



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:52 PM EDT

PDB ID : 7FSD / pdb_00007fsd
Title : Structure of liver pyruvate kinase in complex with allosteric modulator 44
Authors : Lulla, A.; Nilsson, O.; Brear, P.; Nain-Perez, A.; Grotli, M.; Hyvonen, M.
Deposited on : 2022-12-18
Resolution : 1.77 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

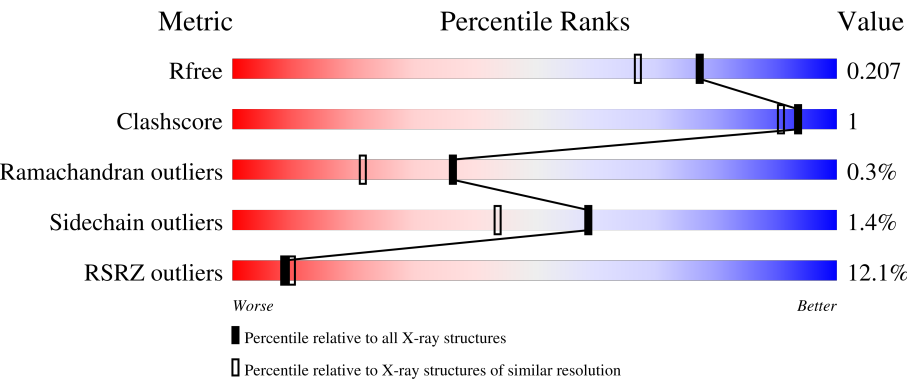
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.77 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	15% 90%6%
1	B	447	28% 91%6%
1	C	447	7% 91%5%
1	D	447	5% 91%5%
1	E	447	15% 89%5%6%

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXL	A	602	-	X	-	-
3	OXL	B	602	-	X	-	-
3	OXL	C	602	-	X	-	-
3	OXL	D	602	-	X	-	-
3	OXL	E	602	-	X	-	-
3	OXL	F	602	-	X	-	-
3	OXL	G	602	-	X	-	-
3	OXL	H	602	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 29414 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

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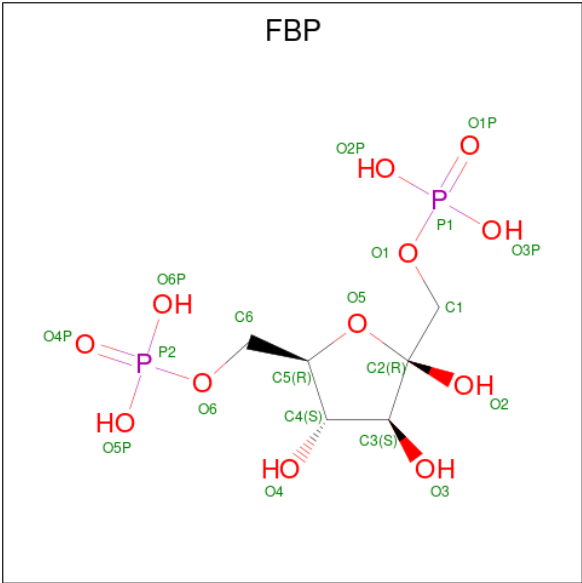
Chain	Residue	Modelled	Actual	Comment	Reference
B	130	GLY	-	linker	UNP P30613
B	131	SER	-	linker	UNP P30613
B	132	GLY	-	linker	UNP P30613
C	-1	GLY	-	expression tag	UNP P30613
C	0	SER	-	expression tag	UNP P30613
C	1	MET	-	expression tag	UNP P30613
C	2	GLU	-	expression tag	UNP P30613
C	12	ASP	SER	conflict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

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

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



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	O	P	0	0
			20	6	12	2		
2	H	1	Total	C	O	P	0	0
			20	6	12	2		

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



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

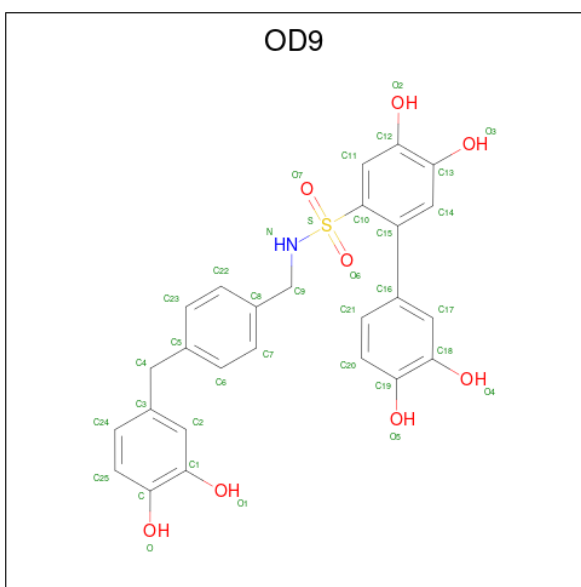
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

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

- Molecule 6 is (1M)-N-({4-[(3,4-dihydroxyphenyl)methyl]phenyl}methyl)-3',4,4',5-tetrahydroxy[1,1'-biphenyl]-2-sulfonamide (CCD ID: OD9) (formula: C₂₆H₂₃NO₈S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total 59	C 26	H 23	N 1	O 8	S 1	23	0
6	B	1	Total 59	C 26	H 23	N 1	O 8	S 1	23	0
6	E	1	Total 59	C 26	H 23	N 1	O 8	S 1	23	0
6	H	1	Total 59	C 26	H 23	N 1	O 8	S 1	23	0

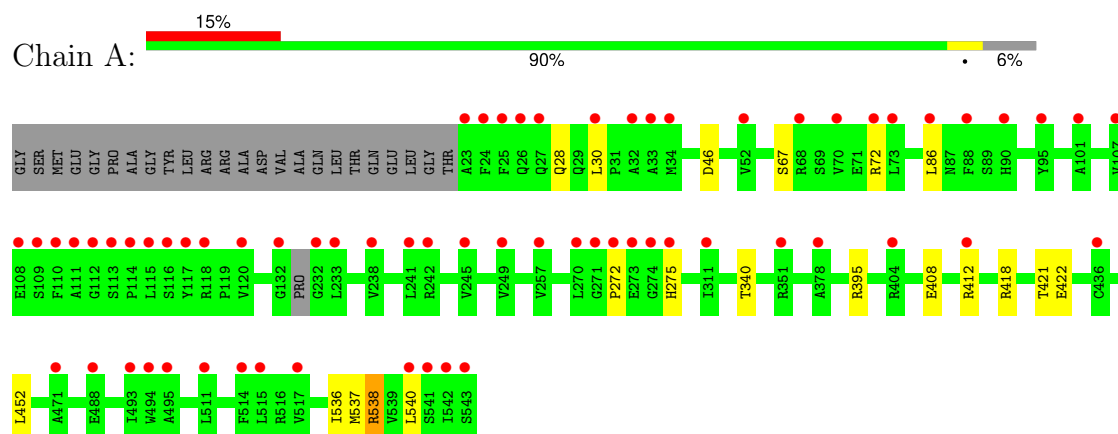
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	292	Total	O	0	0
			292	292		
7	B	248	Total	O	0	0
			248	248		
7	C	392	Total	O	0	0
			392	392		
7	D	420	Total	O	0	0
			420	420		
7	E	289	Total	O	0	0
			289	289		
7	F	351	Total	O	0	0
			351	351		
7	G	410	Total	O	0	0
			410	410		
7	H	475	Total	O	0	0
			475	475		

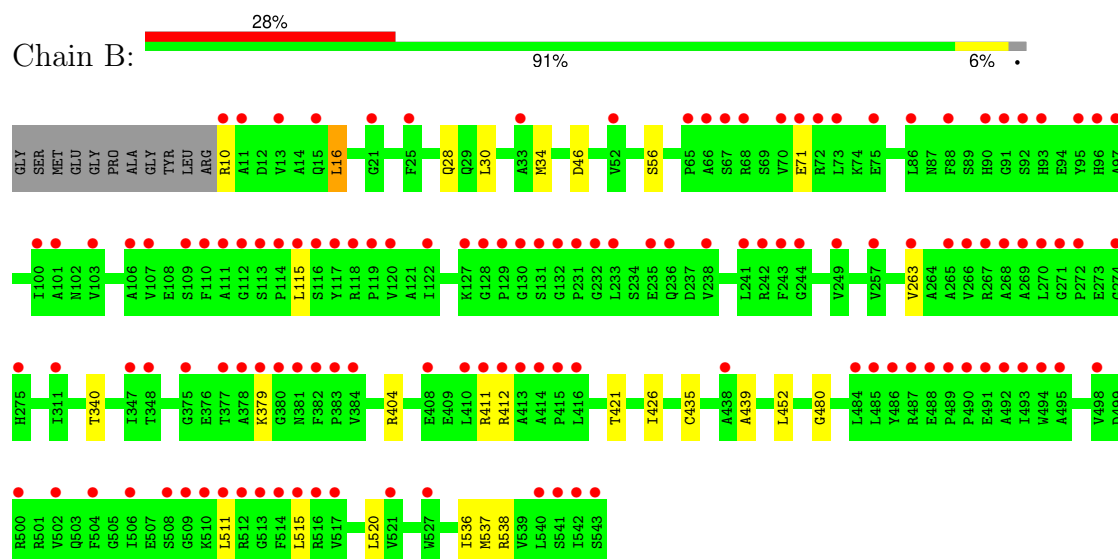
3 Residue-property plots [i](#)

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

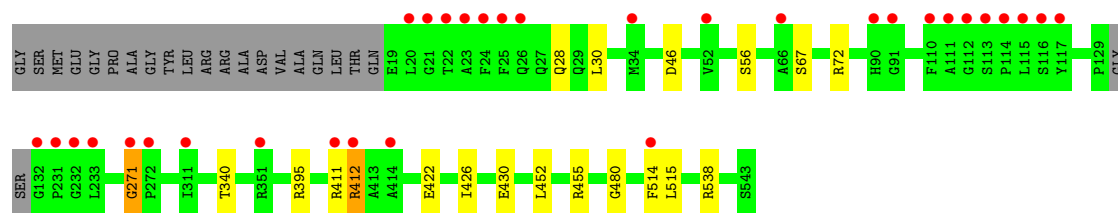


• Molecule 1: Pyruvate kinase PKLR

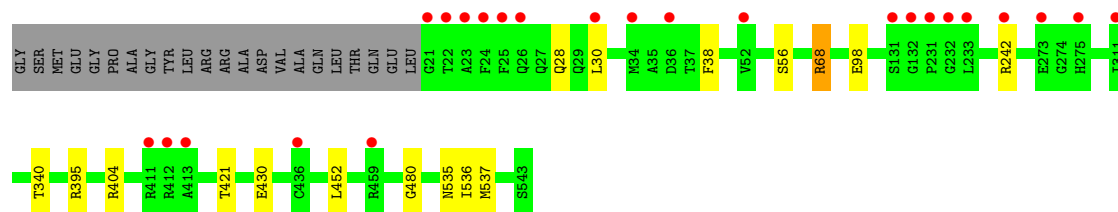
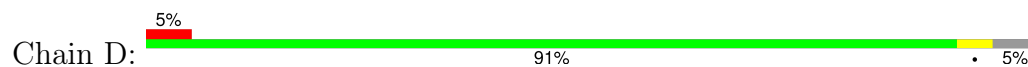


• Molecule 1: Pyruvate kinase PKLR

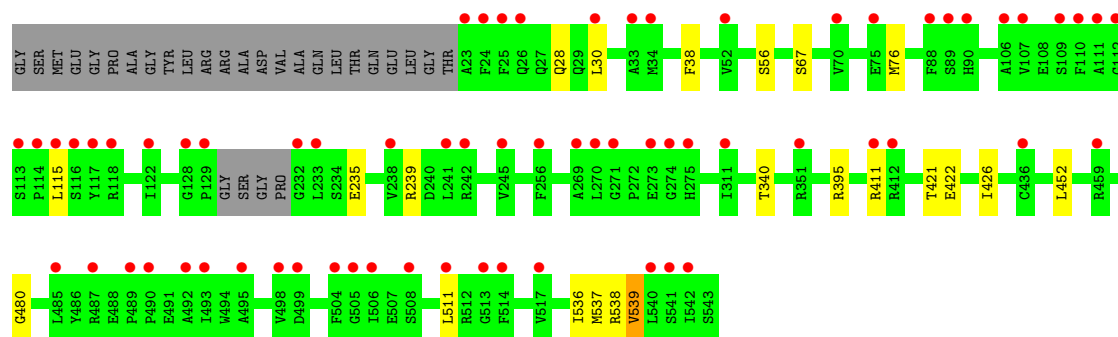
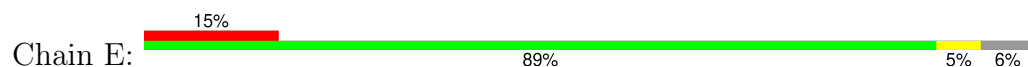




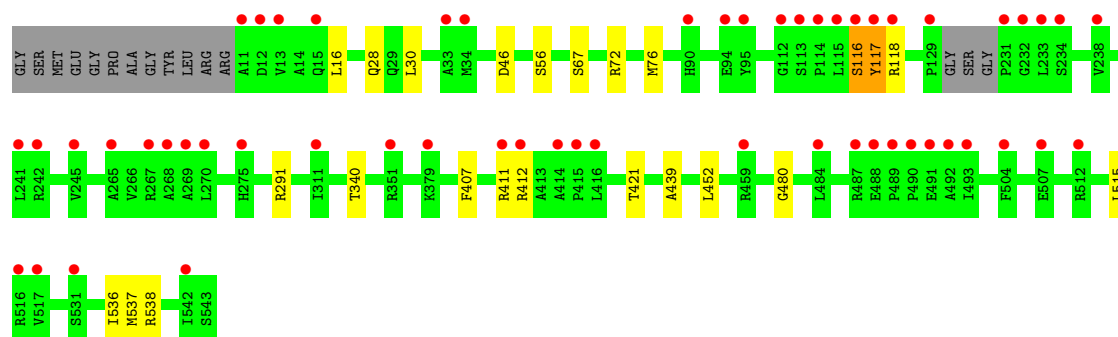
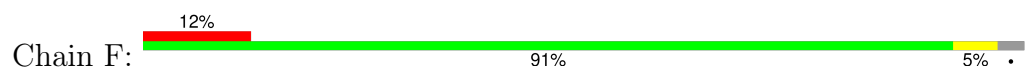
• Molecule 1: Pyruvate kinase PKLR



