



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:57 AM UTC

PDB ID : 5SCA / pdb_00005sca
Title : Structure of liver pyruvate kinase in complex with anthraquinone derivative 36
Authors : Lulla, A.; Foller, A.; Nain-Perez, A.; Grotli, M.; Brear, P.; Hyvonen, M.
Deposited on : 2021-12-01
Resolution : 1.92 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

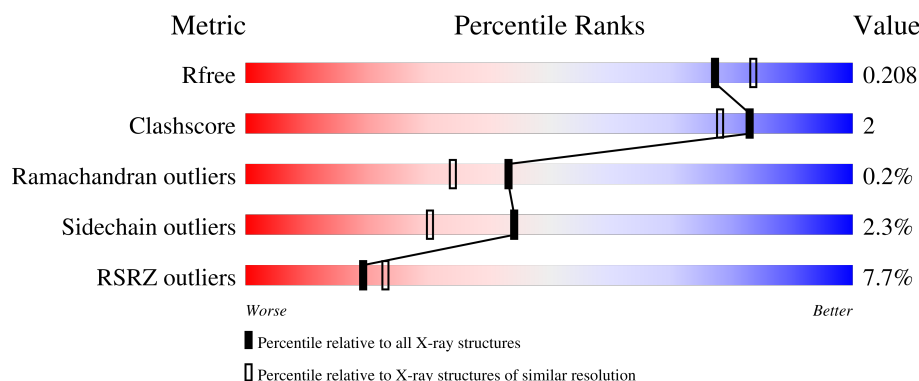
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	6% 85% 8% 6%
1	B	447	25% 90% 7% .
1	C	447	5% 88% 6% 5%
1	D	447	3% 88% 6% 5%
1	E	447	6% 87% 7% 6%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXL	A	602	-	X	-	-
3	OXL	B	602	-	X	-	-
3	OXL	C	603	-	X	-	-
3	OXL	D	602	-	X	-	-
3	OXL	E	602	-	X	-	-
3	OXL	F	603	-	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 29195 atoms, of which 88 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	13	0
			3242	2035	582	605	20			
1	B	436	Total	C	N	O	S	3	8	0
			3350	2104	604	622	20			
1	C	424	Total	C	N	O	S	0	8	0
			3263	2053	584	607	19			
1	D	425	Total	C	N	O	S	0	8	0
			3261	2048	590	604	19			
1	E	419	Total	C	N	O	S	0	13	0
			3257	2049	584	604	20			
1	F	432	Total	C	N	O	S	0	7	0
			3322	2089	597	616	20			
1	G	423	Total	C	N	O	S	0	7	0
			3247	2042	583	603	19			
1	H	425	Total	C	N	O	S	0	9	0
			3277	2057	597	604	19			

There are 48 discrepancies between the modelled and reference sequences:

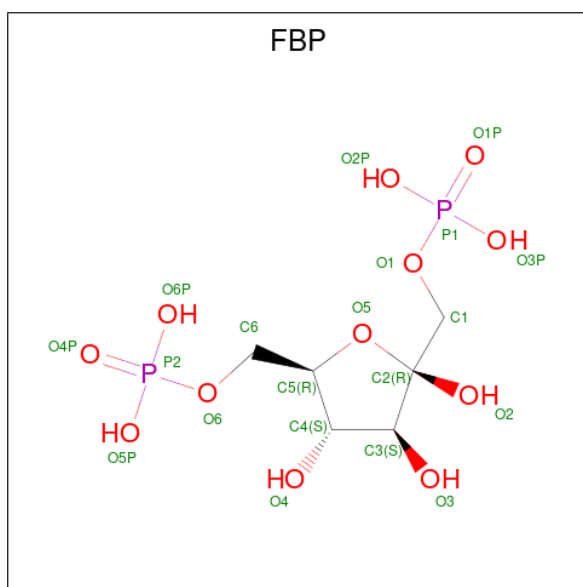
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q16716
A	0	SER	-	expression tag	UNP Q16716
A	12	ASP	SER	conflict	UNP Q16716
A	130	GLY	-	linker	UNP Q16716
A	131	SER	-	linker	UNP Q16716
A	132	GLY	-	linker	UNP Q16716
B	-1	GLY	-	expression tag	UNP Q16716
B	0	SER	-	expression tag	UNP Q16716
B	12	ASP	SER	conflict	UNP Q16716
B	130	GLY	-	linker	UNP Q16716
B	131	SER	-	linker	UNP Q16716
B	132	GLY	-	linker	UNP Q16716
C	-1	GLY	-	expression tag	UNP Q16716

