



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 01:52 PM UTC

PDB ID : 7FSA / pdb_00007fsa
Title : Structure of liver pyruvate kinase in complex with allosteric modulator 24
Authors : Lulla, A.; Nilsson, O.; Brear, P.; Nain-Perez, A.; Grotli, M.; Hyvonen, M.
Deposited on : 2022-12-18
Resolution : 1.91 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

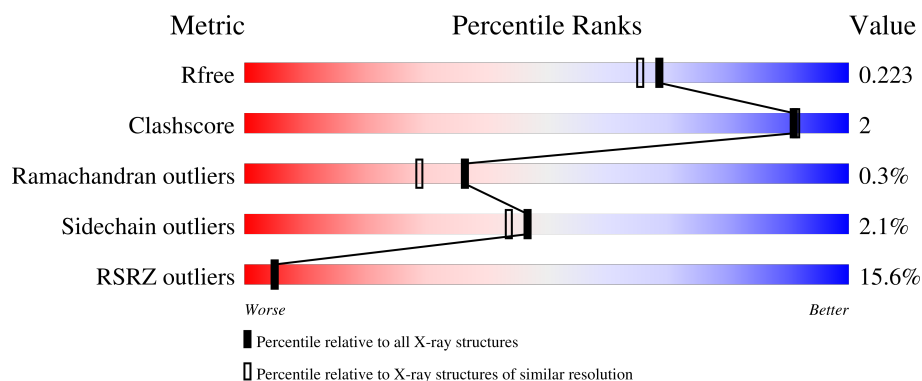
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	24% 88% 6% 6%
1	B	447	18% 91% 7% .
1	C	447	12% 89% 6% 5%
1	D	447	4% 90% 5% 5%
1	E	447	35% 88% 5% 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	603	-	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 28878 atoms, of which 92 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...

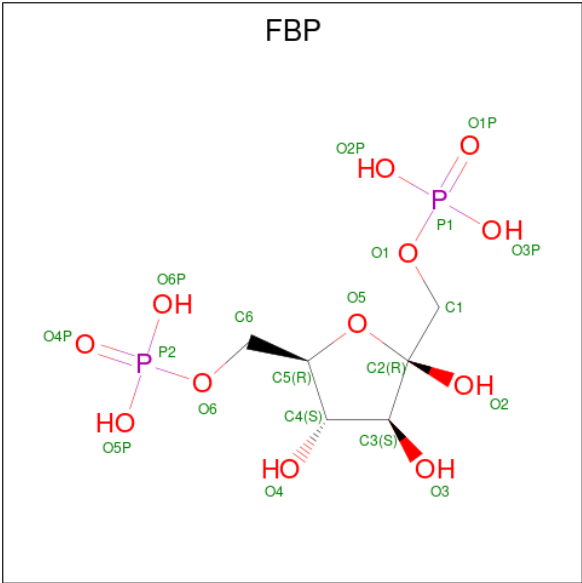
Chain	Residue	Modelled	Actual	Comment	Reference
B	130	GLY	-	linker	UNP P30613
B	131	SER	-	linker	UNP P30613
B	132	GLY	-	linker	UNP P30613
C	-1	GLY	-	expression tag	UNP P30613
C	0	SER	-	expression tag	UNP P30613
C	1	MET	-	expression tag	UNP P30613
C	2	GLU	-	expression tag	UNP P30613
C	12	ASP	SER	conflict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

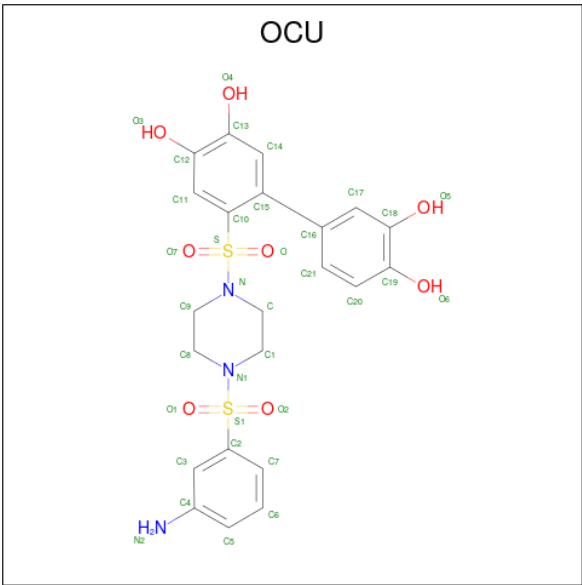
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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 (1M)-6-[4-(3-aminobenzene-1-sulfonyl)piperazine-1-sulfonyl][1,1'-biphenyl]-3,3',4,4'-tetrol (CCD ID: OCU) (formula: C₂₂H₂₃N₃O₈S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total	C	H	N	O	S	23	0
			58	22	23	3	8	2		
6	C	1	Total	C	H	N	O	S	23	0
			58	22	23	3	8	2		
6	G	1	Total	C	H	N	O	S	23	0
			58	22	23	3	8	2		
6	H	1	Total	C	H	N	O	S	23	0
			58	22	23	3	8	2		

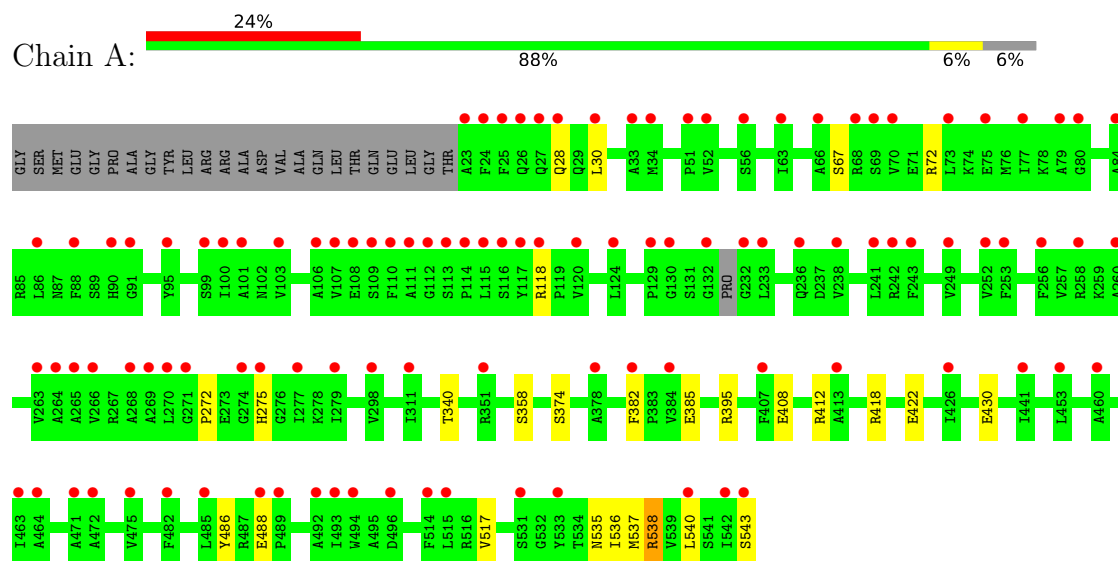
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	212	Total	O	0	0
			212	212		
7	B	236	Total	O	0	0
			236	236		
7	C	296	Total	O	0	0
			296	296		
7	D	385	Total	O	0	0
			385	385		
7	E	180	Total	O	0	0
			180	180		
7	F	258	Total	O	0	0
			258	258		
7	G	370	Total	O	0	0
			370	370		
7	H	408	Total	O	0	0
			408	408		

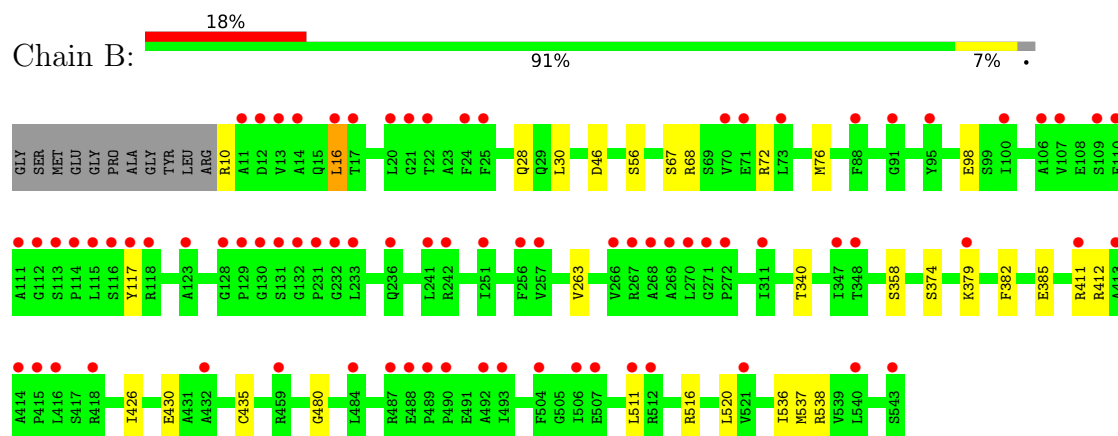
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

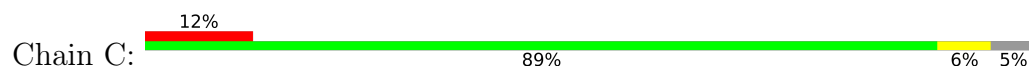
- Molecule 1: Pyruvate kinase PKLR

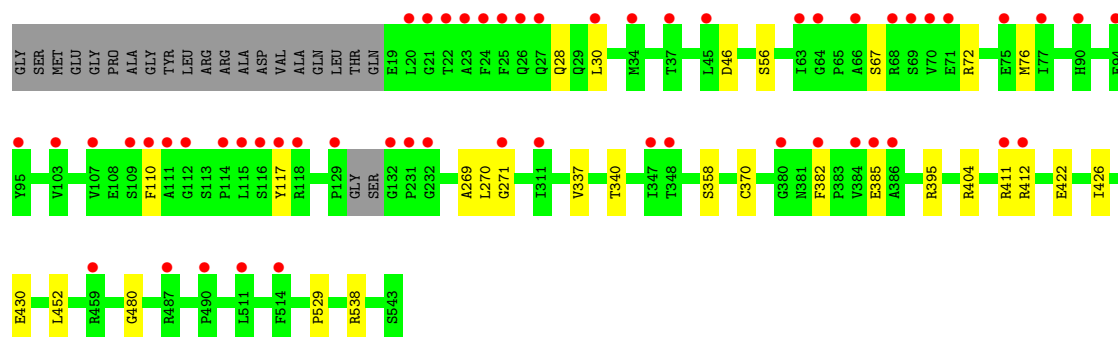


- Molecule 1: Pyruvate kinase PKLR

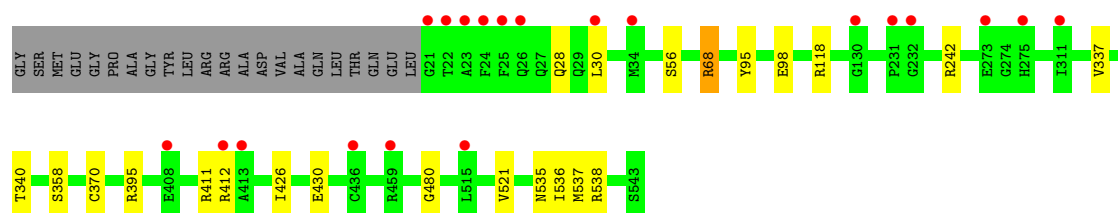


- Molecule 1: Pyruvate kinase PKLR

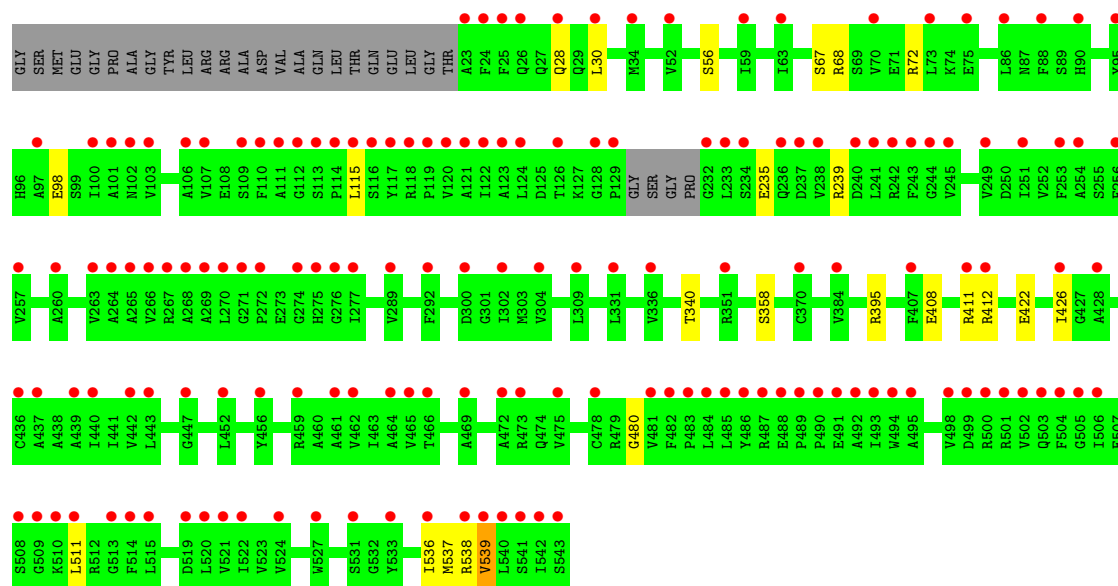
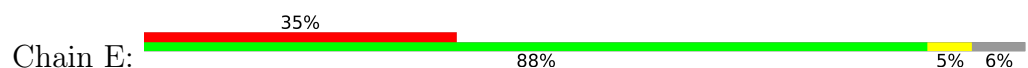




• Molecule 1: Pyruvate kinase PKLR

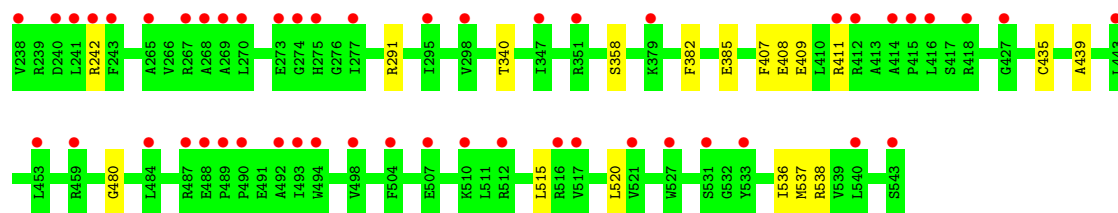


• Molecule 1: Pyruvate kinase PKLR

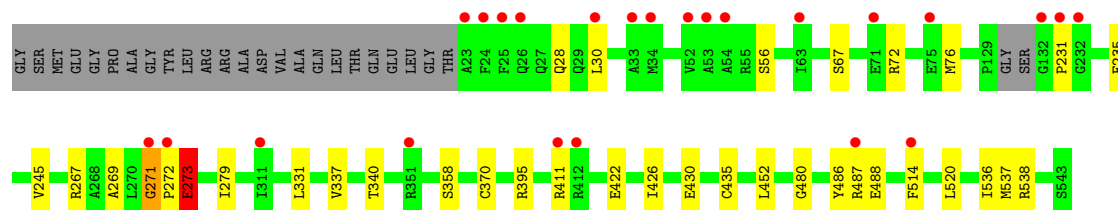
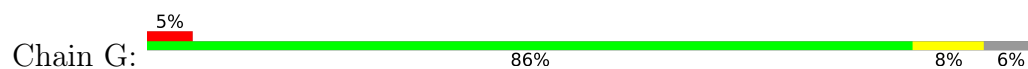


• Molecule 1: Pyruvate kinase PKLR

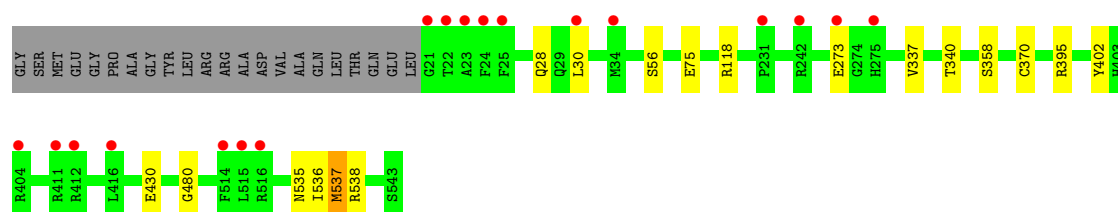
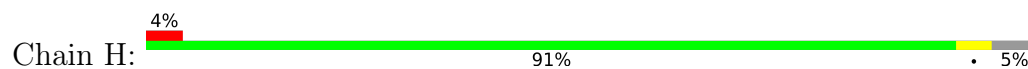




