHE	2.1
1	F	243	PHE	2.1
1	A	245	VAL	2.1
1	B	521	VAL	2.1
1	E	505	GLY	2.1
1	E	242	ARG	2.1
1	F	118	ARG	2.1
1	B	111	ALA	2.1
1	B	438	ALA	2.1
1	G	54	ALA	2.1
1	B	343	LEU	2.1
1	B	510	LYS	2.1
1	C	115	LEU	2.1
1	G	115	LEU	2.1
1	B	105	GLU	2.1
1	D	235	GLU	2.1
1	A	274	GLY	2.1
1	C	24	PHE	2.1
1	E	52	VAL	2.1
1	B	349	LYS	2.1
1	B	99	SER	2.1
1	B	131	SER	2.1
1	F	408	GLU	2.1
1	F	499	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	68	ARG	2.1
1	A	117	TYR	2.1
1	F	412	ARG	2.1
1	C	380	GLY	2.1
1	B	77	ILE	2.1
1	C	63	ILE	2.1
1	E	88	PHE	2.1
1	G	514	PHE	2.1
1	B	121	ALA	2.1
1	C	109	SER	2.1
1	C	113	SER	2.1
1	B	520	LEU	2.0
1	F	12	ASP	2.0
1	F	240	ASP	2.0
1	A	126	THR	2.0
1	A	91	GLY	2.0
1	B	122	ILE	2.0
1	A	103	VAL	2.0
1	A	120	VAL	2.0
1	B	25	PHE	2.0
1	A	265	ALA	2.0
1	E	26	GLN	2.0
1	E	499	ASP	2.0
1	G	411	ARG	2.0
1	A	275	HIS	2.0
1	C	348	THR	2.0
1	D	232	GLY	2.0
1	F	232	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,

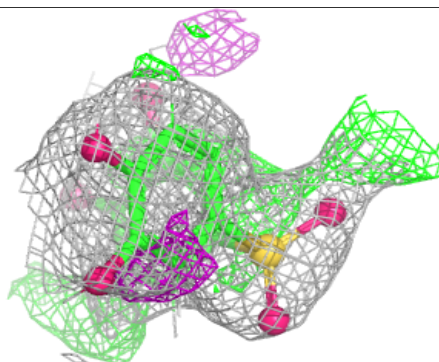
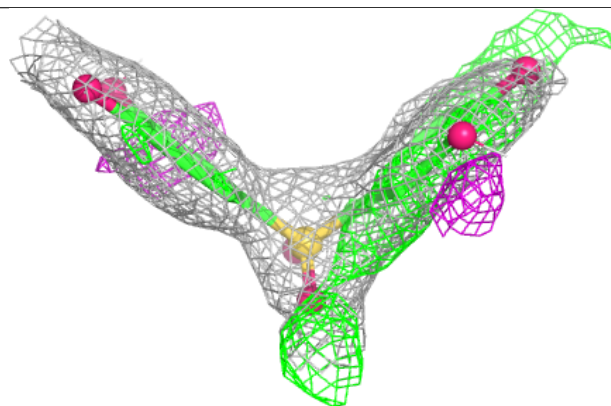
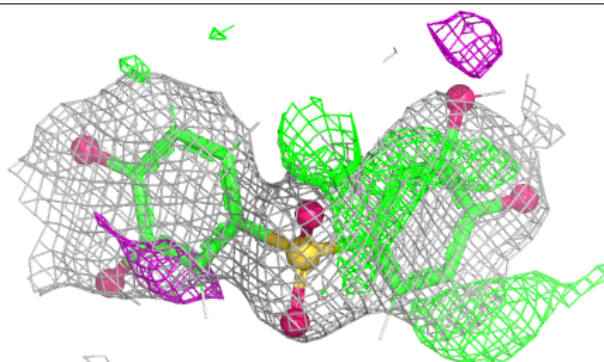
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	OXL	E	602	6/6	0.78	0.17	75,75,76,76	0
3	OXL	F	602	6/6	0.82	0.17	65,65,66,67	0
3	OXL	H	602	6/6	0.82	0.15	50,50,51,52	0
6	OD5	F	605[A]	19/19	0.83	0.23	34,37,40,41	29
6	OD5	F	605[B]	19/19	0.83	0.23	34,35,38,39	29
6	OD5	D	605[A]	19/19	0.84	0.21	30,33,34,35	29
6	OD5	D	605[B]	19/19	0.84	0.21	32,35,37,37	29
3	OXL	D	602	6/6	0.84	0.16	57,58,59,59	0
3	OXL	A	602	6/6	0.84	0.15	85,85,85,86	0
3	OXL	B	602	6/6	0.85	0.16	67,68,69,69	0
4	MG	A	603	1/1	0.85	0.09	84,84,84,84	0
3	OXL	G	603	6/6	0.85	0.13	62,62,63,63	0
6	OD5	A	605[A]	19/19	0.86	0.27	45,46,48,48	29
6	OD5	A	605[B]	19/19	0.86	0.27	38,41,43,44	29
4	MG	B	603	1/1	0.87	0.13	85,85,85,85	0
4	MG	E	603	1/1	0.87	0.08	68,68,68,68	0
3	OXL	C	602	6/6	0.88	0.14	76,76,77,77	0
4	MG	F	603	1/1	0.89	0.08	51,51,51,51	0
6	OD5	G	601[A]	19/19	0.89	0.22	41,42,44,45	29
6	OD5	G	601[B]	19/19	0.89	0.22	38,40,43,43	29
4	MG	D	603	1/1	0.91	0.08	54,54,54,54	0
2	FBP	B	601	20/20	0.92	0.10	48,49,53,53	0
5	K	E	604	1/1	0.94	0.23	83,83,83,83	0
2	FBP	F	601	20/20	0.94	0.08	38,43,48,48	0
2	FBP	A	601	20/20	0.94	0.09	50,51,52,52	0
5	K	A	604	1/1	0.95	0.14	84,84,84,84	0
2	FBP	E	601	20/20	0.95	0.08	46,47,50,50	0
5	K	F	604	1/1	0.95	0.11	71,71,71,71	0
5	K	G	605	1/1	0.95	0.11	54,54,54,54	0
5	K	C	604	1/1	0.96	0.16	56,56,56,56	0
5	K	B	604	1/1	0.96	0.15	73,73,73,73	0
4	MG	C	603	1/1	0.97	0.05	64,64,64,64	0
2	FBP	G	602	20/20	0.97	0.06	27,28,30,31	0
4	MG	H	603	1/1	0.98	0.04	44,44,44,44	0
2	FBP	D	601	20/20	0.98	0.04	25,26,29,30	0
2	FBP	H	601	20/20	0.98	0.05	21,23,25,26	0
2	FBP	C	601	20/20	0.99	0.04	29,30,32,33	0
4	MG	G	604	1/1	0.99	0.03	46,46,46,46	0
5	K	D	604	1/1	0.99	0.08	45,45,45,45	0
5	K	H	604	1/1	0.99	0.06	47,47,47,47	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.