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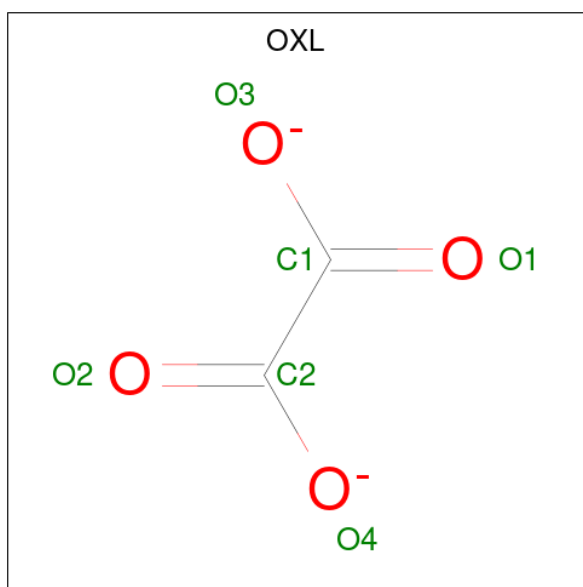
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP Q16716
C	12	ASP	SER	conflict	UNP Q16716
C	228	GLY	-	linker	UNP Q16716
C	229	SER	-	linker	UNP Q16716
C	230	GLY	-	linker	UNP Q16716
D	-1	GLY	-	expression tag	UNP Q16716
D	0	SER	-	expression tag	UNP Q16716
D	12	ASP	SER	conflict	UNP Q16716
D	130	GLY	-	linker	UNP Q16716
D	131	SER	-	linker	UNP Q16716
D	132	GLY	-	linker	UNP Q16716
E	-1	GLY	-	expression tag	UNP Q16716
E	0	SER	-	expression tag	UNP Q16716
E	12	ASP	SER	conflict	UNP Q16716
E	228	GLY	-	linker	UNP Q16716
E	229	SER	-	linker	UNP Q16716
E	230	GLY	-	linker	UNP Q16716
F	-1	GLY	-	expression tag	UNP Q16716
F	0	SER	-	expression tag	UNP Q16716
F	12	ASP	SER	conflict	UNP Q16716
F	228	GLY	-	linker	UNP Q16716
F	229	SER	-	linker	UNP Q16716
F	230	GLY	-	linker	UNP Q16716
G	-1	GLY	-	expression tag	UNP Q16716
G	0	SER	-	expression tag	UNP Q16716
G	12	ASP	SER	conflict	UNP Q16716
G	228	GLY	-	linker	UNP Q16716
G	229	SER	-	linker	UNP Q16716
G	230	GLY	-	linker	UNP Q16716
H	-1	GLY	-	expression tag	UNP Q16716
H	0	SER	-	expression tag	UNP Q16716
H	12	ASP	SER	conflict	UNP Q16716
H	130	GLY	-	linker	UNP Q16716
H	131	SER	-	linker	UNP Q16716
H	132	GLY	-	linker	UNP Q16716

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: $C_6H_{14}O_{12}P_2$).



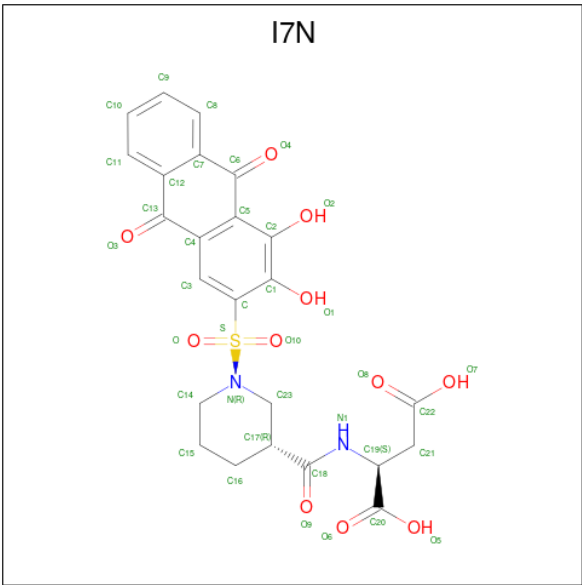
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		
2	E	1	Total	C	O	P	0	0
			20	6	12	2		
2	F	1	Total	C	O	P	0	0
			20	6	12	2		
2	G	1	Total	C	O	P	0	0
			20	6	12	2		
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 N-[(3R)-1-(3,4-dihydroxy-9,10-dioxo-9,10-dihydroanthracene-2-sulfonyl)pyridine-3-carbonyl]-L-aspartic acid (CCD ID: I7N) (formula: C₂₄H₂₂N₂O₁₁S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	S	22	0
			60	24	22	2	11	1		
4	C	1	Total	C	H	N	O	S	22	0
			60	24	22	2	11	1		
4	E	1	Total	C	H	N	O	S	22	0
			60	24	22	2	11	1		
4	F	1	Total	C	H	N	O	S	22	0
			60	24	22	2	11	1		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