● Molecule 1: Pyruvate kinase PKLR



● Molecule 1: Pyruvate kinase PKLR



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	208.13Å 112.69Å 189.16Å 90.00° 91.49° 90.00°	Depositor
Resolution (Å)	189.09 – 1.91 189.09 – 1.91	Depositor EDS
% Data completeness (in resolution range)	82.5 (189.09-1.91) 82.6 (189.09-1.91)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 1.91Å)	Xtriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, R_{free}	0.208 , 0.232 0.200 , 0.223	Depositor DCC
R_{free} test set	14050 reflections (4.16%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	28878	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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 67.04 % 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 5.4845e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.64	1/3307 (0.0%)	0.97	1/4469 (0.0%)
1	B	0.69	1/3396 (0.0%)	0.96	1/4592 (0.0%)
1	C	0.70	0/3313	0.96	3/4479 (0.1%)
1	D	0.73	0/3326	0.96	0/4497
1	E	0.64	0/3278	0.96	2/4430 (0.0%)
1	F	0.68	0/3396	0.97	1/4591 (0.0%)
1	G	0.70	0/3303	0.96	2/4465 (0.0%)
1	H	0.75	0/3316	0.95	0/4483
All	All	0.69	2/26635 (0.0%)	0.96	10/36006 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	374	SER	CA-C	6.47	1.55	1.52
1	A	374	SER	CA-C	5.29	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	422	GLU	CB-CG-CD	7.60	125.52	112.60
1	A	422	GLU	CB-CG-CD	7.11	124.69	112.60
1	G	514	PHE	CA-CB-CG	5.46	119.26	113.80
1	G	273	GLU	CB-CG-CD	5.44	121.85	112.60
1	E	539	VAL	N-CA-CB	5.40	117.52	111.21
1	F	46	ASP	CA-CB-CG	5.18	117.78	112.60
1	C	46	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	46	ASP	CA-CB-CG	5.06	117.66	112.60
1	C	270	LEU	CA-C-N	5.00	129.72	121.87
1	C	270	LEU	C-N-CA	5.00	129.72	121.87

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	12	0
1	B	3329	0	3394	11	0
1	C	3247	0	3299	15	0
1	D	3252	0	3310	13	0
1	E	3210	0	3270	8	0
1	F	3321	0	3393	11	0
1	G	3231	0	3284	20	0
1	H	3251	0	3306	11	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

Continued on next page...

Continued from previous page...

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	B	35	23	0	2	0
6	C	35	23	0	1	0
6	G	35	23	0	1	0
6	H	35	23	0	3	0
7	A	212	0	0	0	0
7	B	236	0	0	1	0
7	C	296	0	0	1	0
7	D	385	0	0	0	0
7	E	180	0	0	0	0
7	F	258	0	0	0	0
7	G	370	0	0	0	0
7	H	408	0	0	1	0
All	All	28786	92	26635	90	0

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

All (90) 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	1.48	0.92
1:B:411:ARG:HG3	1:B:426:ILE:HD11	1.52	0.90
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.60	0.84
1:C:422[A]:GLU:HG3	1:C:452:LEU:HD13	1.65	0.78
1:G:538:ARG:HG2	1:H:536:ILE:HG12	1.65	0.78
1:E:411:ARG:HG3	1:E:426:ILE:HD11	1.66	0.77
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.68	0.75
1:D:68:ARG:NH2	1:D:95:TYR:O	2.22	0.73
1:D:411:ARG:HG3	1:D:426:ILE:HD11	1.69	0.72
1:C:538:ARG:HG2	1:D:536:ILE:HG12	1.73	0.71
1:A:538:ARG:HG3	1:B:536:ILE:HG12	1.76	0.66
1:E:235:GLU:O	1:E:239:ARG:HD3	1.96	0.65
1:D:68:ARG:HH22	1:D:98:GLU:HB2	1.65	0.62
6:C:601:OCU:O7	6:C:601:OCU:C21	2.47	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:PRO:HA	1:A:275:HIS:CE1	2.35	0.61
1:E:538:ARG:HG2	1:F:536:ILE:HG12	1.80	0.61
1:F:407:PHE:CE2	1:F:411:ARG:NH1	2.69	0.60
1:E:536:ILE:HG12	1:F:538:ARG:HG2	1.85	0.59
1:A:418[A]:ARG:HG3	1:B:16:LEU:HD11	1.87	0.57
1:G:536:ILE:HG12	1:H:538[A]:ARG:HG2	1.86	0.56
1:F:409:GLU:OE1	6:H:605:OCU:N2	2.39	0.56
1:A:272:PRO:HA	1:A:275:HIS:NE2	2.21	0.55
1:G:411:ARG:HG3	1:G:426:ILE:HD11	1.89	0.54
1:A:517:VAL:HG13	1:A:543:SER:HB3	1.90	0.54
1:C:529:PRO:HG3	1:G:235:GLU:HG2	1.91	0.53
1:G:56:SER:HB2	1:G:480:GLY:HA2	1.90	0.53
6:B:605:OCU:O7	6:B:605:OCU:C17	2.56	0.52
1:C:538:ARG:HD3	7:C:778:HOH:O	2.10	0.52
1:D:535:ASN:OD1	1:D:536:ILE:HG13	2.10	0.51
1:G:430[B]:GLU:OE2	1:H:430:GLU:OE1	2.28	0.51
1:G:411:ARG:CG	1:G:426:ILE:HD11	2.41	0.51
1:F:407:PHE:CD2	1:F:411:ARG:NH1	2.78	0.51
1:G:267:ARG:HG2	1:G:279:ILE:CD1	2.41	0.51
1:G:245:VAL:CG1	1:G:273:GLU:HG2	2.41	0.50
1:H:56:SER:HB2	1:H:480:GLY:HA2	1.94	0.50
6:B:605:OCU:C21	7:B:887:HOH:O	2.61	0.49
1:C:430[A]:GLU:OE1	1:D:430[A]:GLU:OE1	2.30	0.49
1:F:56:SER:HB2	1:F:480:GLY:HA2	1.95	0.48
1:G:269:ALA:C	1:G:271:GLY:H	2.21	0.48
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.96	0.48
1:G:267:ARG:HG2	1:G:279:ILE:HD12	1.95	0.48
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.96	0.48
1:G:272:PRO:HD2	1:G:273:GLU:OE1	2.14	0.47
1:G:430[A]:GLU:OE1	1:H:430:GLU:OE1	2.32	0.47
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.96	0.47
1:A:67:SER:HA	1:A:72:ARG:HG2	1.95	0.47
6:H:605:OCU:O7	6:H:605:OCU:C16	2.62	0.47
1:A:430:GLU:OE2	1:B:430:GLU:OE1	2.33	0.46
1:C:404:ARG:HD3	1:D:412:ARG:NH2	2.30	0.46
1:C:67:SER:HA	1:C:72:ARG:HG2	1.98	0.46
1:G:28:GLN:HG3	1:G:30:LEU:HG	1.98	0.46
1:B:28:GLN:HG3	1:B:30:LEU:HG	1.98	0.45
1:B:435:CYS:HB2	1:B:520:LEU:HD12	1.99	0.45
1:F:382:PHE:HB3	1:F:385:GLU:HB2	1.98	0.45
1:A:28:GLN:HG3	1:A:30:LEU:HG	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430[B]:GLU:OE2	1:D:430[B]:GLU:OE1	2.35	0.45
1:E:56:SER:HB2	1:E:480:GLY:HA2	1.98	0.44
1:D:28:GLN:HG3	1:D:30:LEU:HG	1.99	0.44
1:H:535:ASN:OD1	1:H:536:ILE:HG13	2.17	0.44
1:F:28:GLN:HG3	1:F:30:LEU:HG	2.00	0.44
1:C:110:PHE:O	1:C:117:TYR:HB2	2.18	0.44
1:H:28:GLN:HG3	1:H:30:LEU:HG	2.00	0.43
1:C:28:GLN:HG3	1:C:30:LEU:HG	2.00	0.43
1:G:537:MET:HE3	1:H:537:MET:HG2	2.00	0.43
1:E:28:GLN:HG3	1:E:30:LEU:HG	1.99	0.43
1:A:486:TYR:CZ	1:A:488[B]:GLU:HB2	2.54	0.43
1:B:382:PHE:HB3	1:B:385:GLU:HB2	2.01	0.42
1:F:439:ALA:HB3	1:F:515:LEU:HD21	2.00	0.42
1:H:402:TYR:H	6:H:605:OCU:C20	2.32	0.42
1:D:411:ARG:CG	1:D:426:ILE:HD11	2.45	0.42
1:G:67:SER:HA	1:G:72:ARG:HG2	2.01	0.42
1:H:75:GLU:HG3	7:H:1060:HOH:O	2.20	0.42
1:A:382:PHE:HB3	1:A:385:GLU:HB2	2.02	0.42
1:F:435:CYS:HB2	1:F:520:LEU:HD12	2.01	0.42
1:C:269:ALA:C	1:C:271:GLY:H	2.28	0.41
1:C:337:VAL:HG22	1:C:370:CYS:HB2	2.03	0.41
6:G:601:OCU:C17	6:G:601:OCU:O7	2.68	0.41
1:A:535:ASN:OD1	1:A:536:ILE:HG13	2.21	0.41
1:B:68:ARG:NH2	1:B:98:GLU:HB3	2.35	0.41
1:H:337:VAL:HG22	1:H:370:CYS:HB2	2.03	0.41
1:B:67:SER:HA	1:B:72:ARG:HG2	2.02	0.41
1:F:67:SER:HA	1:F:72:ARG:HG2	2.02	0.41
1:E:67:SER:HA	1:E:72:ARG:HG2	2.01	0.40
1:G:435:CYS:HB2	1:G:520:LEU:HD12	2.04	0.40
1:E:68:ARG:NH2	1:E:98:GLU:HB3	2.36	0.40
1:D:30:LEU:HD23	1:D:30:LEU:HA	1.99	0.40
1:D:337:VAL:HG22	1:D:370:CYS:HB2	2.04	0.40
1:G:486:TYR:CZ	1:G:488:GLU:HB2	2.57	0.40
1:C:382:PHE:HB3	1:C:385:GLU:HB2	2.04	0.40
1:G:337:VAL:HG22	1:G:370:CYS:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	424/447 (95%)	418 (99%)	5 (1%)	1 (0%)	43	36
1	B	438/447 (98%)	432 (99%)	4 (1%)	2 (0%)	24	16
1	C	425/447 (95%)	417 (98%)	7 (2%)	1 (0%)	43	36
1	D	429/447 (96%)	425 (99%)	3 (1%)	1 (0%)	43	36
1	E	420/447 (94%)	414 (99%)	5 (1%)	1 (0%)	43	36
1	F	435/447 (97%)	430 (99%)	4 (1%)	1 (0%)	43	36
1	G	423/447 (95%)	413 (98%)	7 (2%)	3 (1%)	18	10
1	H	427/447 (96%)	423 (99%)	3 (1%)	1 (0%)	43	36
All	All	3421/3576 (96%)	3372 (99%)	38 (1%)	11 (0%)	36	29

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	117	TYR
1	A	340	THR
1	B	340	THR
1	C	340	THR
1	D	340	THR
1	E	340	THR
1	F	340	THR
1	G	340	THR
1	H	340	THR
1	G	271	GLY
1	G	231	PRO

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	35
1	B	349/352 (99%)	337 (97%)	12 (3%)	32	25
1	C	341/352 (97%)	336 (98%)	5 (2%)	57	56
1	D	342/352 (97%)	333 (97%)	9 (3%)	40	35
1	E	338/352 (96%)	329 (97%)	9 (3%)	39	34
1	F	350/352 (99%)	341 (97%)	9 (3%)	40	35
1	G	340/352 (97%)	333 (98%)	7 (2%)	47	44
1	H	340/352 (97%)	335 (98%)	5 (2%)	57	56
All	All	2740/2816 (97%)	2675 (98%)	65 (2%)	47	38

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	ARG
1	A	358	SER
1	A	395	ARG
1	A	408	GLU
1	A	412	ARG
1	A	537[A]	MET
1	A	537[B]	MET
1	A	538	ARG
1	A	540	LEU
1	B	10	ARG
1	B	16	LEU
1	B	76[A]	MET
1	B	76[B]	MET
1	B	263	VAL
1	B	358	SER
1	B	379	LYS
1	B	412	ARG
1	B	511	LEU
1	B	516	ARG
1	B	537[A]	MET
1	B	537[B]	MET
1	C	76[A]	MET
1	C	76[B]	MET
1	C	358	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	395	ARG
1	C	412	ARG
1	D	68	ARG
1	D	118	ARG
1	D	242[A]	ARG
1	D	242[B]	ARG
1	D	358	SER
1	D	395	ARG
1	D	521	VAL
1	D	537	MET
1	D	538	ARG
1	E	115	LEU
1	E	358	SER
1	E	395	ARG
1	E	408	GLU
1	E	412	ARG
1	E	511	LEU
1	E	537[A]	MET
1	E	537[B]	MET
1	E	539	VAL
1	F	16	LEU
1	F	76[A]	MET
1	F	76[B]	MET
1	F	242	ARG
1	F	291	ARG
1	F	358	SER
1	F	408	GLU
1	F	537[A]	MET
1	F	537[B]	MET
1	G	76[A]	MET
1	G	76[B]	MET
1	G	273	GLU
1	G	331	LEU
1	G	358	SER
1	G	395	ARG
1	G	487	ARG
1	H	118	ARG
1	H	273	GLU
1	H	358	SER
1	H	395	ARG
1	H	537	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	A	236	GLN
1	B	90	HIS
1	C	90	HIS
1	D	26	GLN
1	D	90	HIS
1	E	90	HIS
1	F	90	HIS
1	F	403	HIS
1	G	90	HIS
1	G	470	GLN
1	H	90	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 16 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	OXL	F	602	4	5,5,5	2.97	4 (80%)	6,6,6	2.51	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FBP	C	602	-	18,20,20	0.67	1 (5%)	21,32,32	0.83	0
2	FBP	B	601	-	18,20,20	0.81	1 (5%)	21,32,32	0.86	1 (4%)
2	FBP	F	601	-	18,20,20	0.34	0	21,32,32	0.61	0
3	OXL	B	602	4	5,5,5	2.37	2 (40%)	6,6,6	1.20	1 (16%)
2	FBP	E	601	-	18,20,20	0.44	0	21,32,32	0.77	1 (4%)
3	OXL	A	602	4	5,5,5	1.98	2 (40%)	6,6,6	1.93	3 (50%)
3	OXL	H	602	4	5,5,5	1.85	2 (40%)	6,6,6	1.63	1 (16%)
3	OXL	G	603	4	5,5,5	2.16	2 (40%)	6,6,6	1.92	2 (33%)
6	OCU	G	601	-	38,38,38	0.26	0	58,58,58	0.46	0
2	FBP	H	601	-	18,20,20	0.85	1 (5%)	21,32,32	0.65	0
3	OXL	D	602	4	5,5,5	2.07	2 (40%)	6,6,6	2.11	2 (33%)
2	FBP	G	602	-	18,20,20	0.72	0	21,32,32	0.91	0
3	OXL	E	602	4	5,5,5	2.29	2 (40%)	6,6,6	1.77	2 (33%)
6	OCU	C	601	-	38,38,38	0.38	0	58,58,58	0.56	0
2	FBP	A	601	-	18,20,20	0.53	0	21,32,32	0.66	0
6	OCU	H	605	-	38,38,38	0.40	0	58,58,58	0.75	2 (3%)
3	OXL	C	603	4	5,5,5	1.96	2 (40%)	6,6,6	1.80	2 (33%)
6	OCU	B	605	-	38,38,38	0.35	0	58,58,58	0.53	0
2	FBP	D	601	-	18,20,20	0.58	1 (5%)	21,32,32	0.70	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OXL	F	602	4	-	4/4/4/4	-
2	FBP	C	602	-	-	2/13/32/32	0/1/1/1
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
3	OXL	B	602	4	-	4/4/4/4	-
2	FBP	E	601	-	-	2/13/32/32	0/1/1/1
3	OXL	A	602	4	-	4/4/4/4	-
3	OXL	H	602	4	-	4/4/4/4	-
3	OXL	G	603	4	-	4/4/4/4	-
6	OCU	G	601	-	-	14/28/38/38	0/4/4/4
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OXL	D	602	4	-	4/4/4/4	-
2	FBP	G	602	-	-	2/13/32/32	0/1/1/1
3	OXL	E	602	4	-	4/4/4/4	-
6	OCU	C	601	-	-	0/28/38/38	0/4/4/4
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
6	OCU	H	605	-	-	12/28/38/38	0/4/4/4
3	OXL	C	603	4	-	4/4/4/4	-
6	OCU	B	605	-	-	13/28/38/38	0/4/4/4
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	OXL	O1-C1	4.44	1.33	1.22
3	B	602	OXL	O2-C2	4.15	1.32	1.22
3	C	603	OXL	O1-C1	3.66	1.31	1.22
3	F	602	OXL	O1-C1	3.64	1.31	1.22
3	A	602	OXL	O2-C2	3.62	1.31	1.22
3	F	602	OXL	O3-C1	-3.60	1.20	1.30
3	G	603	OXL	O1-C1	3.49	1.31	1.22
3	F	602	OXL	O2-C2	3.26	1.30	1.22
3	B	602	OXL	O4-C2	-3.25	1.21	1.30
3	D	602	OXL	O2-C2	3.23	1.30	1.22
3	H	602	OXL	O4-C2	-3.15	1.22	1.30
3	G	603	OXL	O3-C1	-3.07	1.22	1.30
3	D	602	OXL	O4-C2	-3.02	1.22	1.30
3	H	602	OXL	O2-C2	2.67	1.29	1.22
3	A	602	OXL	O4-C2	-2.55	1.23	1.30
3	E	602	OXL	O3-C1	-2.46	1.23	1.30
3	C	603	OXL	O3-C1	-2.34	1.24	1.30
2	C	602	FBP	P1-O3P	-2.31	1.46	1.54
2	D	601	FBP	P2-O5P	-2.21	1.46	1.54
3	F	602	OXL	O4-C2	-2.16	1.24	1.30
2	H	601	FBP	P2-O5P	-2.12	1.46	1.54
2	B	601	FBP	P2-O5P	-2.04	1.47	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	602	OXL	O4-C2-C1	4.49	121.54	112.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	603	OXL	O3-C1-C2	3.62	119.86	112.83
3	A	602	OXL	O4-C2-C1	3.62	119.85	112.83
3	D	602	OXL	O4-C2-C1	3.54	119.69	112.83
3	H	602	OXL	O4-C2-C1	3.40	119.43	112.83
3	G	603	OXL	O3-C1-C2	3.38	119.38	112.83
3	F	602	OXL	O3-C1-C2	3.02	118.68	112.83
6	H	605	OCU	C11-C10-C15	2.95	123.56	120.25
3	E	602	OXL	O3-C1-C2	2.89	118.43	112.83
3	F	602	OXL	O2-C2-C1	-2.74	114.92	120.63
2	E	601	FBP	O3P-P1-O2P	2.72	118.00	107.80
3	D	602	OXL	O3-C1-C2	2.69	118.04	112.83
2	B	601	FBP	O3P-P1-O2P	2.65	117.74	107.80
3	E	602	OXL	O4-C2-C1	2.63	117.94	112.83
3	G	603	OXL	O4-C2-C1	2.60	117.86	112.83
2	D	601	FBP	O5P-P2-O6	2.50	113.18	106.67
6	H	605	OCU	C15-C10-S	-2.38	119.81	122.63
3	B	602	OXL	O3-C1-C2	2.36	117.40	112.83
3	A	602	OXL	O2-C2-C1	-2.17	116.10	120.63
3	A	602	OXL	O3-C1-C2	2.08	116.86	112.83
3	C	603	OXL	O1-C1-C2	-2.04	116.38	120.63

