



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:48 PM UTC

PDB ID : 7FRX / pdb_00007frx
Title : Structure of liver pyruvate kinase in complex with allosteric modulator 5
Authors : Lulla, A.; Nilsson, O.; Brear, P.; Nain-Perez, A.; Grotli, M.; Hyvonen, M.
Deposited on : 2022-12-18
Resolution : 1.85 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

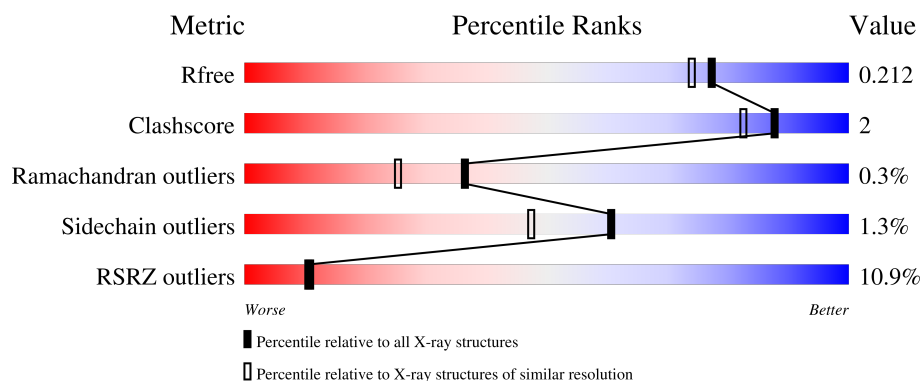
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	22% 88% 6% 6%
1	B	447	16% 90% 7% .
1	C	447	6% 90% 5% 5%
1	D	447	3% 90% . 5%
1	E	447	13% 88% 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 29187 atoms, of which 68 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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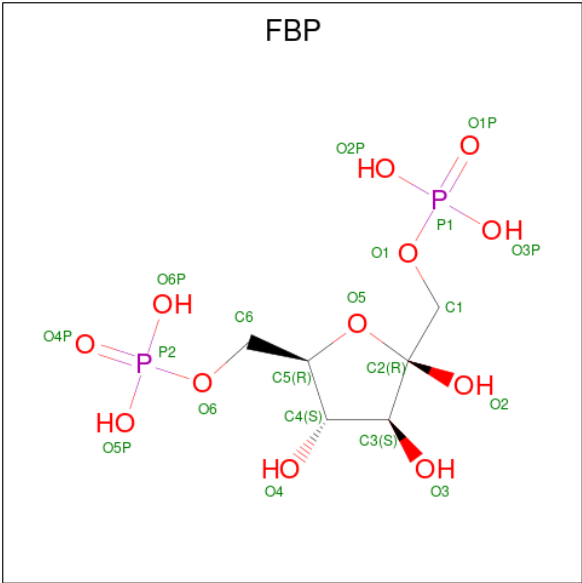
Chain	Residue	Modelled	Actual	Comment	Reference
B	130	GLY	-	linker	UNP P30613
B	131	SER	-	linker	UNP P30613
B	132	GLY	-	linker	UNP P30613
C	-1	GLY	-	expression tag	UNP P30613
C	0	SER	-	expression tag	UNP P30613
C	1	MET	-	expression tag	UNP P30613
C	2	GLU	-	expression tag	UNP P30613
C	12	ASP	SER	conflict	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		

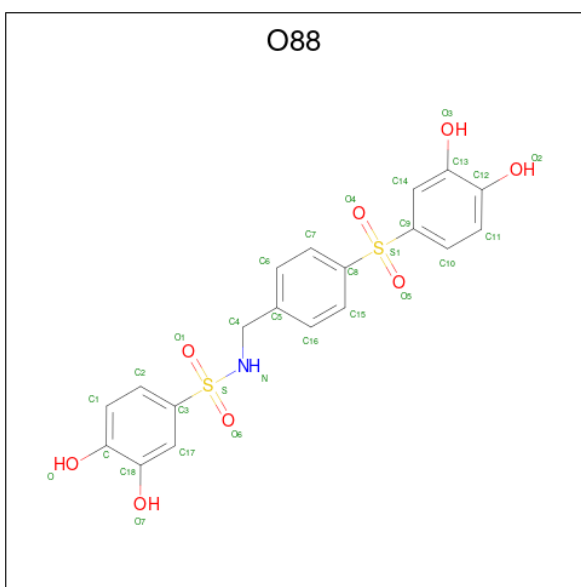
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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 N-{[4-(3,4-dihydroxybenzene-1-sulfonyl)phenyl]methyl}-3,4-dihydroxybenzene-1-sulfonamide (CCD ID: O88) (formula: C₁₉H₁₇NO₈S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total 47	C 19	H 17	N 1	O 8	S 2	17	0
6	B	1	Total 47	C 19	H 17	N 1	O 8	S 2	17	0
6	E	1	Total 47	C 19	H 17	N 1	O 8	S 2	17	0
6	F	1	Total 47	C 19	H 17	N 1	O 8	S 2	17	0

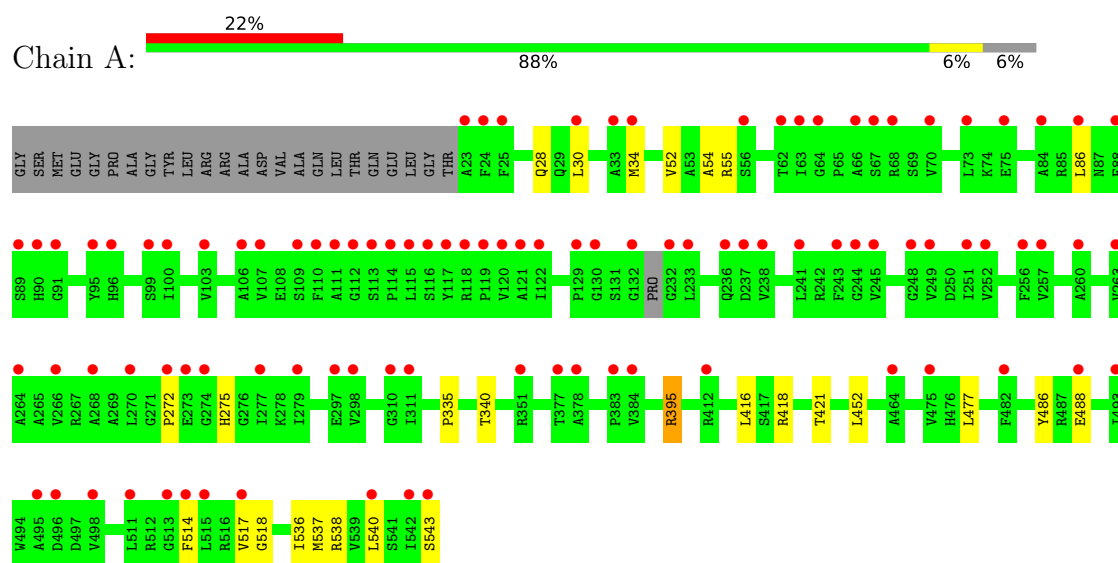
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	235	Total O 235 235	0	0
7	B	260	Total O 260 260	0	0
7	C	377	Total O 377 377	0	0
7	D	421	Total O 421 421	0	0
7	E	250	Total O 250 250	0	0
7	F	326	Total O 326 326	0	0
7	G	380	Total O 380 380	0	0
7	H	449	Total O 449 449	0	0

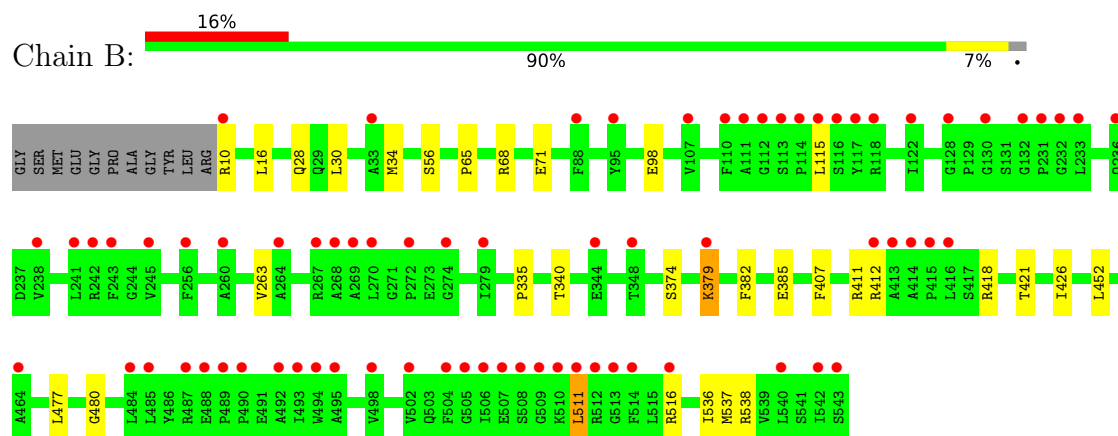
3 Residue-property plots [i](#)

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

• Molecule 1: Pyruvate kinase PKLR

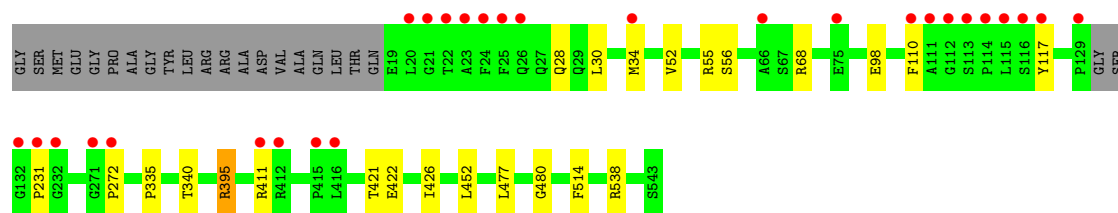


• Molecule 1: Pyruvate kinase PKLR

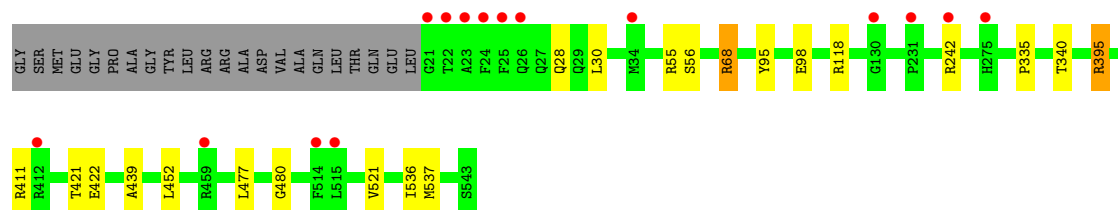
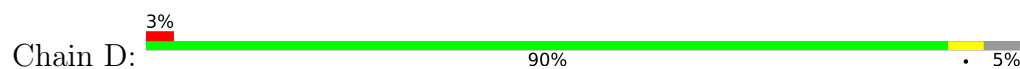


• Molecule 1: Pyruvate kinase PKLR

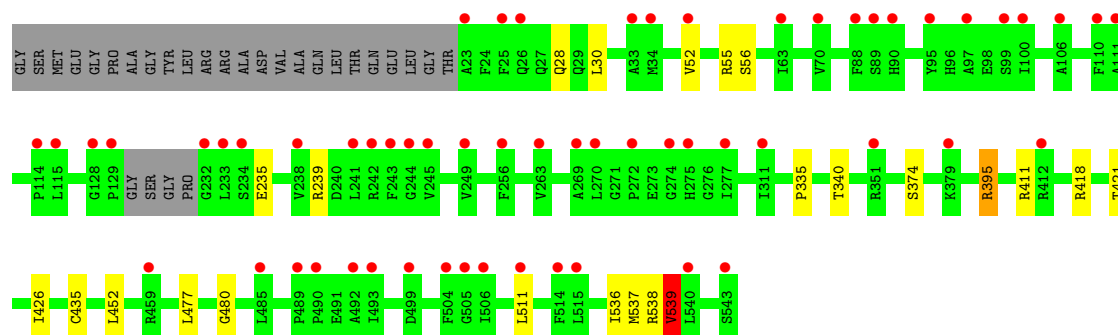
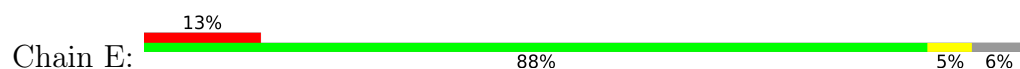




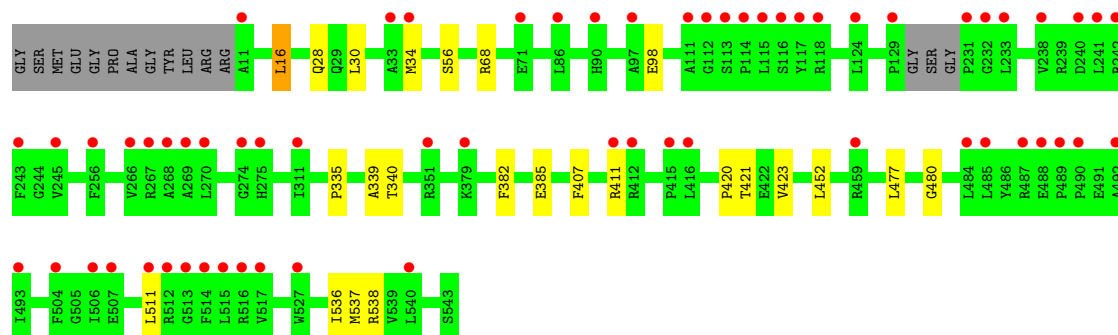
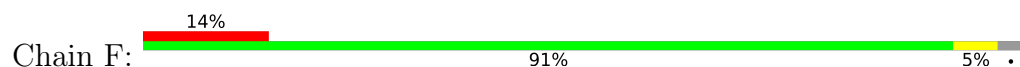
• Molecule 1: Pyruvate kinase PKLR



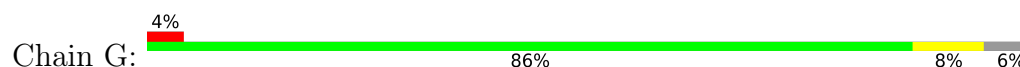
• Molecule 1: Pyruvate kinase PKLR

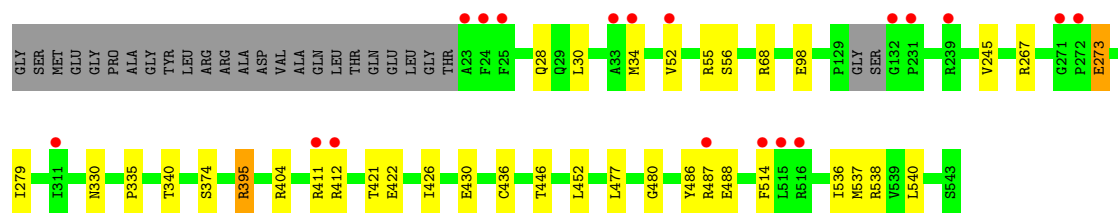


• Molecule 1: Pyruvate kinase PKLR

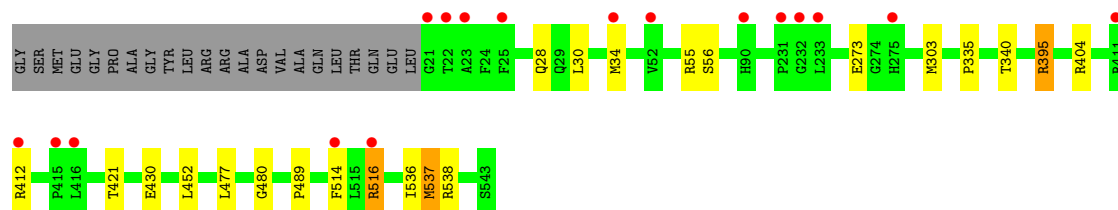
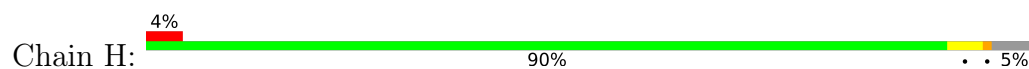