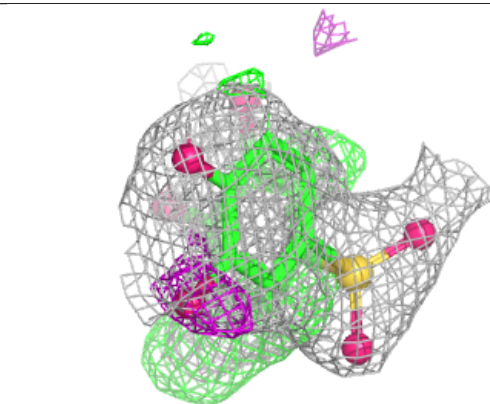
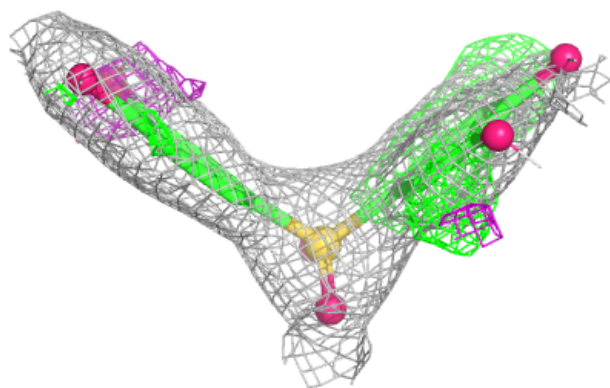
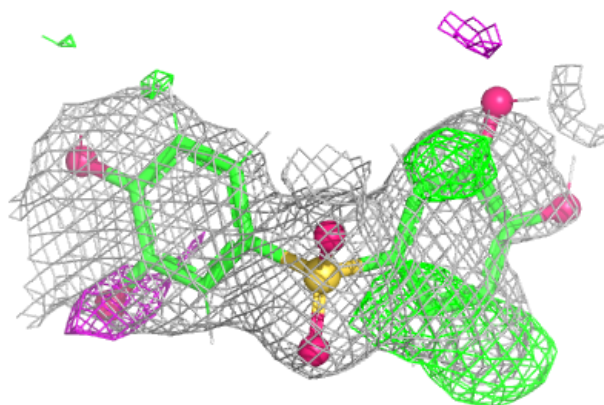
Electron density around OD5 F 605 (A):

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

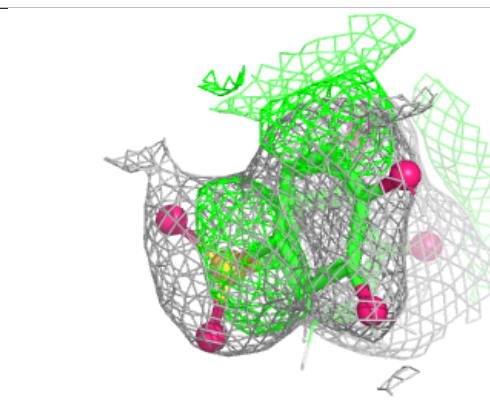
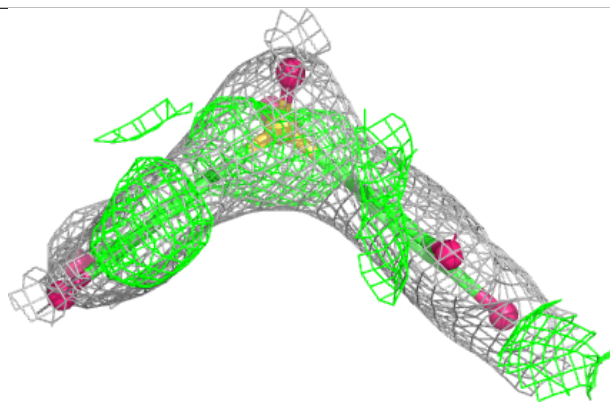
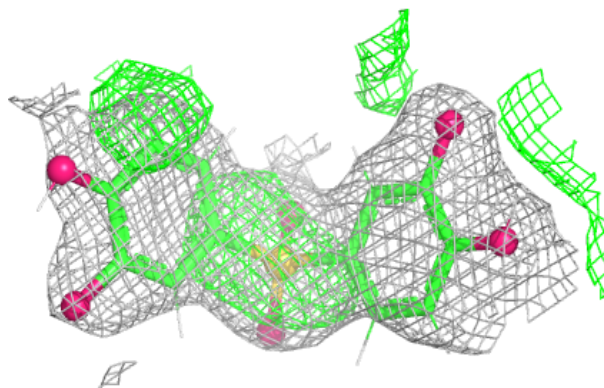