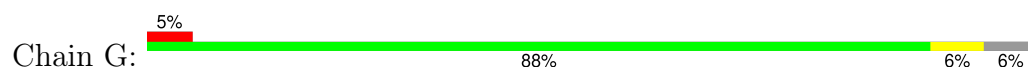
• Molecule 1: Pyruvate kinase PKLR

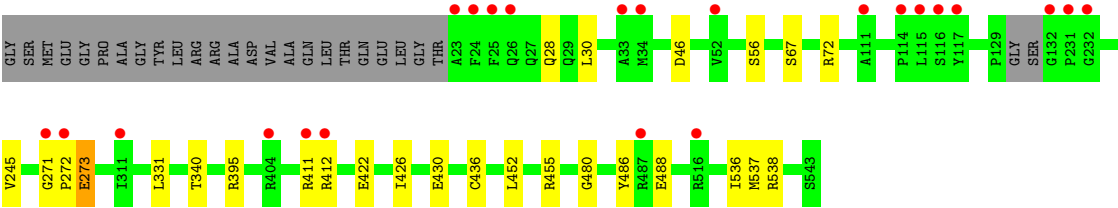


• Molecule 1: Pyruvate kinase PKLR

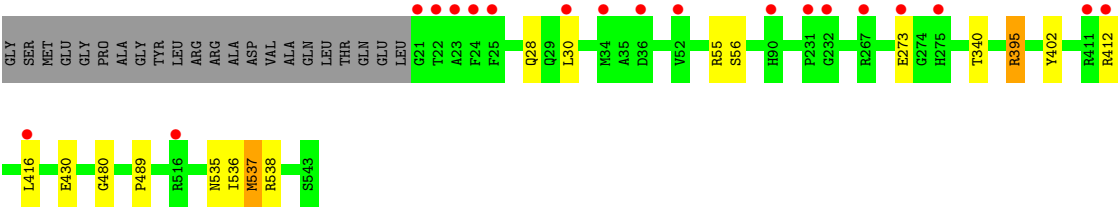


• Molecule 1: Pyruvate kinase PKLR





● 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	208.22Å 112.81Å 188.75Å 90.00° 91.85° 90.00°	Depositor
Resolution (Å)	104.06 – 1.77 104.06 – 1.77	Depositor EDS
% Data completeness (in resolution range)	79.7 (104.06-1.77) 79.6 (104.06-1.77)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.77Å)	Xtriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, R_{free}	0.200 , 0.217 0.193 , 0.207	Depositor DCC
R_{free} test set	17037 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	29414	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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 45.18 % 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 1.3723e-04. 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: OXL, K, FBP, MG, OD9

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	0/3307	0.94	2/4469 (0.0%)
1	B	0.66	0/3396	0.96	1/4592 (0.0%)
1	C	0.69	0/3313	0.94	3/4479 (0.1%)
1	D	0.71	0/3326	0.93	0/4497
1	E	0.63	0/3278	0.94	2/4430 (0.0%)
1	F	0.69	0/3396	0.94	1/4591 (0.0%)
1	G	0.68	0/3303	0.93	1/4465 (0.0%)
1	H	0.73	1/3316 (0.0%)	0.93	0/4483
All	All	0.68	1/26635 (0.0%)	0.94	10/36006 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	489	PRO	CA-C	5.62	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	514	PHE	CA-CB-CG	5.74	119.54	113.80
1	E	422	GLU	CB-CG-CD	5.63	122.17	112.60
1	E	539	VAL	N-CA-CB	5.43	118.30	111.46
1	C	46	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	422	GLU	CB-CG-CD	5.38	121.74	112.60
1	B	46	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	46	ASP	CA-CB-CG	5.17	117.77	112.60
1	C	515	LEU	N-CA-C	5.14	117.62	109.50
1	G	46	ASP	CA-CB-CG	5.08	117.68	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	11	0
1	B	3329	0	3394	13	0
1	C	3247	0	3299	13	0
1	D	3252	0	3310	10	0
1	E	3210	0	3270	9	0
1	F	3321	0	3393	10	0
1	G	3231	0	3284	16	0
1	H	3251	0	3306	10	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

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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	36	23	0	0	0
6	B	36	23	0	1	0
6	E	36	23	0	2	0
6	H	36	23	0	1	0
7	A	292	0	0	0	0
7	B	248	0	0	0	0
7	C	392	0	0	2	0
7	D	420	0	0	0	0
7	E	289	0	0	0	1
7	F	351	0	0	0	2
7	G	410	0	0	1	0
7	H	475	0	0	0	0
All	All	29322	92	26635	76	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (76) 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	1.56	0.87
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.60	0.84
1:B:411:ARG:HG3	1:B:426:ILE:HD11	1.60	0.81
1:C:422[A]:GLU:HG3	1:C:452:LEU:HD13	1.62	0.81
1:C:412:ARG:NH1	1:D:404:ARG:HE	1.85	0.74
1:A:412:ARG:NH1	1:B:404:ARG:HH11	1.85	0.73
1:A:272:PRO:HA	1:A:275:HIS:CE1	2.26	0.70
1:G:538:ARG:HG2	1:H:536:ILE:HG12	1.73	0.70
1:E:536:ILE:HG12	1:F:538:ARG:HG2	1.75	0.69
1:H:402:TYR:HB3	6:H:605:OD9:O6	1.94	0.67
1:A:538:ARG:HG3	1:B:536:ILE:HG12	1.77	0.67
1:C:412:ARG:HH11	1:D:404:ARG:HE	1.42	0.67
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.77	0.66
1:A:412:ARG:NH1	1:B:404:ARG:NH1	2.46	0.62
1:E:38:PHE:HE2	6:E:605:OD9:C21	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:407:PHE:CE2	1:F:411:ARG:NH1	2.68	0.60
1:A:418[A]:ARG:HG3	1:B:16:LEU:HD11	1.83	0.60
1:A:272:PRO:HA	1:A:275:HIS:NE2	2.14	0.60
1:G:271:GLY:HA2	7:G:847:HOH:O	2.02	0.60
1:E:411:ARG:HG3	1:E:426:ILE:HD11	1.82	0.59
1:C:538:ARG:HD3	7:C:867:HOH:O	2.03	0.58
1:F:439:ALA:HB3	1:F:515:LEU:HD21	1.85	0.58
1:E:538:ARG:HG2	1:F:536:ILE:HG12	1.85	0.57
1:A:408:GLU:OE2	1:B:411:ARG:NH2	2.38	0.57
1:E:235:GLU:O	1:E:239:ARG:HD3	2.05	0.56
1:C:538:ARG:HG2	1:D:536:ILE:HG12	1.88	0.56
1:G:537:MET:HE3	1:H:537:MET:HG2	1.87	0.56
1:B:30:LEU:O	1:B:34:MET:HG2	2.09	0.53
1:G:536:ILE:HG12	1:H:538[A]:ARG:HG2	1.91	0.53
6:E:605:OD9:C17	6:E:605:OD9:O7	2.59	0.51
1:G:245:VAL:CG1	1:G:273:GLU:HG2	2.41	0.51
1:G:272:PRO:HD2	1:G:273:GLU:OE1	2.12	0.50
1:G:430[B]:GLU:OE2	1:H:430:GLU:OE1	2.30	0.50
1:F:116:SER:O	1:F:117:TYR:O	2.29	0.49
1:A:67:SER:HA	1:A:72:ARG:HG2	1.93	0.49
1:C:430[B]:GLU:OE2	1:D:430[B]:GLU:OE1	2.31	0.49
1:G:56:SER:HB2	1:G:480:GLY:HA2	1.95	0.48
1:C:271:GLY:HA2	7:C:719:HOH:O	2.11	0.48
1:F:28:GLN:HG3	1:F:30:LEU:HG	1.95	0.48
1:B:28:GLN:HG3	1:B:30:LEU:HG	1.96	0.48
1:A:28:GLN:HG3	1:A:30:LEU:HG	1.96	0.48
1:D:28:GLN:HG3	1:D:30:LEU:HG	1.96	0.48
1:G:411:ARG:HG3	1:G:426:ILE:HD11	1.96	0.47
1:H:28:GLN:HG3	1:H:30:LEU:HG	1.97	0.47
1:H:56:SER:HB2	1:H:480:GLY:HA2	1.97	0.46
1:E:28:GLN:HG3	1:E:30:LEU:HG	1.97	0.46
1:C:28:GLN:HG3	1:C:30:LEU:HG	1.97	0.46
1:G:28:GLN:HG3	1:G:30:LEU:HG	1.96	0.46
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.98	0.46
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.98	0.46
1:G:486:TYR:CZ	1:G:488:GLU:HB2	2.51	0.46
1:H:535:ASN:OD1	1:H:536:ILE:HG13	2.16	0.45
1:C:67:SER:HA	1:C:72:ARG:HG2	1.99	0.45
1:F:56:SER:HB2	1:F:480:GLY:HA2	1.99	0.44
1:G:436:CYS:SG	1:H:416:LEU:HD13	2.57	0.44
1:D:535:ASN:OD1	1:D:536:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:SER:HB2	1:E:76[A]:MET:SD	2.58	0.43
1:D:68:ARG:NH2	1:D:98:GLU:HB2	2.34	0.43
1:F:421:THR:HG22	1:F:452:LEU:HD12	2.00	0.43
1:G:67:SER:HA	1:G:72:ARG:HG2	2.00	0.43
1:A:421:THR:HG22	1:A:452:LEU:HD12	2.01	0.42
1:B:421:THR:HG22	1:B:452:LEU:HD12	2.01	0.42
1:B:439:ALA:HB3	1:B:515:LEU:HD21	2.01	0.42
1:D:56:SER:HB2	1:D:480:GLY:HA2	2.02	0.42
6:B:605:OD9:C17	1:D:38:PHE:CE2	3.02	0.42
1:F:67:SER:HB2	1:F:76[B]:MET:SD	2.60	0.42
1:F:67:SER:HA	1:F:72:ARG:HG2	2.01	0.41
1:C:452:LEU:O	1:C:455:ARG:HG2	2.20	0.41
1:E:56:SER:HB2	1:E:480:GLY:HA2	2.01	0.41
1:E:421:THR:HG22	1:E:452:LEU:HD12	2.01	0.41
1:G:56:SER:HB2	1:G:480:GLY:CA	2.50	0.41
1:H:55:ARG:HB2	1:H:395:ARG:HG3	2.03	0.41
1:B:435:CYS:HB2	1:B:520:LEU:HD12	2.03	0.40
1:G:452:LEU:O	1:G:455:ARG:HG2	2.21	0.40
1:C:30:LEU:HD23	1:C:30:LEU:HA	1.99	0.40
1:D:421:THR:HG22	1:D:452:LEU:HD12	2.04	0.40

All (2) 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)
7:F:1030:HOH:O	7:F:1030:HOH:O[2_656]	0.70	1.50
7:E:923:HOH:O	7:F:836:HOH:O[2_656]	2.13	0.07

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	27
1	B	438/447 (98%)	432 (99%)	5 (1%)	1 (0%)	43	27
1	C	425/447 (95%)	417 (98%)	6 (1%)	2 (0%)	24	11
1	D	429/447 (96%)	423 (99%)	5 (1%)	1 (0%)	43	27
1	E	420/447 (94%)	414 (99%)	5 (1%)	1 (0%)	43	27
1	F	435/447 (97%)	428 (98%)	5 (1%)	2 (0%)	24	11
1	G	423/447 (95%)	414 (98%)	8 (2%)	1 (0%)	43	27
1	H	427/447 (96%)	421 (99%)	5 (1%)	1 (0%)	43	27
All	All	3421/3576 (96%)	3367 (98%)	44 (1%)	10 (0%)	36	21

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	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	C	271	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	340/352 (97%)	334 (98%)	6 (2%)	51	33
1	B	349/352 (99%)	339 (97%)	10 (3%)	37	17
1	C	341/352 (97%)	339 (99%)	2 (1%)	78	71
1	D	342/352 (97%)	337 (98%)	5 (2%)	57	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	338/352 (96%)	332 (98%)	6 (2%)	51	33
1	F	350/352 (99%)	343 (98%)	7 (2%)	48	29
1	G	340/352 (97%)	336 (99%)	4 (1%)	63	49
1	H	340/352 (97%)	336 (99%)	4 (1%)	63	49
All	All	2740/2816 (97%)	2696 (98%)	44 (2%)	59	38

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	395	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	71	GLU
1	B	115	LEU
1	B	263	VAL
1	B	379	LYS
1	B	412	ARG
1	B	511	LEU
1	B	537[A]	MET
1	B	537[B]	MET
1	C	395	ARG
1	C	412	ARG
1	D	68	ARG
1	D	242[A]	ARG
1	D	242[B]	ARG
1	D	395	ARG
1	D	537	MET
1	E	115	LEU
1	E	395	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	116	SER
1	F	118	ARG