• Molecule 1: Pyruvate kinase PKLR





- 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	208.84Å 113.20Å 189.15Å 90.00° 90.99° 90.00°	Depositor
Resolution (Å)	189.12 – 1.85 189.12 – 1.85	Depositor EDS
% Data completeness (in resolution range)	79.2 (189.12-1.85) 79.2 (189.12-1.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 1.84Å)	Xtriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, R_{free}	0.200 , 0.222 0.192 , 0.212	Depositor DCC
R_{free} test set	14973 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.7	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	29187	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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 43.84 % 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 1.6636e-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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, K, O88, OXL, FBP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.64	0/3307	0.95	0/4469
1	B	0.67	1/3396 (0.0%)	0.95	0/4592
1	C	0.71	0/3313	0.95	1/4479 (0.0%)
1	D	0.71	0/3326	0.94	0/4497
1	E	0.63	1/3278 (0.0%)	0.95	1/4430 (0.0%)
1	F	0.67	0/3396	0.95	2/4591 (0.0%)
1	G	0.72	2/3303 (0.1%)	0.94	2/4465 (0.0%)
1	H	0.73	2/3316 (0.1%)	0.94	1/4483 (0.0%)
All	All	0.69	6/26635 (0.0%)	0.95	7/36006 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	374	SER	CA-C	5.99	1.55	1.52
1	G	374[A]	SER	CA-C	5.52	1.55	1.52
1	G	374[B]	SER	CA-C	5.52	1.55	1.52
1	H	489	PRO	CA-C	5.11	1.55	1.52
1	H	303	MET	SD-CE	-5.07	1.66	1.79
1	E	374	SER	CA-C	5.01	1.54	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	330	ASN	CA-CB-CG	6.00	118.60	112.60
1	H	514	PHE	CA-CB-CG	5.64	119.44	113.80
1	F	339	ALA	CA-C-N	5.52	132.09	121.54
1	F	339	ALA	C-N-CA	5.52	132.09	121.54
1	E	539	VAL	N-CA-CB	5.26	117.37	111.21
1	C	514	PHE	CA-CB-CG	5.21	119.01	113.80
1	G	514	PHE	CA-CB-CG	5.02	118.82	113.80

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	16	0
1	B	3329	0	3394	16	1
1	C	3247	0	3299	17	0
1	D	3252	0	3310	13	0
1	E	3210	0	3270	13	0
1	F	3321	0	3393	13	0
1	G	3231	0	3284	23	0
1	H	3251	0	3306	15	0
2	A	20	0	10	0	0
2	B	20	0	10	0	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
2	E	20	0	10	0	0
2	F	20	0	10	0	0
2	G	20	0	10	0	0
2	H	20	0	10	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0
3	G	6	0	0	0	0
3	H	6	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	30	17	0	0	0
6	B	30	17	0	0	0
6	E	30	17	0	0	0
6	F	30	17	0	0	0
7	A	235	0	0	0	0
7	B	260	0	0	0	0
7	C	377	0	0	1	0
7	D	421	0	0	1	0
7	E	250	0	0	0	0
7	F	326	0	0	0	0
7	G	380	0	0	0	0
7	H	449	0	0	1	0
All	All	29119	68	26635	105	1

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

All (105) 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:D:422:GLU:HG3	7:D:703:HOH:O	1.73	0.88
1:G:538:ARG:HG2	1:H:536:ILE:HG12	1.62	0.81
1:C:538:ARG:HG2	1:D:536:ILE:HG12	1.62	0.80
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.66	0.77
1:C:422[A]:GLU:HG3	1:C:452:LEU:HD13	1.67	0.77
1:B:411:ARG:HG2	1:B:426:ILE:HD11	1.68	0.75
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.69	0.73
1:D:68:ARG:NH2	1:D:98:GLU:HB2	2.10	0.66
1:F:407:PHE:CE2	1:F:411:ARG:NH1	2.65	0.65
1:A:418[A]:ARG:HG3	1:B:16:LEU:HD11	1.80	0.63
1:C:411:ARG:HG2	1:C:426:ILE:HD11	1.83	0.60
1:A:272:PRO:HA	1:A:275:HIS:CE1	2.37	0.59
1:G:536:ILE:HG12	1:H:538[A]:ARG:HG2	1.84	0.58
1:A:28:GLN:HB3	1:A:52:VAL:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:ARG:HH12	1:D:411:ARG:NH2	2.03	0.57
1:C:28:GLN:HB3	1:C:52:VAL:HG22	1.87	0.56
1:G:411:ARG:HG3	1:G:426:ILE:HD11	1.86	0.56
1:E:28:GLN:HB3	1:E:52:VAL:HG22	1.88	0.55
1:G:28:GLN:HB3	1:G:52:VAL:HG22	1.88	0.55
1:E:235:GLU:O	1:E:239:ARG:HD3	2.07	0.54
1:E:536:ILE:HG12	1:F:538:ARG:HG2	1.90	0.54
1:G:267:ARG:HG2	1:G:279:ILE:HD12	1.91	0.53
1:E:538:ARG:HG2	1:F:536:ILE:HG12	1.89	0.53
1:D:68:ARG:NH2	1:D:95:TYR:O	2.40	0.52
1:A:272:PRO:HA	1:A:275:HIS:NE2	2.23	0.52
1:G:267:ARG:HG2	1:G:279:ILE:CD1	2.39	0.52
1:F:28:GLN:HG3	1:F:30:LEU:HG	1.90	0.52
1:G:56:SER:HB2	1:G:480:GLY:HA2	1.92	0.51
1:A:518:GLY:O	1:B:418:ARG:NH2	2.44	0.51
1:H:56:SER:HB2	1:H:480:GLY:HA2	1.92	0.51
1:A:538:ARG:HG3	1:B:536:ILE:HG12	1.92	0.51
1:A:517:VAL:HG13	1:A:543:SER:HB3	1.94	0.50
1:B:28:GLN:HG3	1:B:30:LEU:HG	1.93	0.50
1:C:272:PRO:HD3	1:G:446:THR:HG22	1.93	0.50
1:C:110:PHE:O	1:C:117:TYR:HB2	2.11	0.50
1:B:407:PHE:CZ	1:B:411:ARG:HD2	2.47	0.50
1:E:418:ARG:HD3	1:F:16:LEU:HD11	1.94	0.50
1:G:537:MET:HE3	1:H:537:MET:HG2	1.94	0.50
1:A:28:GLN:HG3	1:A:30:LEU:HG	1.93	0.49
1:D:68:ARG:HH22	1:D:98:GLU:HB2	1.74	0.49
1:D:28:GLN:HG3	1:D:30:LEU:HG	1.95	0.49
1:G:486:TYR:CZ	1:G:488:GLU:HB2	2.47	0.49
1:G:245:VAL:CG1	1:G:273:GLU:HG2	2.42	0.49
1:D:439:ALA:O	1:D:521:VAL:HG23	2.12	0.48
1:G:28:GLN:HG3	1:G:30:LEU:HG	1.96	0.48
1:B:407:PHE:CE2	1:B:411:ARG:HD2	2.48	0.48
1:H:28:GLN:HG3	1:H:30:LEU:HG	1.96	0.48
1:E:411:ARG:HG3	1:E:426:ILE:HD11	1.94	0.47
1:G:430[B]:GLU:OE2	1:H:430:GLU:OE1	2.32	0.47
1:E:28:GLN:HG3	1:E:30:LEU:HG	1.96	0.47
1:G:430[A]:GLU:OE1	1:H:430:GLU:OE1	2.33	0.47
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.97	0.47
1:E:56:SER:HB2	1:E:480:GLY:HA2	1.96	0.46
1:H:55:ARG:HB2	1:H:395:ARG:HG3	1.97	0.46
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:ARG:NH1	1:D:411:ARG:NH2	2.63	0.46
1:F:56:SER:HB2	1:F:480:GLY:HA2	1.98	0.46
1:C:538:ARG:HD3	7:C:748:HOH:O	2.14	0.46
1:F:421:THR:HG22	1:F:452:LEU:HD12	1.98	0.46
1:G:55:ARG:HB2	1:G:395:ARG:HG3	1.98	0.46
1:C:28:GLN:HG3	1:C:30:LEU:HG	1.97	0.46
1:A:335:PRO:HB3	1:A:477:LEU:O	2.16	0.45
1:E:335:PRO:HB3	1:E:477:LEU:O	2.16	0.45
1:C:68:ARG:NH2	1:C:98:GLU:HB3	2.32	0.45
1:B:335:PRO:HB3	1:B:477:LEU:O	2.17	0.45
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.99	0.45
1:B:421:THR:HG22	1:B:452:LEU:HD12	1.99	0.45
1:B:68:ARG:NH2	1:B:98:GLU:HB3	2.31	0.45
1:H:335:PRO:HB3	1:H:477:LEU:O	2.17	0.45
1:A:55:ARG:HB2	1:A:395:ARG:HG3	1.97	0.45
1:A:421:THR:HG22	1:A:452:LEU:HD12	2.00	0.44
1:F:68:ARG:NH2	1:F:98:GLU:HB3	2.33	0.44
1:F:335:PRO:HB3	1:F:477:LEU:O	2.17	0.44
1:C:421:THR:HG22	1:C:452:LEU:HD12	1.98	0.44
1:G:421:THR:HG22	1:G:452:LEU:HD12	2.00	0.44
1:B:382:PHE:HB3	1:B:385:GLU:HB2	1.99	0.44
1:H:421:THR:HG22	1:H:452:LEU:HD12	2.00	0.43
1:A:486:TYR:CZ	1:A:488[B]:GLU:HB2	2.54	0.43
1:C:55:ARG:HB2	1:C:395:ARG:HG3	2.00	0.43
1:D:335:PRO:HB3	1:D:477:LEU:O	2.18	0.43
1:E:539:VAL:HG22	1:F:420:PRO:HB3	2.01	0.43
1:H:56:SER:HB2	1:H:480:GLY:CA	2.48	0.43
1:E:55:ARG:HB2	1:E:395:ARG:HG3	1.99	0.43
1:F:30:LEU:O	1:F:34:MET:HG2	2.18	0.43
1:C:411:ARG:CG	1:C:426:ILE:HD11	2.48	0.43
1:D:55:ARG:HB2	1:D:395:ARG:HG3	2.00	0.42
1:G:335:PRO:HB3	1:G:477:LEU:O	2.20	0.42
1:A:54:ALA:CB	1:A:514:PHE:HE1	2.32	0.42
1:B:30:LEU:O	1:B:34:MET:HG2	2.20	0.42
1:B:65:PRO:HG2	1:B:379:LYS:HG2	2.02	0.42
1:C:335:PRO:HB3	1:C:477:LEU:O	2.19	0.42
1:A:416:LEU:HB3	1:B:16:LEU:HD22	2.01	0.42
1:G:404:ARG:HD3	1:H:412:ARG:CZ	2.49	0.42
1:C:30:LEU:O	1:C:34:MET:HG2	2.20	0.41
1:E:421:THR:HG22	1:E:452:LEU:HD12	2.00	0.41
1:D:421:THR:HG22	1:D:452:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:56:SER:HB2	1:G:480:GLY:CA	2.50	0.41
1:G:412:ARG:CZ	1:H:404:ARG:HD3	2.51	0.41
1:A:30:LEU:O	1:A:34:MET:HG2	2.20	0.41
1:H:30:LEU:O	1:H:34:MET:HG2	2.20	0.41
1:G:68:ARG:NH2	1:G:98[B]:GLU:HB3	2.36	0.41
1:E:435:CYS:HB3	1:F:423:VAL:HG21	2.03	0.40
1:G:30:LEU:O	1:G:34:MET:HG2	2.22	0.40
1:H:516:ARG:HD3	7:H:906:HOH:O	2.20	0.40
1:F:382:PHE:HB3	1:F:385:GLU:HB2	2.02	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:LEU:O	1:B:511:LEU:O[2_555]	2.18	0.02

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%)	420 (99%)	3 (1%)	1 (0%)	43	34
1	B	438/447 (98%)	435 (99%)	2 (0%)	1 (0%)	43	34
1	C	425/447 (95%)	418 (98%)	5 (1%)	2 (0%)	24	12
1	D	429/447 (96%)	426 (99%)	2 (0%)	1 (0%)	43	34
1	E	420/447 (94%)	415 (99%)	4 (1%)	1 (0%)	43	34
1	F	435/447 (97%)	432 (99%)	2 (0%)	1 (0%)	43	34
1	G	423/447 (95%)	414 (98%)	8 (2%)	1 (0%)	43	34
1	H	427/447 (96%)	423 (99%)	3 (1%)	1 (0%)	43	34
All	All	3421/3576 (96%)	3383 (99%)	29 (1%)	9 (0%)	36	25

All (9) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	340/352 (97%)	335 (98%)	5 (2%)	57	42
1	B	349/352 (99%)	339 (97%)	10 (3%)	37	20
1	C	341/352 (97%)	340 (100%)	1 (0%)	86	81
1	D	342/352 (97%)	336 (98%)	6 (2%)	51	35
1	E	338/352 (96%)	333 (98%)	5 (2%)	57	42
1	F	350/352 (99%)	346 (99%)	4 (1%)	65	54
1	G	340/352 (97%)	335 (98%)	5 (2%)	57	42
1	H	340/352 (97%)	336 (99%)	4 (1%)	63	51
All	All	2740/2816 (97%)	2700 (98%)	40 (2%)	61	42

All (40) 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	540	LEU

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Mol	Chain	Res	Type
1	B	10	ARG
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	516	ARG
1	B	537[A]	MET
1	B	537[B]	MET
1	C	395	ARG
1	D	68	ARG
1	D	118	ARG
1	D	242[A]	ARG
1	D	242[B]	ARG
1	D	395	ARG
1	D	537	MET
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	511	LEU
1	F	537[A]	MET
1	F	537[B]	MET
1	G	273	GLU
1	G	395	ARG
1	G	436	CYS
1	G	487	ARG
1	G	540	LEU
1	H	273	GLU
1	H	395	ARG
1	H	516	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	27	GLN
1	A	236	GLN
1	B	27	GLN