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

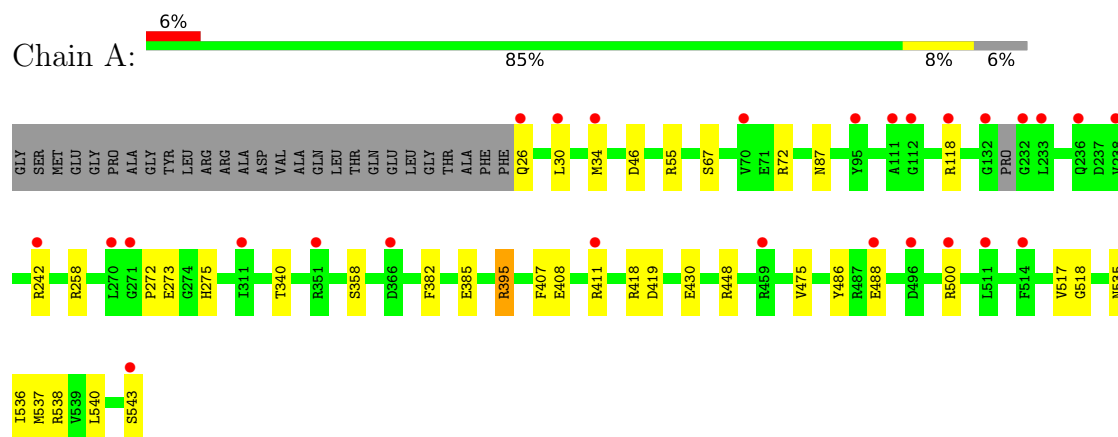
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	252	Total O 252 252	0	0
7	B	216	Total O 216 216	0	0
7	C	344	Total O 344 344	0	0
7	D	376	Total O 376 376	0	0
7	E	266	Total O 266 266	0	0
7	F	276	Total O 276 276	0	0
7	G	388	Total O 388 388	0	0
7	H	394	Total O 394 394	0	0

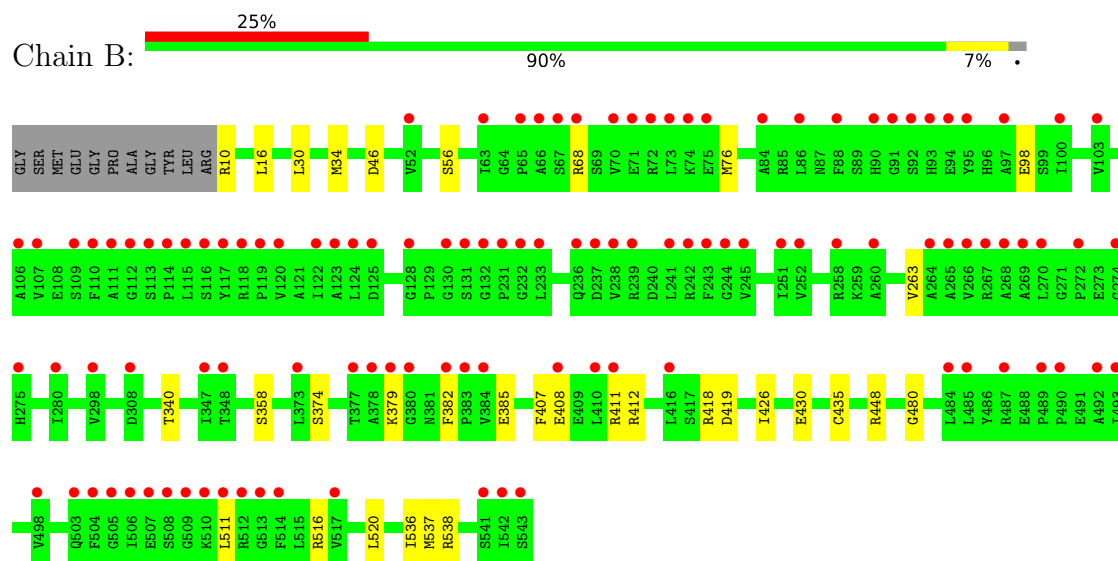
3 Residue-property plots [i](#)

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.