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Mol	Chain	Res	Type
1	F	291	ARG
1	F	412	ARG
1	F	537[A]	MET
1	F	537[B]	MET
1	G	273	GLU
1	G	331	LEU
1	G	395	ARG
1	G	412	ARG
1	H	273	GLU
1	H	395	ARG
1	H	412	ARG
1	H	537	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	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	$\# Z > 2$
2	FBP	A	601	-	18,20,20	0.50	0	21,32,32	0.58	0
2	FBP	E	601	-	18,20,20	0.49	0	21,32,32	0.82	1 (4%)
3	OXL	D	602	4	5,5,5	2.06	2 (40%)	6,6,6	2.06	2 (33%)
6	OD9	B	605	-	39,39,39	0.32	0	57,57,57	0.91	3 (5%)
6	OD9	A	605	-	39,39,39	0.22	0	57,57,57	0.53	0
2	FBP	C	601	-	18,20,20	0.63	0	21,32,32	0.64	0
3	OXL	H	602	4	5,5,5	1.70	2 (40%)	6,6,6	1.90	1 (16%)
3	OXL	B	602	4	5,5,5	2.14	2 (40%)	6,6,6	1.52	2 (33%)
3	OXL	A	602	4	5,5,5	1.97	2 (40%)	6,6,6	2.33	3 (50%)
6	OD9	E	605	-	39,39,39	0.27	0	57,57,57	0.66	2 (3%)
2	FBP	H	601	-	18,20,20	0.69	0	21,32,32	0.88	1 (4%)
3	OXL	F	602	4	5,5,5	2.89	4 (80%)	6,6,6	2.39	3 (50%)
3	OXL	C	602	4	5,5,5	1.90	2 (40%)	6,6,6	1.55	1 (16%)
3	OXL	G	602	4	5,5,5	2.09	2 (40%)	6,6,6	2.21	2 (33%)
2	FBP	B	601	-	18,20,20	0.81	1 (5%)	21,32,32	0.80	1 (4%)
2	FBP	F	601	-	18,20,20	0.45	0	21,32,32	0.58	0
2	FBP	G	601	-	18,20,20	0.66	0	21,32,32	0.81	0
2	FBP	D	601	-	18,20,20	0.43	0	21,32,32	0.89	1 (4%)
6	OD9	H	605	-	39,39,39	0.24	0	57,57,57	0.74	2 (3%)
3	OXL	E	602	4	5,5,5	2.08	2 (40%)	6,6,6	1.70	2 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
2	FBP	E	601	-	-	2/13/32/32	0/1/1/1
3	OXL	D	602	4	-	4/4/4/4	-
6	OD9	B	605	-	-	5/20/20/20	0/4/4/4
6	OD9	A	605	-	-	2/20/20/20	0/4/4/4
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
3	OXL	H	602	4	-	4/4/4/4	-
3	OXL	B	602	4	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OXL	A	602	4	-	4/4/4/4	-
6	OD9	E	605	-	-	0/20/20/20	0/4/4/4
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1
3	OXL	F	602	4	-	4/4/4/4	-
3	OXL	C	602	4	-	4/4/4/4	-
3	OXL	G	602	4	-	4/4/4/4	-
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
2	FBP	G	601	-	-	2/13/32/32	0/1/1/1
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
6	OD9	H	605	-	-	7/20/20/20	0/4/4/4
3	OXL	E	602	4	-	4/4/4/4	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	OXL	O1-C1	3.86	1.32	1.22
3	B	602	OXL	O2-C2	3.73	1.31	1.22
3	A	602	OXL	O2-C2	3.56	1.31	1.22
3	F	602	OXL	O1-C1	3.50	1.31	1.22
3	F	602	OXL	O2-C2	3.32	1.30	1.22
3	G	602	OXL	O1-C1	3.29	1.30	1.22
3	F	602	OXL	O3-C1	-3.26	1.21	1.30
3	C	602	OXL	O1-C1	3.26	1.30	1.22
3	D	602	OXL	O4-C2	-3.19	1.21	1.30
3	G	602	OXL	O3-C1	-3.17	1.21	1.30
3	D	602	OXL	O2-C2	3.14	1.30	1.22
3	B	602	OXL	O4-C2	-2.97	1.22	1.30
3	H	602	OXL	O4-C2	-2.76	1.23	1.30
3	F	602	OXL	O4-C2	-2.61	1.23	1.30
3	E	602	OXL	O3-C1	-2.59	1.23	1.30
3	C	602	OXL	O3-C1	-2.59	1.23	1.30
3	A	602	OXL	O4-C2	-2.58	1.23	1.30
3	H	602	OXL	O2-C2	2.40	1.28	1.22
2	B	601	FBP	P2-O5P	-2.34	1.46	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	OXL	O4-C2-C1	4.08	120.74	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	602	OXL	O4-C2-C1	4.02	120.63	112.83
3	H	602	OXL	O4-C2-C1	4.00	120.58	112.83
3	G	602	OXL	O3-C1-C2	3.87	120.35	112.83
3	D	602	OXL	O4-C2-C1	3.77	120.14	112.83
6	B	605	OD9	C10-S-N	-3.54	103.04	107.86
3	F	602	OXL	O3-C1-C2	3.36	119.35	112.83
3	C	602	OXL	O3-C1-C2	3.24	119.11	112.83
2	D	601	FBP	O5P-P2-O6	3.09	114.72	106.67
2	H	601	FBP	O5P-P2-O6	3.03	114.58	106.67
3	G	602	OXL	O4-C2-C1	3.00	118.66	112.83
3	E	602	OXL	O3-C1-C2	2.91	118.47	112.83
3	A	602	OXL	O3-C1-C2	2.85	118.36	112.83
2	E	601	FBP	O3P-P1-O2P	2.62	117.64	107.80
6	B	605	OD9	C11-C10-S	-2.59	113.84	118.59
3	A	602	OXL	O2-C2-C1	-2.58	115.26	120.63
6	H	605	OD9	C8-C9-N	2.56	117.67	112.08
3	D	602	OXL	O3-C1-C2	2.51	117.69	112.83
3	B	602	OXL	O3-C1-C2	2.50	117.68	112.83
3	B	602	OXL	O4-C2-C1	2.48	117.65	112.83
6	B	605	OD9	C5-C4-C3	-2.45	105.38	113.76
3	E	602	OXL	O4-C2-C1	2.41	117.51	112.83
6	H	605	OD9	C10-S-N	2.36	111.06	107.86
3	F	602	OXL	O2-C2-C1	-2.24	115.97	120.63
2	B	601	FBP	O3P-P1-O2P	2.23	116.16	107.80
6	E	605	OD9	C11-C10-S	-2.18	114.58	118.59
6	E	605	OD9	C15-C10-S	2.06	125.05	122.56

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	605	OD9	C9-N-S-O6
6	B	605	OD9	C9-N-S-C10
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	G	601	FBP	C4-C5-C6-O6
2	H	601	FBP	C4-C5-C6-O6
6	H	605	OD9	C9-N-S-O7

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Mol	Chain	Res	Type	Atoms
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	G	601	FBP	O5-C5-C6-O6
2	H	601	FBP	O5-C5-C6-O6
6	H	605	OD9	C9-N-S-C10
6	H	605	OD9	C15-C10-S-O6
6	H	605	OD9	C15-C10-S-N
6	A	605	OD9	C10-C15-C16-C21
3	E	602	OXL	O1-C1-C2-O2
3	H	602	OXL	O3-C1-C2-O4
3	B	602	OXL	O3-C1-C2-O4
3	G	602	OXL	O3-C1-C2-O4
6	B	605	OD9	C11-C10-S-O7
6	H	605	OD9	C11-C10-S-O6
3	C	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	O3-C1-C2-O4
3	D	602	OXL	O3-C1-C2-O4
3	A	602	OXL	O1-C1-C2-O2
3	B	602	OXL	O1-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O2
3	F	602	OXL	O1-C1-C2-O2
3	G	602	OXL	O1-C1-C2-O2
3	C	602	OXL	O1-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O2
6	A	605	OD9	C10-C15-C16-C17
6	B	605	OD9	C11-C10-S-O6
3	H	602	OXL	O3-C1-C2-O2
6	H	605	OD9	C11-C10-S-N
3	B	602	OXL	O1-C1-C2-O4
3	B	602	OXL	O3-C1-C2-O2
3	F	602	OXL	O3-C1-C2-O2
3	G	602	OXL	O1-C1-C2-O4
3	C	602	OXL	O3-C1-C2-O2
3	G	602	OXL	O3-C1-C2-O2
3	A	602	OXL	O1-C1-C2-O4
3	A	602	OXL	O3-C1-C2-O2

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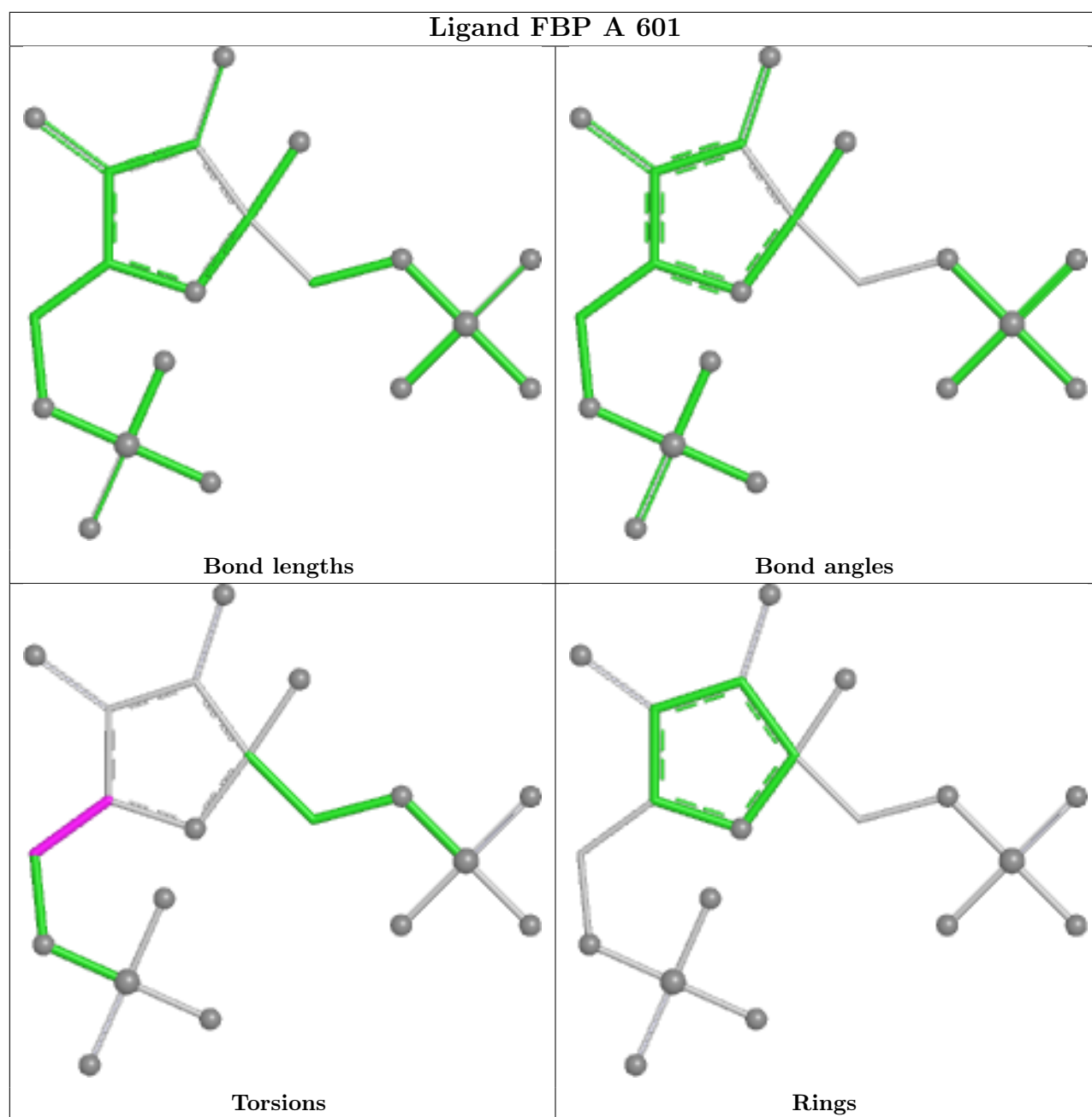
Mol	Chain	Res	Type	Atoms
3	C	602	OXL	O1-C1-C2-O4
3	D	602	OXL	O1-C1-C2-O4
3	D	602	OXL	O3-C1-C2-O2
3	F	602	OXL	O1-C1-C2-O4
3	H	602	OXL	O1-C1-C2-O4
3	E	602	OXL	O1-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O2
6	B	605	OD9	C11-C10-S-N
6	H	605	OD9	C9-N-S-O6

There are no ring outliers.

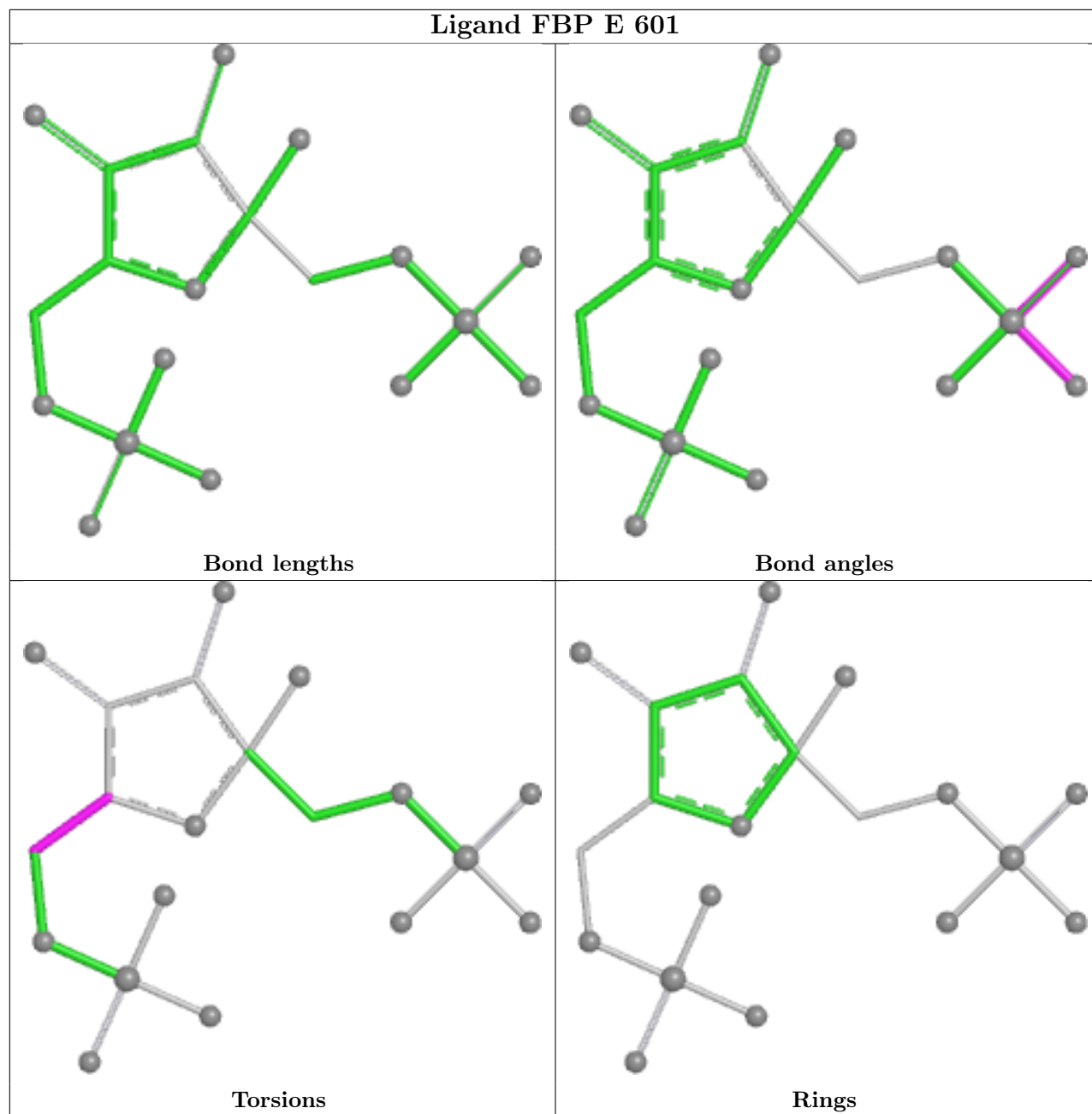
3 monomers are involved in 4 short contacts:

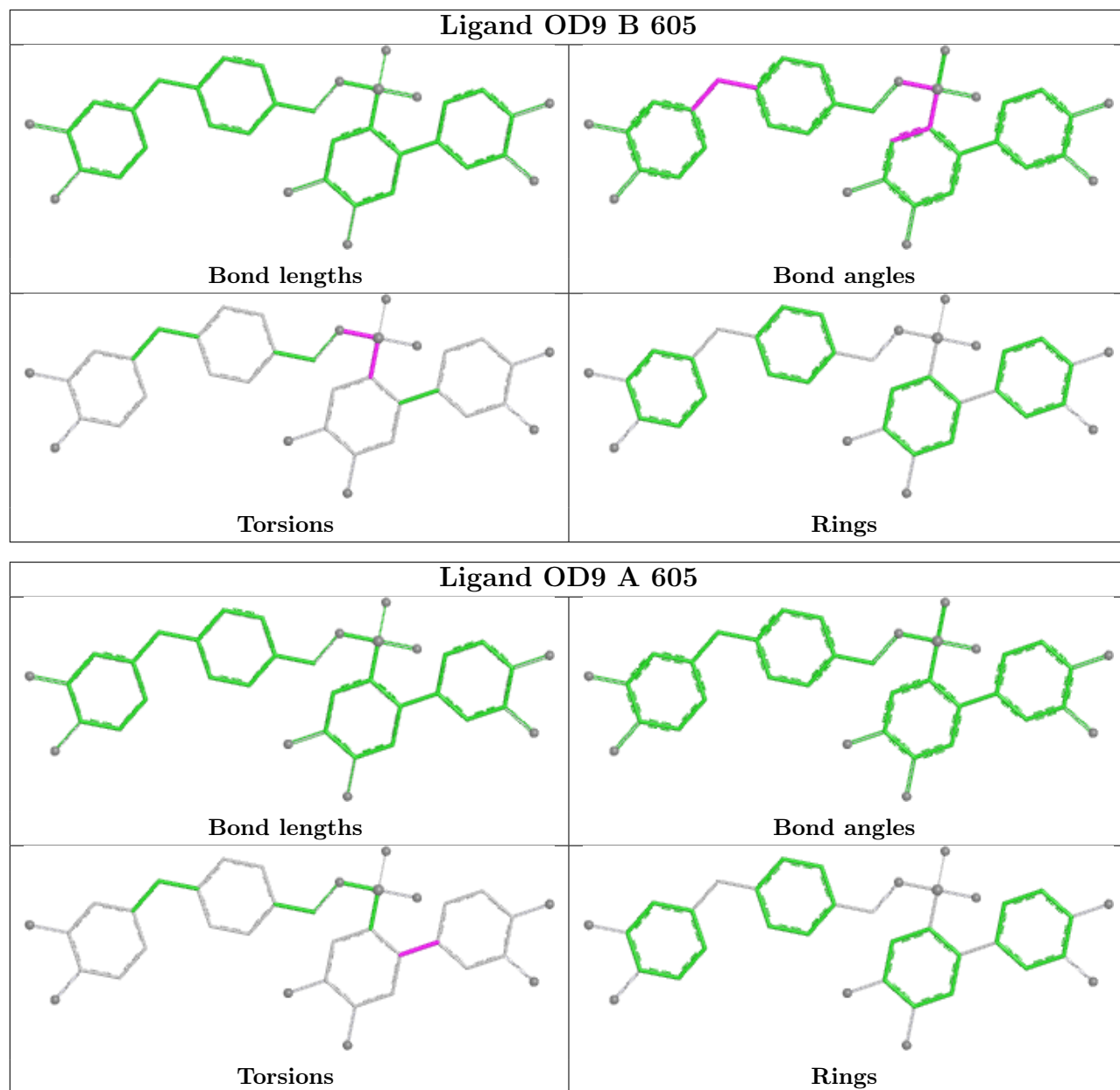
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	605	OD9	1	0
6	E	605	OD9	2	0
6	H	605	OD9	1	0

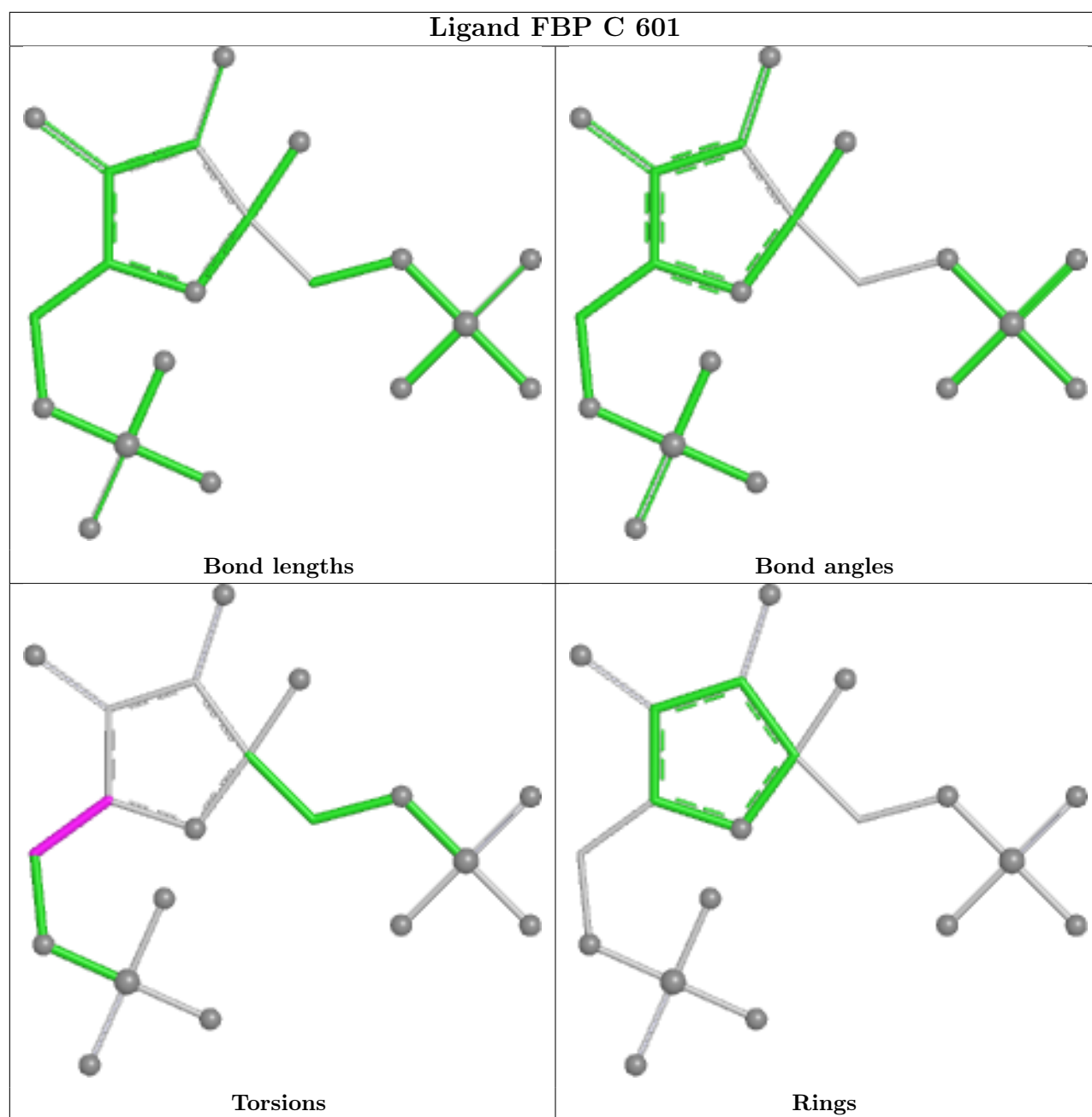
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