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Mol	Chain	Res	Type
1	C	27	GLN
1	C	470	GLN
1	D	27	GLN
1	E	27	GLN
1	F	26	GLN
1	G	27	GLN
1	G	275	HIS
1	H	27	GLN
1	H	390	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	0.46	0	21,32,32	0.67	0
6	O88	F	605	-	32,32,32	2.26	7 (21%)	46,48,48	1.81	17 (36%)
3	OXL	E	602	4	5,5,5	2.14	2 (40%)	6,6,6	1.97	2 (33%)
3	OXL	G	602	4	5,5,5	1.97	2 (40%)	6,6,6	2.12	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OXL	D	602	4	5,5,5	2.12	2 (40%)	6,6,6	1.74	2 (33%)
2	FBP	G	601	-	18,20,20	0.58	0	21,32,32	0.84	1 (4%)
3	OXL	A	602	4	5,5,5	2.00	2 (40%)	6,6,6	2.10	3 (50%)
3	OXL	H	602	4	5,5,5	1.92	2 (40%)	6,6,6	1.91	2 (33%)
6	O88	E	605	-	32,32,32	2.28	6 (18%)	46,48,48	1.94	18 (39%)
3	OXL	C	602	4	5,5,5	1.89	2 (40%)	6,6,6	1.99	2 (33%)
2	FBP	B	601	-	18,20,20	0.83	1 (5%)	21,32,32	0.81	1 (4%)
2	FBP	C	601	-	18,20,20	0.56	0	21,32,32	0.62	0
6	O88	B	605	-	32,32,32	2.19	5 (15%)	46,48,48	2.00	22 (47%)
6	O88	A	605	-	32,32,32	2.12	6 (18%)	46,48,48	2.26	21 (45%)
2	FBP	H	601	-	18,20,20	0.69	0	21,32,32	0.73	1 (4%)
3	OXL	B	602	4	5,5,5	2.20	2 (40%)	6,6,6	1.95	2 (33%)
3	OXL	F	602	4	5,5,5	2.88	4 (80%)	6,6,6	2.08	2 (33%)
2	FBP	F	601	-	18,20,20	0.50	0	21,32,32	0.57	0
2	FBP	E	601	-	18,20,20	0.55	0	21,32,32	0.73	1 (4%)
2	FBP	D	601	-	18,20,20	0.53	0	21,32,32	0.73	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
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
6	O88	F	605	-	-	1/24/24/24	0/3/3/3
3	OXL	E	602	4	-	4/4/4/4	-
3	OXL	G	602	4	-	4/4/4/4	-
3	OXL	D	602	4	-	4/4/4/4	-
2	FBP	G	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	-
6	O88	E	605	-	-	2/24/24/24	0/3/3/3
3	OXL	C	602	4	-	4/4/4/4	-
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
6	O88	B	605	-	-	3/24/24/24	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	O88	A	605	-	-	2/24/24/24	0/3/3/3
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1
3	OXL	B	602	4	-	4/4/4/4	-
3	OXL	F	602	4	-	4/4/4/4	-
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
2	FBP	E	601	-	-	2/13/32/32	0/1/1/1
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	605	O88	C8-S1	-7.71	1.65	1.77
6	F	605	O88	C8-S1	-7.61	1.65	1.77
6	B	605	O88	C8-S1	-7.03	1.66	1.77
6	A	605	O88	C9-S1	-6.28	1.67	1.77
6	E	605	O88	C3-S	-5.82	1.67	1.76
6	B	605	O88	C3-S	-5.73	1.67	1.76
6	A	605	O88	C8-S1	-5.30	1.68	1.77
6	A	605	O88	C3-S	-5.12	1.68	1.76
6	F	605	O88	C9-S1	-5.04	1.69	1.77
6	F	605	O88	C3-S	-4.90	1.68	1.76
6	E	605	O88	C9-S1	-4.83	1.69	1.77
6	B	605	O88	C9-S1	-4.23	1.70	1.77
6	A	605	O88	C2-C3	3.84	1.44	1.38
6	B	605	O88	O1-S	-3.84	1.39	1.43
3	E	602	OXL	O1-C1	3.81	1.32	1.22
3	B	602	OXL	O2-C2	3.78	1.31	1.22
3	F	602	OXL	O3-C1	-3.68	1.20	1.30
3	F	602	OXL	O2-C2	3.59	1.31	1.22
3	A	602	OXL	O2-C2	3.57	1.31	1.22
3	D	602	OXL	O2-C2	3.50	1.31	1.22
6	E	605	O88	C2-C3	3.29	1.44	1.38
3	C	602	OXL	O1-C1	3.15	1.30	1.22
3	H	602	OXL	O2-C2	3.14	1.30	1.22
6	F	605	O88	O6-S	-3.09	1.40	1.43
6	F	605	O88	O1-S	-3.07	1.40	1.43
3	F	602	OXL	O1-C1	3.05	1.30	1.22
3	G	602	OXL	O3-C1	-3.02	1.22	1.30
3	D	602	OXL	O4-C2	-3.01	1.22	1.30
3	G	602	OXL	O1-C1	2.95	1.29	1.22
3	B	602	OXL	O4-C2	-2.86	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	OXL	O3-C1	-2.67	1.23	1.30
3	H	602	OXL	O4-C2	-2.65	1.23	1.30
6	B	605	O88	C2-C3	2.59	1.42	1.38
6	A	605	O88	C6-C7	2.53	1.42	1.38
3	A	602	OXL	O4-C2	-2.52	1.23	1.30
6	F	605	O88	S-N	2.49	1.65	1.61
3	C	602	OXL	O3-C1	-2.40	1.24	1.30
6	E	605	O88	S-N	2.39	1.65	1.61
3	F	602	OXL	O4-C2	-2.37	1.24	1.30
6	E	605	O88	C10-C9	2.31	1.42	1.38
2	B	601	FBP	P2-O5P	-2.22	1.46	1.54
6	F	605	O88	C2-C3	2.20	1.42	1.38
6	A	605	O88	O5-S1	-2.14	1.40	1.44

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	605	O88	C3-S-N	-5.05	100.58	107.54
6	A	605	O88	O1-S-N	-4.62	99.83	107.03
6	A	605	O88	C1-C2-C3	4.09	123.41	119.44
3	C	602	OXL	O3-C1-C2	4.07	120.72	112.83
3	G	602	OXL	O3-C1-C2	3.96	120.50	112.83
6	A	605	O88	C16-C15-C8	3.92	123.25	119.44
6	A	605	O88	C4-C5-C16	-3.92	112.94	120.94
3	H	602	OXL	O4-C2-C1	3.88	120.36	112.83
6	A	605	O88	C7-C8-S1	3.88	124.54	119.49
3	A	602	OXL	O4-C2-C1	3.87	120.34	112.83
6	E	605	O88	C11-C10-C9	3.76	123.09	119.44
6	A	605	O88	C4-C5-C6	3.74	128.57	120.94
6	E	605	O88	C4-C5-C16	-3.71	113.38	120.94
3	F	602	OXL	O4-C2-C1	3.60	119.81	112.83
6	B	605	O88	C11-C10-C9	3.59	122.93	119.44
6	A	605	O88	C11-C10-C9	3.58	122.92	119.44
6	A	605	O88	C10-C9-S1	3.51	124.06	119.49
6	E	605	O88	C10-C9-S1	3.47	124.01	119.49
6	E	605	O88	C3-S-N	-3.44	102.80	107.54
3	E	602	OXL	O3-C1-C2	3.43	119.49	112.83
6	A	605	O88	C7-C8-C15	-3.26	116.22	120.47
6	A	605	O88	O6-S-O1	3.25	123.46	119.52
6	A	605	O88	C2-C1-C	-3.22	117.28	120.50
6	B	605	O88	C1-C2-C3	3.22	122.57	119.44
6	B	605	O88	C3-S-N	-3.21	103.12	107.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	605	O88	O6-S-N	-3.20	102.05	107.03
6	A	605	O88	C17-C18-C	3.18	122.83	119.89
3	B	602	OXL	O4-C2-C1	3.17	118.97	112.83
6	B	605	O88	C4-C5-C6	-3.16	114.50	120.94
3	B	602	OXL	O3-C1-C2	3.11	118.86	112.83
6	F	605	O88	C1-C2-C3	3.10	122.46	119.44
3	D	602	OXL	O4-C2-C1	3.06	118.77	112.83
6	F	605	O88	C16-C15-C8	2.97	122.33	119.44
6	B	605	O88	C16-C15-C8	2.97	122.33	119.44
6	F	605	O88	C11-C10-C9	2.95	122.31	119.44
6	E	605	O88	C1-C2-C3	2.91	122.27	119.44
6	E	605	O88	C5-C4-N	2.89	118.38	112.08
6	E	605	O88	C4-C5-C6	2.89	126.83	120.94
3	F	602	OXL	O3-C1-C2	2.84	118.35	112.83
6	E	605	O88	C10-C11-C12	-2.83	117.67	120.50
6	B	605	O88	C4-C5-C16	2.80	126.65	120.94
6	E	605	O88	C17-C18-C	2.80	122.47	119.89
6	B	605	O88	C2-C3-S	2.79	122.82	119.76
6	F	605	O88	O6-S-O1	2.75	122.86	119.52
3	E	602	OXL	O4-C2-C1	2.73	118.13	112.83
6	B	605	O88	C10-C9-S1	2.73	123.05	119.49
3	G	602	OXL	O4-C2-C1	2.71	118.08	112.83
6	B	605	O88	C10-C9-C14	-2.70	117.34	120.68
6	B	605	O88	C2-C1-C	-2.64	117.86	120.50
6	B	605	O88	C15-C8-S1	2.61	122.89	119.49
6	A	605	O88	C10-C11-C12	-2.60	117.90	120.50
2	H	601	FBP	O5P-P2-O6	2.55	113.32	106.67
6	F	605	O88	C4-C5-C16	2.52	126.09	120.94
2	B	601	FBP	O3P-P1-O2P	2.51	117.19	107.80
6	E	605	O88	O6-S-N	-2.49	103.14	107.03
6	E	605	O88	C2-C1-C	-2.49	118.00	120.50
6	A	605	O88	C2-C3-S	2.48	122.49	119.76
6	B	605	O88	C17-C18-C	2.48	122.18	119.89
3	D	602	OXL	O3-C1-C2	2.48	117.64	112.83
6	E	605	O88	C7-C8-S1	2.47	122.70	119.49
6	F	605	O88	C4-C5-C6	-2.46	115.92	120.94
6	E	605	O88	C6-C7-C8	2.44	121.82	119.44
6	A	605	O88	C2-C3-C17	-2.43	117.67	120.68
6	B	605	O88	C2-C3-C17	-2.43	117.67	120.68
3	A	602	OXL	O3-C1-C2	2.42	117.52	112.83
6	F	605	O88	C2-C3-S	2.42	122.41	119.76
6	B	605	O88	C5-C4-N	2.41	117.33	112.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	605	O88	O4-S1-C8	2.41	110.92	107.96
6	E	605	O88	C10-C9-C14	-2.40	117.71	120.68
6	F	605	O88	C2-C1-C	-2.39	118.11	120.50
6	B	605	O88	C7-C8-C15	-2.39	117.35	120.47
6	A	605	O88	C3-S-N	-2.37	104.28	107.54
6	E	605	O88	O6-S-C3	2.34	110.93	107.98
2	E	601	FBP	O3P-P1-O2P	2.32	116.48	107.80
6	F	605	O88	O1-S-C3	2.30	110.88	107.98
6	B	605	O88	O1-S-N	2.29	110.60	107.03
3	C	602	OXL	O1-C1-C2	-2.28	115.87	120.63
2	D	601	FBP	O5P-P2-O6	2.28	112.62	106.67
6	E	605	O88	O-C-C18	2.28	124.51	118.42
3	A	602	OXL	O2-C2-C1	-2.26	115.92	120.63
6	F	605	O88	C10-C9-S1	2.25	122.42	119.49
6	A	605	O88	C5-C4-N	2.23	116.95	112.08
6	F	605	O88	C7-C8-C15	-2.18	117.62	120.47
6	A	605	O88	O2-C12-C13	2.15	124.17	118.42
6	F	605	O88	C10-C11-C12	-2.14	118.36	120.50
6	B	605	O88	O1-S-C3	2.13	110.67	107.98
6	A	605	O88	O6-S-N	2.11	110.32	107.03
6	F	605	O88	C5-C4-N	2.11	116.68	112.08
6	F	605	O88	O-C-C18	2.10	124.04	118.42
3	H	602	OXL	O2-C2-C1	-2.10	116.26	120.63
6	E	605	O88	C2-C3-S	2.09	122.06	119.76
6	A	605	O88	C6-C7-C8	2.09	121.47	119.44
6	B	605	O88	O6-S-O1	2.08	122.04	119.52
6	B	605	O88	O2-C12-C13	2.07	123.96	118.42
2	G	601	FBP	O3P-P1-O1	2.06	112.03	106.67
6	F	605	O88	C2-C3-C17	-2.05	118.14	120.68
6	B	605	O88	O-C-C18	2.05	123.91	118.42
6	E	605	O88	C2-C3-C17	-2.04	118.15	120.68
6	F	605	O88	C4-N-S	2.03	124.39	120.26
6	A	605	O88	C10-C9-C14	-2.02	118.18	120.68

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	601	FBP	C4-C5-C6-O6
2	A	601	FBP	C4-C5-C6-O6
2	B	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	D	601	FBP	C4-C5-C6-O6
2	E	601	FBP	C4-C5-C6-O6
2	F	601	FBP	C4-C5-C6-O6
2	H	601	FBP	C4-C5-C6-O6
2	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	G	601	FBP	O5-C5-C6-O6
2	A	601	FBP	O5-C5-C6-O6
2	F	601	FBP	O5-C5-C6-O6
2	H	601	FBP	O5-C5-C6-O6
3	H	602	OXL	O3-C1-C2-O4
3	B	602	OXL	O3-C1-C2-O4
3	C	602	OXL	O3-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O4
3	F	602	OXL	O3-C1-C2-O4
3	G	602	OXL	O3-C1-C2-O4
3	B	602	OXL	O1-C1-C2-O2
3	C	602	OXL	O1-C1-C2-O2
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	D	602	OXL	O1-C1-C2-O2
3	F	602	OXL	O1-C1-C2-O2
3	G	602	OXL	O1-C1-C2-O2
3	E	602	OXL	O1-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O2
3	H	602	OXL	O3-C1-C2-O2
6	E	605	O88	C4-N-S-O1
6	E	605	O88	C4-N-S-O6
6	A	605	O88	C4-N-S-O6
3	B	602	OXL	O1-C1-C2-O4
3	B	602	OXL	O3-C1-C2-O2
3	C	602	OXL	O1-C1-C2-O4
3	C	602	OXL	O3-C1-C2-O2
3	E	602	OXL	O1-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O2
3	F	602	OXL	O3-C1-C2-O2
3	G	602	OXL	O1-C1-C2-O4
3	G	602	OXL	O3-C1-C2-O2
6	B	605	O88	C4-N-S-O1