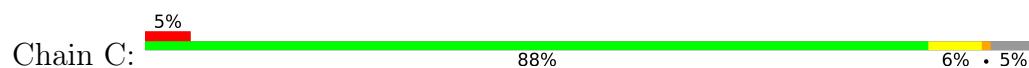
• Molecule 1: Pyruvate kinase

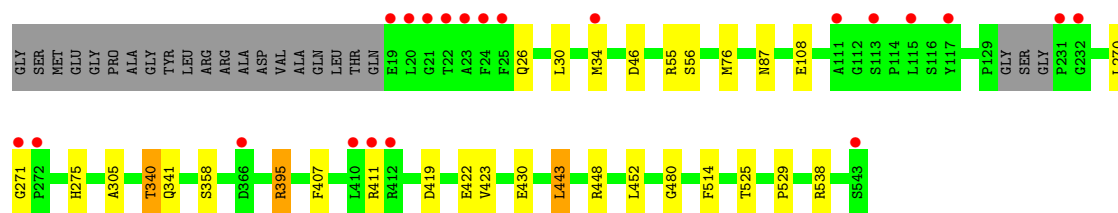


• Molecule 1: Pyruvate kinase

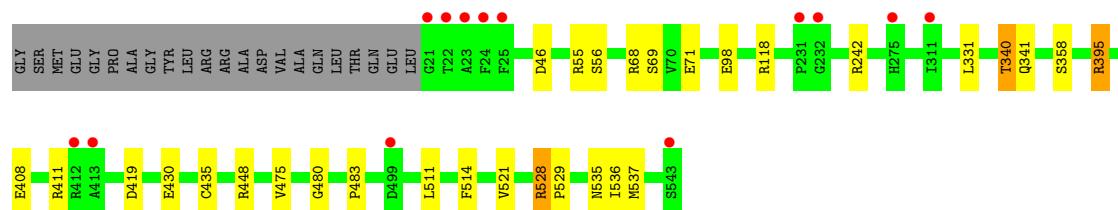
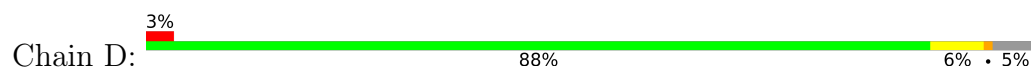


• Molecule 1: Pyruvate kinase

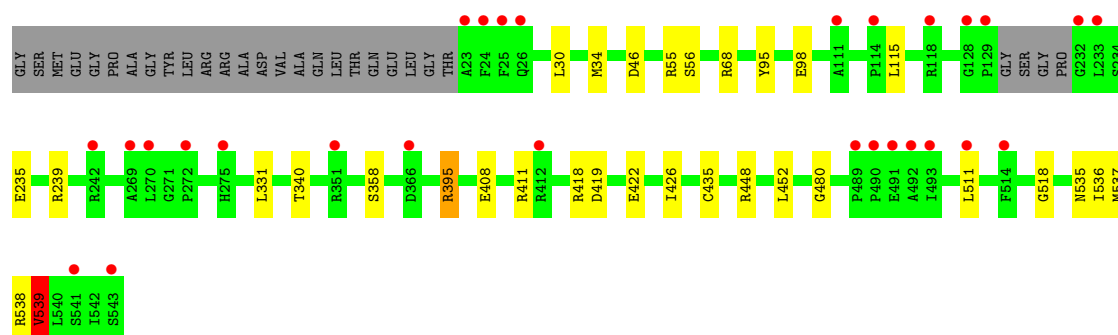
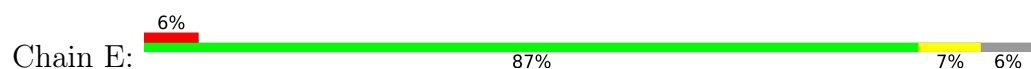




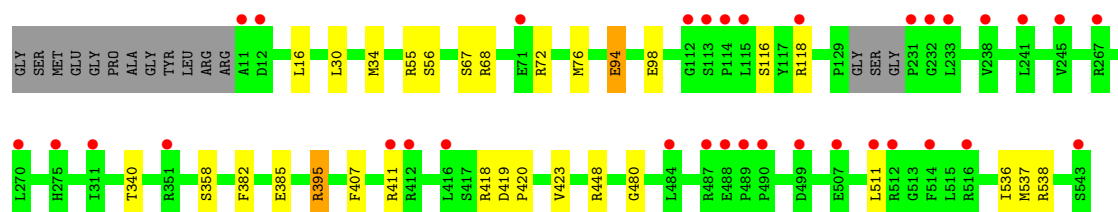
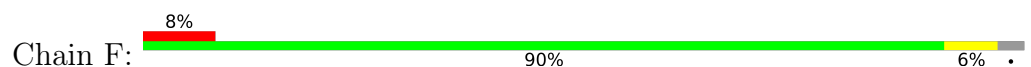
• Molecule 1: Pyruvate kinase