Electron density around OD5 F 605 (B):

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

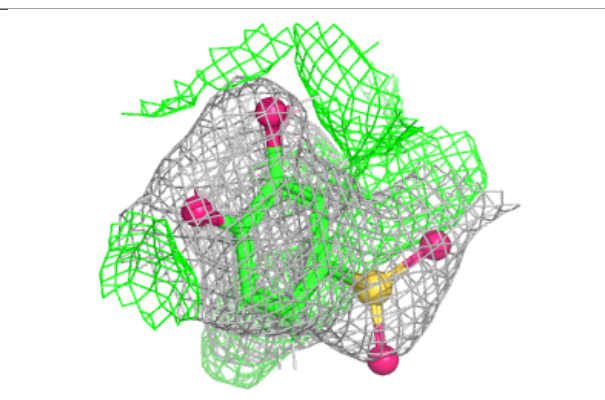
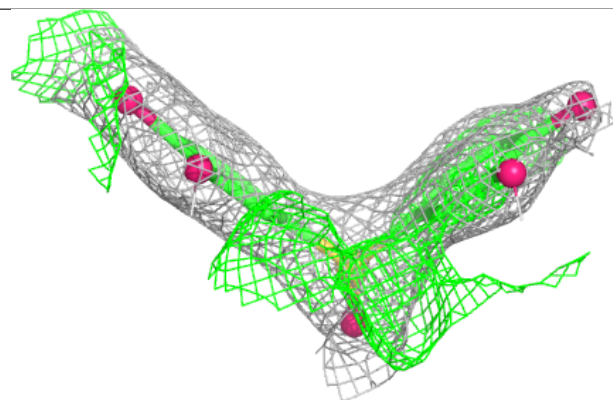
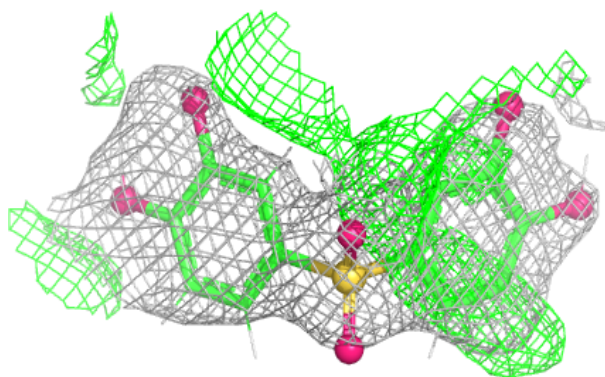
**Electron density around OD5 D 605 (A):**

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

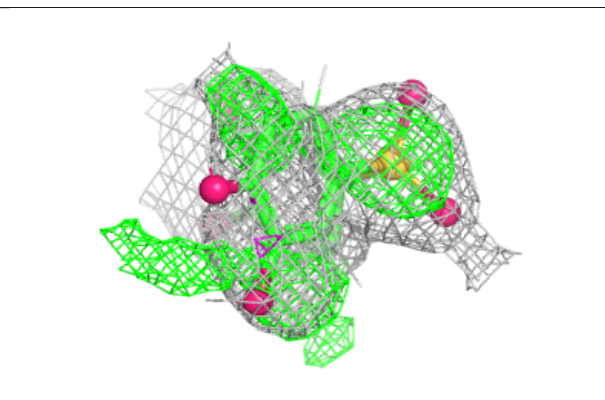
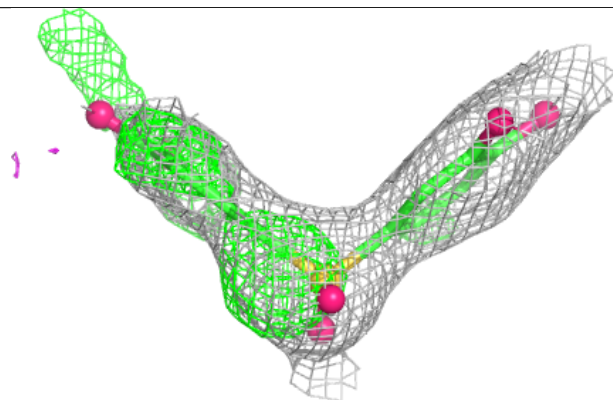
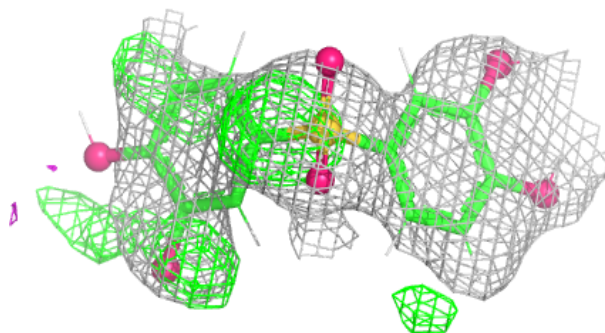