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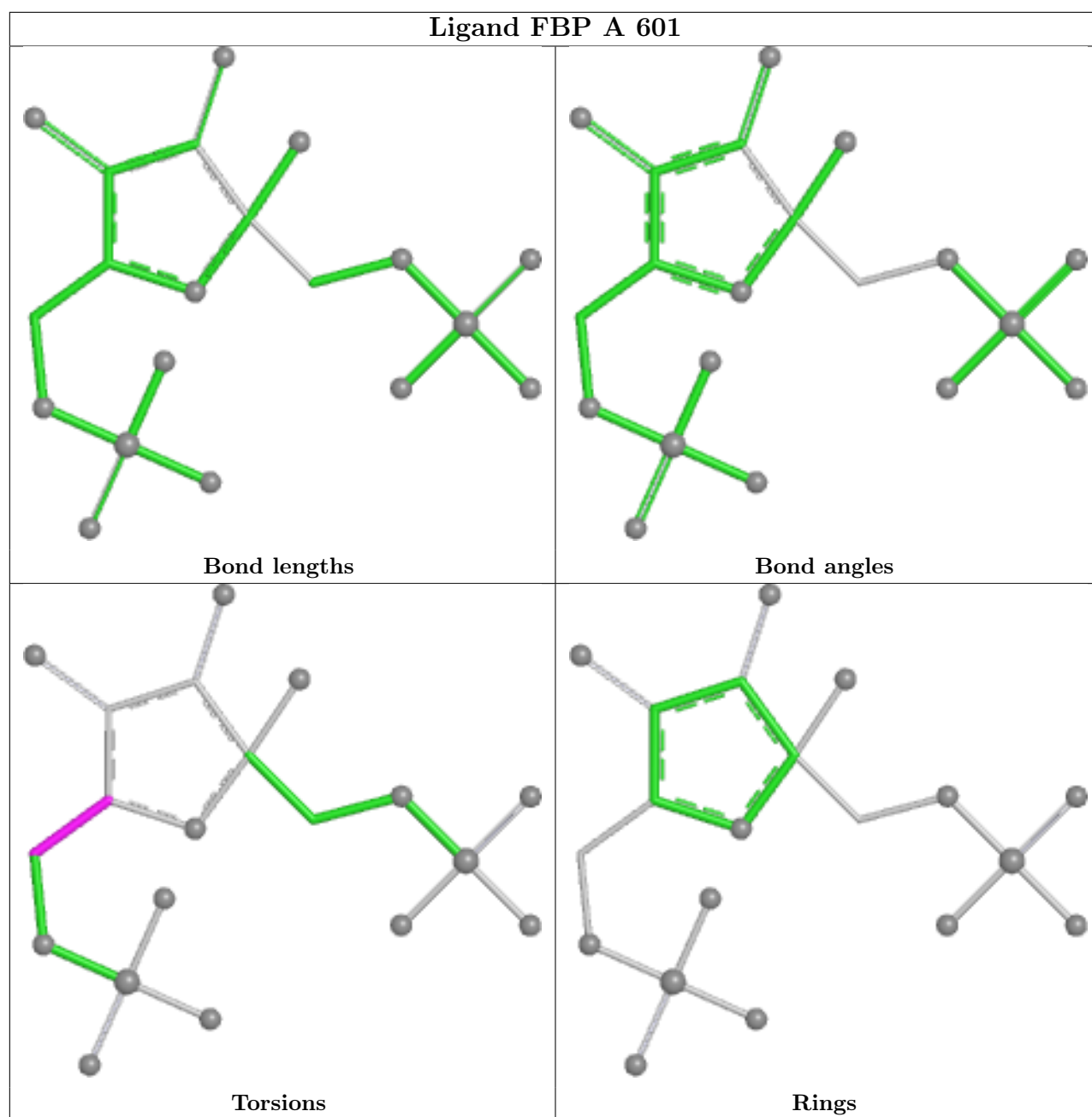
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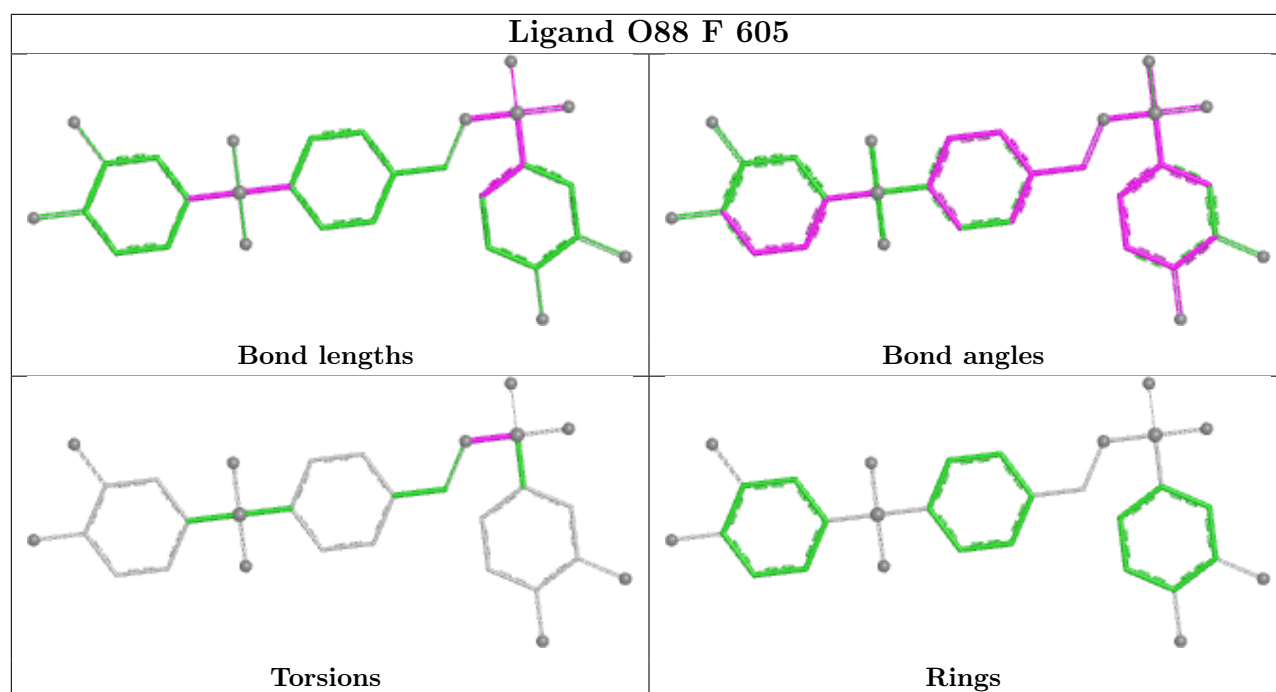
Mol	Chain	Res	Type	Atoms
3	D	602	OXL	O1-C1-C2-O4
3	D	602	OXL	O3-C1-C2-O2
3	F	602	OXL	O1-C1-C2-O4
3	A	602	OXL	O1-C1-C2-O4
3	A	602	OXL	O3-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O4
6	A	605	O88	C4-N-S-O1
6	B	605	O88	C4-N-S-O6
6	B	605	O88	C4-N-S-C3
6	F	605	O88	C4-N-S-O1

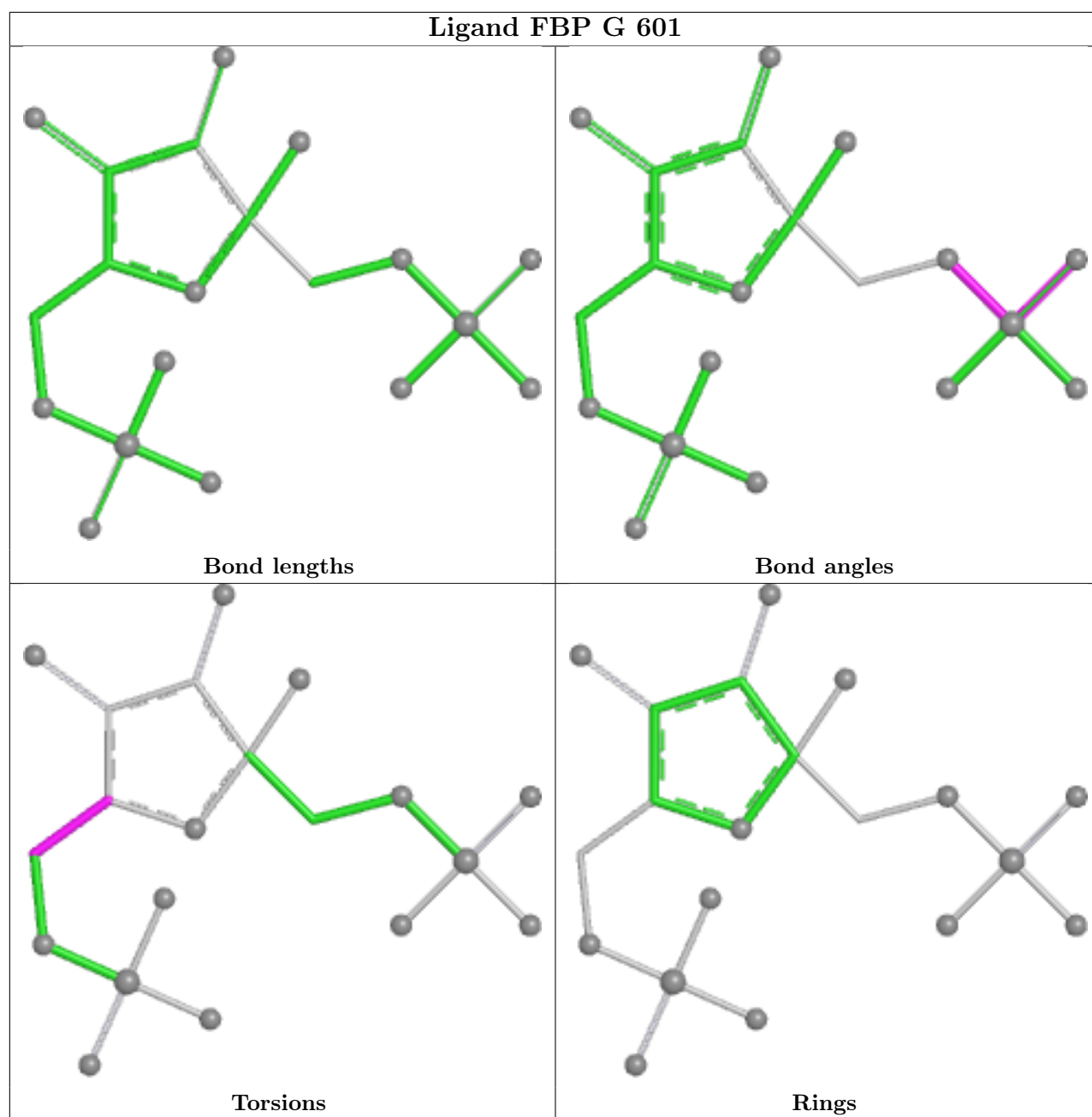
There are no ring outliers.

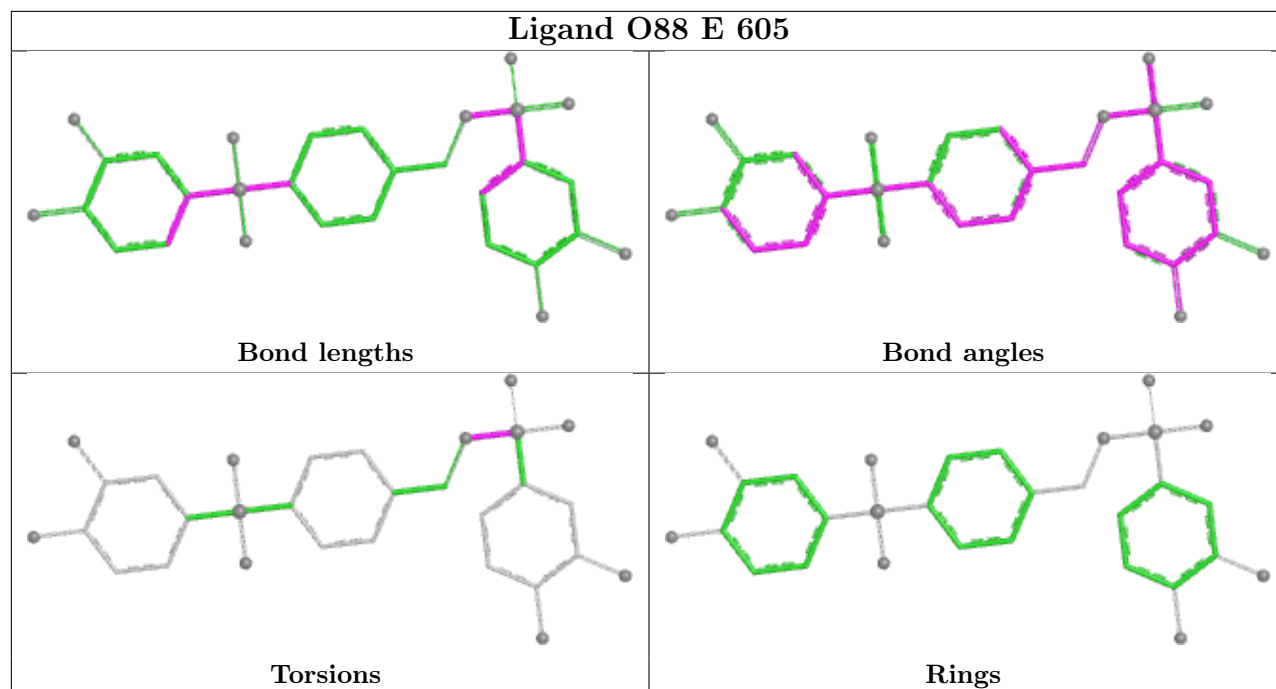
No monomer is involved in short contacts.