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	605	OCU	C8-N1-S1-O1
6	B	605	OCU	C8-N1-S1-O2
6	G	601	OCU	C-N-S-O7
6	H	605	OCU	C8-N1-S1-O2
6	G	601	OCU	C-N-S-C10
6	H	605	OCU	C8-N1-S1-C2
6	B	605	OCU	C1-N1-S1-O1
6	B	605	OCU	C1-N1-S1-O2
6	G	601	OCU	C1-N1-S1-O1
6	B	605	OCU	C8-N1-S1-C2
6	H	605	OCU	C8-N1-S1-O1
6	B	605	OCU	C9-N-S-O7
6	G	601	OCU	C-N-S-O
6	H	605	OCU	C9-N-S-O7
6	B	605	OCU	C1-N1-S1-C2
6	G	601	OCU	C1-N1-S1-C2
2	A	601	FBP	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	601	FBP	C4-C5-C6-O6
2	C	602	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	G	602	FBP	C4-C5-C6-O6
2	H	601	FBP	C4-C5-C6-O6
6	B	605	OCU	C9-N-S-C10
6	H	605	OCU	C9-N-S-C10
6	G	601	OCU	C9-N-S-O
6	H	605	OCU	C1-N1-S1-O1
6	H	605	OCU	C1-N1-S1-O2
6	G	601	OCU	C9-N-S-O7
6	G	601	OCU	C1-N1-S1-O2
6	G	601	OCU	C9-N-S-C10
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	F	601	FBP	O5-C5-C6-O6
2	G	602	FBP	O5-C5-C6-O6
6	H	605	OCU	C1-N1-S1-C2
6	G	601	OCU	C8-N1-S1-O2
2	H	601	FBP	O5-C5-C6-O6
6	G	601	OCU	C8-N1-S1-O1
6	B	605	OCU	C9-N-S-O
3	C	603	OXL	O3-C1-C2-O4
3	D	602	OXL	O3-C1-C2-O4
3	G	603	OXL	O3-C1-C2-O4
3	A	602	OXL	O3-C1-C2-O4
3	B	602	OXL	O3-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O4
3	F	602	OXL	O3-C1-C2-O4
3	A	602	OXL	O1-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O2
3	H	602	OXL	O3-C1-C2-O4
6	H	605	OCU	C9-N-S-O
3	B	602	OXL	O1-C1-C2-O2
3	C	603	OXL	O1-C1-C2-O2
3	F	602	OXL	O1-C1-C2-O2
3	G	603	OXL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	H	602	OXL	O1-C1-C2-O2
6	B	605	OCU	C-N-S-O
3	E	602	OXL	O1-C1-C2-O2
6	G	601	OCU	C8-N1-S1-C2
6	B	605	OCU	C-N-S-O7
3	A	602	OXL	O1-C1-C2-O4
3	A	602	OXL	O3-C1-C2-O2
3	C	603	OXL	O1-C1-C2-O4
3	C	603	OXL	O3-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O4
3	D	602	OXL	O3-C1-C2-O2
3	F	602	OXL	O3-C1-C2-O2
3	G	603	OXL	O1-C1-C2-O4
3	G	603	OXL	O3-C1-C2-O2
6	G	601	OCU	C10-C15-C16-C21
3	B	602	OXL	O1-C1-C2-O4
3	B	602	OXL	O3-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O4
6	G	601	OCU	C14-C15-C16-C21
6	H	605	OCU	C14-C15-C16-C17
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	H	602	OXL	O3-C1-C2-O2
6	B	605	OCU	C14-C15-C16-C21
6	H	605	OCU	C-N-S-O7
6	H	605	OCU	C-N-S-O
6	B	605	OCU	C-N-S-C10

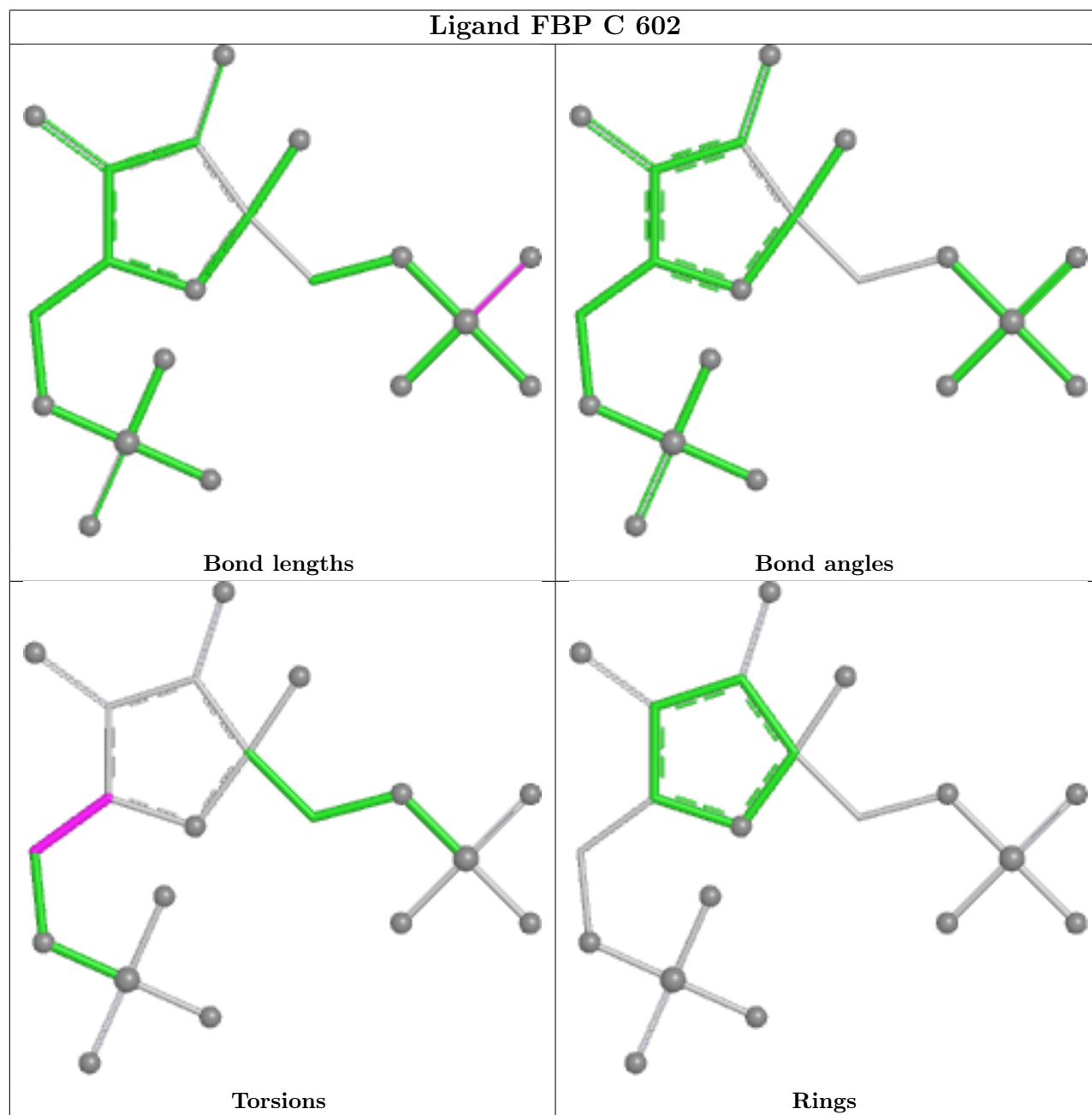
There are no ring outliers.

4 monomers are involved in 7 short contacts:

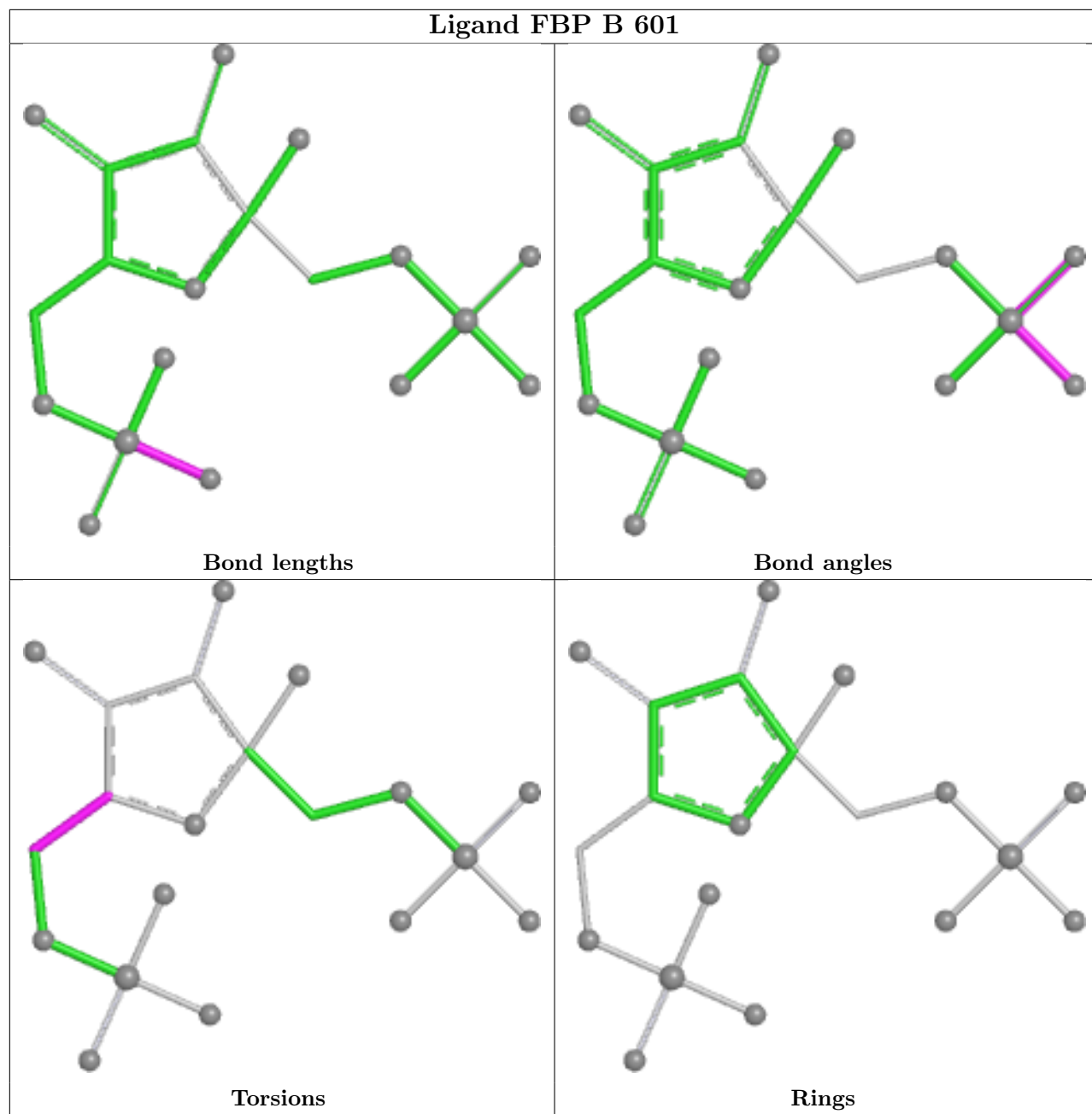
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	601	OCU	1	0
6	C	601	OCU	1	0
6	H	605	OCU	3	0
6	B	605	OCU	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