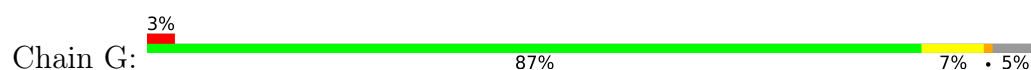
• Molecule 1: Pyruvate kinase

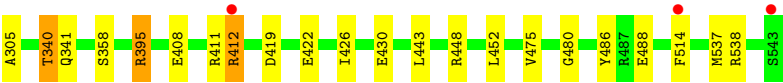


• Molecule 1: Pyruvate kinase

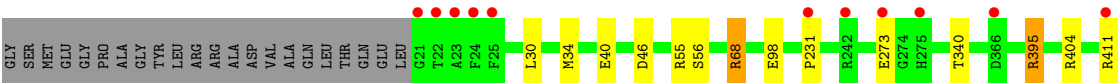
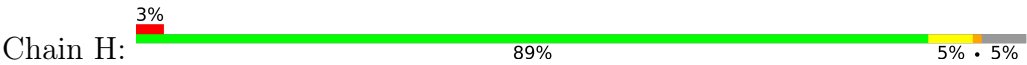


• Molecule 1: Pyruvate kinase





● Molecule 1: Pyruvate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	208.32Å 112.52Å 188.73Å 90.00° 91.75° 90.00°	Depositor
Resolution (Å)	188.64 – 1.92 188.64 – 1.92	Depositor EDS
% Data completeness (in resolution range)	81.1 (188.64-1.92) 81.1 (188.64-1.92)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 1.92Å)	Xtriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, R_{free}	0.192 , 0.216 0.185 , 0.208	Depositor DCC
R_{free} test set	13593 reflections (4.09%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.001 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	29195	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 30.86 % 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 1.2178e-03. 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: FBP, OXL, MG, I7N, K

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.70	0/3332	0.96	3/4502 (0.1%)
1	B	0.70	2/3429 (0.1%)	0.97	1/4636 (0.0%)
1	C	0.76	0/3341	0.96	2/4516 (0.0%)
1	D	0.76	0/3341	0.98	2/4517 (0.0%)
1	E	0.69	0/3350	0.95	2/4527 (0.0%)
1	F	0.71	0/3397	0.96	0/4592
1	G	0.76	0/3322	0.97	3/4490 (0.1%)
1	H	0.79	1/3357 (0.0%)	0.96	3/4537 (0.1%)
All	All	0.73	3/26869 (0.0%)	0.96	16/36317 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	374[A]	SER	CA-C	6.20	1.55	1.52
1	B	374[B]	SER	CA-C	6.20	1.55	1.52
1	H	489	PRO	CA-C	5.48	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	539	VAL	N-CA-CB	5.94	118.16	111.21
1	A	46	ASP	CA-CB-CG	5.90	118.50	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	ASP	CA-CB-CG	5.76	118.36	112.60
1	H	514	PHE	CA-CB-CG	5.76	119.56	113.80
1	G	514	PHE	CA-CB-CG	5.73	119.53	113.80
1	G	273	GLU	CB-CG-CD	5.43	121.84	112.60
1	A	26	GLN	CA-C-N	5.41	131.23	121.06
1	A	26	GLN	C-N-CA	5.41	131.23	121.06
1	H	46	ASP	CA-CB-CG	5.39	118.00	112.60
1	D	46	ASP	CA-CB-CG	5.37	117.97	112.60
1	G	46	ASP	CA-CB-CG	5.32	117.92	112.60
1	C	46	ASP	CA-CB-CG	5.25	117.85	112.60
1	H	40	GLU	CB-CG-CD	5.19	121.43	112.60
1	E	46	ASP	CA-CB-CG	5.15	117.75	112.60
1	D	514	PHE	CA-CB-CG	5.13	118.93	113.80
1	C	514	PHE	CA-CB-CG	5.05	118.86	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	231	PRO	Peptide