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

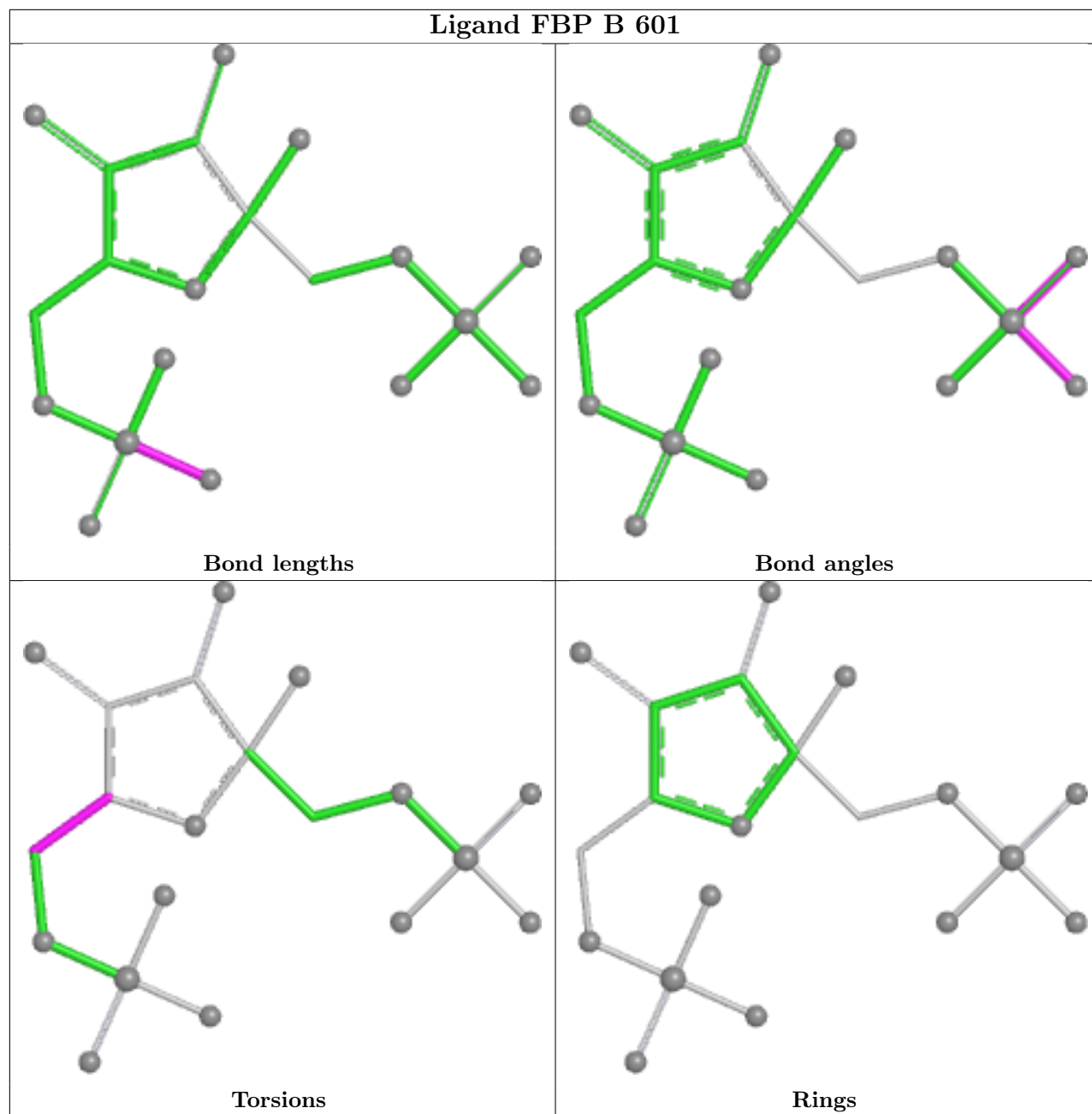




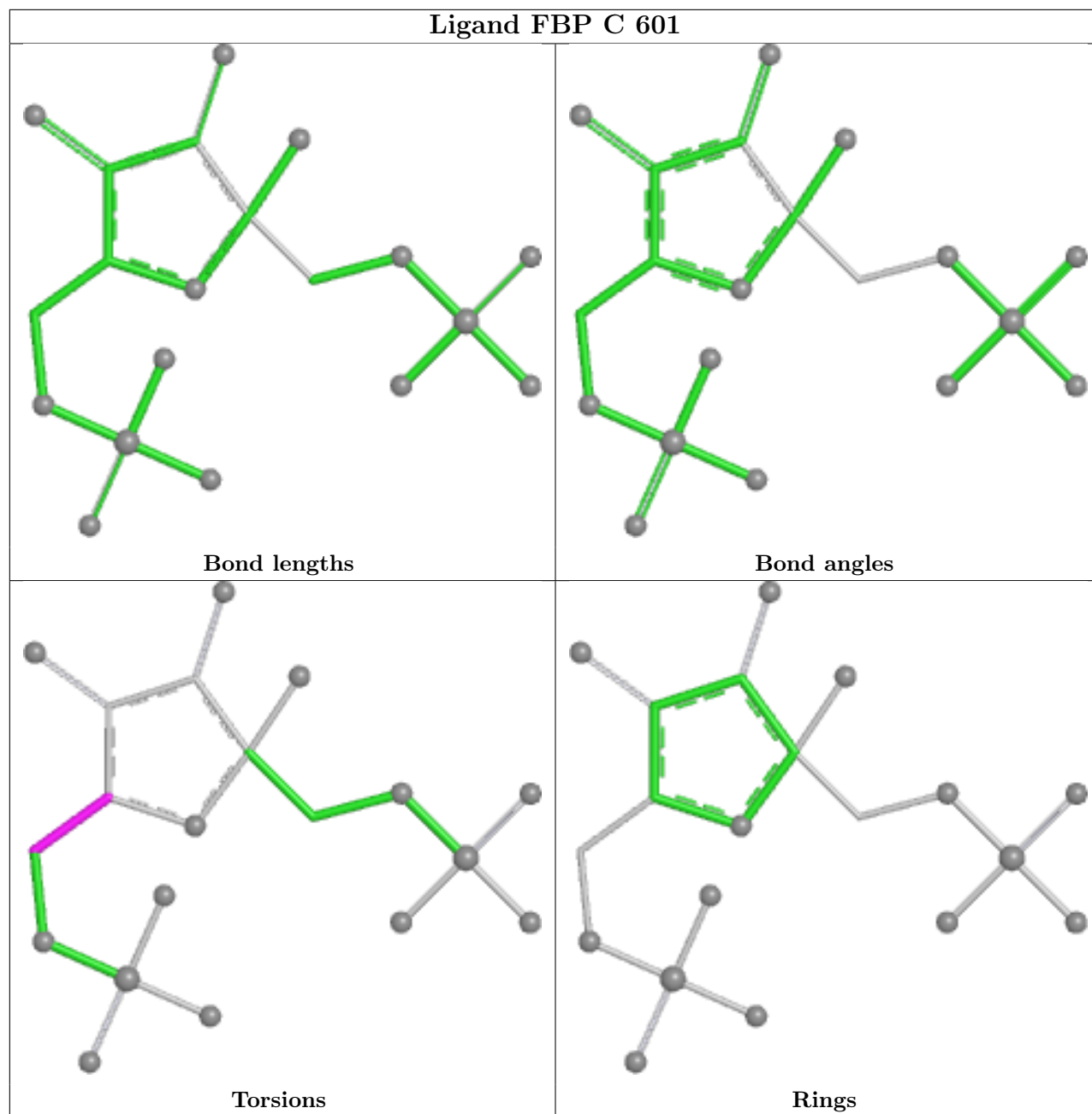




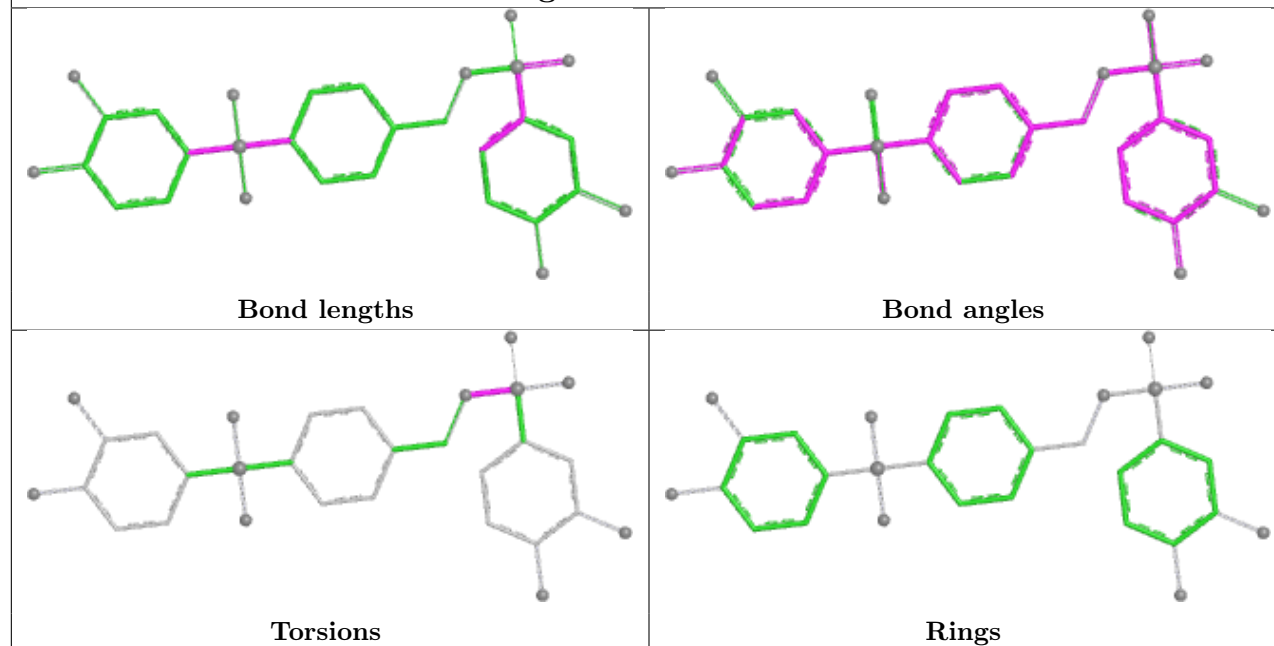
Ligand FBP B 601



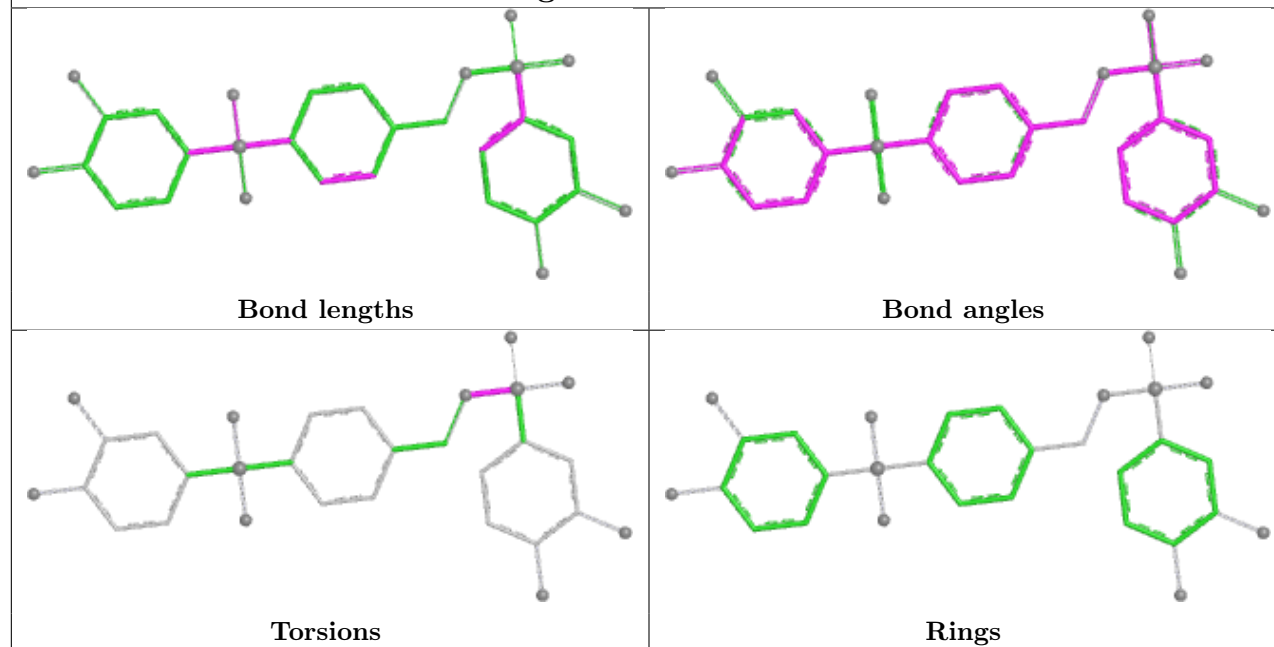
Ligand FBP C 601

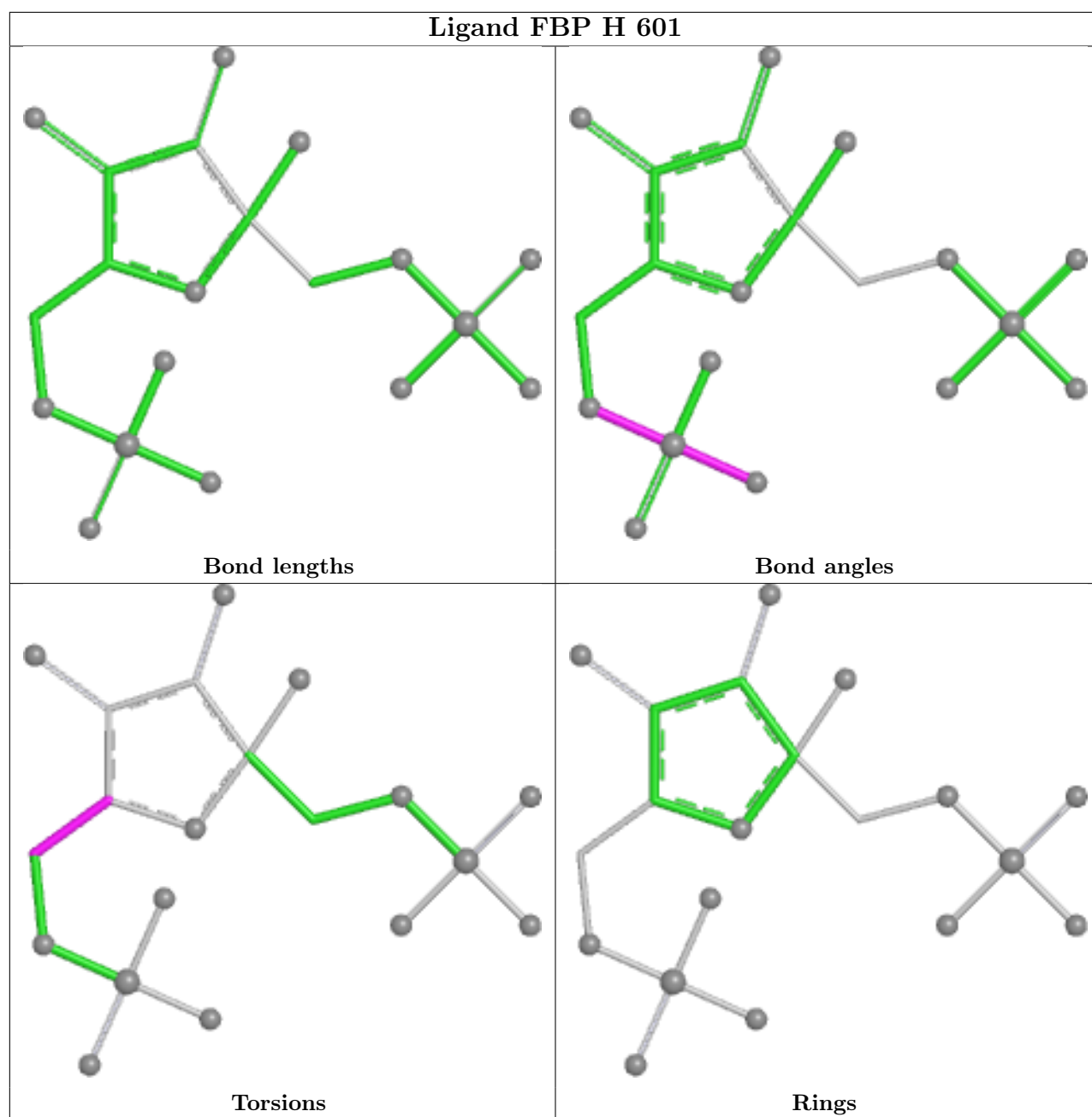


Ligand O88 B 605

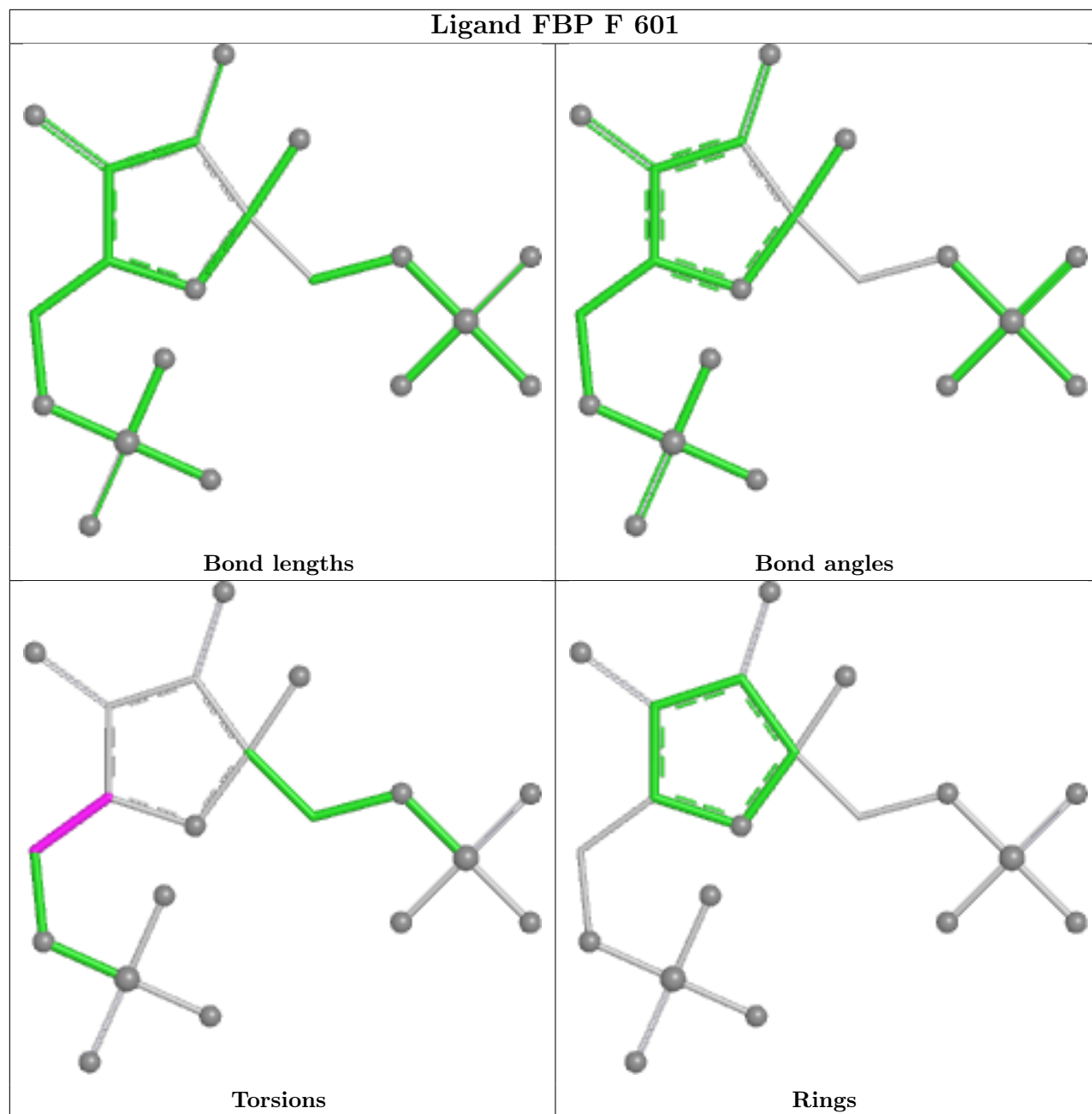


Ligand O88 A 605

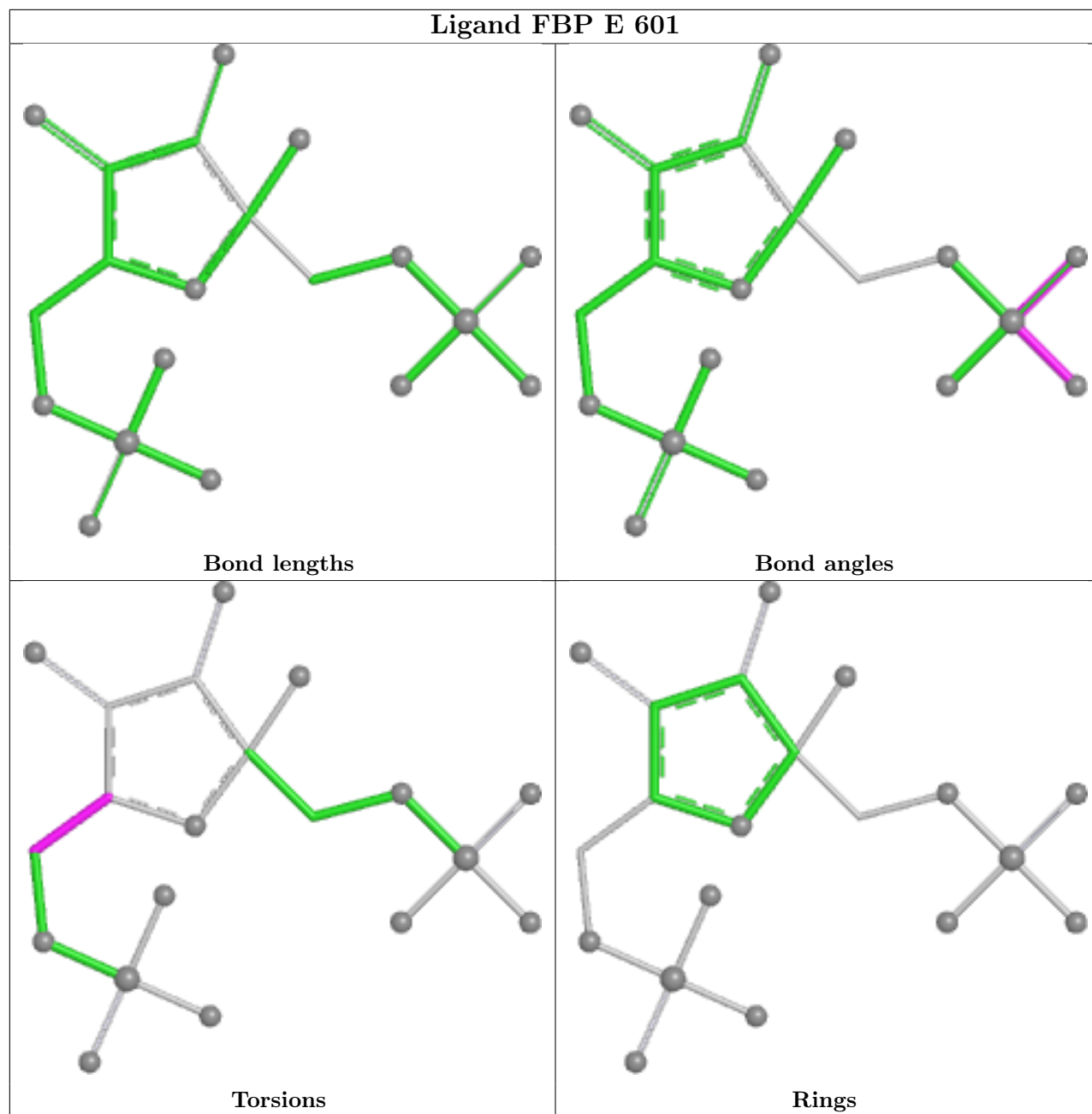


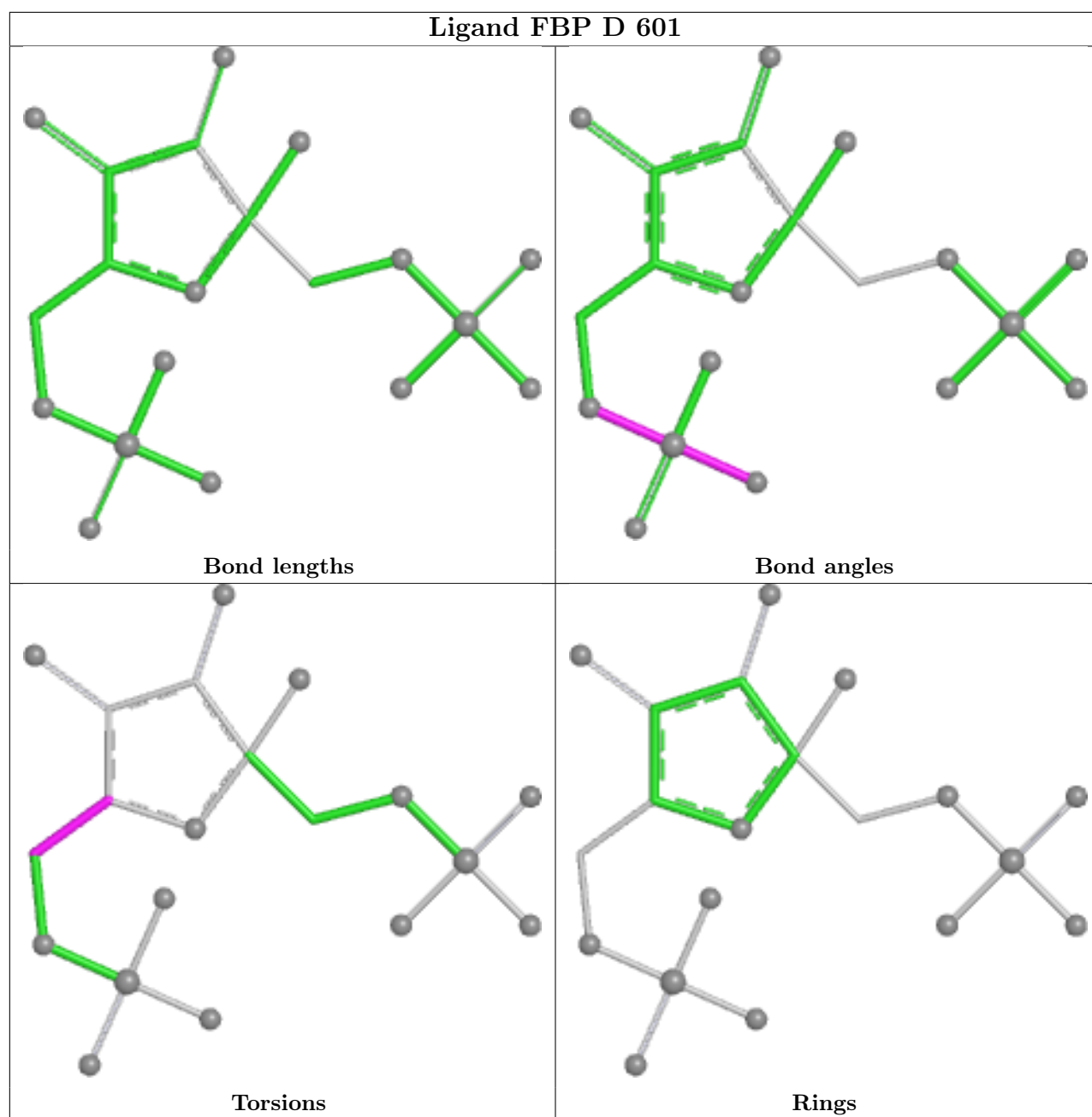


Ligand FBP F 601



Ligand FBP E 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%)	1.25	98 (23%)	2 2	22, 43, 69, 86	6 (1%)
1	B	436/447 (97%)	0.94	73 (16%)	4 4	20, 39, 67, 76	4 (0%)
1	C	425/447 (95%)	0.33	28 (6%)	24 25	18, 31, 53, 86	4 (0%)
1	D	425/447 (95%)	0.03	15 (3%)	47 51	13, 27, 48, 76	6 (1%)
1	E	419/447 (93%)	0.95	59 (14%)	6 6	19, 42, 65, 82	5 (1%)
1	F	432/447 (96%)	0.72	62 (14%)	6 6	22, 35, 62, 73	7 (1%)
1	G	421/447 (94%)	0.20	18 (4%)	40 42	17, 29, 46, 58	7 (1%)
1	H	425/447 (95%)	-0.09	17 (4%)	42 45	13, 25, 47, 62	4 (0%)
All	All	3405/3576 (95%)	0.54	370 (10%)	10 11	13, 34, 61, 86	43 (1%)

All (370) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	115	LEU	9.2
1	B	511	LEU	7.3
1	F	115	LEU	6.9
1	A	25	PHE	6.9
1	G	271	GLY	6.5
1	C	271	GLY	6.4
1	F	116	SER	6.1
1	F	511	LEU	5.9
1	B	116	SER	5.8
1	E	23	ALA	5.7
1	D	21	GLY	5.7
1	H	21	GLY	5.4
1	G	25	PHE	5.4
1	B	416	LEU	5.4
1	B	114	PRO	5.3
1	A	132	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
1	F	114	PRO	5.2
1	E	129	PRO	5.2
1	D	25	PHE	5.1
1	A	232	GLY	5.0
1	F	231	PRO	4.8
1	B	117	TYR	4.8
1	A	34	MET	4.8
1	A	114	PRO	4.8
1	F	117	TYR	4.7
1	B	118	ARG	4.6
1	E	232	GLY	4.6
1	H	514	PHE	4.6
1	E	25	PHE	4.5
1	A	115	LEU	4.5
1	B	415	PRO	4.4
1	A	238	VAL	4.4
1	C	25	PHE	4.4
1	C	20	LEU	4.3
1	D	22	THR	4.3
1	C	34	MET	4.3
1	C	132	GLY	4.3
1	H	25	PHE	4.2
1	A	118	ARG	4.2
1	C	117	TYR	4.2
1	E	490	PRO	4.2
1	D	24	PHE	4.1
1	G	272	PRO	4.1
1	A	514	PHE	4.0
1	A	233	LEU	4.0
1	D	23	ALA	4.0
1	C	272	PRO	4.0
1	B	267[A]	ARG	4.0
1	H	231	PRO	3.9
1	D	275[A]	HIS	3.9
1	B	270	LEU	3.8
1	B	130	GLY	3.8
1	C	114	PRO	3.8
1	A	543	SER	3.8
1	G	514	PHE	3.7
1	C	232	GLY	3.7
1	E	115	LEU	3.7
1	A	241	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	482	PHE	3.6
1	E	514	PHE	3.6
1	A	73	LEU	3.6
1	F	233	LEU	3.6
1	F	415	PRO	3.6
1	B	233	LEU	3.6
1	F	112	GLY	3.5
1	B	489	PRO	3.5
1	H	411	ARG	3.5
1	B	256	PHE	3.5
1	C	21	GLY	3.5
1	B	512	ARG	3.4
1	B	269	ALA	3.4
1	B	493	ILE	3.4
1	A	488[A]	GLU	3.4
1	F	493	ILE	3.4
1	G	23	ALA	3.4
1	A	24	PHE	3.4
1	E	275	HIS	3.3
1	E	493	ILE	3.3
1	A	515	LEU	3.3
1	C	113	SER	3.3
1	B	232	GLY	3.3
1	A	70	VAL	3.3
1	B	414	ALA	3.3
1	C	111	ALA	3.3
1	E	249	VAL	3.3
1	A	496	ASP	3.3
1	A	110	PHE	3.3
1	F	516	ARG	3.2
1	G	132	GLY	3.2
1	B	379	LYS	3.2
1	A	30	LEU	3.2
1	A	270	LEU	3.2
1	H	516	ARG	3.2
1	A	63	ILE	3.1
1	F	489	PRO	3.1
1	A	56	SER	3.1
1	B	113	SER	3.1
1	E	269	ALA	3.1
1	A	95	TYR	3.1
1	F	267[A]	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	231	PRO	3.1
1	B	509	GLY	3.1
1	A	100	ILE	3.0
1	A	120	VAL	3.0
1	A	475	VAL	3.0
1	A	311	ILE	3.0
1	F	275	HIS	3.0
1	B	508	SER	3.0
1	F	487	ARG	3.0
1	G	411	ARG	3.0
1	C	23	ALA	3.0
1	F	416	LEU	2.9
1	A	91	GLY	2.9
1	B	490	PRO	2.9
1	G	34	MET	2.9
1	F	506	ILE	2.9
1	C	416	LEU	2.9
1	F	379	LYS	2.9
1	E	351	ARG	2.9
1	C	412	ARG	2.9
1	A	511	LEU	2.9
1	C	110	PHE	2.9
1	F	514	PHE	2.9
1	H	275[A]	HIS	2.9
1	G	33	ALA	2.9
1	E	241	LEU	2.9
1	B	487	ARG	2.8
1	C	116	SER	2.8
1	H	416	LEU	2.8
1	A	249	VAL	2.8
1	G	52	VAL	2.8
1	D	514	PHE	2.8
1	E	274	GLY	2.8
1	F	90	HIS	2.8
1	E	114	PRO	2.8
1	E	33	ALA	2.8
1	F	111	ALA	2.8
1	A	88	PHE	2.8
1	A	236	GLN	2.8
1	A	130	GLY	2.8
1	B	542	ILE	2.8
1	E	272	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	489	PRO	2.8
1	E	238	VAL	2.8
1	A	23	ALA	2.7
1	A	68	ARG	2.7
1	A	111	ALA	2.7
1	B	111	ALA	2.7
1	B	506	ILE	2.7
1	E	89	SER	2.7
1	A	252	VAL	2.7
1	A	268	ALA	2.7
1	B	128	GLY	2.7
1	E	26	GLN	2.7
1	F	118	ARG	2.7
1	E	111	ALA	2.7
1	A	117	TYR	2.7
1	H	34	MET	2.7