Electron density around OD5 D 605 (B):

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

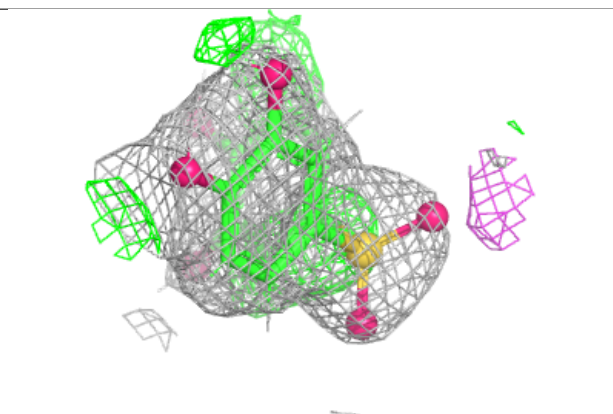
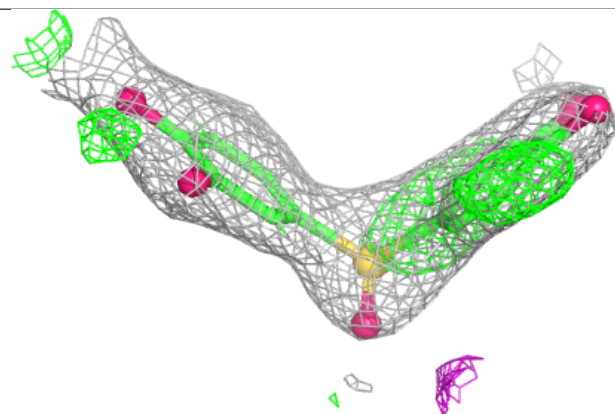
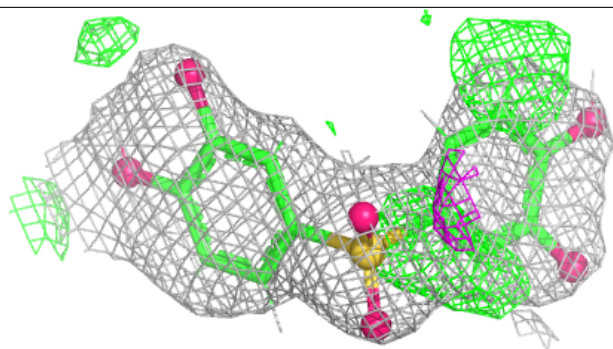
**Electron density around OD5 A 605 (A):**

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

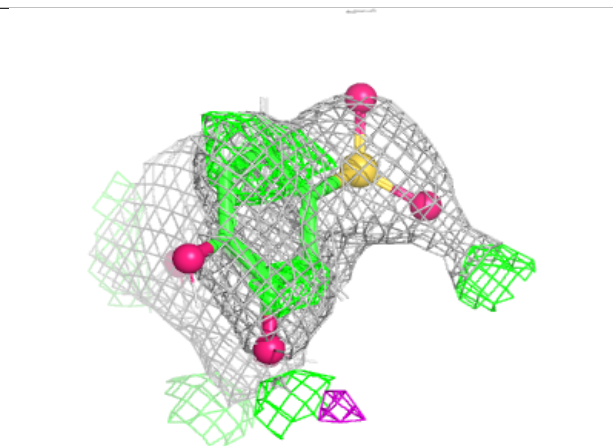
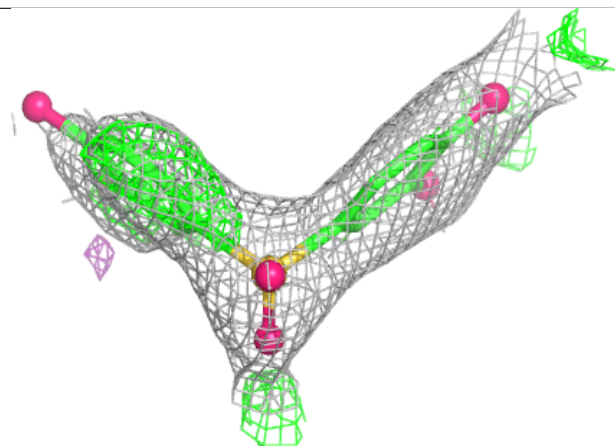
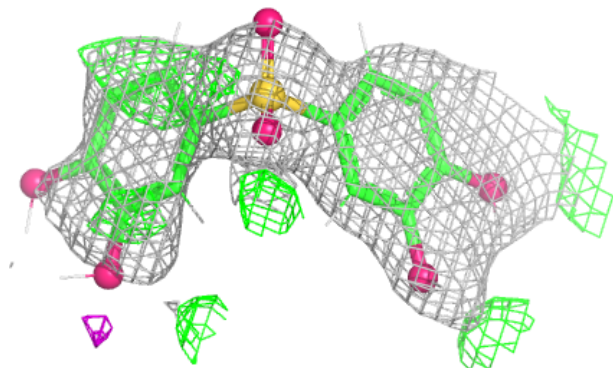


Electron density around OD5 A 605 (B):