5.2 Too-close contacts [i](#)

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	3242	0	3315	21	0
1	B	3350	0	3417	17	0
1	C	3263	0	3325	23	0
1	D	3261	0	3321	19	0
1	E	3257	0	3323	19	0
1	F	3322	0	3388	20	0
1	G	3247	0	3304	22	0
1	H	3277	0	3341	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	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	1	0
3	H	6	0	0	0	0
4	A	38	22	0	1	0
4	C	38	22	0	1	0
4	E	38	22	0	1	0
4	F	38	22	0	0	0
5	A	1	0	0	0	0
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	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	A	252	0	0	1	0
7	B	216	0	0	0	1
7	C	344	0	0	2	0
7	D	376	0	0	0	0
7	E	266	0	0	0	1
7	F	276	0	0	0	0
7	G	388	0	0	0	0
7	H	394	0	0	1	0
All	All	29107	88	26814	127	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 (127) 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:G:538:ARG:HG2	1:H:536:ILE:HG12	1.45	0.96
1:C:538:ARG:HG2	1:D:536:ILE:HG12	1.69	0.74
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.71	0.71
1:E:418[B]:ARG:HG3	1:F:16:LEU:HD11	1.72	0.70
1:A:418[B]:ARG:HG3	1:B:16:LEU:HD11	1.74	0.69
1:F:407:PHE:CD2	1:F:411:ARG:NH1	2.64	0.66
1:A:87:ASN:HB3	4:A:603:I7N:O2	1.96	0.66
1:E:411:ARG:HG3	1:E:426:ILE:HD11	1.78	0.65
1:A:272:PRO:HA	1:A:275:HIS:NE2	2.13	0.64
1:B:407:PHE:CE2	1:B:411:ARG:NH1	2.66	0.64
1:D:71[B]:GLU:H	1:D:71[B]:GLU:CD	2.06	0.64
1:E:538:ARG:HG2	1:F:536:ILE:HG12	1.80	0.63
1:C:108:GLU:HG2	7:C:797:HOH:O	1.97	0.63
1:A:407:PHE:CE2	1:A:411:ARG:NH1	2.67	0.63
1:C:538:ARG:HD3	7:C:805:HOH:O	1.99	0.62
1:H:56:SER:HB2	1:H:480:GLY:HA2	1.83	0.60
1:G:56:SER:HB2	1:G:480:GLY:HA2	1.84	0.60
1:C:407:PHE:CD2	1:C:411:ARG:NH1	2.70	0.60
1:G:245:VAL:CG1	1:G:273:GLU:HG2	2.34	0.57
1:E:536:ILE:HG12	1:F:538:ARG:HG2	1.86	0.57
1:H:516:ARG:HD3	7:H:822:HOH:O	2.05	0.56
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.87	0.56
1:E:235:GLU:O	1:E:239:ARG:HD3	2.05	0.56
1:E:539:VAL:HG22	1:F:420:PRO:HB3	1.87	0.56
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.88	0.56
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.88	0.56
1:B:411:ARG:HG2	1:B:426:ILE:HD11	1.87	0.55
1:D:535:ASN:OD1	1:D:536:ILE:HG13	2.07	0.55
1:A:517:VAL:HG22	1:A:543:SER:HB3	1.89	0.54
1:F:407:PHE:CE2	1:F:411:ARG:NH1	2.75	0.54
1:E:56:SER:HB2	1:E:480:GLY:HA2	1.89	0.54
1:G:537:MET:HE3	1:H:537:MET:HG2	1.90	0.54
1:C:411:ARG:HH22	1:D:411:ARG:NH2	2.05	0.54
1:D:68:ARG:NH2	1:D:98:GLU:HB2	2.23	0.53
1:C:407:PHE:CE2	1:C:411:ARG:NH1	2.77	0.53
1:F:56:SER:HB2	1:F:480:GLY:HA2	1.91	0.53
1:E:408[B]:GLU:CD	1:F:411:ARG:HH21	2.16	0.52
1:B:407:PHE:CD2	1:B:411:ARG:NH1	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.91	0.52
1:C:411:ARG:NH2	1:D:411:ARG:NH2	2.59	0.51
1:A:538:ARG:HG3	1:B:536:ILE:HG12	1.93	0.51
1:D:419:ASP:OD2	1:D:448:ARG:NH2	2.43	0.50
1:A:419:ASP:OD2	1:A:448:ARG:NH2	2.44	0.50
1:C:422[A]:GLU:HG3	1:C:452:LEU:HD13	1.93	0.50
1:H:56:SER:HB2	1:H:480:GLY:CA	2.41	0.50
1:E:422:GLU:HG2	1:E:452:LEU:HD13	1.93	0.50
1:H:419:ASP:OD2	1:H:448:ARG:NH2	2.45	0.50
1:D:528:ARG:HD2	1:D:529:PRO:O	2.11	0.50
1:E:418[A]:ARG:HD3	1:F:16:LEU:HD11	1.93	0.49
1:A:430:GLU:OE2	1:B:430[B]:GLU:OE1	2.30	0.49
1:C:411:ARG:NH2	1:D:411:ARG:HH21	2.10	0.49
1:F:116:SER:O	1:F:118:ARG:HD2	2.14	0.48
1:G:419:ASP:OD2	1:G:448:ARG:NH2	2.45	0.47
1:G:430[A]:GLU:OE1	1:H:430[A]:GLU:OE1	2.32	0.47
1:H:68:ARG:NH2	1:H:98:GLU:HB2	2.28	0.47
1:F:67:SER:HA	1:F:72:ARG:HG2	1.97	0.47
1:H:535:ASN:OD1	1:H:536:ILE:HG13	2.14	0.47
1:E:419:ASP:OD2	1:E:448:ARG:NH2	2.45	0.46
1:G:430[B]:GLU:OE2	1:H:430[B]:GLU:OE1	2.33	0.46
1:C:443:LEU:HD22	1:C:525:THR:HG22	1.97	0.46
1:B:56:SER:HB2	1:B:480:GLY:CA	2.45	0.46
1:G:55:ARG:HB2	1:G:395:ARG:HG3	1.98	0.46
1:E:535:ASN:OD1	1:E:536:ILE:HG13	2.16	0.45
1:G:411:ARG:CG	1:G:426:ILE:HD11	2.46	0.45