1	E	233	LEU	2.7
1	E	511	LEU	2.7
1	B	507	GLU	2.7
1	B	245	VAL	2.7
1	B	112	GLY	2.6
1	F	269	ALA	2.6
1	B	504	PHE	2.6
1	E	270	LEU	2.6
1	A	107	VAL	2.6
1	A	274	GLY	2.6
1	B	238	VAL	2.6
1	H	52	VAL	2.6
1	A	377	THR	2.6
1	F	129	PRO	2.6
1	A	96	HIS	2.6
1	B	241	LEU	2.6
1	B	484	LEU	2.6
1	B	485	LEU	2.6
1	C	115	LEU	2.6
1	G	515	LEU	2.6
1	E	506	ILE	2.6
1	A	244	GLY	2.6
1	A	513	GLY	2.6
1	A	121	ALA	2.6
1	E	263	VAL	2.6
1	A	243	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	540	LEU	2.6
1	E	515	LEU	2.6
1	F	232	GLY	2.6
1	F	33	ALA	2.6
1	E	95	TYR	2.5
1	B	243	PHE	2.5
1	F	515	LEU	2.5
1	C	112	GLY	2.5
1	F	492	ALA	2.5
1	A	298	VAL	2.5
1	F	238	VAL	2.5
1	F	512	ARG	2.5
1	H	412	ARG	2.5
1	E	110	PHE	2.5
1	E	243	PHE	2.5
1	A	493	ILE	2.5
1	B	10	ARG	2.5
1	E	543	SER	2.5
1	B	344	GLU	2.5
1	E	34	MET	2.5
1	E	70	VAL	2.5
1	H	22	THR	2.5
1	A	237	ASP	2.5
1	A	112	GLY	2.5
1	A	351	ARG	2.5
1	F	411	ARG	2.5
1	G	516	ARG	2.5
1	H	90	HIS	2.5
1	A	251	ILE	2.5
1	D	26	GLN	2.5
1	F	268	ALA	2.5
1	A	498	VAL	2.5
1	A	64	GLY	2.4
1	C	22	THR	2.4
1	A	119	PRO	2.4
1	H	232	GLY	2.4
1	F	71	GLU	2.4
1	A	116	SER	2.4
1	F	113	SER	2.4
1	F	540[A]	LEU	2.4
1	E	88	PHE	2.4
1	F	504	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	100	ILE	2.4
1	F	97	ALA	2.4
1	F	412	ARG	2.4
1	B	272	PRO	2.4
1	C	415	PRO	2.4
1	A	103	VAL	2.4
1	E	245	VAL	2.4
1	B	505	GLY	2.4
1	A	86	LEU	2.4
1	D	515	LEU	2.4
1	B	95	TYR	2.4
1	A	277	ILE	2.4
1	D	412	ARG	2.4
1	F	351	ARG	2.4
1	A	84	ALA	2.4
1	A	264	ALA	2.4
1	A	378	ALA	2.4
1	H	23	ALA	2.4
1	B	488	GLU	2.4
1	A	266	VAL	2.4
1	A	99	SER	2.4
1	F	270	LEU	2.3
1	B	110	PHE	2.3
1	C	24	PHE	2.3
1	E	504	PHE	2.3
1	F	507	GLU	2.3
1	C	26	GLN	2.3
1	A	279	ILE	2.3
1	B	122	ILE	2.3
1	E	277	ILE	2.3
1	G	311	ILE	2.3
1	A	310	GLY	2.3
1	A	263	VAL	2.3
1	B	107	VAL	2.3
1	F	245	VAL	2.3
1	F	124	LEU	2.3
1	A	256	PHE	2.3
1	A	542	ILE	2.3
1	D	130	GLY	2.3
1	E	505	GLY	2.3
1	E	242	ARG	2.3
1	G	412	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	266	VAL	2.3
1	E	540	LEU	2.3
1	D	34	MET	2.3
1	E	97	ALA	2.3
1	A	122	ILE	2.3
1	G	239	ARG	2.3
1	A	113	SER	2.3
1	B	502	VAL	2.3
1	B	540[A]	LEU	2.3
1	A	412	ARG	2.2
1	B	33	ALA	2.2
1	B	88	PHE	2.2
1	F	243	PHE	2.2
1	A	67	SER	2.2
1	B	242	ARG	2.2
1	E	412	ARG	2.2
1	F	241	LEU	2.2
1	A	383	PRO	2.2
1	B	132	GLY	2.2
1	B	231	PRO	2.2
1	G	231	PRO	2.2
1	A	66	ALA	2.2
1	B	492	ALA	2.2
1	E	492	ALA	2.2
1	G	24	PHE	2.2
1	A	90	HIS	2.2
1	F	34	MET	2.2
1	A	384	VAL	2.2
1	B	274	GLY	2.2
1	D	231	PRO	2.2
1	F	490	PRO	2.2
1	A	495	ALA	2.2
1	B	260	ALA	2.2
1	B	464	ALA	2.2
1	E	256	PHE	2.2
1	B	543	SER	2.2
1	F	86	LEU	2.2
1	F	484	LEU	2.2
1	A	272	PRO	2.2
1	C	129	PRO	2.2
1	A	33	ALA	2.2
1	B	413	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	412	ARG	2.2
1	B	510	LYS	2.2
1	C	411	ARG	2.2
1	E	90	HIS	2.1
1	F	242	ARG	2.2
1	G	487	ARG	2.2
1	B	514	PHE	2.1
1	F	256	PHE	2.1
1	F	488	GLU	2.1
1	B	494	TRP	2.1
1	A	245	VAL	2.1
1	B	513	GLY	2.1
1	E	244	GLY	2.1
1	A	129	PRO	2.1
1	H	233	LEU	2.1
1	A	75	GLU	2.1
1	A	106	ALA	2.1
1	A	260	ALA	2.1
1	A	464	ALA	2.1
1	B	495	ALA	2.1
1	F	11	ALA	2.1
1	B	279	ILE	2.1
1	A	62	THR	2.1
1	B	348	THR	2.1
1	F	527	TRP	2.1
1	A	517	VAL	2.1
1	D	242[A]	ARG	2.1
1	D	459	ARG	2.1
1	F	459	ARG	2.1
1	F	517	VAL	2.1
1	B	236	GLN	2.1
1	B	268	ALA	2.1
1	E	106	ALA	2.1
1	A	89	SER	2.1
1	E	459	ARG	2.1
1	E	128	GLY	2.1
1	F	274	GLY	2.1
1	A	257	VAL	2.1
1	H	415	PRO	2.1
1	E	485	LEU	2.1
1	F	485	LEU	2.1
1	B	264	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	66	ALA	2.1
1	E	499	ASP	2.1
1	A	273	GLU	2.0
1	A	297	GLU	2.0
1	E	234	SER	2.0
1	E	311	ILE	2.0
1	A	248	GLY	2.0
1	F	513	GLY	2.0
1	B	498	VAL	2.0
1	F	240	ASP	2.0
1	C	75	GLU	2.0
1	E	379	LYS	2.0
1	A	109	SER	2.0
1	E	99	SER	2.0
1	E	63	ILE	2.0
1	F	311	ILE	2.0
1	B	516	ARG	2.0
1	E	52	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	K	E	604	1/1	0.87	0.31	77,77,77,77	0
3	OXL	A	602	6/6	0.90	0.11	52,52,53,53	0
3	OXL	E	602	6/6	0.91	0.10	51,52,52,52	0
5	K	A	604	1/1	0.92	0.26	71,71,71,71	0
3	OXL	C	602	6/6	0.92	0.09	39,40,40,40	0