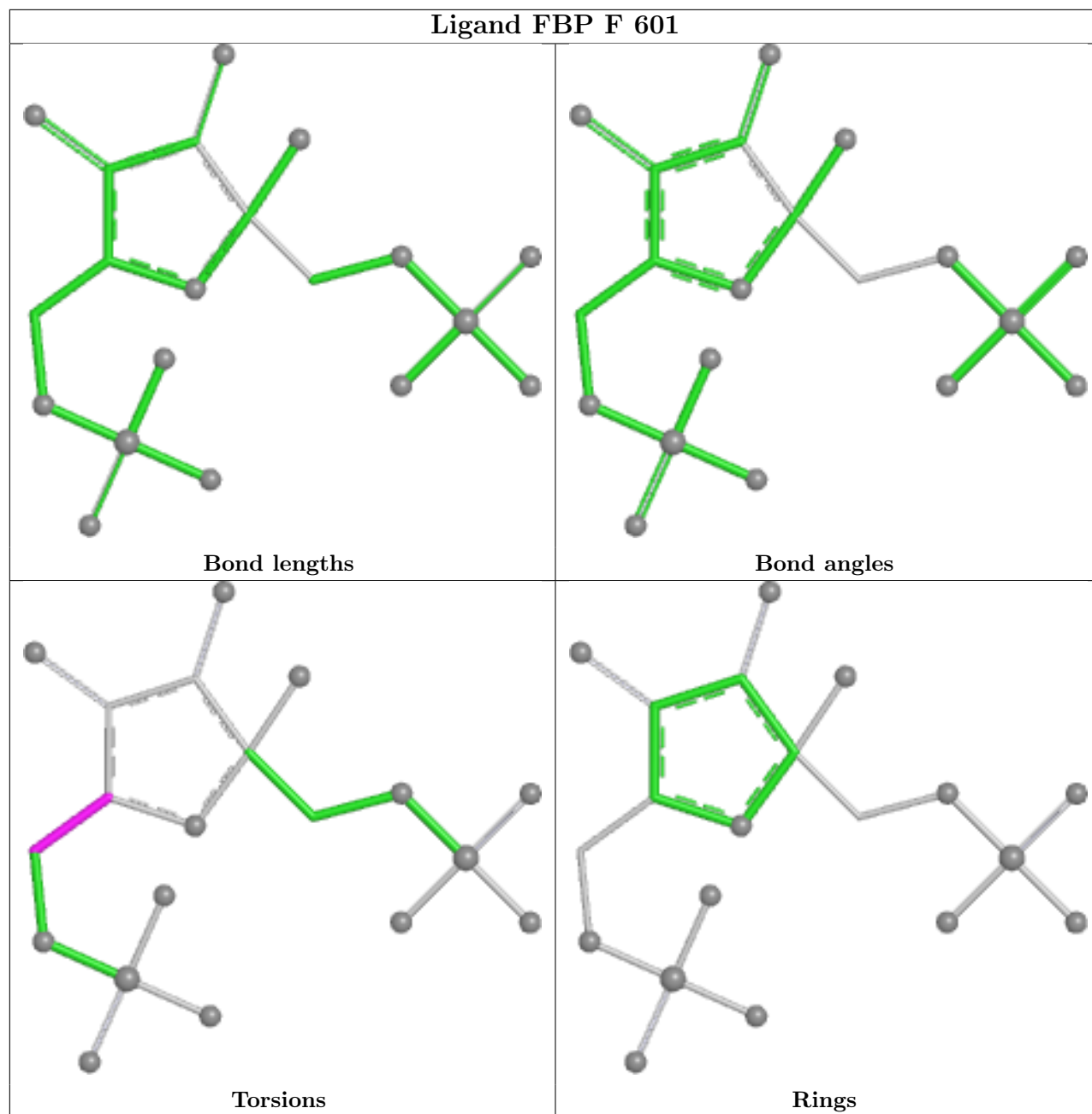
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