1:A:486:TYR:CZ	1:A:488[B]:GLU:HB2	2.51	0.45
1:G:56:SER:HB2	1:G:480:GLY:CA	2.46	0.45
1:F:419:ASP:OD2	1:F:448:ARG:NH2	2.47	0.45
1:H:55:ARG:HB2	1:H:395:ARG:HG3	1.99	0.45
1:C:411:ARG:HH22	1:D:411:ARG:HH21	1.65	0.45
1:A:67:SER:HA	1:A:72:ARG:HG2	1.98	0.44
1:C:419:ASP:OD2	1:C:448:ARG:NH2	2.50	0.44
1:G:340:THR:HG22	1:G:341:GLN:HG3	1.99	0.44
1:G:411:ARG:HG2	1:G:426:ILE:HD11	2.00	0.44
1:C:529:PRO:HG2	1:G:235:GLU:HG2	2.00	0.44
1:A:55:ARG:HB2	1:A:395:ARG:HG3	1.99	0.43
1:A:518:GLY:O	1:B:418:ARG:NH2	2.49	0.43
1:D:56:SER:HB2	1:D:480:GLY:CA	2.47	0.43
1:F:30:LEU:O	1:F:34:MET:HG2	2.18	0.43
1:F:56:SER:HB2	1:F:480:GLY:CA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:ARG:HB2	1:E:395:ARG:HG3	2.00	0.43
1:C:55:ARG:HB2	1:C:395:ARG:HG3	1.99	0.43
1:A:535:ASN:OD1	1:A:536:ILE:HG13	2.19	0.43
1:D:340:THR:HG22	1:D:341:GLN:HG3	2.01	0.43
1:G:411:ARG:HH21	1:H:411:ARG:NH2	2.15	0.43
1:A:408[B]:GLU:HG2	1:A:411:ARG:HH21	1.83	0.43
1:C:56:SER:HB2	1:C:480:GLY:CA	2.48	0.43
1:C:87:ASN:ND2	4:C:602:I7N:O5	2.41	0.42
1:D:475:VAL:CG2	1:D:483:PRO:HB3	2.49	0.42
1:E:95:TYR:CE2	4:E:603:I7N:C10	3.02	0.42
1:G:538:ARG:CG	1:H:536:ILE:HG12	2.33	0.42
1:B:68:ARG:NH2	1:B:98:GLU:HB3	2.34	0.42
1:A:272:PRO:HA	1:A:275:HIS:CE1	2.53	0.42
1:G:305:ALA:HB1	3:G:602:OXL:C1	2.49	0.42
1:B:419:ASP:OD2	1:B:448:ARG:NH2	2.50	0.42
1:F:68:ARG:NH2	1:F:98:GLU:HB3	2.35	0.42
1:A:30:LEU:O	1:A:34:MET:HG2	2.20	0.42
1:A:242:ARG:HG2	7:A:712:HOH:O	2.19	0.42
1:A:430:GLU:OE2	1:B:430[A]:GLU:OE1	2.37	0.42
1:B:30:LEU:O	1:B:34:MET:HG2	2.20	0.42
1:E:56:SER:HB2	1:E:480:GLY:CA	2.48	0.42
1:E:518:GLY:O	1:F:418:ARG:NH2	2.53	0.42
1:G:267:ARG:HG2	1:G:279:ILE:CD1	2.50	0.42
1:C:30:LEU:O	1:C:34:MET:HG2	2.19	0.42
1:F:55:ARG:HB2	1:F:395:ARG:HG3	2.02	0.41
1:C:271:GLY:O	1:C:275:HIS:CE1	2.74	0.41
1:H:30:LEU:O	1:H:34:MET:HG2	2.21	0.41
1:A:382:PHE:HB3	1:A:385:GLU:HB2	2.02	0.41
1:B:382:PHE:HB3	1:B:385:GLU:HB2	2.02	0.41
1:C:305:ALA:HB1	3:C:603:OXL:C1	2.50	0.41
1:C:430[B]:GLU:OE2	1:D:430[B]:GLU:OE1	2.39	0.41
1:G:422[A]:GLU:CG	1:G:452:LEU:HD13	2.50	0.41
1:B:408:GLU:HG3	1:B:411:ARG:NH2	2.35	0.41
1:C:340:THR:HG22	1:C:341:GLN:HG3	2.03	0.41
1:D:242[A]:ARG:HE	1:D:242[A]:ARG:HA	1.85	0.41
1:G:30:LEU:O	1:G:34:MET:HG2	2.20	0.41
1:E:435:CYS:HB3	1:F:423:VAL:HG21	2.03	0.40
1:F:94:GLU:CD	1:F:94:GLU:H	2.29	0.40
1:F:382:PHE:HB3	1:F:385:GLU:HB2	2.02	0.40
1:C:423:VAL:HG21	1:D:435:CYS:HB3	2.03	0.40
1:D:55:ARG:HB2	1:D:395:ARG:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:LEU:O	1:E:34:MET:HG3	2.21	0.40
1:E:68:ARG:NH2	1:E:98:GLU:HB3	2.36	0.40
1:A:407:PHE:HE2	1:A:411:ARG:HH12	1.66	0.40
1:B:435:CYS:HB2	1:B:520:LEU:HD12	2.03	0.40
1:G:412:ARG:CZ	1:H:404:ARG:HD3	2.51	0.40
1:G:486:TYR:CZ	1:G:488:GLU:HB2	2.57	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:893:HOH:O	7:E:715:HOH:O[3_455]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	428/447 (96%)	424 (99%)	3 (1%)	1 (0%)	43	34
1	B	442/447 (99%)	437 (99%)	4 (1%)	1 (0%)	43	34
1	C	428/447 (96%)	425 (99%)	2 (0%)	1 (0%)	43	34
1	D	431/447 (96%)	427 (99%)	3 (1%)	1 (0%)	43	34
1	E	428/447 (96%)	424 (99%)	3 (1%)	1 (0%)	43	34
1	F	435/447 (97%)	431 (99%)	3 (1%)	1 (0%)	43	34
1	G	426/447 (95%)	420 (99%)	5 (1%)	1 (0%)	43	34
1	H	432/447 (97%)	428 (99%)	3 (1%)	1 (0%)	43	34
All	All	3450/3576 (96%)	3416 (99%)	26 (1%)	8 (0%)	43	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	345/352 (98%)	335 (97%)	10 (3%)	37	21
1	B	353/352 (100%)	342 (97%)	11 (3%)	35	19
1	C	345/352 (98%)	337 (98%)	8 (2%)	44	30
1	D	344/352 (98%)	334 (97%)	10 (3%)	37	21
1	E	346/352 (98%)	338 (98%)	8 (2%)	44	30
1	F	350/352 (99%)	342 (98%)	8 (2%)	44	30
1	G	342/352 (97%)	332 (97%)	10 (3%)	37	21
1	H	345/352 (98%)	339 (98%)	6 (2%)	53	41
All	All	2770/2816 (98%)	2699 (97%)	71 (3%)	44	24