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

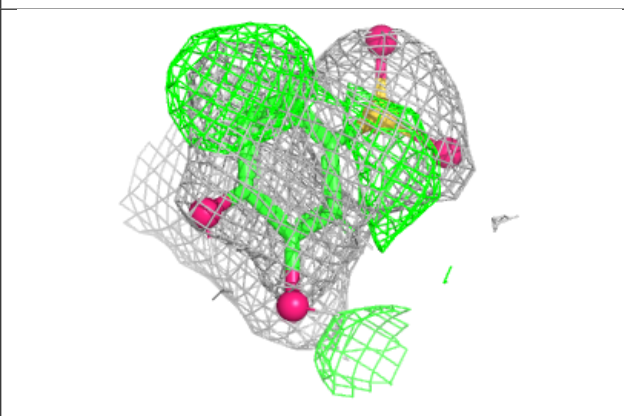
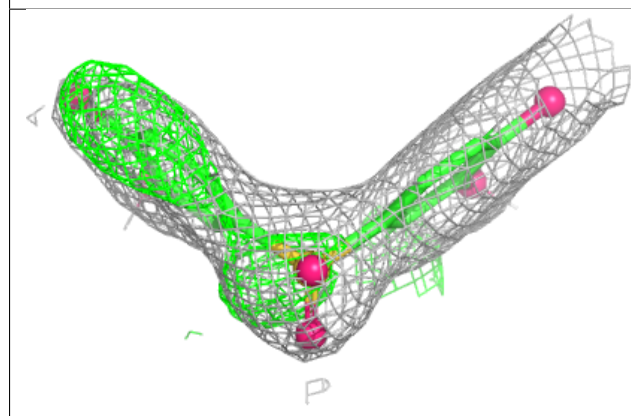
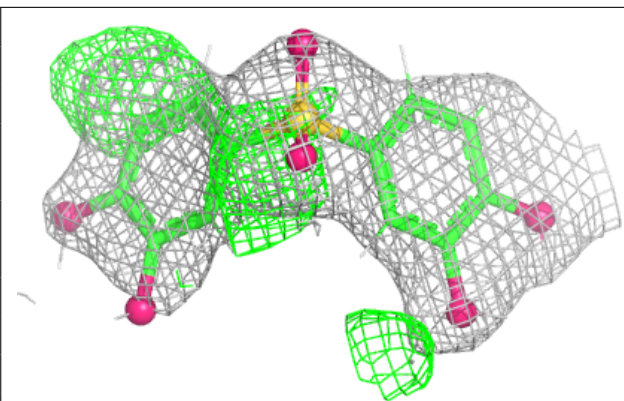
**Electron density around OD5 G 601 (A):**

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

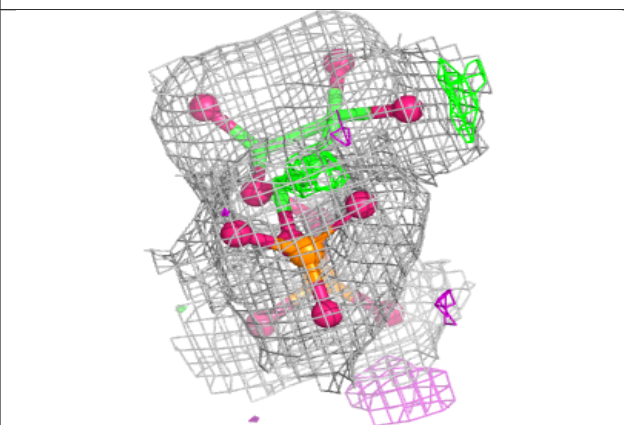
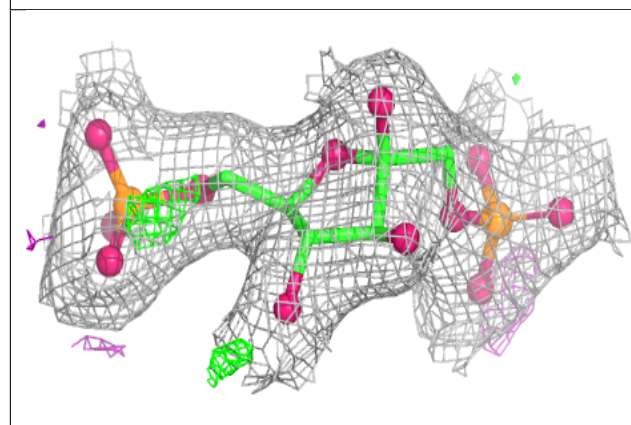
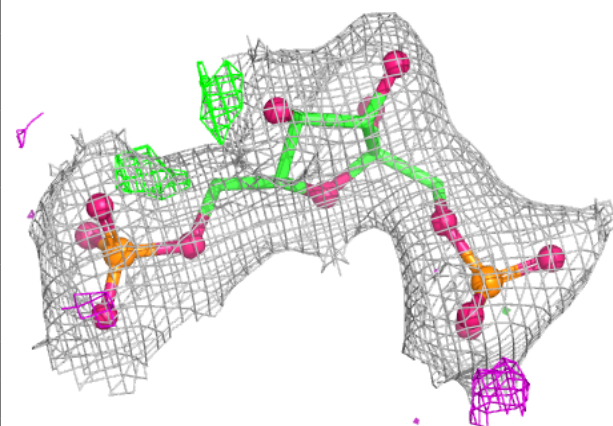


Electron density around OD5 G 601 (B):