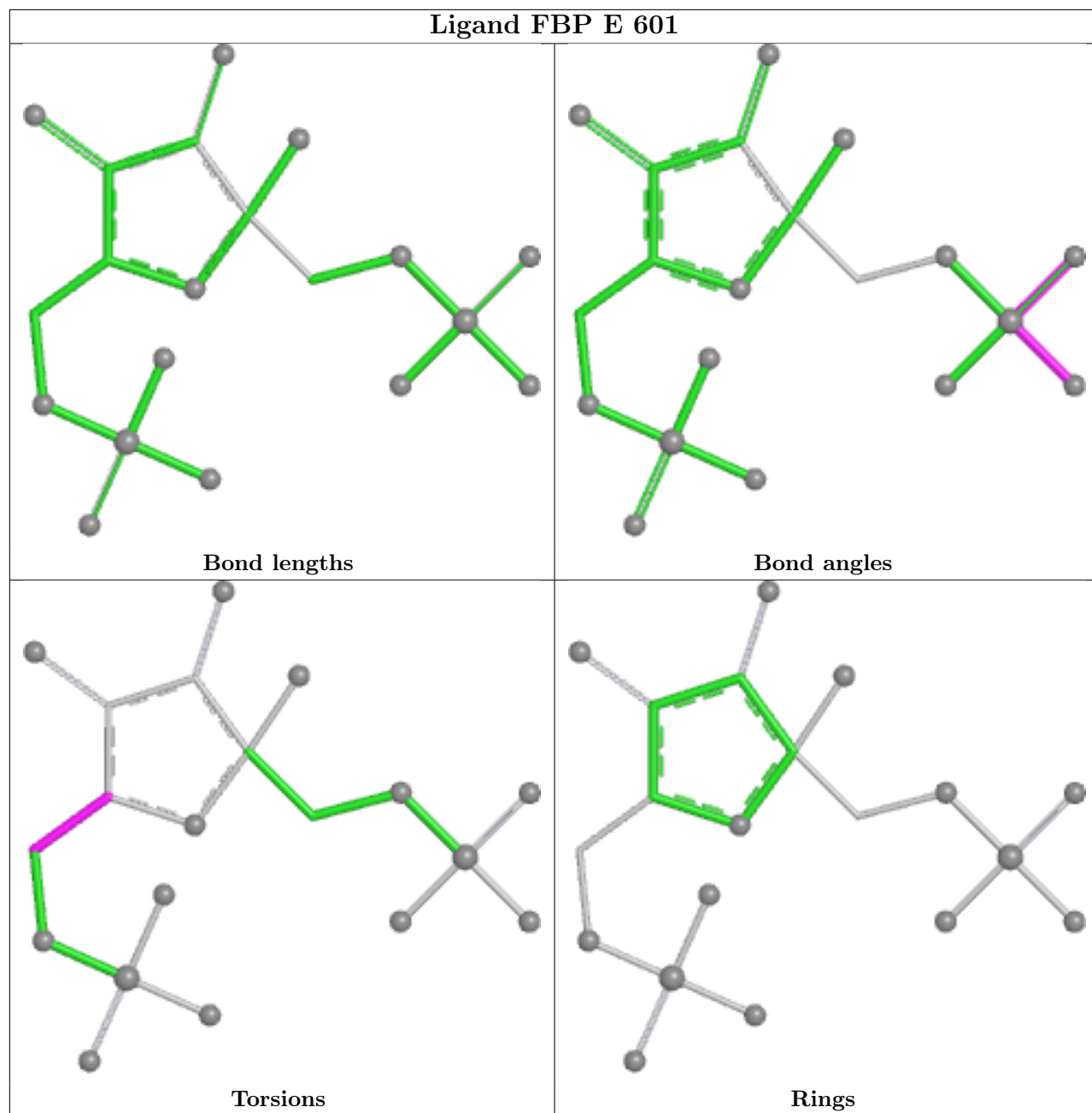
Ligand FBP B 601

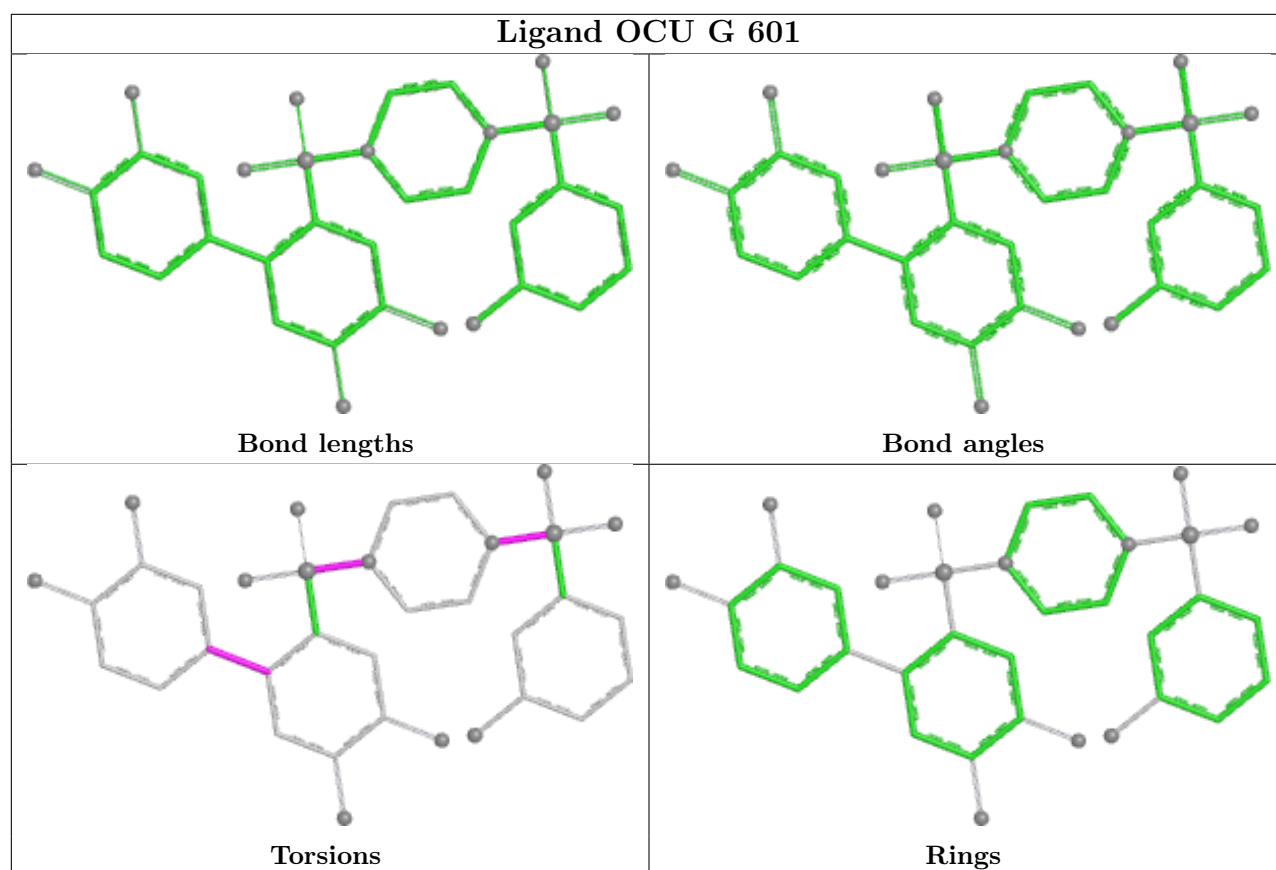


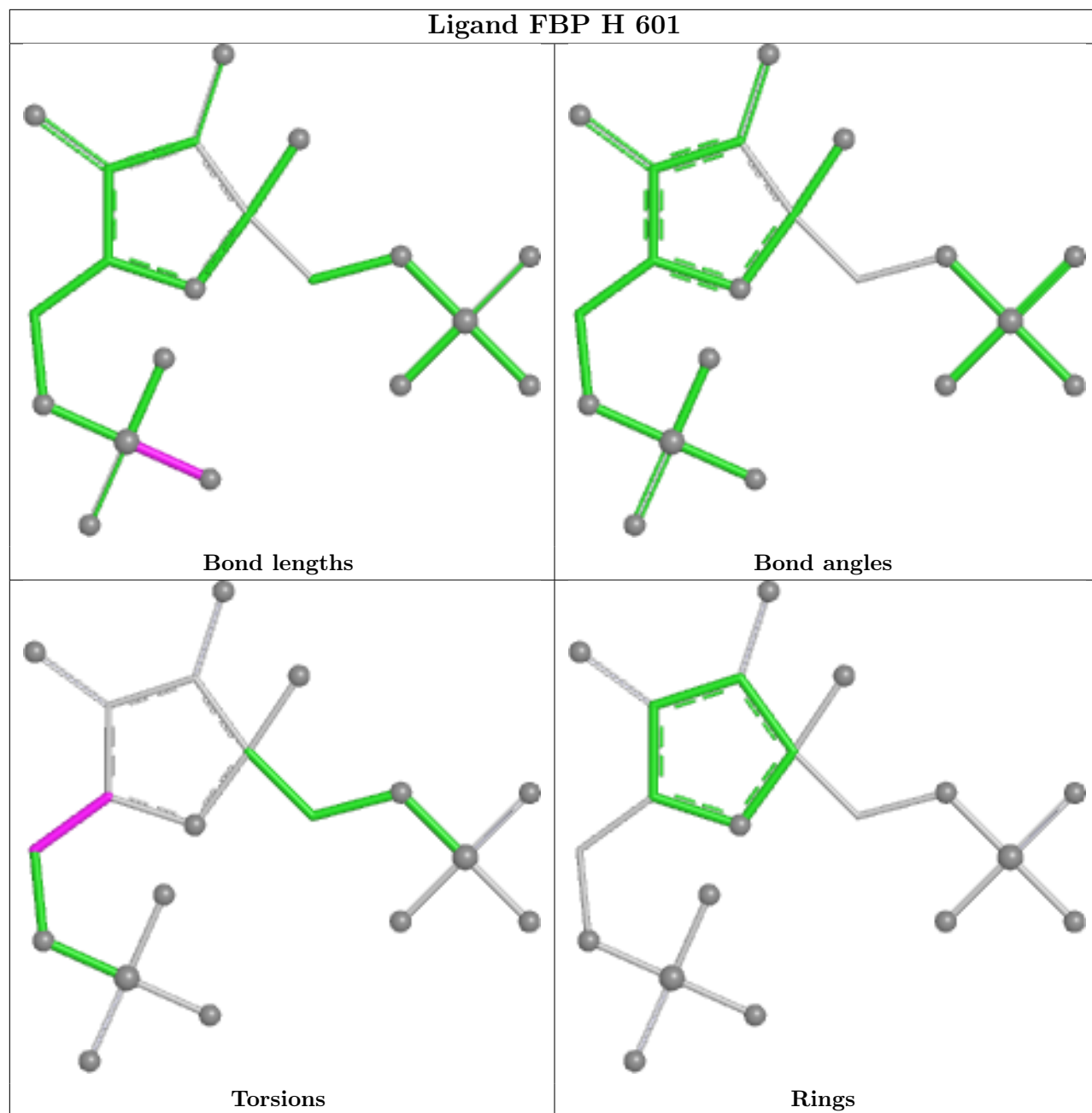
Ligand FBP F 601

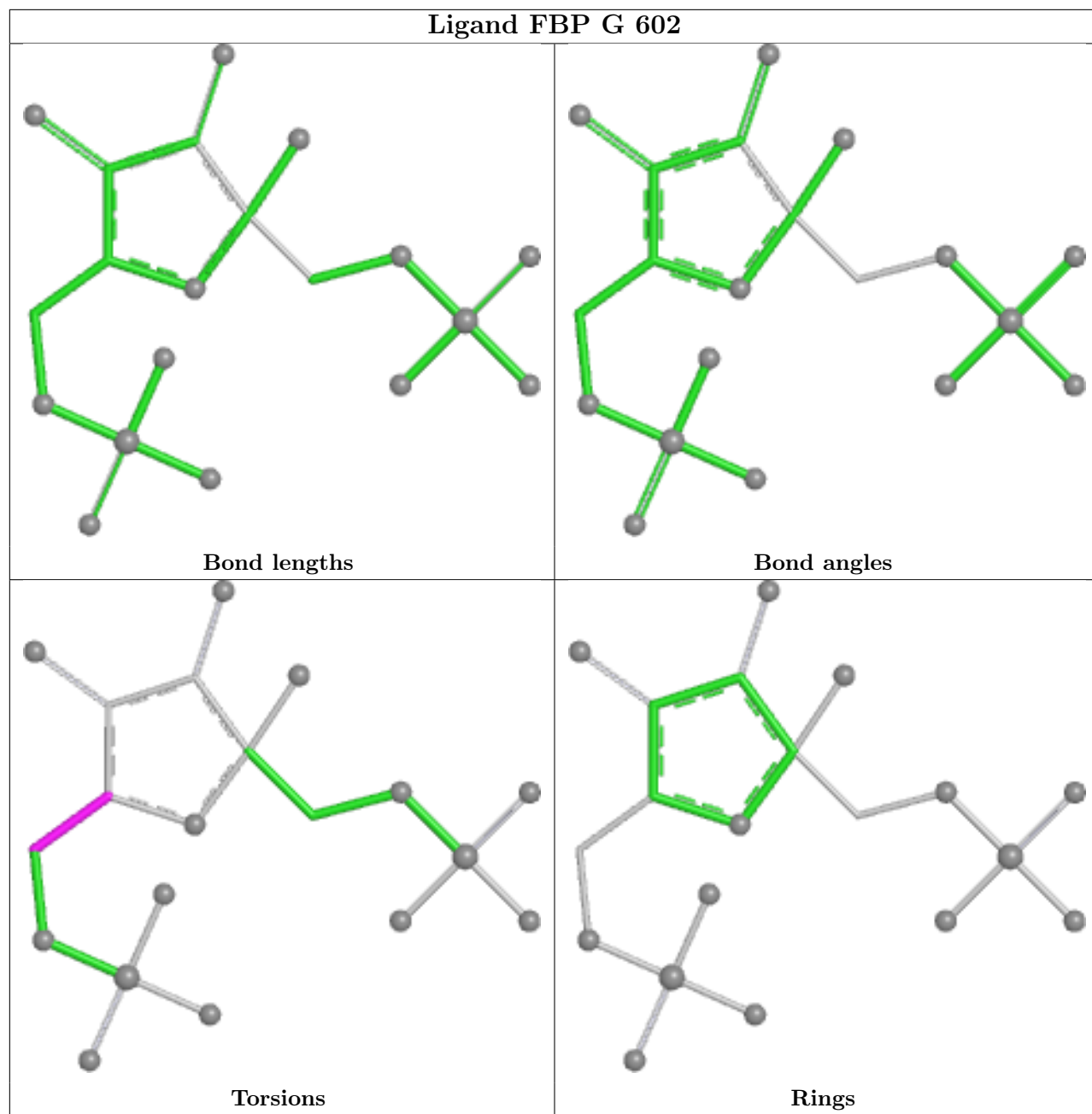


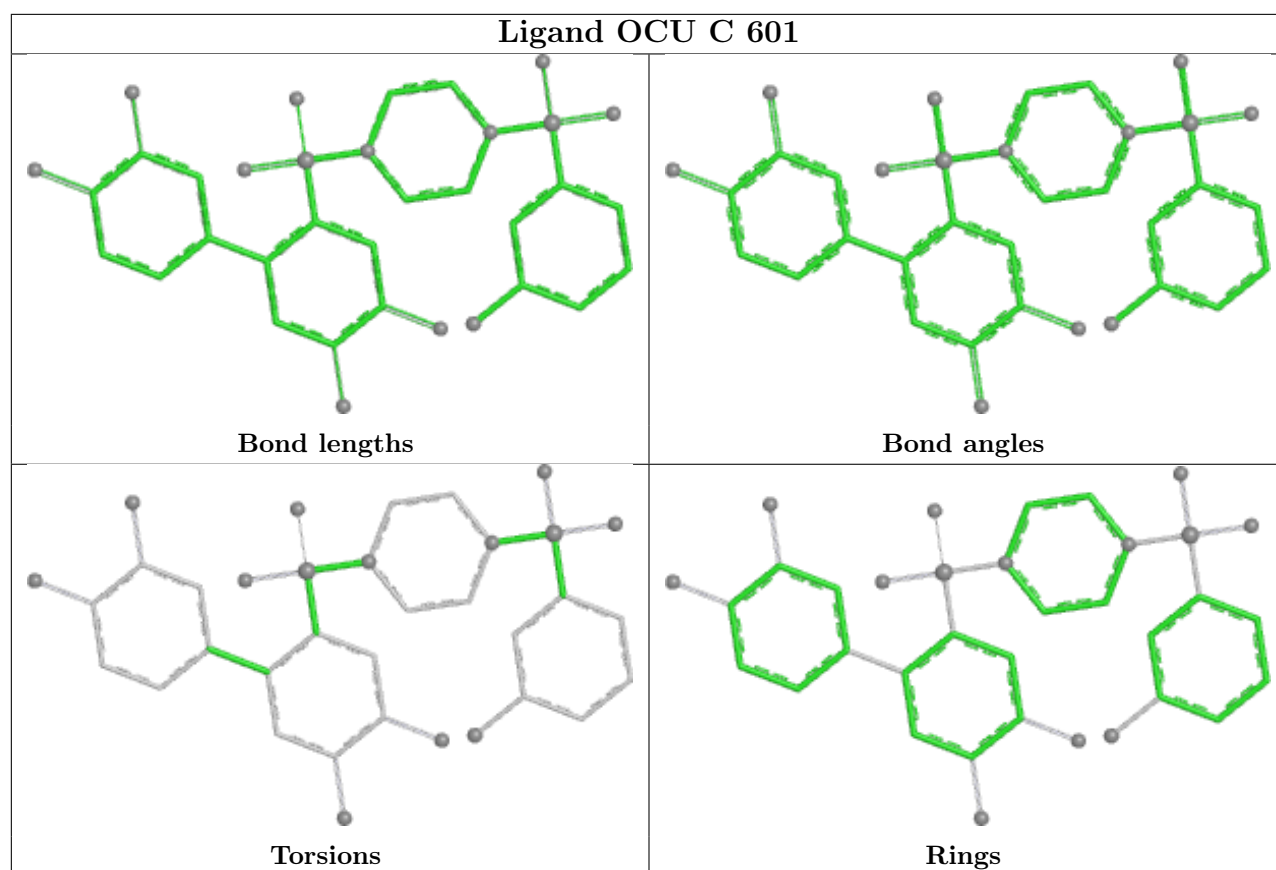
Ligand FBP E 601



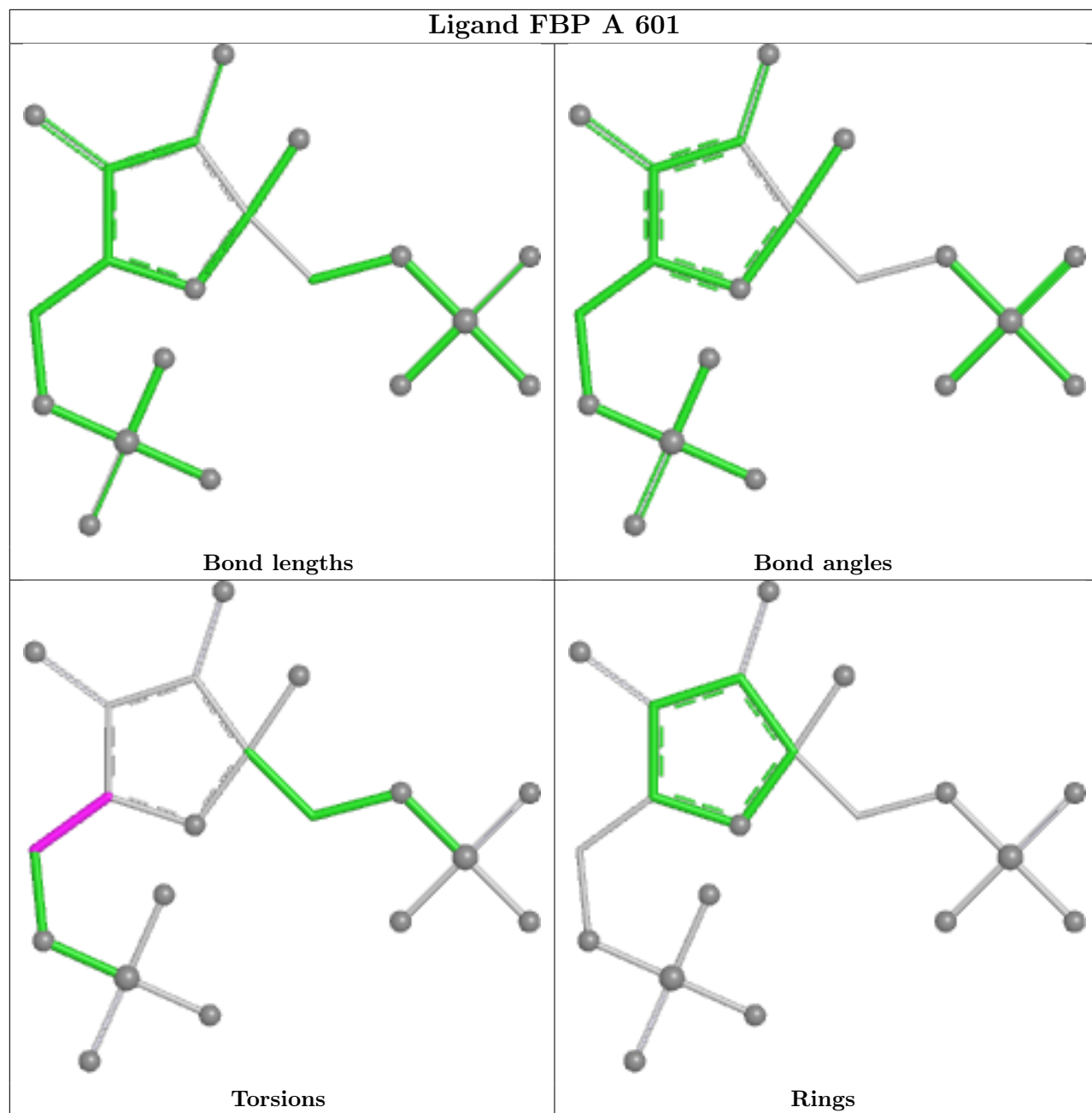


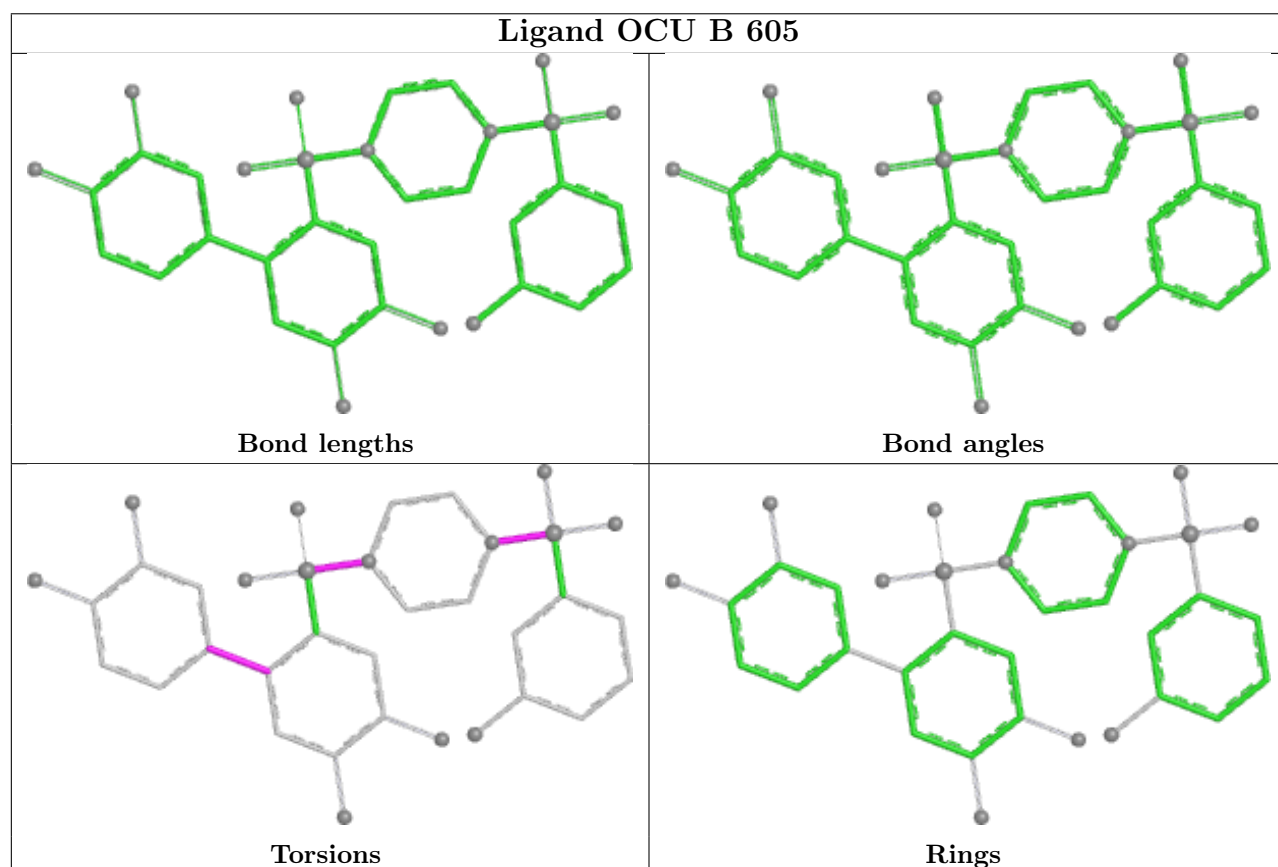
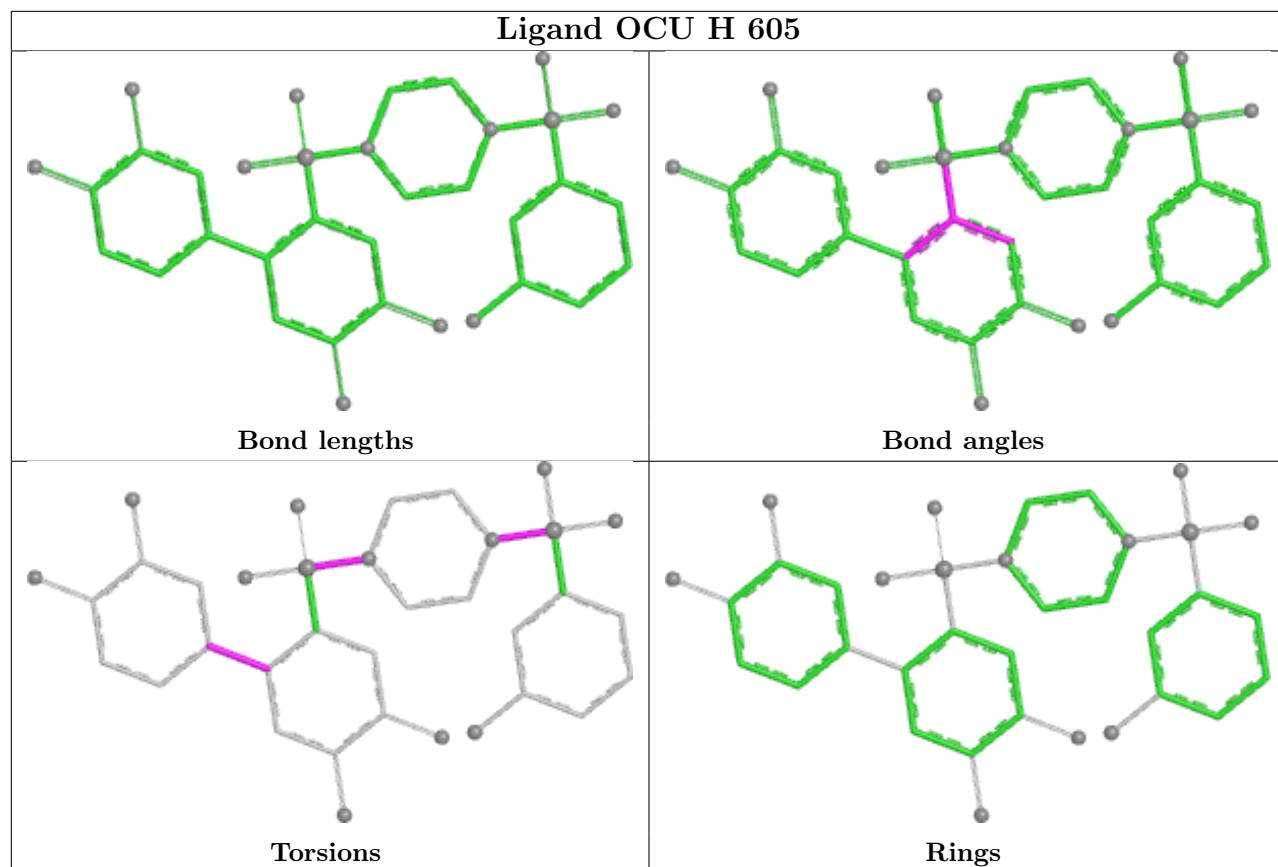