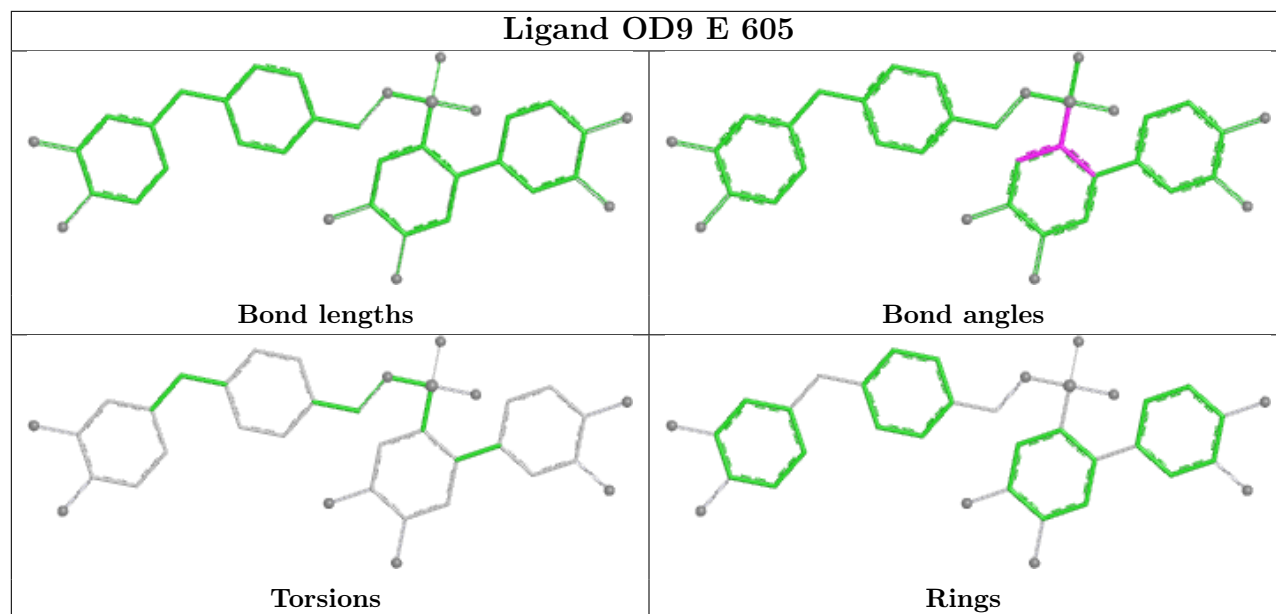


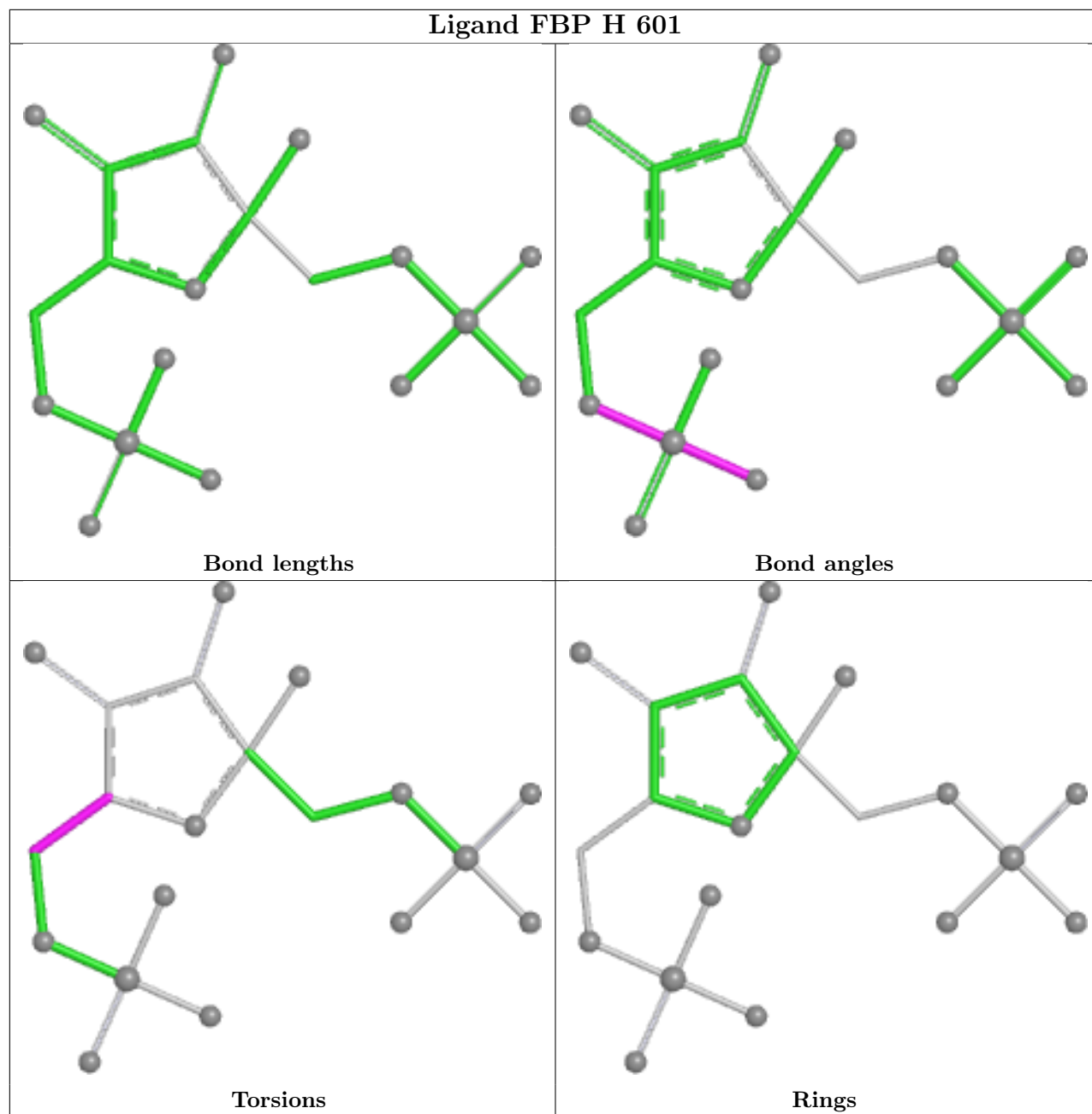
Ligand FBP E 601



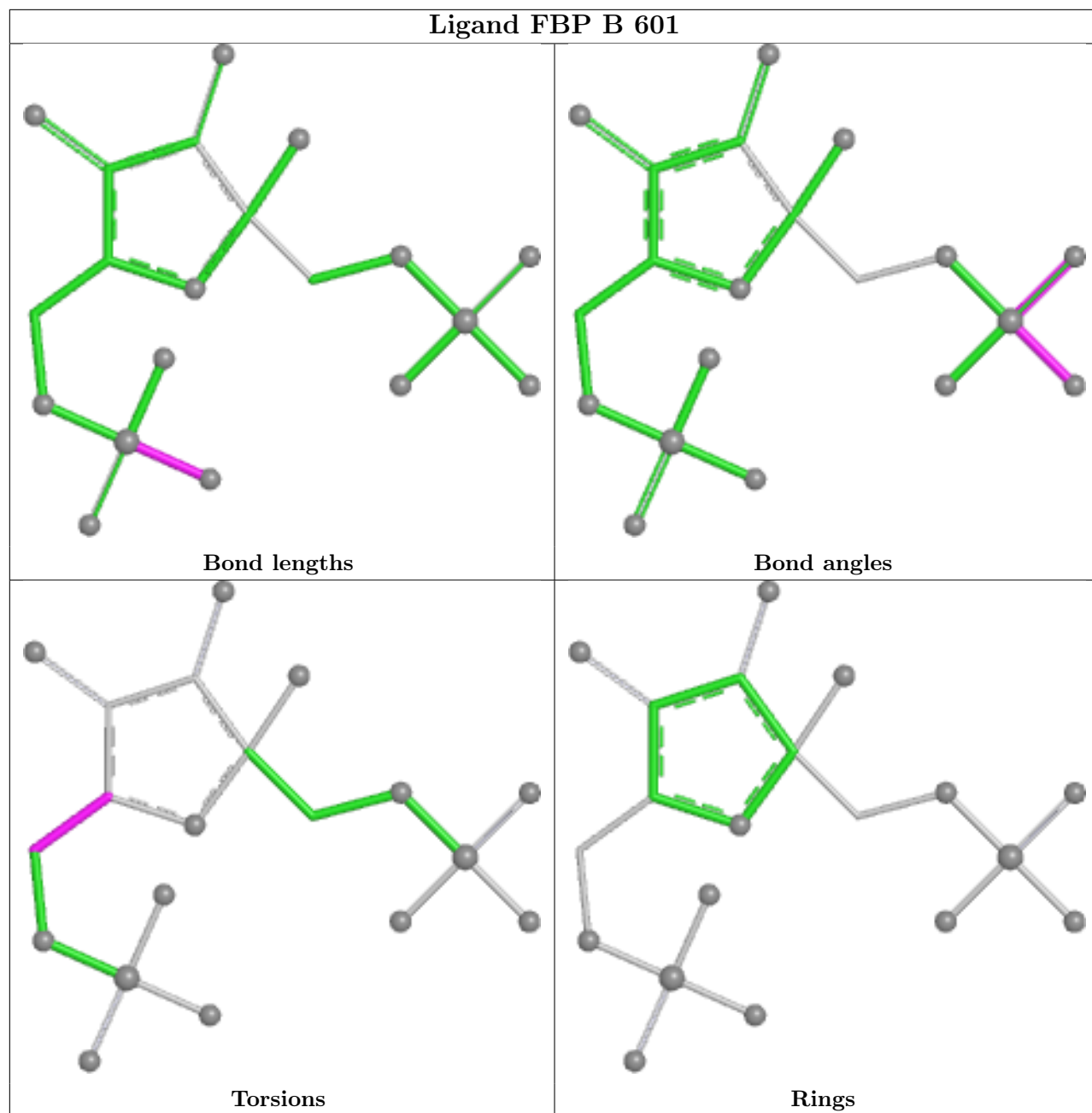




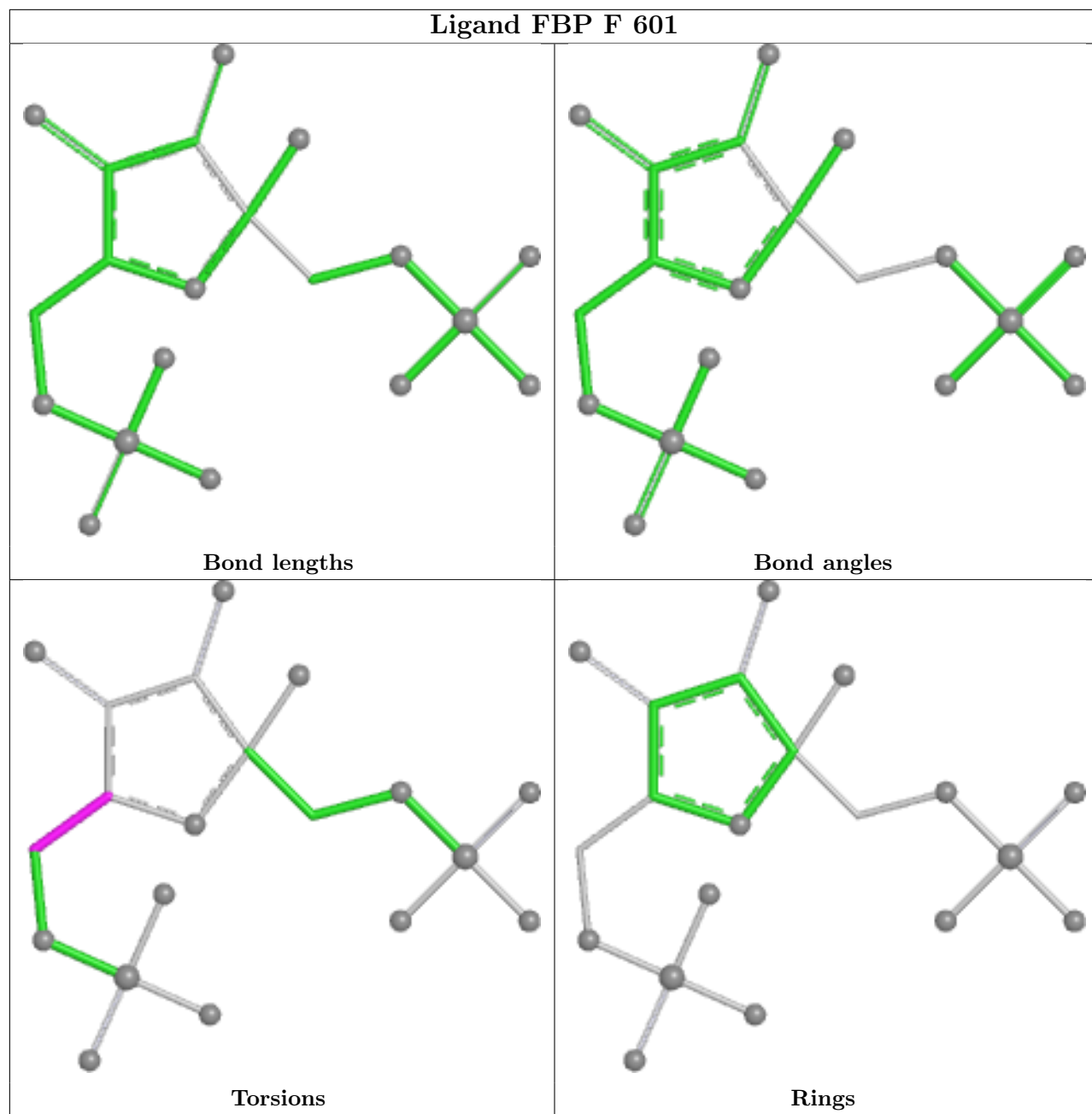


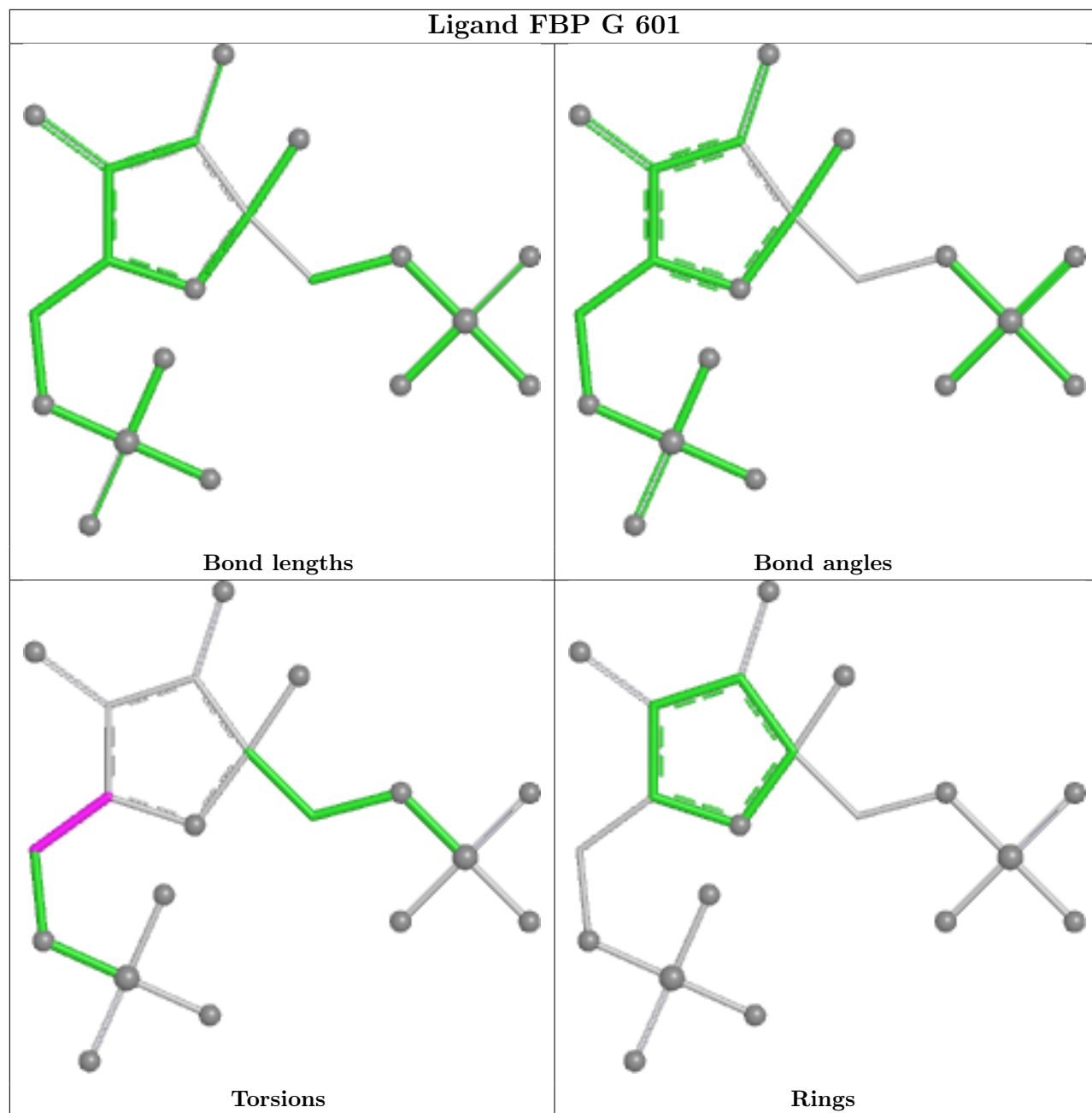


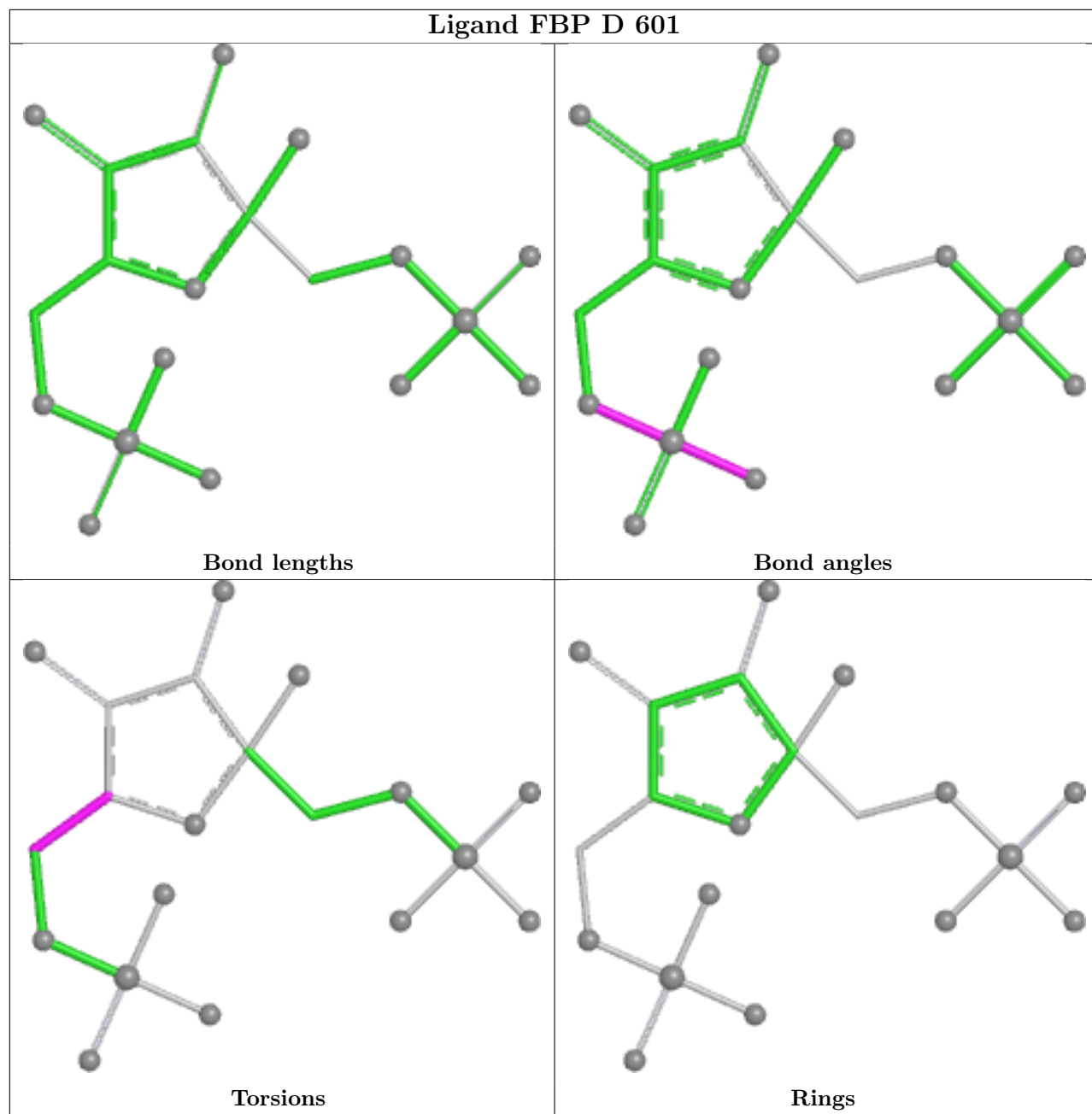
Ligand FBP B 601

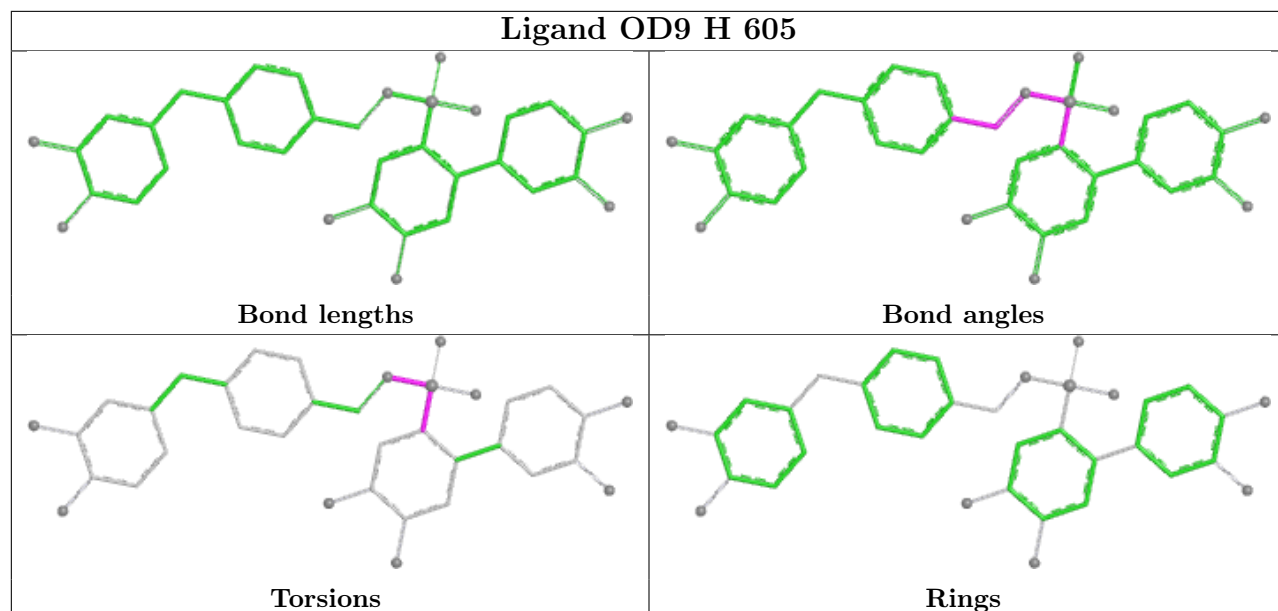


Ligand FBP F 601









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%)	1.02	66 (15%) 5 5	20, 38, 62, 75	6 (1%)
1	B	436/447 (97%)	1.35	127 (29%) 1 1	19, 38, 66, 75	4 (0%)
1	C	425/447 (95%)	0.40	32 (7%) 20 23	18, 29, 49, 87	4 (0%)
1	D	425/447 (95%)	0.24	24 (5%) 30 34	14, 27, 48, 84	6 (1%)
1	E	419/447 (93%)	0.98	67 (15%) 5 5	19, 37, 63, 74	5 (1%)
1	F	432/447 (96%)	0.70	55 (12%) 8 8	19, 31, 53, 69	7 (1%)
1	G	421/447 (94%)	0.22	23 (5%) 30 35	16, 27, 44, 58	7 (1%)
1	H	425/447 (95%)	0.02	19 (4%) 38 44	13, 24, 45, 71	4 (0%)
All	All	3405/3576 (95%)	0.62	413 (12%) 8 10	13, 32, 58, 87	43 (1%)

All (413) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	115	LEU	15.1
1	F	115	LEU	13.8
1	F	116	SER	10.4
1	A	25	PHE	9.7
1	F	114	PRO	8.7
1	D	25	PHE	8.7
1	B	511	LEU	8.7
1	G	271	GLY	8.6
1	B	116	SER	7.8
1	B	114	PRO	7.7
1	B	117	TYR	7.1
1	H	21	GLY	6.8
1	C	271	GLY	6.6
1	E	114	PRO	6.4
1	F	489	PRO	6.4
1	D	24	PHE	6.3

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Mol	Chain	Res	Type	RSRZ
1	E	25	PHE	6.2
1	A	24	PHE	6.0
1	G	25	PHE	6.0
1	B	489	PRO	5.7
1	B	118	ARG	5.6
1	D	21	GLY	5.5
1	C	20	LEU	5.4
1	D	22	THR	5.3
1	C	232	GLY	5.3
1	C	21	GLY	5.2
1	H	25	PHE	5.2
1	D	23	ALA	5.2
1	C	231	PRO	5.1
1	F	488	GLU	5.0
1	E	115	LEU	5.0
1	E	23	ALA	5.0
1	A	132	GLY	4.9
1	B	490	PRO	4.9
1	B	113	SER	4.9
1	F	231	PRO	4.8
1	B	348	THR	4.8
1	C	25	PHE	4.7
1	C	132	GLY	4.7
1	A	30	LEU	4.6
1	E	116	SER	4.6
1	B	512	ARG	4.5
1	H	22	THR	4.5
1	C	22	THR	4.5
1	A	543	SER	4.4
1	B	231	PRO	4.4
1	E	24	PHE	4.4
1	E	110	PHE	4.4
1	H	24	PHE	4.3
1	F	512	ARG	4.2
1	F	516	ARG	4.2
1	F	490	PRO	4.2
1	A	23	ALA	4.2
1	E	117	TYR	4.2
1	E	111	ALA	4.2
1	A	115	LEU	4.1
1	H	411	ARG	4.0
1	E	232	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	112	GLY	4.0
1	F	484	LEU	3.9
1	E	269	ALA	3.9
1	E	26	GLN	3.9
1	B	504	PHE	3.9
1	D	30	LEU	3.9
1	A	514	PHE	3.9
1	F	492	ALA	3.8
1	E	129	PRO	3.8
1	G	24	PHE	3.8
1	G	23	ALA	3.8
1	G	132	GLY	3.8
1	F	267[A]	ARG	3.8
1	B	484	LEU	3.8
1	B	508	SER	3.7
1	B	492	ALA	3.7
1	A	540	LEU	3.7
1	E	490	PRO	3.7
1	B	111	ALA	3.7
1	B	132	GLY	3.7
1	A	238	VAL	3.7
1	B	97	ALA	3.7
1	B	517	VAL	3.6
1	A	116	SER	3.6
1	B	267[A]	ARG	3.6
1	D	34	MET	3.6
1	E	489	PRO	3.6
1	B	416	LEU	3.6
1	B	506	ILE	3.6
1	A	34	MET	3.6
1	B	100	ILE	3.5
1	A	232	GLY	3.5
1	B	268	ALA	3.5
1	E	118	ARG	3.5
1	A	117	TYR	3.5
1	B	543	SER	3.5
1	B	236	GLN	3.5
1	A	118	ARG	3.5
1	F	487	ARG	3.5
1	H	516	ARG	3.5
1	A	70	VAL	3.5
1	D	275[A]	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	270	LEU	3.4
1	E	30	LEU	3.4
1	A	114	PRO	3.4
1	F	517	VAL	3.4
1	B	513	GLY	3.4
1	F	459	ARG	3.4
1	B	493	ILE	3.4
1	E	511	LEU	3.4
1	B	52	VAL	3.4
1	G	116	SER	3.4
1	B	233	LEU	3.3
1	F	233	LEU	3.3
1	E	487	ARG	3.3
1	F	414	ALA	3.3
1	C	117	TYR	3.3
1	B	107	VAL	3.3
1	B	438	ALA	3.3
1	E	112	GLY	3.3
1	B	488	GLU	3.3
1	C	411	ARG	3.2
1	H	412	ARG	3.2
1	A	73	LEU	3.2
1	C	115	LEU	3.2
1	B	487	ARG	3.2
1	F	118	ARG	3.2
1	F	117	TYR	3.2
1	B	272	PRO	3.2
1	C	34	MET	3.2
1	B	241	LEU	3.2
1	B	130	GLY	3.2
1	B	411	ARG	3.2
1	B	516	ARG	3.2
1	B	88	PHE	3.2
1	E	238	VAL	3.2
1	B	95	TYR	3.1
1	B	379	LYS	3.1
1	E	542	ILE	3.1
1	B	413	ALA	3.1
1	B	70	VAL	3.1
1	E	275	HIS	3.1
1	E	493	ILE	3.1
1	A	33	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	113	SER	3.1
1	E	540	LEU	3.1
1	B	243	PHE	3.1
1	B	93	HIS	3.0
1	E	34	MET	3.0
1	G	412	ARG	3.0
1	B	271	GLY	3.0
1	B	509	GLY	3.0
1	B	510	LYS	3.0
1	F	412	ARG	3.0
1	H	273	GLU	3.0
1	A	233	LEU	3.0
1	B	270	LEU	3.0
1	B	414	ALA	3.0
1	B	515	LEU	3.0
1	C	110	PHE	3.0
1	F	112	GLY	3.0
1	B	249	VAL	3.0
1	B	541	SER	3.0
1	E	233	LEU	3.0
1	A	273	GLU	3.0
1	B	91	GLY	3.0
1	B	514	PHE	3.0
1	F	504	PHE	3.0
1	B	13	VAL	2.9
1	E	109	SER	2.9
1	E	270	LEU	2.9
1	B	382	PHE	2.9
1	B	90	HIS	2.9
1	A	249	VAL	2.9
1	E	492	ALA	2.9
1	F	11	ALA	2.9
1	H	23	ALA	2.9
1	E	311	ILE	2.9
1	F	415	PRO	2.9
1	H	231	PRO	2.9
1	E	242	ARG	2.9
1	H	34	MET	2.9
1	F	275	HIS	2.9
1	C	23	ALA	2.9
1	A	26	GLN	2.9