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

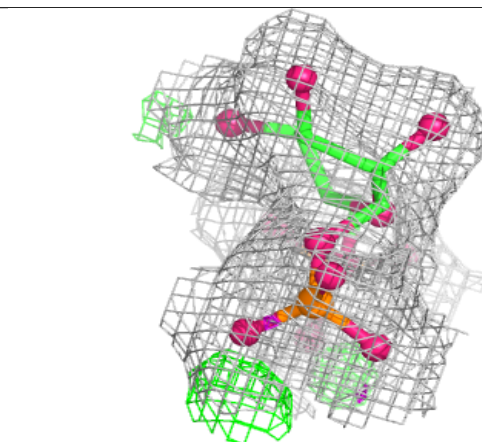
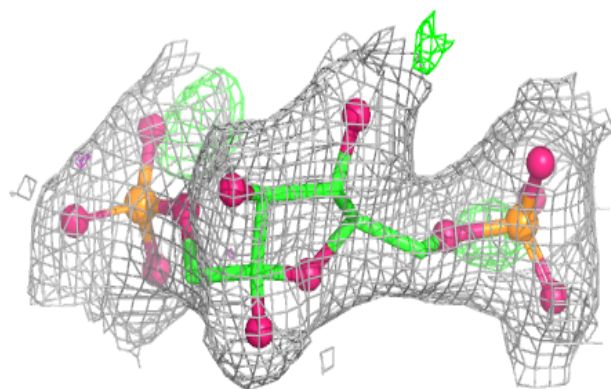
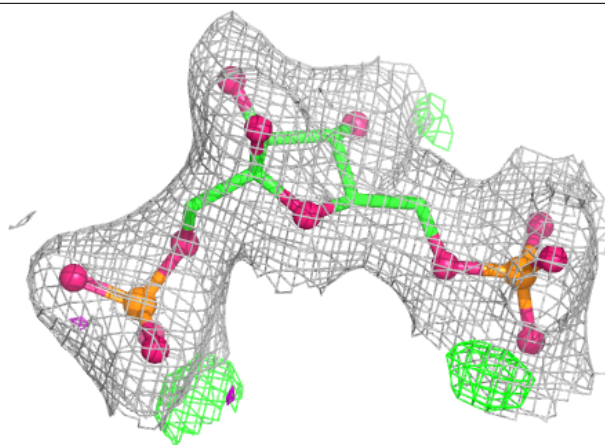
**Electron density around FBP B 601:**

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

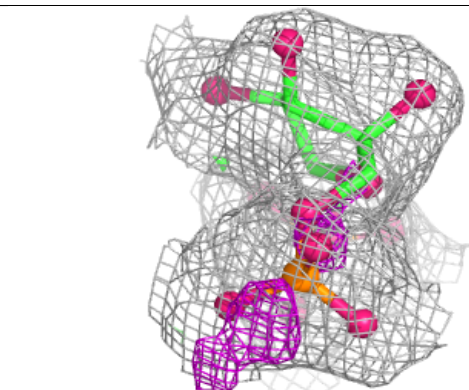
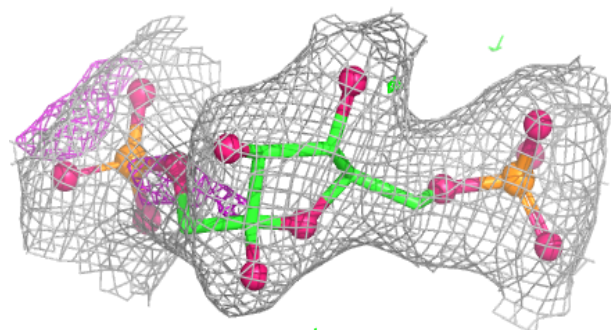
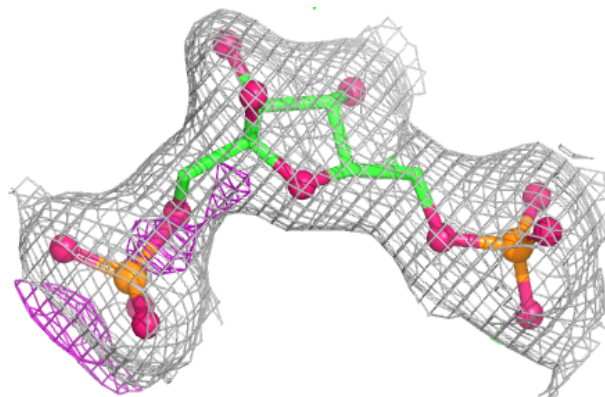


Electron density around FBP F 601:

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

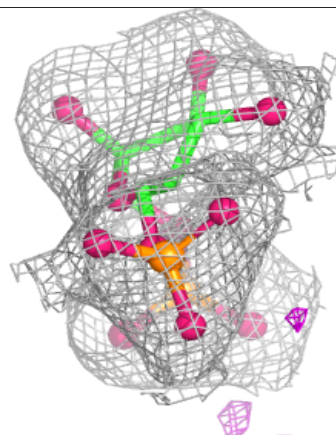
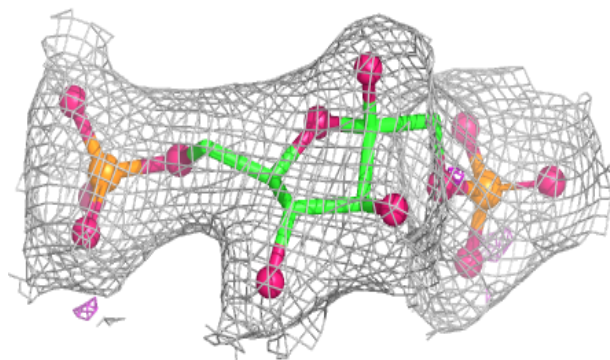
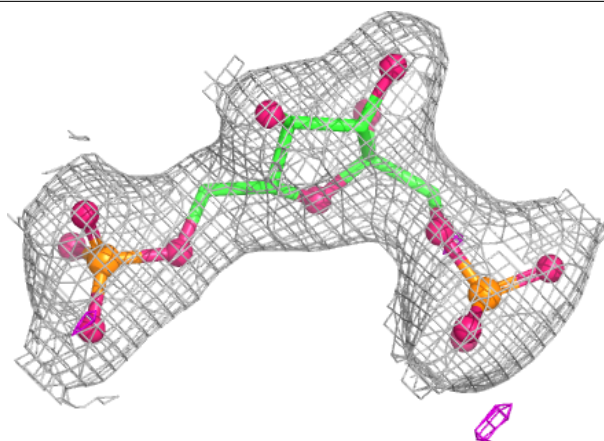
**Electron density around FBP A 601:**

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

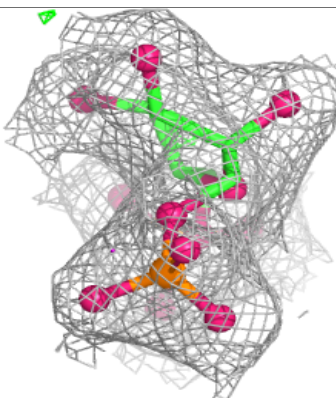
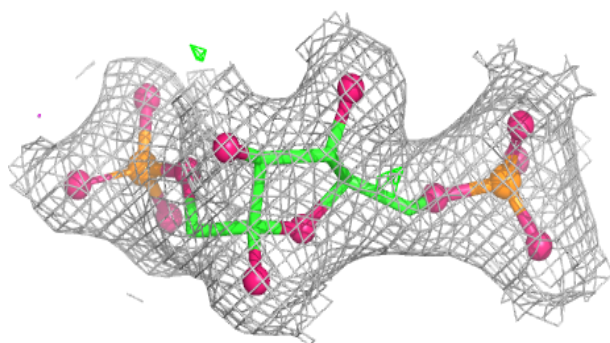
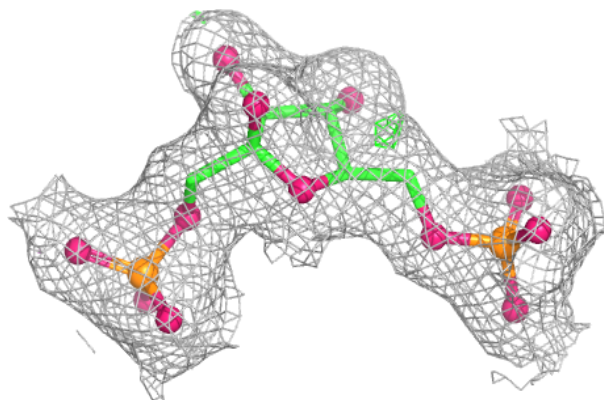


Electron density around FBP E 601:

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

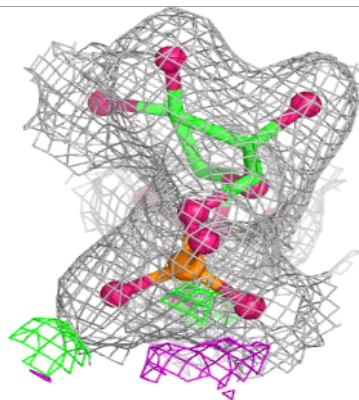
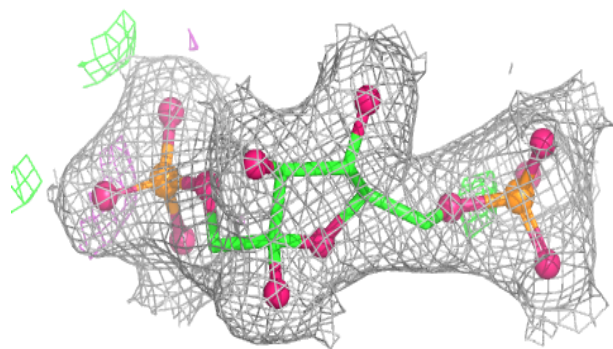
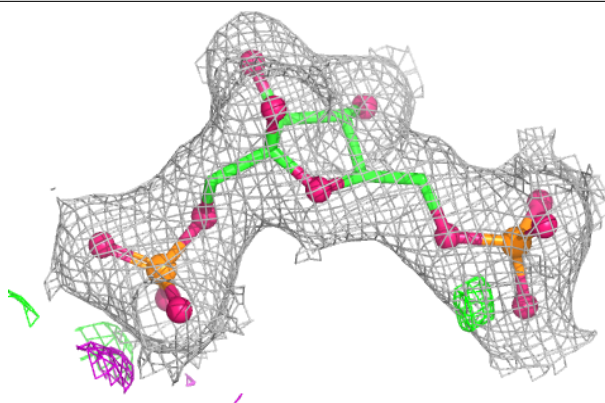
**Electron density around FBP G 602:**