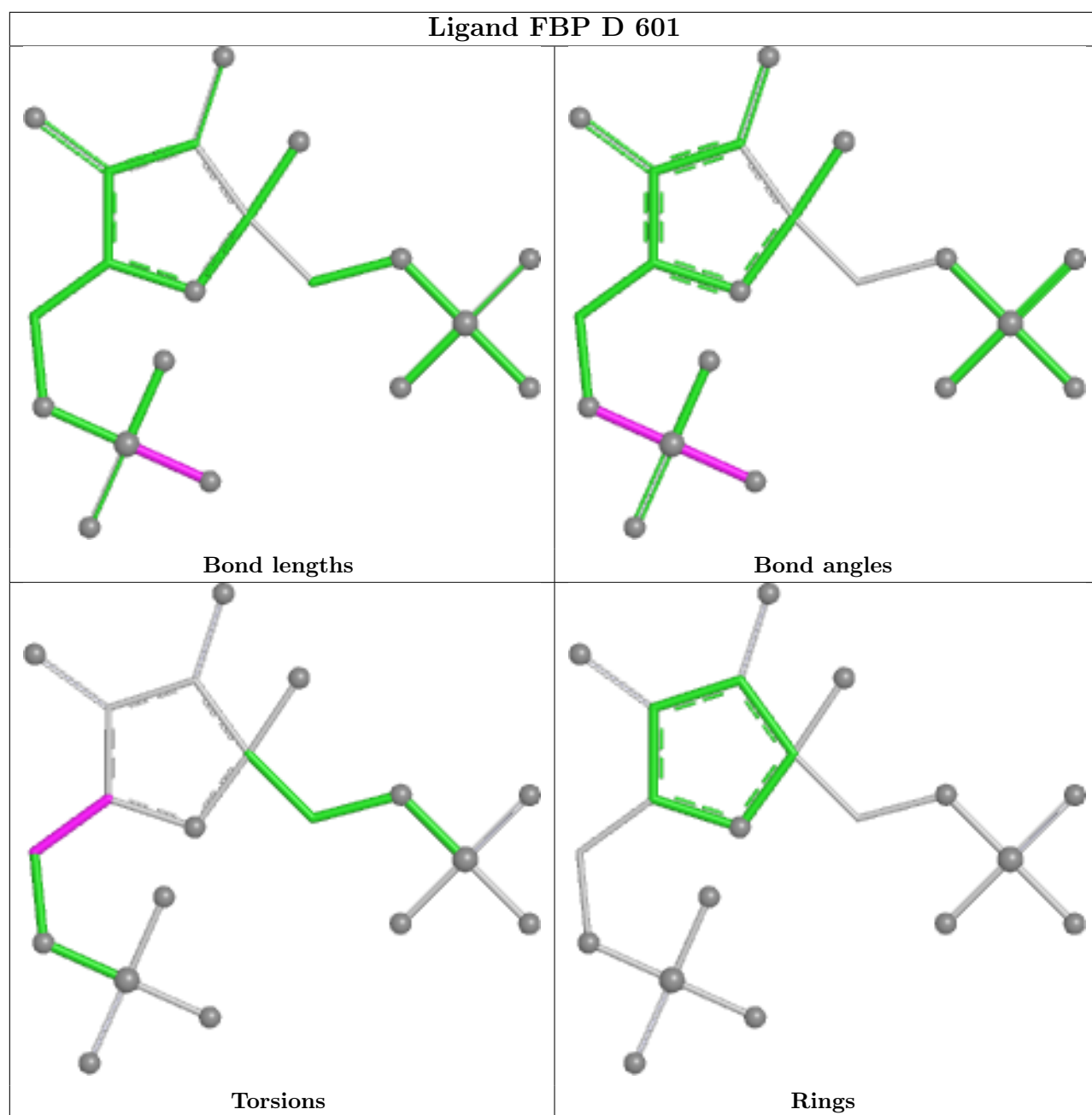




Ligand FBP A 601







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%)	1.47	107 (25%) 1 1	24, 50, 76, 94	6 (1%)
1	B	436/447 (97%)	1.07	79 (18%) 3 3	23, 44, 72, 89	4 (0%)
1	C	425/447 (95%)	0.76	55 (12%) 7 7	21, 38, 64, 117	4 (0%)
1	D	425/447 (95%)	0.19	20 (4%) 36 39	16, 31, 53, 99	6 (1%)
1	E	419/447 (93%)	1.87	158 (37%) 1 0	24, 53, 84, 94	5 (1%)
1	F	432/447 (96%)	1.01	70 (16%) 4 4	24, 41, 67, 81	7 (1%)
1	G	421/447 (94%)	0.47	24 (5%) 29 31	20, 35, 56, 89	7 (1%)
1	H	425/447 (95%)	0.11	18 (4%) 40 43	15, 30, 52, 93	4 (0%)
All	All	3405/3576 (95%)	0.87	531 (15%) 5 5	15, 40, 72, 117	43 (1%)

All (531) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	115	LEU	11.1
1	A	25	PHE	10.4
1	D	25	PHE	10.0
1	F	115	LEU	9.8
1	B	114	PRO	8.4
1	E	25	PHE	8.3
1	C	20	LEU	7.7
1	B	116	SER	7.5
1	C	25	PHE	7.4
1	G	271	GLY	7.2
1	H	25	PHE	7.2
1	F	116	SER	7.0
1	G	25	PHE	6.9
1	E	114	PRO	6.9
1	F	114	PRO	6.5
1	H	21	GLY	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	502	VAL	6.2
1	A	132	GLY	6.1
1	E	115	LEU	6.0
1	D	22	THR	5.9
1	E	129	PRO	5.9
1	E	442	VAL	5.8
1	D	24	PHE	5.7
1	E	485	LEU	5.5
1	E	23	ALA	5.5
1	H	24	PHE	5.5
1	D	21	GLY	5.4
1	B	489	PRO	5.4
1	E	257	VAL	5.3
1	G	24	PHE	5.3
1	B	13	VAL	5.3
1	C	271	GLY	5.3
1	E	249	VAL	5.2
1	E	464	ALA	5.2
1	G	23	ALA	5.1
1	E	270	LEU	5.1
1	B	490	PRO	5.1
1	A	238	VAL	5.1
1	E	504	PHE	5.0
1	E	495	ALA	5.0
1	F	231	PRO	5.0
1	F	489	PRO	4.9
1	E	505	GLY	4.9
1	E	540	LEU	4.9
1	E	232	GLY	4.9
1	E	30	LEU	4.8
1	A	23	ALA	4.7
1	H	23	ALA	4.7
1	C	24	PHE	4.7
1	C	22	THR	4.7
1	H	22	THR	4.7
1	E	233	LEU	4.7
1	A	114	PRO	4.6
1	E	269	ALA	4.5
1	A	115	LEU	4.5
1	B	14	ALA	4.5
1	E	111	ALA	4.4
1	A	112	GLY	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	232	GLY	4.4
1	E	110	PHE	4.3
1	F	484	LEU	4.3
1	E	24	PHE	4.3
1	E	117	TYR	4.3
1	A	540	LEU	4.2
1	B	511	LEU	4.2
1	E	101	ALA	4.2
1	E	238	VAL	4.2
1	D	23	ALA	4.2
1	A	24	PHE	4.2
1	A	270	LEU	4.2
1	F	233	LEU	4.2
1	E	541[A]	SER	4.1
1	C	23	ALA	4.1
1	E	437	ALA	4.1
1	A	34	MET	4.1
1	E	490	PRO	4.1
1	B	411	ARG	4.1
1	F	238	VAL	4.0
1	F	267[A]	ARG	4.0
1	A	30	LEU	4.0
1	A	117	TYR	4.0
1	B	117	TYR	4.0
1	E	26	GLN	4.0
1	E	489	PRO	4.0
1	A	482	PHE	4.0
1	B	112	GLY	3.9
1	E	511	LEU	3.9
1	F	416	LEU	3.9
1	C	231	PRO	3.8
1	F	112	GLY	3.8
1	E	499	ASP	3.8
1	C	117	TYR	3.8
1	E	486	TYR	3.8
1	E	484	LEU	3.8
1	E	264	ALA	3.8
1	E	465	VAL	3.8
1	F	498	VAL	3.8
1	E	514	PHE	3.8
1	B	118	ARG	3.8
1	E	263	VAL	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	256	PHE	3.7
1	C	232	GLY	3.7
1	C	111	ALA	3.7
1	C	115	LEU	3.6
1	C	66	ALA	3.6
1	H	411	ARG	3.6
1	E	124	LEU	3.6
1	B	21	GLY	3.6
1	E	493	ILE	3.6
1	G	231	PRO	3.6
1	H	231	PRO	3.6
1	B	269	ALA	3.6
1	E	487	ARG	3.6
1	B	130	GLY	3.6
1	F	492	ALA	3.5
1	C	75	GLU	3.5
1	E	109	SER	3.5
1	F	516	ARG	3.5
1	F	414	ALA	3.5
1	A	378	ALA	3.5
1	B	432	ALA	3.5
1	B	267[A]	ARG	3.5
1	F	512	ARG	3.5
1	B	25	PHE	3.5
1	F	488	GLU	3.4
1	A	130	GLY	3.4
1	E	70	VAL	3.4
1	C	132	GLY	3.4
1	B	492	ALA	3.4
1	A	116	SER	3.4
1	B	132	GLY	3.4
1	A	111	ALA	3.4
1	E	116	SER	3.4
1	A	118	ARG	3.4
1	H	273	GLU	3.3
1	C	21	GLY	3.3
1	E	120	VAL	3.3
1	A	543	SER	3.3
1	E	122	ILE	3.3
1	B	484	LEU	3.3
1	B	415	PRO	3.3
1	F	427	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	113	SER	3.3
1	B	111	ALA	3.3
1	A	233	LEU	3.3
1	F	487	ARG	3.3
1	E	498	VAL	3.2
1	E	524	VAL	3.2
1	A	86	LEU	3.2
1	D	30	LEU	3.2
1	E	243	PHE	3.2
1	A	488[A]	GLU	3.2
1	F	453	LEU	3.2
1	C	110	PHE	3.2
1	E	292	PHE	3.2
1	A	277	ILE	3.2
1	E	506	ILE	3.2
1	A	70	VAL	3.2
1	E	52	VAL	3.2
1	F	517	VAL	3.2
1	E	275	HIS	3.2
1	B	413	ALA	3.1
1	B	231	PRO	3.1
1	E	245	VAL	3.1
1	E	274	GLY	3.1
1	H	30	LEU	3.1
1	A	88	PHE	3.1
1	A	243	PHE	3.1
1	B	348	THR	3.1
1	E	63	ILE	3.1
1	E	426	ILE	3.1
1	F	490	PRO	3.1
1	E	351	ARG	3.1
1	E	112	GLY	3.1
1	E	28	GLN	3.1
1	E	118	ARG	3.1
1	E	242	ARG	3.1
1	B	414	ALA	3.1
1	A	100	ILE	3.1
1	E	447	GLY	3.1
1	A	241	LEU	3.1
1	F	540[A]	LEU	3.1
1	B	242	ARG	3.1
1	E	500	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	493	ILE	3.0
1	E	277	ILE	3.0
1	E	542	ILE	3.0
1	B	416	LEU	3.0
1	E	241	LEU	3.0
1	F	521	VAL	3.0
1	E	126	THR	3.0
1	C	490	PRO	3.0
1	E	244	GLY	3.0
1	B	11	ALA	3.0
1	E	100	ILE	3.0
1	C	34	MET	3.0
1	G	30	LEU	3.0
1	H	516	ARG	3.0
1	A	51	PRO	3.0
1	E	276	GLY	3.0
1	F	232	GLY	3.0
1	E	97	ALA	3.0
1	F	351	ARG	3.0
1	F	411	ARG	3.0
1	E	309	LEU	3.0
1	E	466	THR	3.0
1	B	487	ARG	3.0
1	G	33	ALA	3.0
1	D	273	GLU	3.0
1	F	270	LEU	2.9
1	C	103	VAL	2.9
1	E	266	VAL	2.9
1	F	379	LYS	2.9
1	B	512	ARG	2.9
1	H	412	ARG	2.9
1	H	34	MET	2.9
1	A	279	ILE	2.9
1	A	426	ILE	2.9
1	E	536	ILE	2.9
1	A	113	SER	2.9
1	E	481	VAL	2.9
1	C	63	ILE	2.9
1	F	493	ILE	2.9
1	A	485	LEU	2.9
1	B	233	LEU	2.9
1	D	275[A]	HIS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	265	ALA	2.9
1	A	73	LEU	2.9
1	A	124	LEU	2.9
1	G	132	GLY	2.9
1	B	107	VAL	2.8
1	B	521	VAL	2.8
1	A	110	PHE	2.8
1	A	260	ALA	2.8
1	E	88	PHE	2.8
1	E	428	ALA	2.8
1	E	436	CYS	2.8
1	E	113	SER	2.8
1	A	249	VAL	2.8
1	E	103	VAL	2.8
1	A	514	PHE	2.8
1	B	110	PHE	2.8
1	C	411	ARG	2.8
1	E	331	LEU	2.8
1	A	95	TYR	2.8
1	F	268	ALA	2.8
1	F	504	PHE	2.8
1	A	275	HIS	2.8
1	A	311	ILE	2.8
1	A	120	VAL	2.8
1	E	482	PHE	2.7
1	B	488	GLU	2.7
1	H	275[A]	HIS	2.7
1	E	271	GLY	2.7
1	E	440	ILE	2.7
1	A	489	PRO	2.7
1	D	34	MET	2.7
1	E	272	PRO	2.7
1	A	63	ILE	2.7
1	A	52	VAL	2.7
1	E	95	TYR	2.7
1	B	504	PHE	2.7
1	E	237	ASP	2.7
1	A	453	LEU	2.7
1	B	543	SER	2.7
1	F	129	PRO	2.7
1	A	542	ILE	2.7
1	B	347	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	302	ILE	2.7
1	A	33	ALA	2.6
1	A	66	ALA	2.6
1	D	232	GLY	2.6
1	C	26	GLN	2.6
1	G	272	PRO	2.6
1	F	241	LEU	2.6
1	B	100	ILE	2.6
1	F	90	HIS	2.6
1	A	266	VAL	2.6
1	C	107	VAL	2.6
1	E	123	ALA	2.6
1	E	254	ALA	2.6
1	E	260	ALA	2.6
1	E	533	TYR	2.6
1	E	234	SER	2.6
1	E	483	PRO	2.6
1	E	411	ARG	2.6
1	A	268	ALA	2.6
1	E	539	VAL	2.6
1	E	510	LYS	2.6
1	E	456	TYR	2.6
1	F	243	PHE	2.6
1	E	494	TRP	2.6
1	C	30	LEU	2.6
1	E	86	LEU	2.6
1	E	443	LEU	2.6
1	H	242	ARG	2.6
1	A	26	GLN	2.6
1	C	385	GLU	2.6
1	A	475	VAL	2.6
1	E	384	VAL	2.6
1	A	382	PHE	2.5
1	B	540[A]	LEU	2.5
1	E	73	LEU	2.5
1	A	274	GLY	2.5
1	A	463	ILE	2.5
1	B	251	ILE	2.5
1	E	251	ILE	2.5
1	E	513	GLY	2.5
1	G	311	ILE	2.5
1	A	264	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	269	ALA	2.5
1	E	475	VAL	2.5
1	A	351	ARG	2.5
1	B	459	ARG	2.5
1	F	412	ARG	2.5
1	G	412	ARG	2.5
1	E	491	GLU	2.5
1	F	527	TRP	2.5
1	E	538	ARG	2.5
1	F	242	ARG	2.5
1	E	492	ALA	2.5
1	F	269	ALA	2.5
1	C	71	GLU	2.5
1	B	12	ASP	2.5
1	C	95	TYR	2.5
1	F	533	TYR	2.5
1	C	380	GLY	2.5
1	E	543	SER	2.5
1	F	295	ILE	2.5
1	A	236	GLN	2.5
1	E	236	GLN	2.5
1	E	488	GLU	2.5
1	G	54	ALA	2.5
1	B	379	LYS	2.5
1	F	117	TYR	2.4
1	F	418	ARG	2.4
1	E	515	LEU	2.4
1	B	71	GLU	2.4
1	F	277	ILE	2.4
1	E	121	ALA	2.4
1	E	268	ALA	2.4
1	A	129	PRO	2.4
1	E	119	PRO	2.4
1	E	473	ARG	2.4
1	F	118	ARG	2.4
1	F	274	GLY	2.4
1	H	514	PHE	2.4
1	A	493	ILE	2.4
1	A	84	ALA	2.4
1	A	101	ALA	2.4
1	A	258	ARG	2.4
1	G	411	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	231	PRO	2.4
1	A	103	VAL	2.4
1	B	70	VAL	2.4
1	E	521	VAL	2.4
1	C	116	SER	2.4
1	E	407	PHE	2.4
1	C	348	THR	2.4
1	A	265	ALA	2.4
1	B	123	ALA	2.4
1	D	413	ALA	2.4
1	A	28	GLN	2.4
1	C	114	PRO	2.4
1	F	415	PRO	2.4
1	A	107	VAL	2.4
1	A	298	VAL	2.4
1	F	12	ASP	2.3
1	B	241	LEU	2.3
1	C	118	ARG	2.3
1	A	533	TYR	2.3
1	C	37	THR	2.3
1	E	75	GLU	2.3
1	A	27	GLN	2.3
1	A	460	ALA	2.3
1	A	492	ALA	2.3
1	E	439	ALA	2.3
1	E	469	ALA	2.3
1	F	265	ALA	2.3
1	C	384	VAL	2.3
1	F	109	SER	2.3
1	A	496	ASP	2.3
1	F	507	GLU	2.3
1	D	26	GLN	2.3
1	G	26	GLN	2.3
1	B	256	PHE	2.3
1	A	106	ALA	2.3
1	A	471	ALA	2.3
1	B	311	ILE	2.3
1	F	347	ILE	2.3
1	B	129	PRO	2.3
1	G	34	MET	2.3
1	A	80	GLY	2.3
1	E	509	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	232	GLY	2.3
1	D	412	ARG	2.3
1	B	266	VAL	2.3
1	A	494	TRP	2.3
1	A	515	LEU	2.3
1	B	16	LEU	2.3
1	B	270	LEU	2.3
1	F	275	HIS	2.3
1	B	232	GLY	2.3
1	C	68	ARG	2.3
1	C	311	ILE	2.3
1	C	412	ARG	2.3
1	A	531	SER	2.3
1	F	237	ASP	2.3
1	G	71	GLU	2.3
1	B	17	THR	2.3
1	H	416	LEU	2.3
1	G	487	ARG	2.2
1	B	24	PHE	2.2
1	B	128	GLY	2.2
1	F	95	TYR	2.2
1	E	508	SER	2.2
1	F	543	SER	2.2
1	D	311	ILE	2.2
1	F	240	ASP	2.2
1	G	63	ILE	2.2
1	A	384	VAL	2.2
1	C	90	HIS	2.2
1	F	34	MET	2.2
1	B	22	THR	2.2
1	C	94	GLU	2.2
1	F	94	GLU	2.2
1	F	124	LEU	2.2
1	B	91	GLY	2.2
1	A	472	ALA	2.2
1	E	300	ASP	2.2
1	A	256	PHE	2.2
1	F	494	TRP	2.2
1	G	514	PHE	2.2
1	E	59	ILE	2.2
1	E	34	MET	2.2
1	E	459	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	263	VAL	2.2
1	E	304	VAL	2.2
1	G	75	GLU	2.2
1	B	236	GLN	2.2
1	A	109	SER	2.2
1	B	131	SER	2.2
1	C	109	SER	2.2
1	A	413	ALA	2.2
1	A	77	ILE	2.2
1	A	242	ARG	2.2
1	E	102	ASN	2.2
1	E	501	ARG	2.2
1	A	75	GLU	2.2
1	A	108	GLU	2.2
1	F	15	GLN	2.2
1	F	298	VAL	2.2
1	E	478	CYS	2.2
1	F	531	SER	2.2
1	B	20	LEU	2.2
1	C	129	PRO	2.2
1	A	464	ALA	2.2
1	B	268	ALA	2.2
1	C	487	ARG	2.2
1	G	351	ARG	2.2
1	B	95	TYR	2.1
1	B	507	GLU	2.1
1	C	382	PHE	2.1
1	D	408	GLU	2.1
1	E	253	PHE	2.1
1	E	522	ILE	2.1
1	C	27	GLN	2.1
1	E	519	ASP	2.1
1	C	70	VAL	2.1
1	E	289	VAL	2.1
1	G	52	VAL	2.1
1	E	531	SER	2.1
1	A	91	GLY	2.1
1	B	271	GLY	2.1
1	C	112	GLY	2.1
1	E	267	ARG	2.1
1	A	79	ALA	2.1
1	C	386	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	11	ALA	2.1
1	B	88	PHE	2.1
1	C	77	ILE	2.1
1	C	347	ILE	2.1
1	A	56	SER	2.1
1	A	99	SER	2.1
1	C	69	SER	2.1
1	E	527	TRP	2.1
1	A	271	GLY	2.1
1	E	412	ARG	2.1
1	A	90	HIS	2.1
1	E	90	HIS	2.1
1	E	370	CYS	2.1
1	C	45	LEU	2.1
1	C	511	LEU	2.1
1	E	461	ALA	2.1
1	G	53	ALA	2.1
1	E	240	ASP	2.1
1	A	69	SER	2.1
1	F	273	GLU	2.1
1	F	510	LYS	2.1
1	C	64	GLY	2.1
1	E	336	VAL	2.1
1	B	272	PRO	2.1
1	E	520	LEU	2.1
1	E	106	ALA	2.1
1	E	472	ALA	2.1
1	A	68	ARG	2.1
1	D	459	ARG	2.1
1	A	253	PHE	2.0
1	A	407	PHE	2.0
1	A	441	ILE	2.0
1	B	109	SER	2.0
1	B	506	ILE	2.0
1	C	514	PHE	2.0
1	D	130	GLY	2.0
1	E	128	GLY	2.0
1	B	257	VAL	2.0
1	B	73	LEU	2.0
1	D	436	CYS	2.0
1	D	515	LEU	2.0
1	E	452	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	443	LEU	2.0
1	H	515	LEU	2.0
1	B	106	ALA	2.0
1	B	418	ARG	2.0
1	F	459	ARG	2.0
1	E	503	GLN	2.0
1	A	252	VAL	2.0
1	C	459	ARG	2.0
1	E	107	VAL	2.0
1	E	462	VAL	2.0
1	H	404	ARG	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
6	OCU	G	601	35/35	0.81	0.21	63,65,71,72	23
6	OCU	C	601	35/35	0.82	0.19	56,59,67,68	23
5	K	E	604	1/1	0.83	0.22	88,88,88,88	0
6	OCU	H	605	35/35	0.83	0.20	52,56,63,64	23
6	OCU	B	605	35/35	0.84	0.19	47,53,64,64	23
3	OXL	E	602	6/6	0.84	0.12	49,50,50,50	0
3	OXL	A	602	6/6	0.85	0.11	60,61,61,61	0
3	OXL	F	602	6/6	0.89	0.10	45,45,46,46	0
3	OXL	D	602	6/6	0.89	0.10	38,39,39,39	0
3	OXL	G	603	6/6	0.90	0.10	40,40,40,41	0
3	OXL	C	603	6/6	0.90	0.10	50,50,50,50	0
3	OXL	B	602	6/6	0.90	0.10	42,43,43,44	0