1	A	511	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	114	PRO	2.9
1	A	351	ARG	2.8
1	B	238	VAL	2.8
1	H	52	VAL	2.8
1	D	231	PRO	2.8
1	E	541[A]	SER	2.8
1	E	506	ILE	2.8
1	D	26	GLN	2.8
1	A	111	ALA	2.8
1	F	232	GLY	2.8
1	B	542	ILE	2.8
1	F	242	ARG	2.8
1	B	106	ALA	2.8
1	B	269	ALA	2.8
1	E	256	PHE	2.8
1	B	383	PRO	2.8
1	F	416	LEU	2.8
1	E	499	ASP	2.8
1	F	90	HIS	2.8
1	G	33	ALA	2.7
1	C	24	PHE	2.7
1	G	34	MET	2.7
1	A	241	LEU	2.7
1	B	73	LEU	2.7
1	G	115	LEU	2.7
1	D	311	ILE	2.7
1	E	351	ARG	2.7
1	F	411	ARG	2.7
1	B	66	ALA	2.7
1	B	378	ALA	2.7
1	D	413	ALA	2.7
1	E	33	ALA	2.7
1	D	36	ASP	2.7
1	A	68	ARG	2.7
1	D	242[A]	ARG	2.7
1	D	412	ARG	2.7
1	F	351	ARG	2.7
1	A	541	SER	2.7
1	B	103	VAL	2.7
1	F	270	LEU	2.7
1	B	33	ALA	2.7
1	B	265	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	111	ALA	2.7
1	B	242	ARG	2.6
1	B	75	GLU	2.6
1	B	86	LEU	2.6
1	B	266	VAL	2.6
1	G	52	VAL	2.6
1	B	10	ARG	2.6
1	D	232	GLY	2.6
1	E	70	VAL	2.6
1	B	347	ILE	2.6
1	E	90	HIS	2.6
1	E	122	ILE	2.6
1	F	15	GLN	2.6
1	F	311	ILE	2.6
1	F	34	MET	2.6
1	A	275	HIS	2.6
1	A	95	TYR	2.6
1	F	129	PRO	2.6
1	B	68	ARG	2.6
1	G	411	ARG	2.5
1	B	101	ALA	2.5
1	B	127	LYS	2.5
1	A	412	ARG	2.5
1	B	110	PHE	2.5
1	A	378	ALA	2.5
1	G	272	PRO	2.5
1	A	488[A]	GLU	2.5
1	B	71	GLU	2.5
1	E	459	ARG	2.5
1	G	26	GLN	2.5
1	B	485	LEU	2.5
1	C	233	LEU	2.5
1	G	117	TYR	2.5
1	B	120	VAL	2.5
1	B	275	HIS	2.5
1	B	498	VAL	2.5
1	F	379	LYS	2.5
1	H	90	HIS	2.5
1	H	232	GLY	2.5
1	C	311	ILE	2.5
1	B	412	ARG	2.5
1	B	491	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	381	ASN	2.4
1	E	241	LEU	2.4
1	E	514	PHE	2.4
1	F	241	LEU	2.4
1	B	72	ARG	2.4
1	C	412	ARG	2.4
1	F	491	GLU	2.4
1	H	275[A]	HIS	2.4
1	A	52	VAL	2.4
1	B	67	SER	2.4
1	E	508	SER	2.4
1	C	26	GLN	2.4
1	D	273	GLU	2.4
1	B	415	PRO	2.4
1	E	504	PHE	2.4
1	B	92	SER	2.4
1	A	107	VAL	2.4
1	A	517	VAL	2.4
1	E	245	VAL	2.4
1	F	238	VAL	2.4
1	C	91	GLY	2.4
1	E	89	SER	2.4
1	E	106	ALA	2.4
1	B	527	TRP	2.4
1	F	245	VAL	2.4
1	A	113	SER	2.3
1	B	274	GLY	2.3
1	B	380	GLY	2.3
1	E	271	GLY	2.3
1	A	101	ALA	2.3
1	C	351	ARG	2.3
1	E	485	LEU	2.3
1	F	542[A]	ILE	2.3
1	A	245	VAL	2.3
1	B	263	VAL	2.3
1	F	113	SER	2.3
1	E	505	GLY	2.3
1	E	273	GLU	2.3
1	H	36	ASP	2.3
1	G	231	PRO	2.3
1	D	233	LEU	2.3
1	D	52	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	112	GLY	2.3
1	A	471	ALA	2.3
1	E	436	CYS	2.3
1	B	410	LEU	2.3
1	A	72	ARG	2.3
1	A	311	ILE	2.3
1	B	122	ILE	2.3
1	B	128	GLY	2.3
1	D	132	GLY	2.3
1	A	120	VAL	2.3
1	B	384	VAL	2.3
1	F	13	VAL	2.3
1	A	27	GLN	2.2
1	A	90	HIS	2.2
1	A	272	PRO	2.2
1	B	235	GLU	2.2
1	E	495	ALA	2.2
1	G	111	ALA	2.2
1	A	86	LEU	2.2
1	A	515	LEU	2.2
1	C	113	SER	2.2
1	F	12	ASP	2.2
1	E	88	PHE	2.2
1	G	232	GLY	2.2
1	F	95	TYR	2.2
1	B	311	ILE	2.2
1	F	493	ILE	2.2
1	E	498	VAL	2.2
1	A	404	ARG	2.2
1	D	411	ARG	2.2
1	E	412	ARG	2.2
1	F	268	ALA	2.2
1	F	269	ALA	2.2
1	F	531	SER	2.2
1	H	30	LEU	2.2
1	A	271	GLY	2.2
1	B	244	GLY	2.2
1	E	75	GLU	2.2
1	B	96	HIS	2.2
1	C	514	PHE	2.2
1	A	493	ILE	2.2
1	D	459	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	119	PRO	2.2
1	B	129	PRO	2.2
1	A	257	VAL	2.2
1	B	502	VAL	2.2
1	C	52	VAL	2.2
1	E	52	VAL	2.2
1	F	265	ALA	2.2
1	A	494	TRP	2.2
1	B	494	TRP	2.2
1	B	408	GLU	2.2
1	H	416	LEU	2.2
1	A	110	PHE	2.2
1	B	109	SER	2.2
1	E	107	VAL	2.1
1	B	11	ALA	2.1
1	E	513	GLY	2.1
1	A	109	SER	2.1
1	G	311	ILE	2.1
1	A	242	ARG	2.1
1	E	411	ARG	2.1
1	C	66	ALA	2.1
1	B	21	GLY	2.1
1	B	375	GLY	2.1
1	B	540[A]	LEU	2.1
1	A	108	GLU	2.1
1	C	116	SER	2.1
1	F	507	GLU	2.1
1	B	15	GLN	2.1
1	B	377	THR	2.1
1	B	65	PRO	2.1
1	A	542	ILE	2.1
1	C	90	HIS	2.1
1	A	32	ALA	2.1
1	A	274	GLY	2.1
1	B	257	VAL	2.1
1	B	521	VAL	2.1
1	B	500	ARG	2.1
1	C	114	PRO	2.1
1	B	486	TYR	2.1
1	B	232	GLY	2.0
1	C	112	GLY	2.0
1	E	128	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	274	GLY	2.0
1	B	495	ALA	2.0
1	E	517	VAL	2.0
1	F	234	SER	2.0
1	G	487	ARG	2.0
1	A	436	CYS	2.0
1	D	436	CYS	2.0
1	C	272	PRO	2.0
1	F	94	GLU	2.0
1	A	88	PHE	2.0
1	B	25	PHE	2.0
1	G	404	ARG	2.0
1	G	516	ARG	2.0
1	H	267[A]	ARG	2.0
1	A	495	ALA	2.0
1	C	414	ALA	2.0
1	F	33	ALA	2.0
1	B	131	SER	2.0
1	D	131	SER	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($\text{\AA}^2$)	Q<0.9
6	OD9	H	605	36/36	0.59	0.26	52,60,62,63	23
6	OD9	E	605	36/36	0.69	0.23	53,58,60,61	23
6	OD9	A	605	36/36	0.78	0.19	50,51,53,53	23
6	OD9	B	605	36/36	0.86	0.15	39,42,44,44	23