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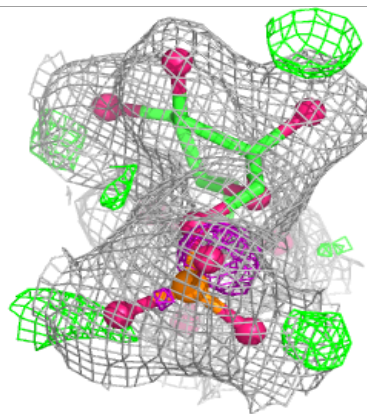
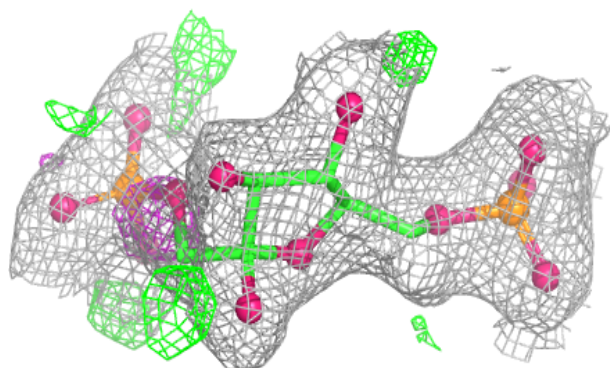
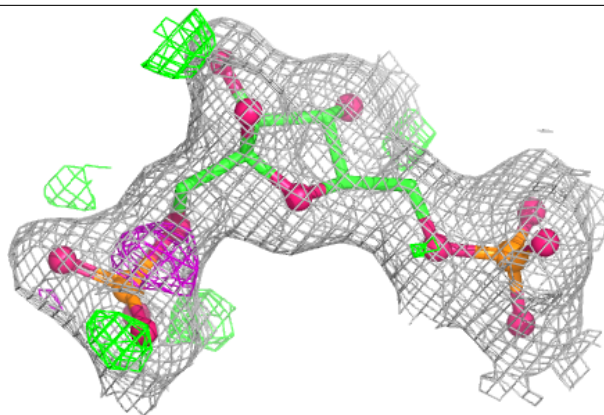
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	OXL	H	602	6/6	0.93	0.14	31,33,34,35	0
2	FBP	A	601	20/20	0.93	0.09	35,37,38,38	0
3	OXL	B	602	6/6	0.93	0.09	46,47,47,48	0
5	K	F	604	1/1	0.94	0.12	71,71,71,71	0
2	FBP	B	601	20/20	0.95	0.08	35,36,42,42	0
3	OXL	D	602	6/6	0.95	0.07	36,36,37,37	0
5	K	B	604	1/1	0.95	0.11	74,74,74,74	0
2	FBP	F	601	20/20	0.95	0.07	34,36,40,40	0
3	OXL	G	602	6/6	0.95	0.06	34,35,35,35	0
5	K	C	604	1/1	0.96	0.22	52,52,52,52	0
2	FBP	E	601	20/20	0.96	0.07	36,37,39,39	0
3	OXL	F	602	6/6	0.96	0.07	40,41,42,43	0
5	K	G	604	1/1	0.96	0.17	50,50,50,50	0
6	O88	A	605	30/30	0.96	0.08	27,31,35,35	17
6	O88	B	605	30/30	0.96	0.07	26,30,33,33	17
6	O88	E	605	30/30	0.96	0.08	27,34,36,37	17
6	O88	F	605	30/30	0.96	0.08	23,30,33,33	17
5	K	D	604	1/1	0.97	0.13	46,46,46,46	0
5	K	H	604	1/1	0.97	0.12	48,48,48,48	0
2	FBP	C	601	20/20	0.98	0.04	22,23,26,27	0
4	MG	E	603	1/1	0.98	0.04	33,33,33,33	0
4	MG	C	603	1/1	0.99	0.09	23,23,23,23	0
4	MG	D	603	1/1	0.99	0.08	23,23,23,23	0
2	FBP	H	601	20/20	0.99	0.04	19,21,23,23	0
4	MG	H	603	1/1	0.99	0.07	20,20,20,20	0
2	FBP	D	601	20/20	0.99	0.04	21,23,25,26	0
2	FBP	G	601	20/20	0.99	0.04	20,22,23,23	0
4	MG	A	603	1/1	0.99	0.03	36,36,36,36	0
4	MG	B	603	1/1	0.99	0.07	32,32,32,32	0
4	MG	G	603	1/1	1.00	0.07	19,19,19,19	0
4	MG	F	603	1/1	1.00	0.02	26,26,26,26	0

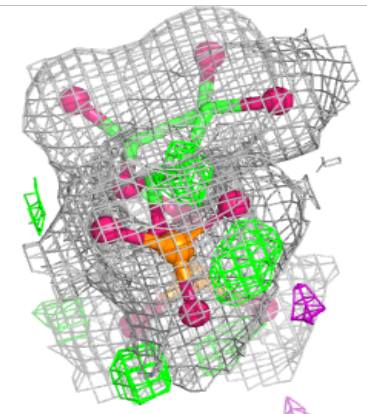
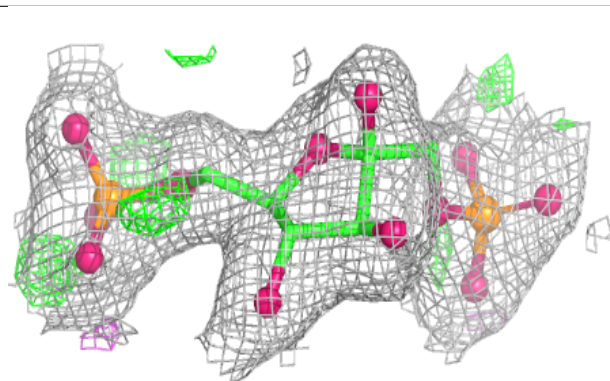
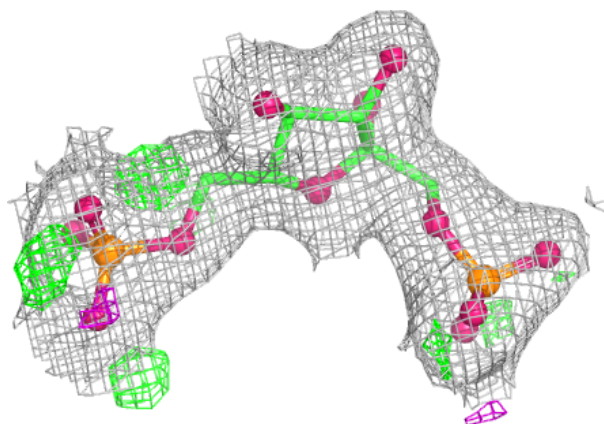
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

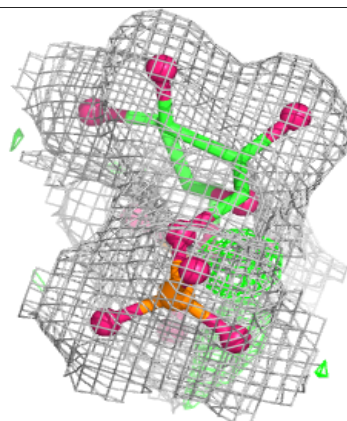
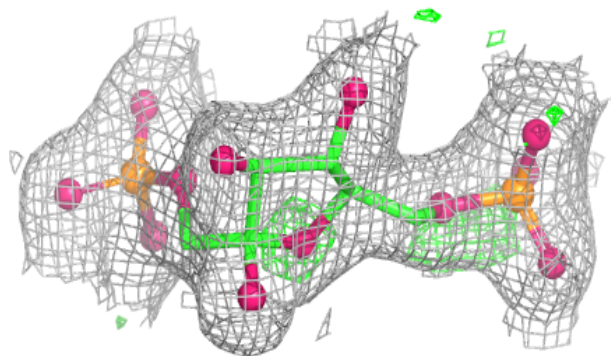
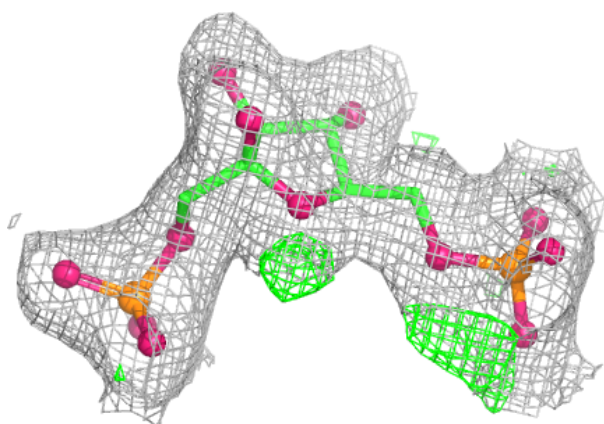
**Electron density around FBP B 601:**