Continued on next page...

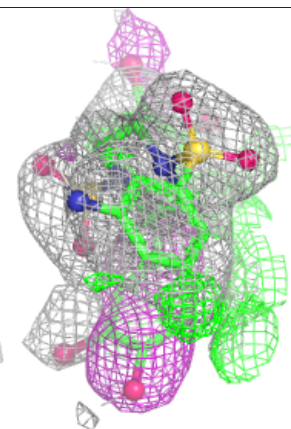
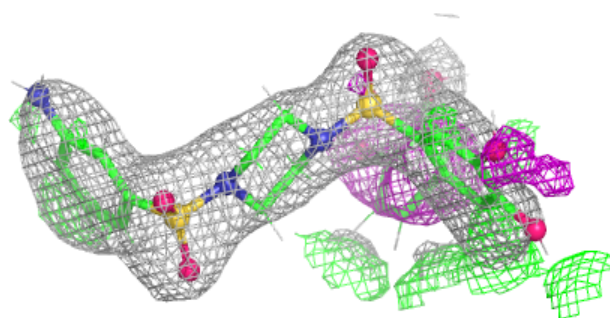
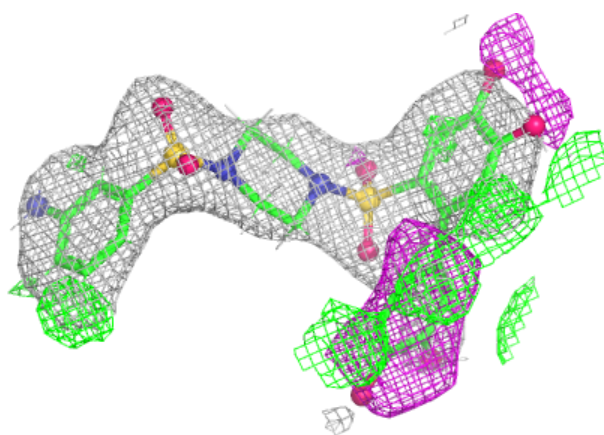
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FBP	E	601	20/20	0.92	0.10	45,46,49,49	0
5	K	A	604	1/1	0.93	0.14	69,69,69,69	0
2	FBP	F	601	20/20	0.93	0.09	39,43,47,47	0
2	FBP	B	601	20/20	0.93	0.09	40,42,44,44	0
2	FBP	A	601	20/20	0.94	0.09	42,42,43,43	0
3	OXL	H	602	6/6	0.94	0.10	34,34,35,36	0
5	K	B	604	1/1	0.95	0.14	68,68,68,68	0
4	MG	E	603	1/1	0.96	0.15	36,36,36,36	0
5	K	C	605	1/1	0.96	0.15	57,57,57,57	0
4	MG	A	603	1/1	0.96	0.12	37,37,37,37	0
5	K	F	604	1/1	0.96	0.10	80,80,80,80	0
4	MG	F	603	1/1	0.97	0.13	25,25,25,25	0
5	K	G	605	1/1	0.97	0.15	54,54,54,54	0
2	FBP	G	602	20/20	0.98	0.05	25,27,28,29	0
5	K	D	604	1/1	0.98	0.11	47,47,47,47	0
4	MG	B	603	1/1	0.98	0.14	30,30,30,30	0
5	K	H	604	1/1	0.99	0.10	51,51,51,51	0
2	FBP	H	601	20/20	0.99	0.04	23,24,26,27	0
2	FBP	D	601	20/20	0.99	0.04	24,25,27,27	0
4	MG	D	603	1/1	0.99	0.12	18,18,18,18	0
2	FBP	C	602	20/20	0.99	0.04	27,28,30,31	0
4	MG	C	604	1/1	1.00	0.11	26,26,26,26	0
4	MG	G	604	1/1	1.00	0.12	21,21,21,21	0
4	MG	H	603	1/1	1.00	0.12	17,17,17,17	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.

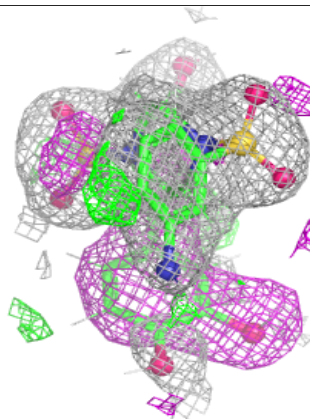
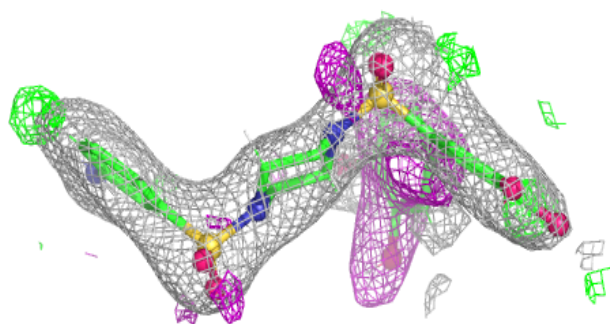
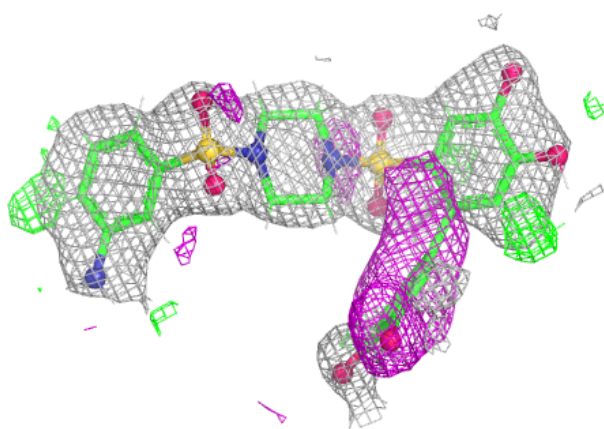
Electron density around OCU G 601:

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



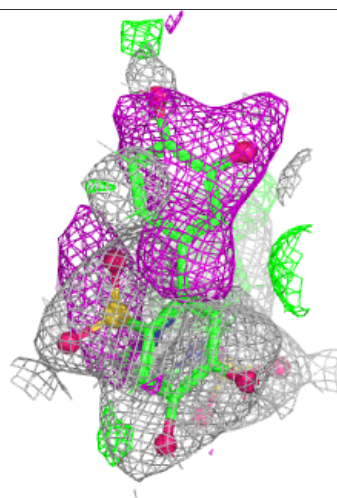
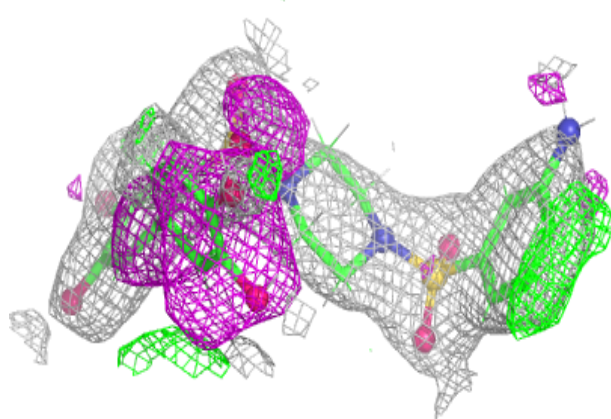
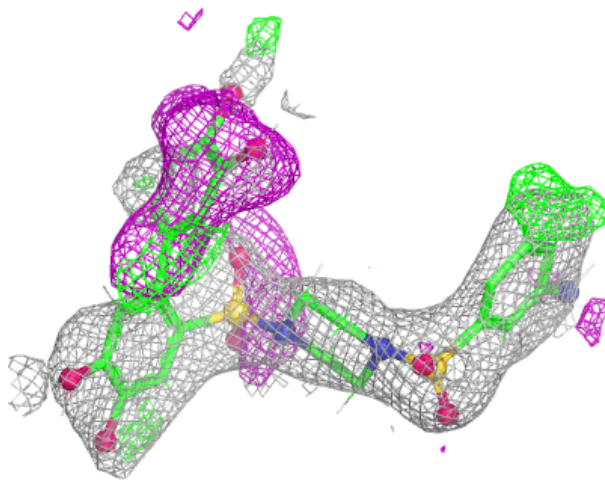
Electron density around OCU C 601:

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



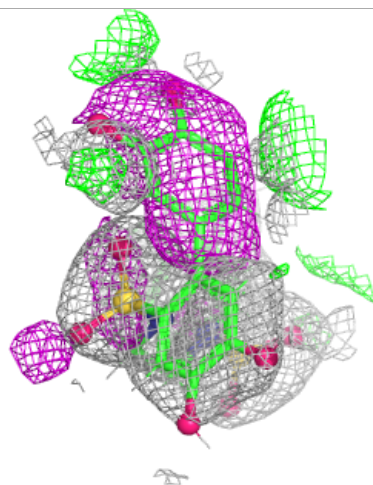
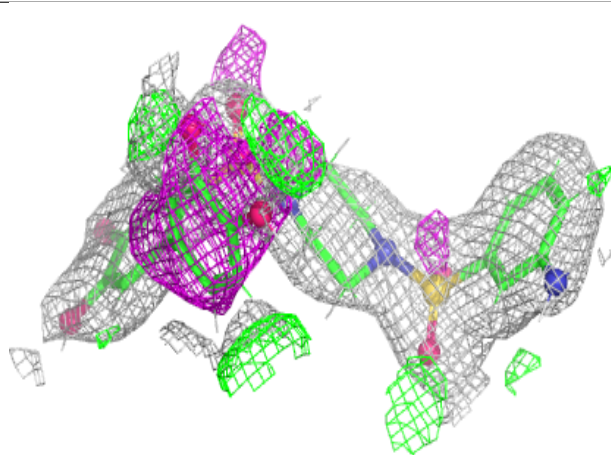
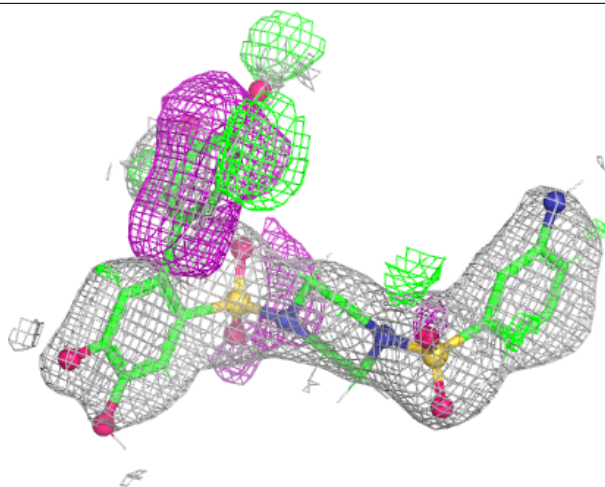
Electron density around OCU H 605:

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



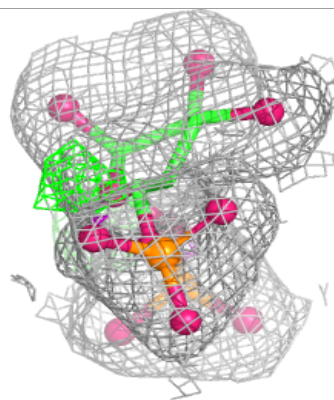
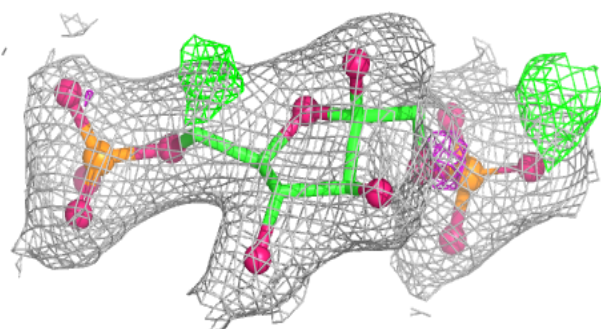
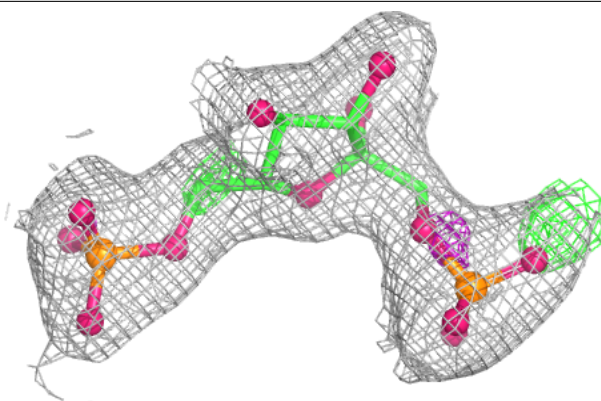
Electron density around OCU B 605:

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



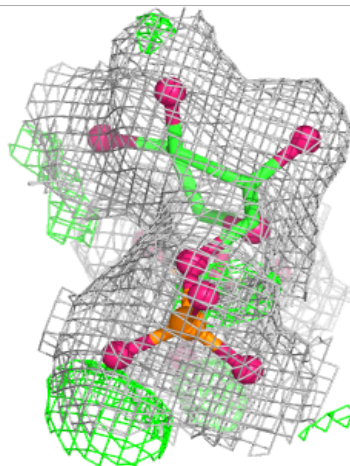
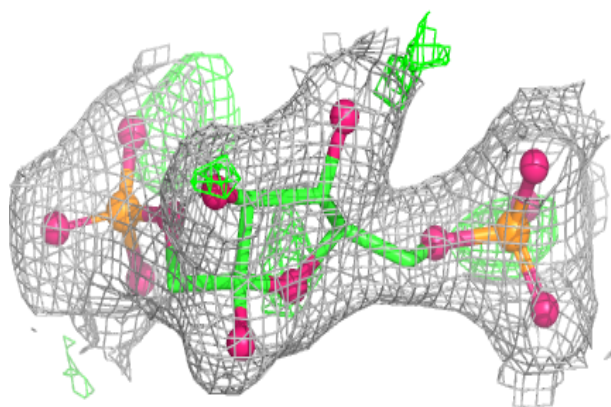
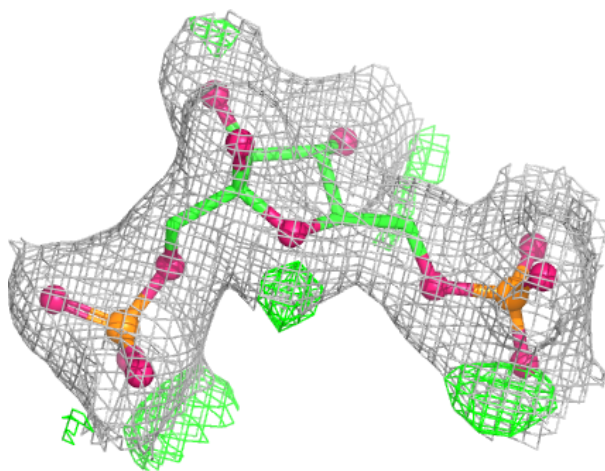
Electron density around FBP E 601:

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



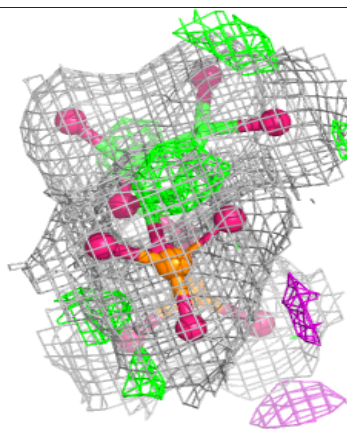
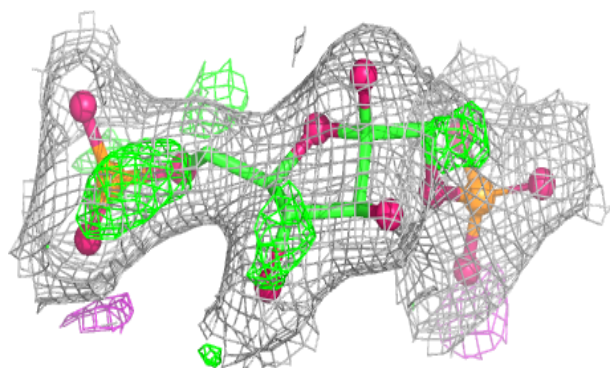
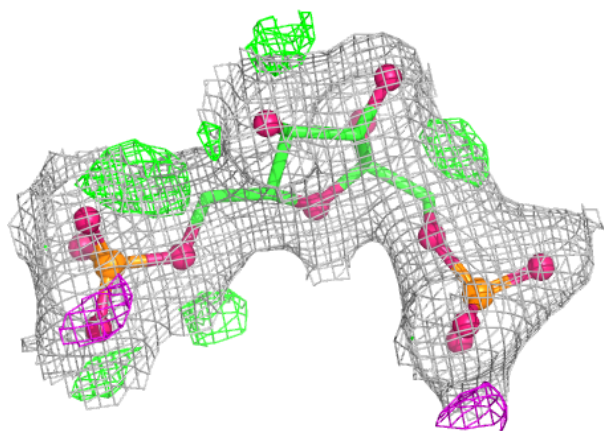
Electron density around FBP F 601:

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

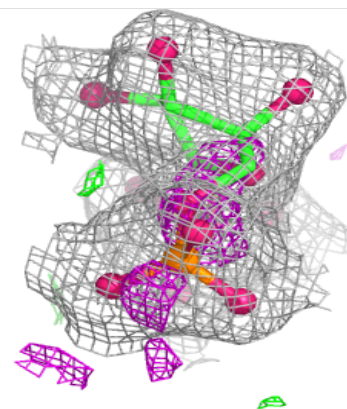
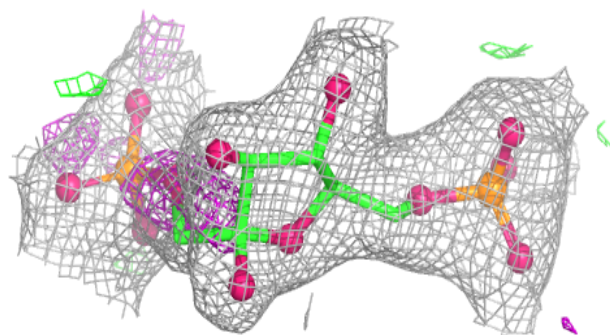
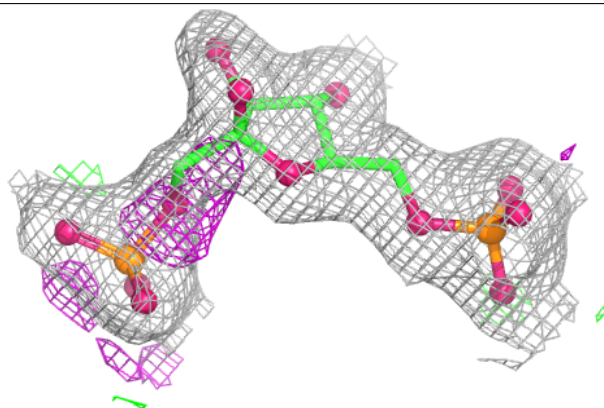


Electron density around FBP B 601:

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

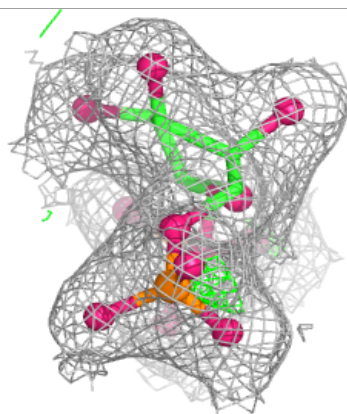
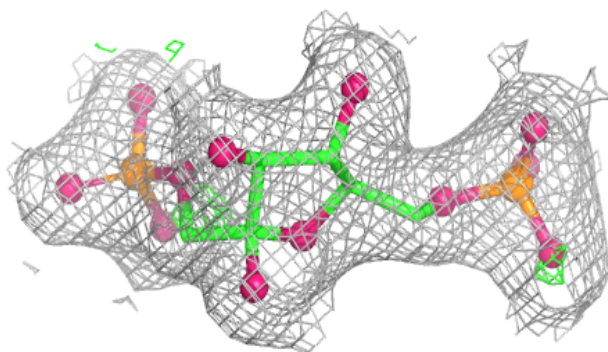
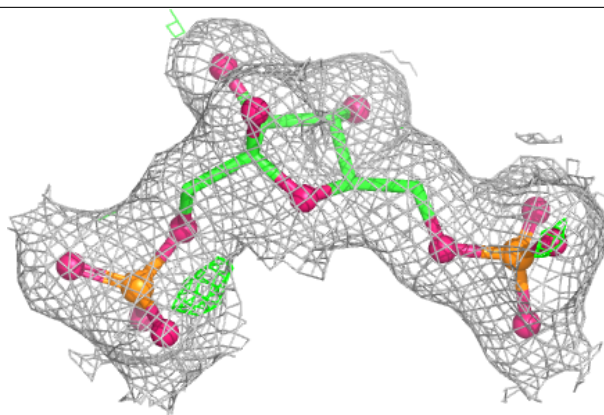
**Electron density around FBP A 601:**

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

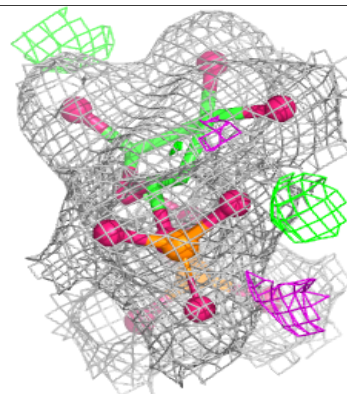
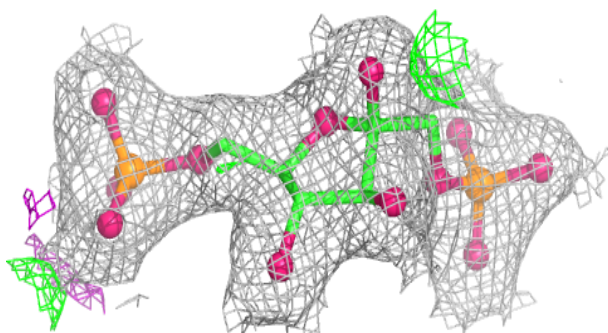
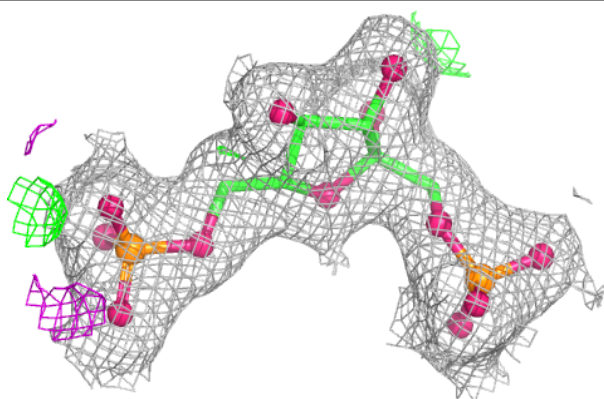


Electron density around FBP G 602:

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

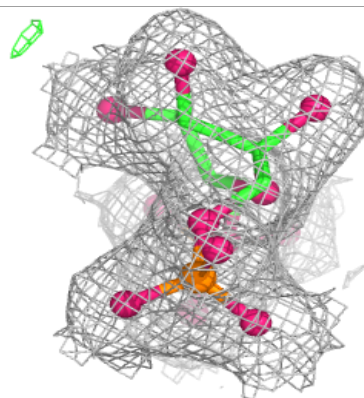
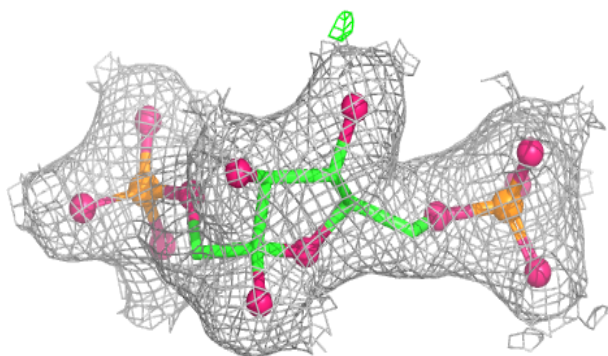
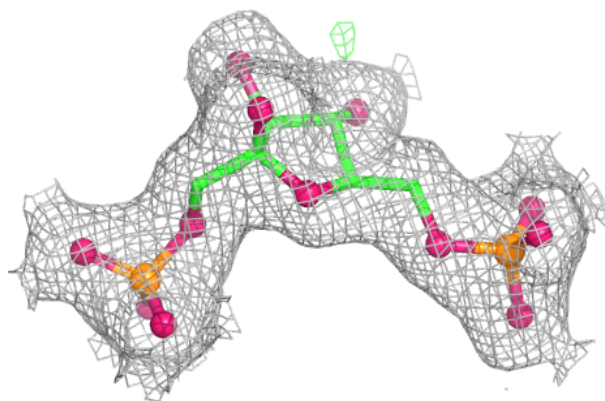
**Electron density around FBP H 601:**

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

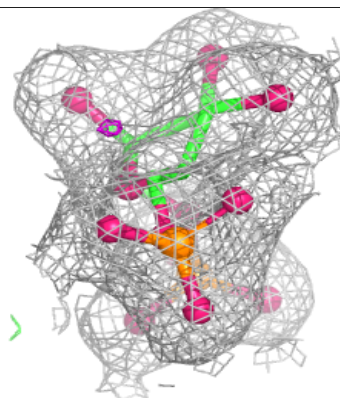
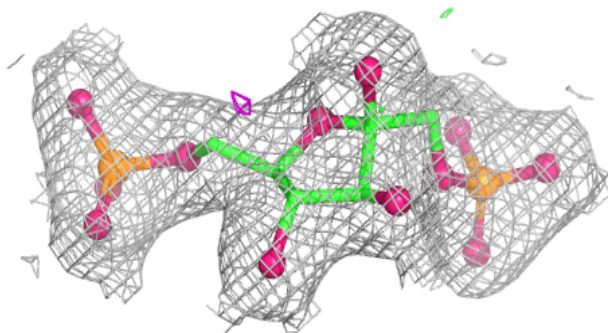
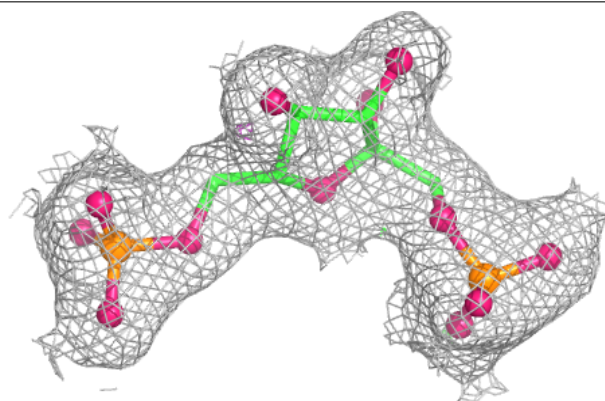


Electron density around FBP D 601:

$2mF_o-DF_c$ (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.