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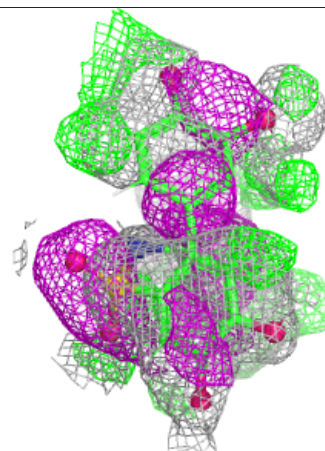
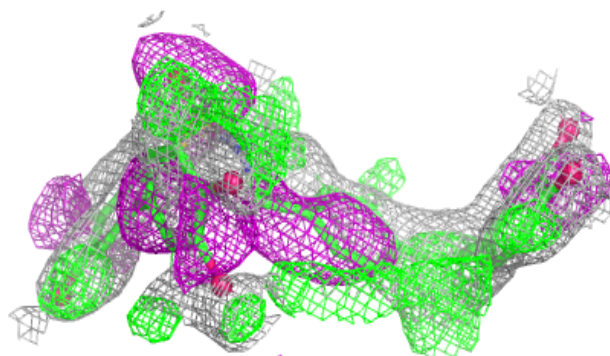
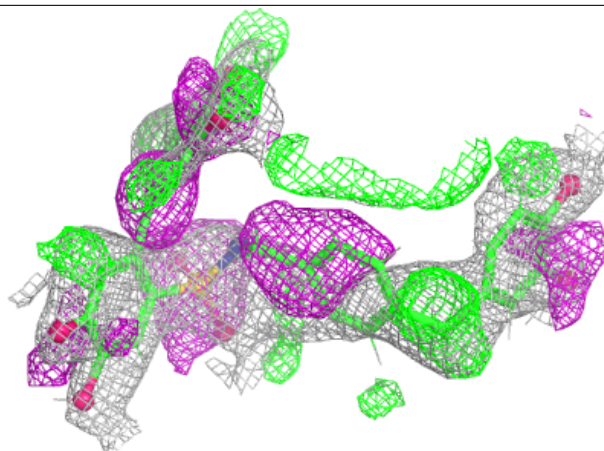
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	OXL	A	602	6/6	0.90	0.10	43,44,44,44	0
3	OXL	E	602	6/6	0.91	0.09	40,41,41,41	0
3	OXL	D	602	6/6	0.92	0.08	31,32,33,33	0
3	OXL	F	602	6/6	0.93	0.10	36,37,38,39	0
3	OXL	G	602	6/6	0.93	0.08	31,31,32,32	0
3	OXL	B	602	6/6	0.93	0.09	37,37,38,39	0
3	OXL	C	602	6/6	0.94	0.07	34,35,36,37	0
5	K	E	604	1/1	0.94	0.22	67,67,67,67	0
3	OXL	H	602	6/6	0.95	0.07	25,27,27,28	0
5	K	F	604	1/1	0.96	0.11	57,57,57,57	0
5	K	H	604	1/1	0.96	0.10	41,41,41,41	0
2	FBP	A	601	20/20	0.96	0.07	33,34,35,35	0
2	FBP	B	601	20/20	0.96	0.08	32,33,37,37	0
5	K	B	604	1/1	0.96	0.14	60,60,60,60	0
2	FBP	E	601	20/20	0.96	0.07	31,32,34,34	0
5	K	A	604	1/1	0.97	0.11	59,59,59,59	0
2	FBP	F	601	20/20	0.97	0.06	28,32,35,35	0
5	K	G	604	1/1	0.97	0.15	47,47,47,47	0
5	K	C	604	1/1	0.97	0.16	47,47,47,47	0
4	MG	A	603	1/1	0.98	0.16	26,26,26,26	0
5	K	D	604	1/1	0.98	0.10	41,41,41,41	0
4	MG	B	603	1/1	0.99	0.13	24,24,24,24	0
4	MG	C	603	1/1	0.99	0.13	19,19,19,19	0
4	MG	E	603	1/1	0.99	0.15	24,24,24,24	0
4	MG	G	603	1/1	0.99	0.15	14,14,14,14	0
2	FBP	D	601	20/20	0.99	0.04	21,22,24,24	0
2	FBP	G	601	20/20	0.99	0.04	20,21,23,23	0
2	FBP	H	601	20/20	0.99	0.04	17,19,21,21	0
2	FBP	C	601	20/20	0.99	0.04	22,23,24,25	0
4	MG	F	603	1/1	1.00	0.13	18,18,18,18	0
4	MG	D	603	1/1	1.00	0.15	16,16,16,16	0
4	MG	H	603	1/1	1.00	0.14	13,13,13,13	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.

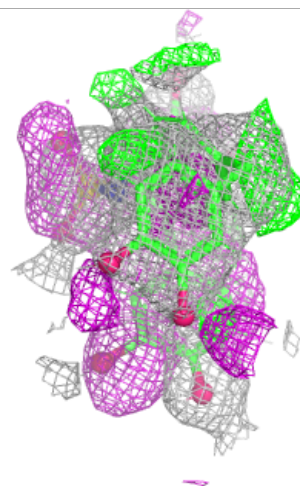
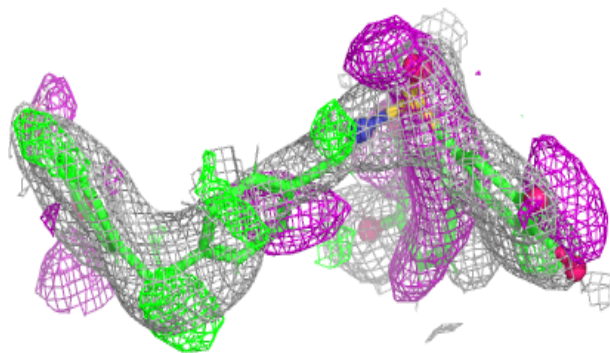
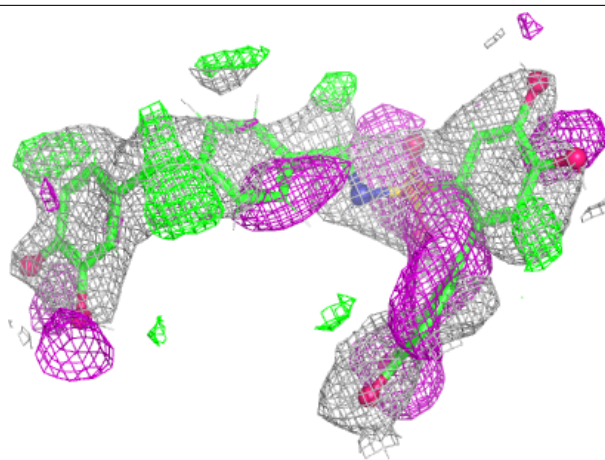
Electron density around OD9 H 605:

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



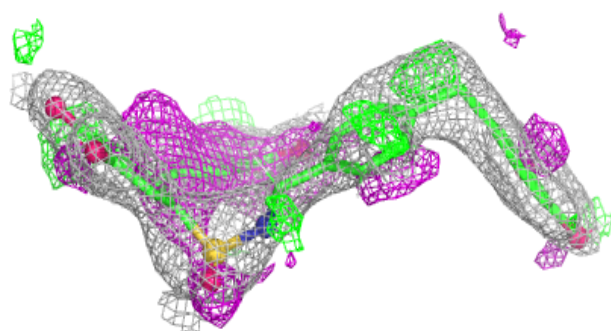
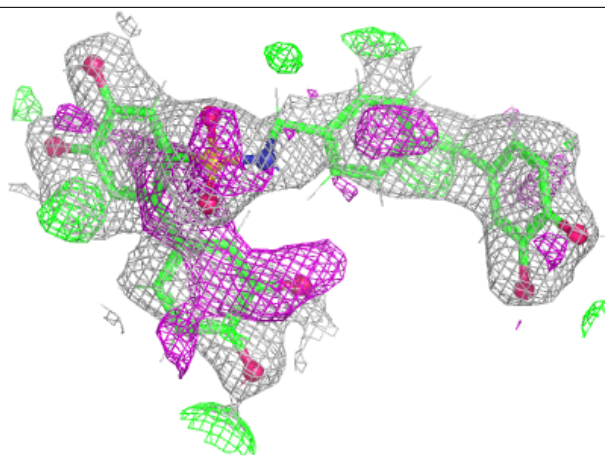
Electron density around OD9 E 605:

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



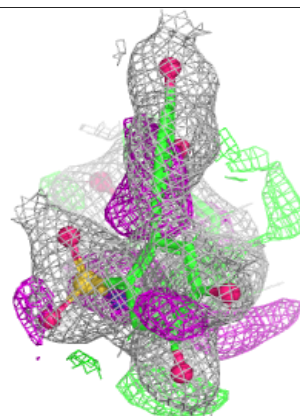
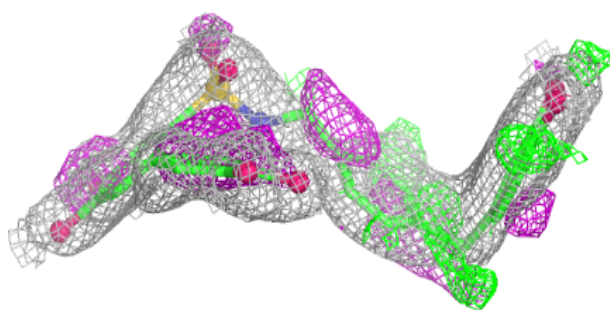
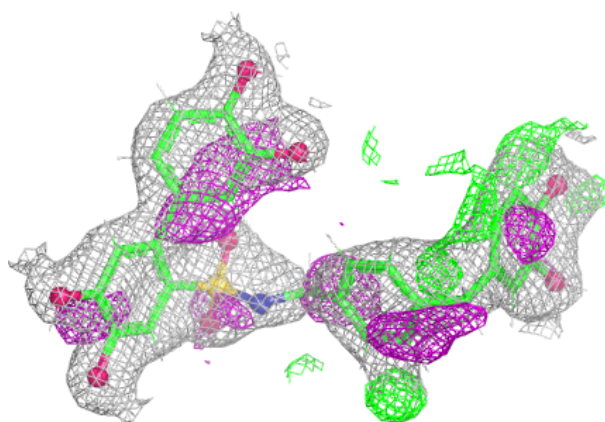
Electron density around OD9 A 605:

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

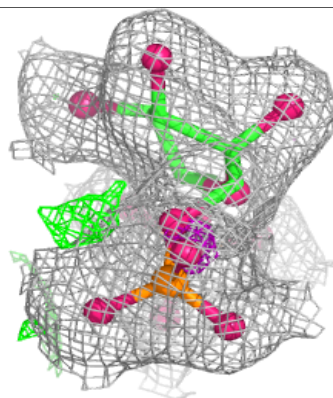
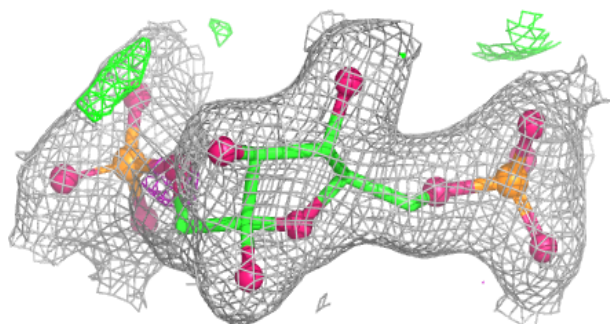
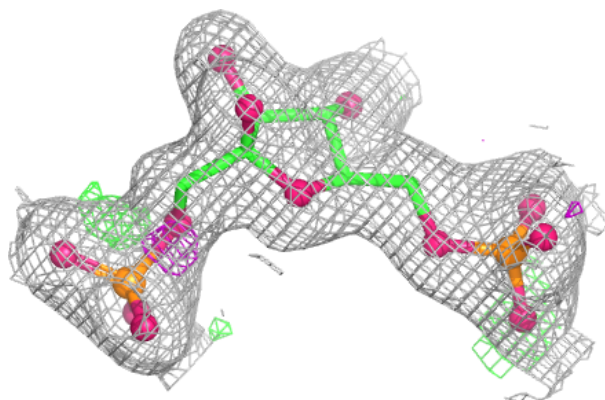