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

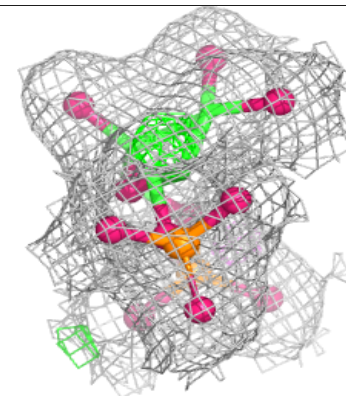
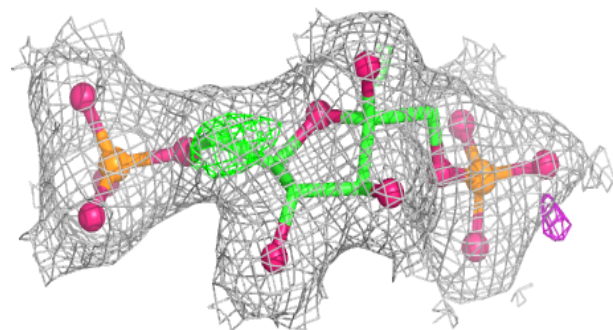
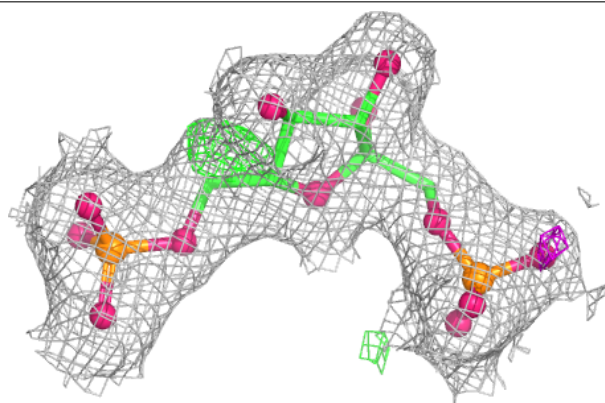


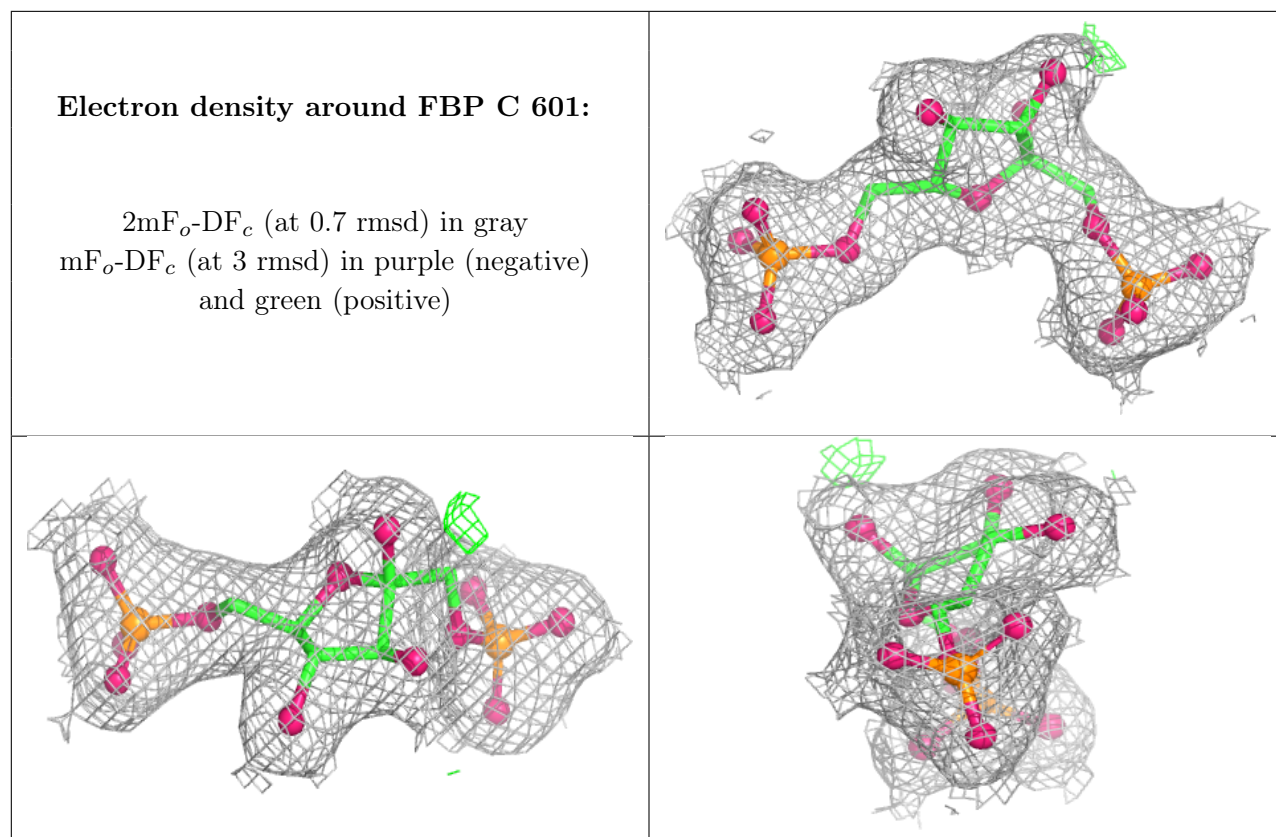
Electron density around FBP D 601:

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

**Electron density around FBP 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.