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

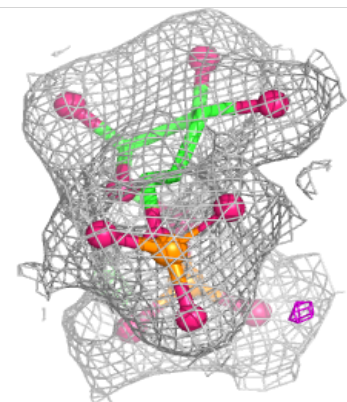
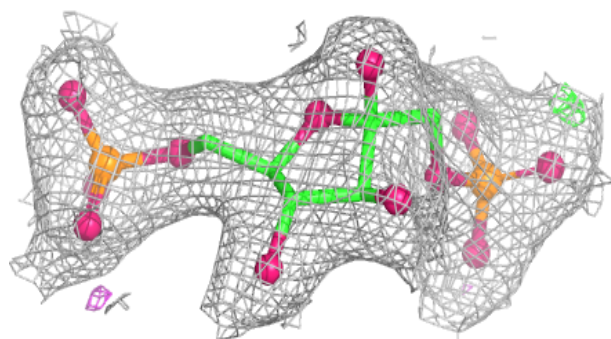
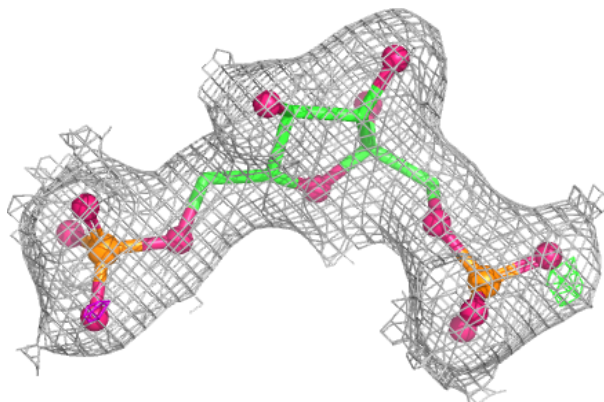


Electron density around FBP F 601:

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

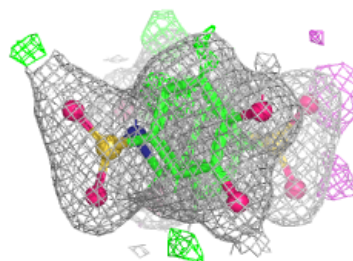
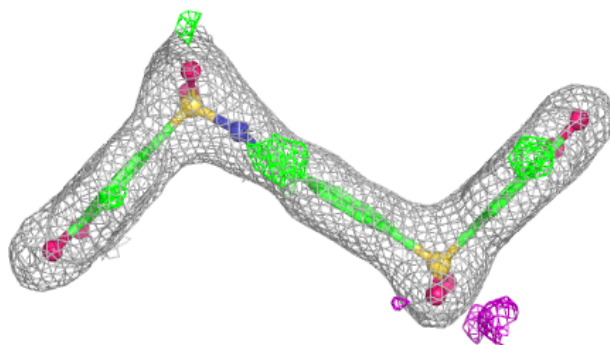
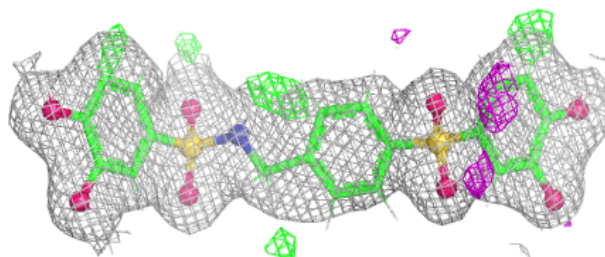
**Electron density around FBP E 601:**

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

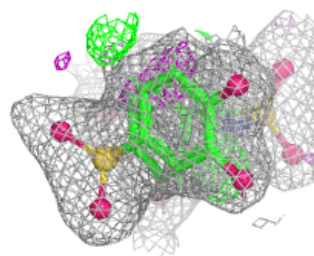
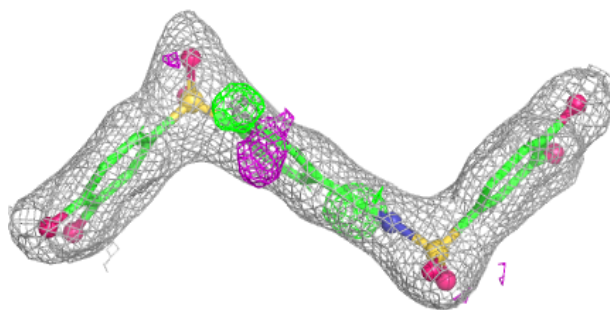
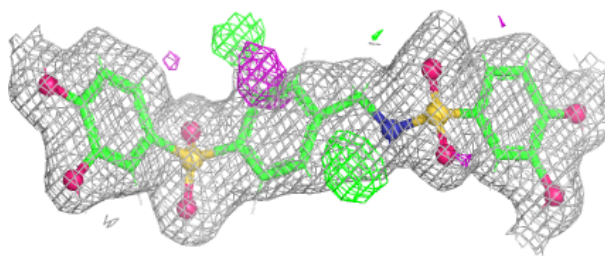


Electron density around O88 A 605:

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

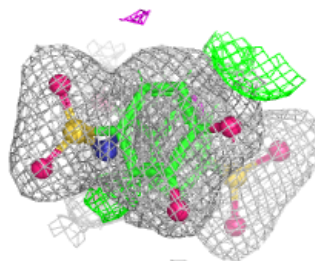
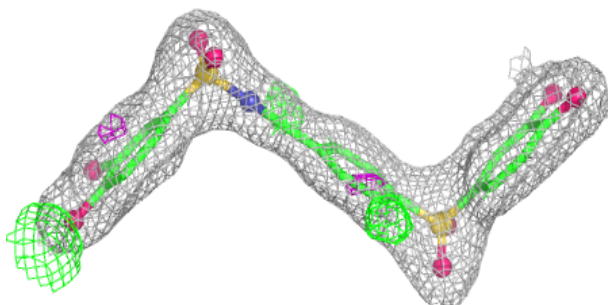
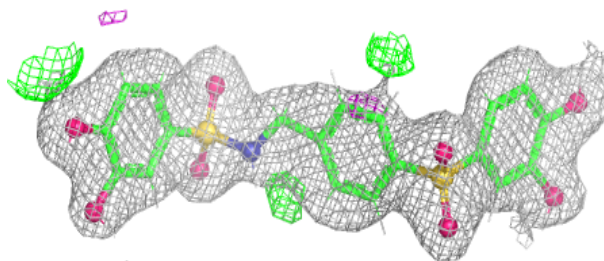
**Electron density around O88 B 605:**

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

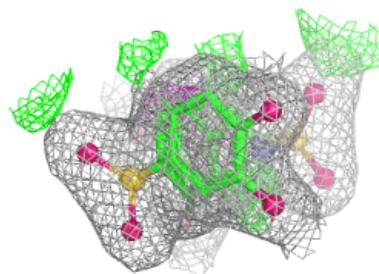
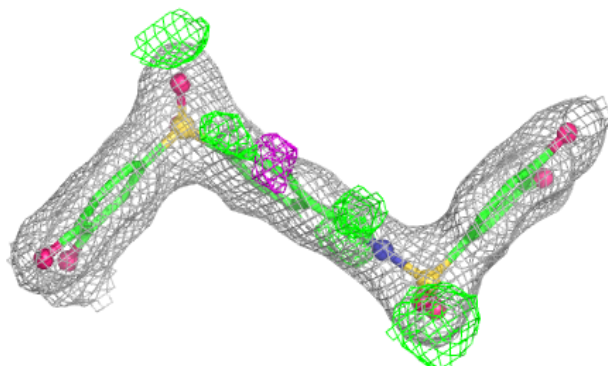
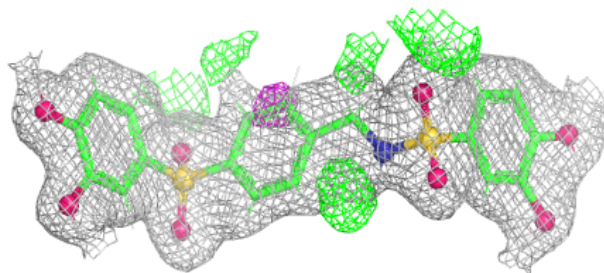


Electron density around O88 E 605:

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

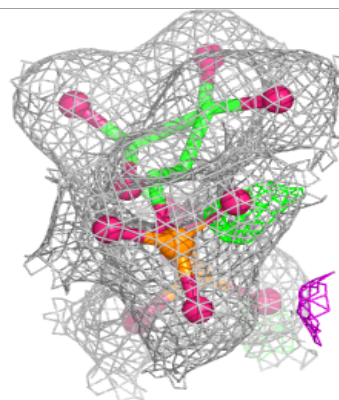
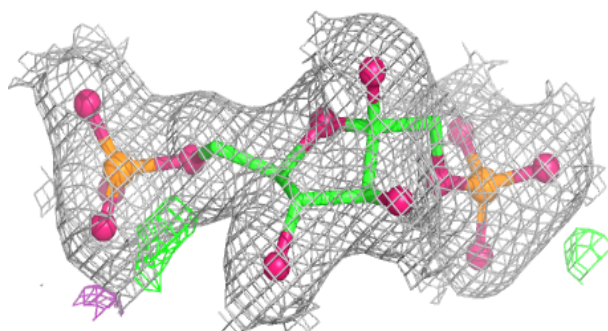
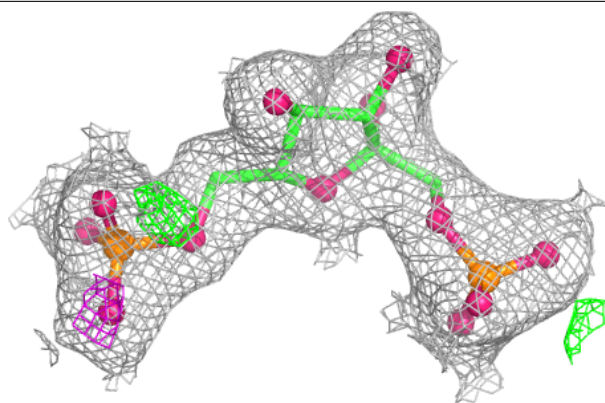
**Electron density around O88 F 605:**

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

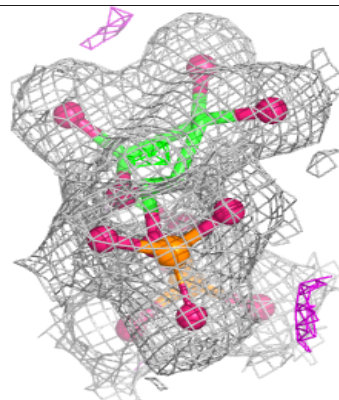
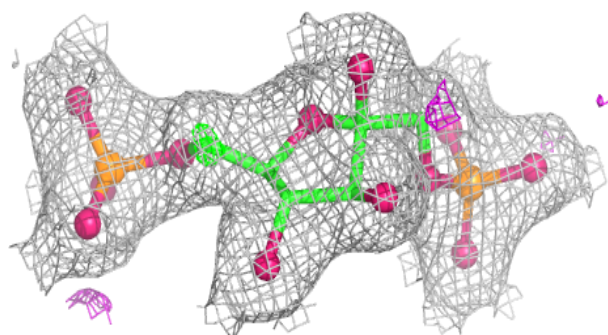
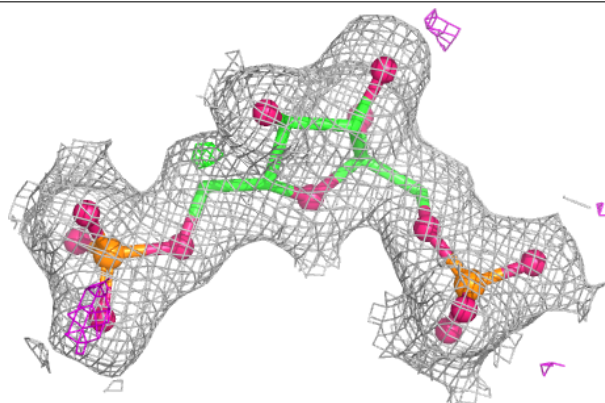


Electron density around FBP C 601:

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

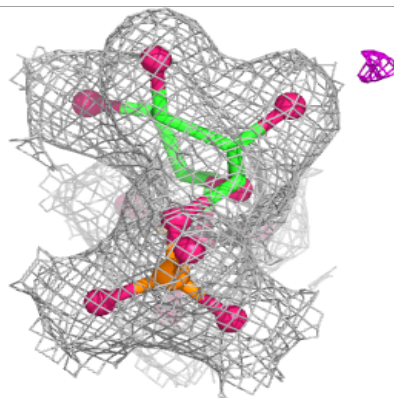
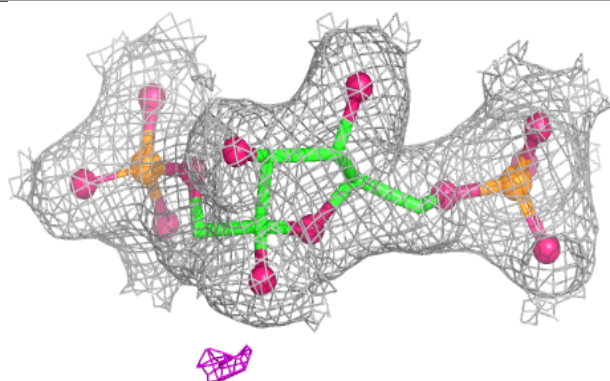
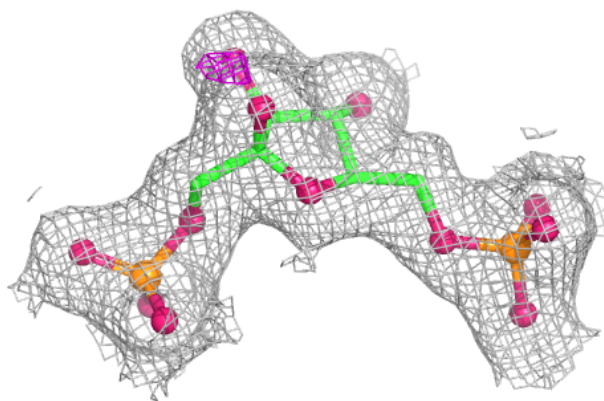
**Electron density around FBP H 601:**

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

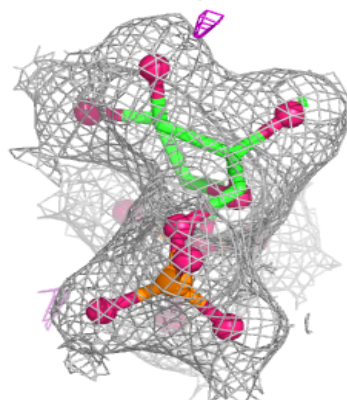
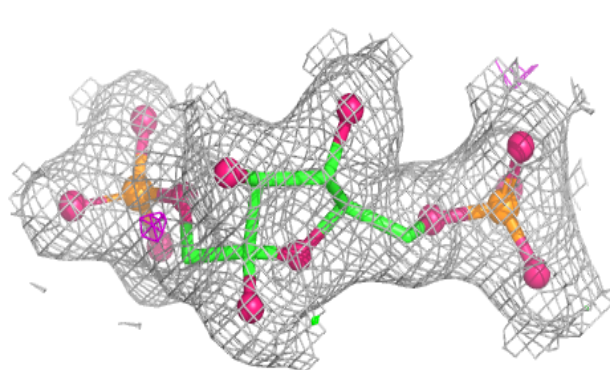
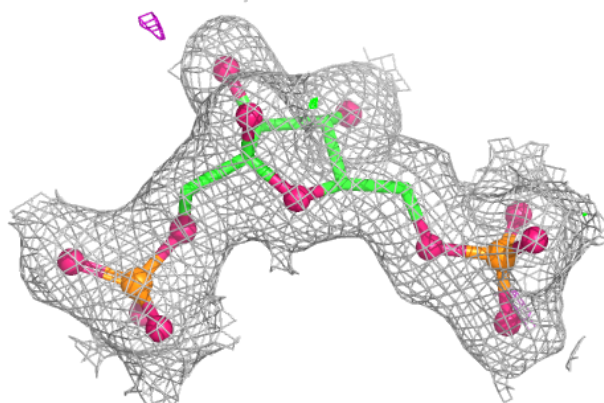


Electron density around FBP D 601:

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

**Electron density around FBP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.