Electron density around OD9 B 605:

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and green (positive)

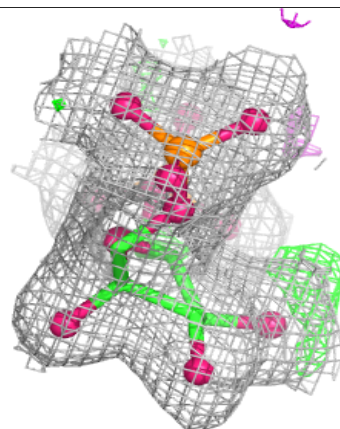
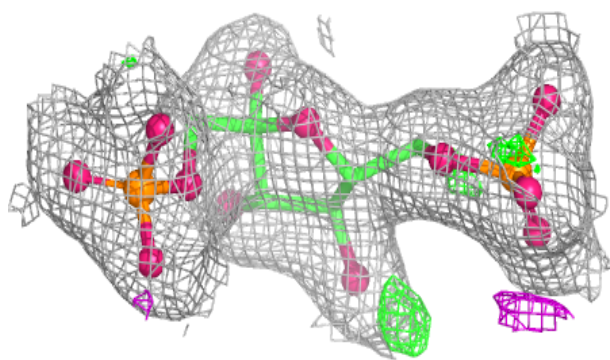
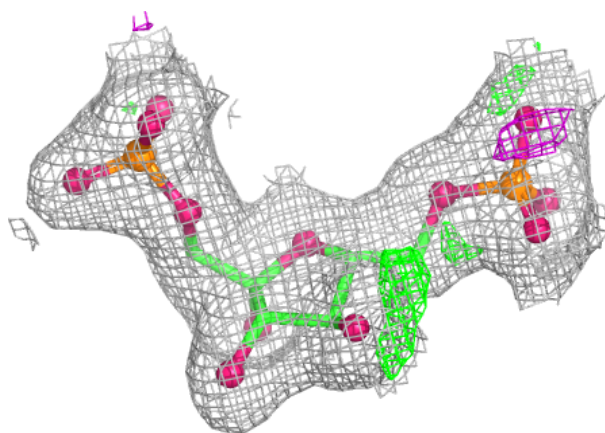
**Electron density around FBP A 601:**

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and green (positive)

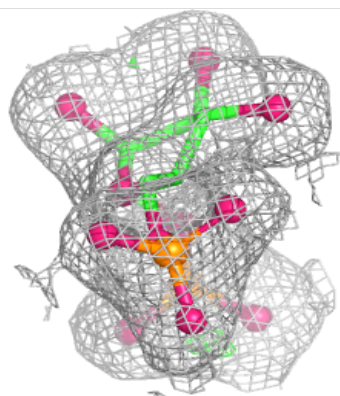
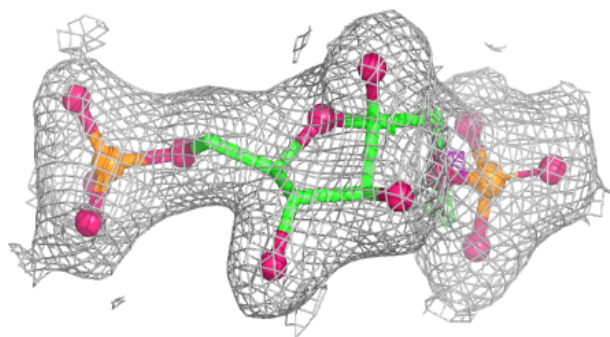
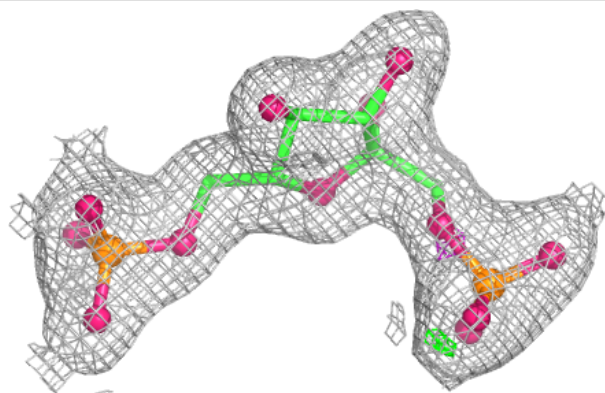


Electron density around FBP B 601:

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and green (positive)

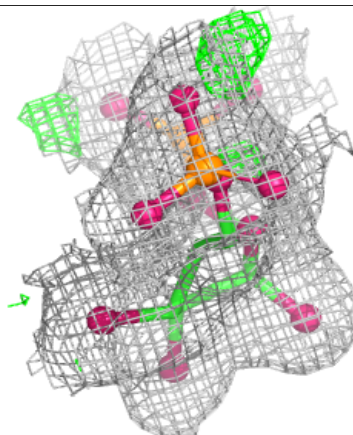
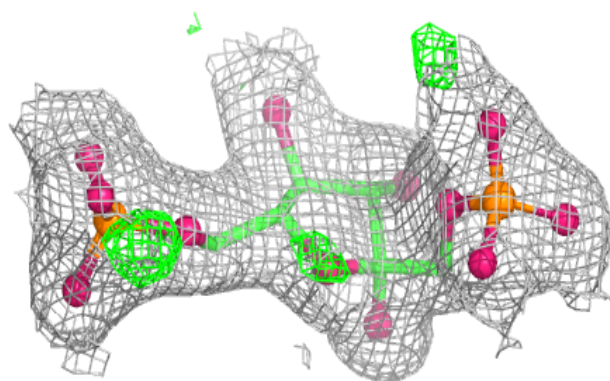
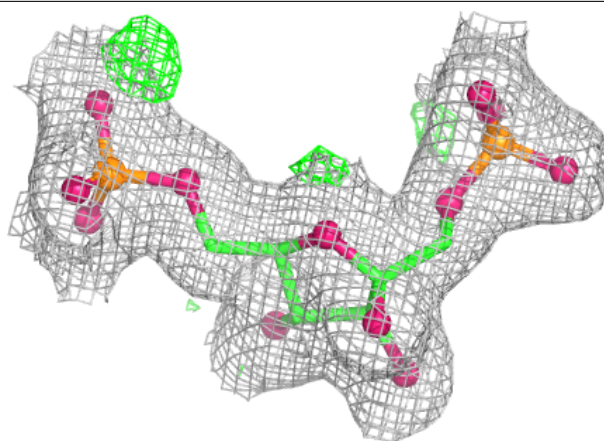
**Electron density around FBP E 601:**

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

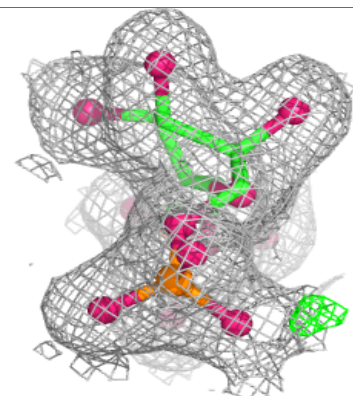
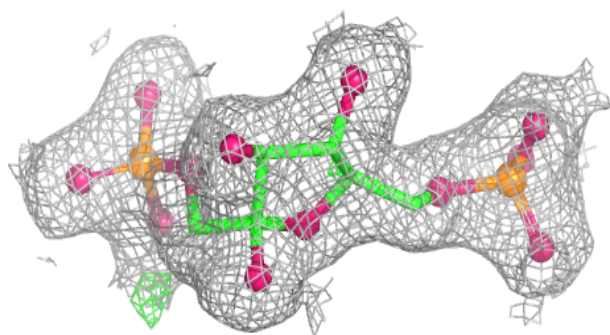
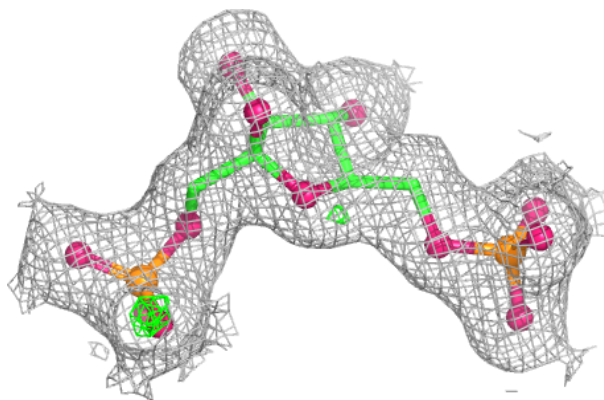


Electron density around FBP F 601:

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

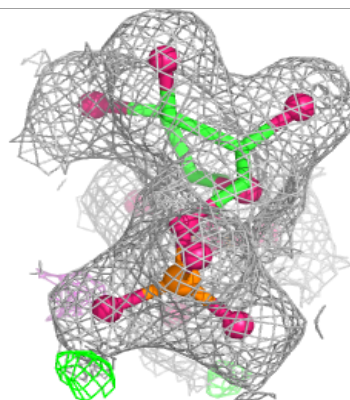
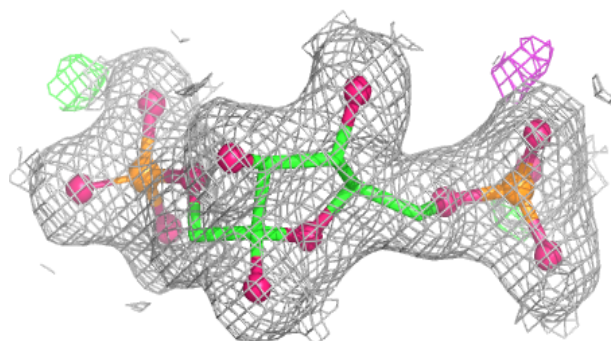
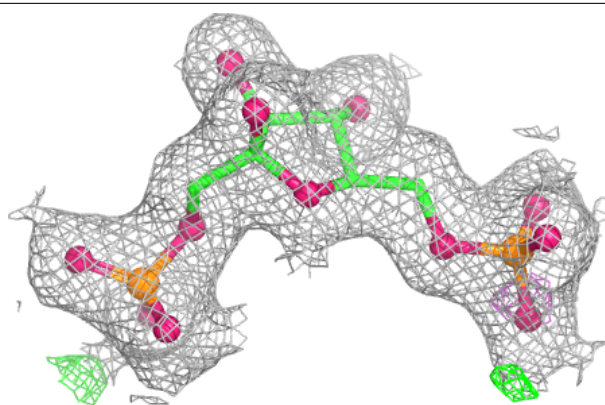
**Electron density around FBP D 601:**

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

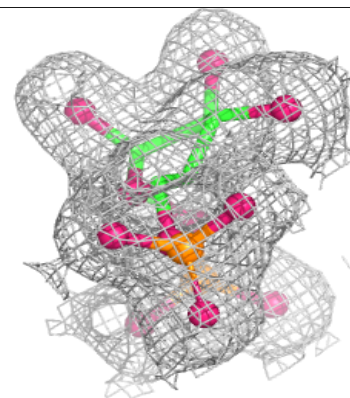
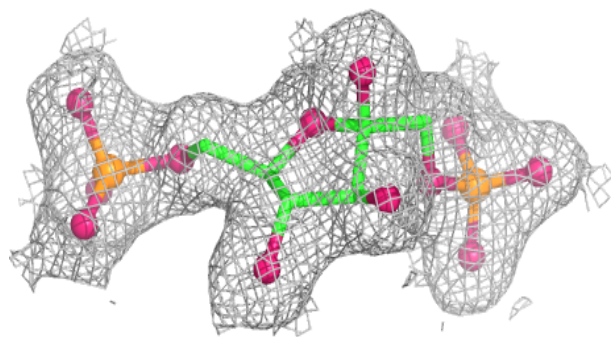
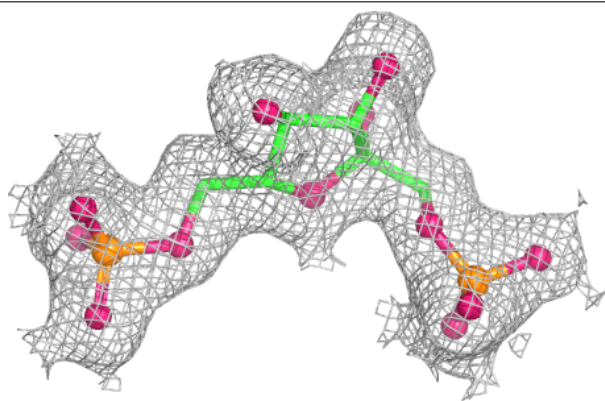


Electron density around FBP G 601:

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and green (positive)

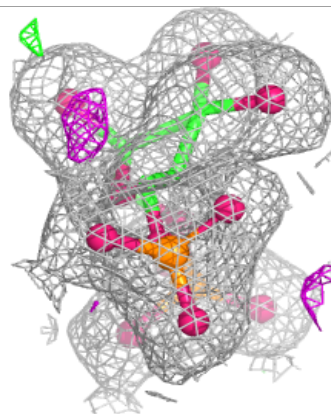
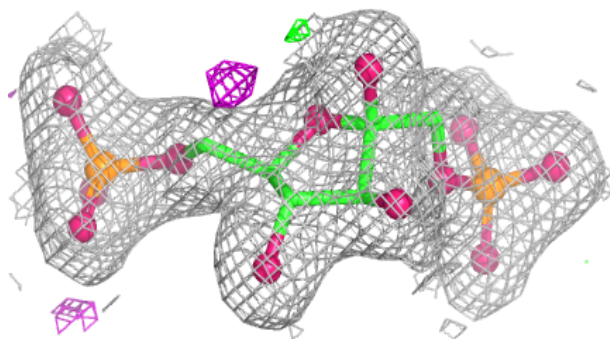
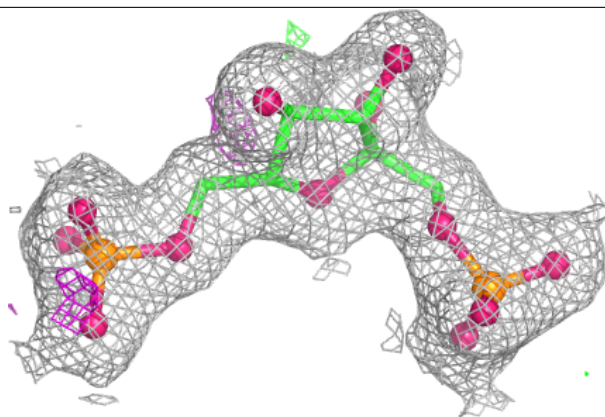
**Electron density around FBP H 601:**

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



Electron density around FBP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.