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	ARG
1	A	258	ARG
1	A	273	GLU
1	A	358	SER
1	A	395	ARG
1	A	475	VAL
1	A	500	ARG
1	A	537[A]	MET

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Mol	Chain	Res	Type
1	A	537[B]	MET
1	A	540	LEU
1	B	10	ARG
1	B	76[A]	MET
1	B	76[B]	MET
1	B	263	VAL
1	B	358	SER
1	B	379	LYS
1	B	412	ARG
1	B	511	LEU
1	B	516	ARG
1	B	537[A]	MET
1	B	537[B]	MET
1	C	26	GLN
1	C	76[A]	MET
1	C	76[B]	MET
1	C	270[A]	LEU
1	C	270[B]	LEU
1	C	358	SER
1	C	395	ARG
1	C	443	LEU
1	D	69	SER
1	D	118	ARG
1	D	331	LEU
1	D	358	SER
1	D	395	ARG
1	D	408	GLU
1	D	511	LEU
1	D	521	VAL
1	D	528	ARG
1	D	537	MET
1	E	115	LEU
1	E	331	LEU
1	E	358	SER
1	E	395	ARG
1	E	511	LEU
1	E	537[A]	MET
1	E	537[B]	MET
1	E	539	VAL
1	F	76[A]	MET
1	F	76[B]	MET
1	F	94	GLU

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Mol	Chain	Res	Type
1	F	358	SER
1	F	395	ARG
1	F	511	LEU
1	F	537[A]	MET
1	F	537[B]	MET
1	G	22	THR
1	G	76[A]	MET
1	G	76[B]	MET
1	G	273	GLU
1	G	358	SER
1	G	395	ARG
1	G	408	GLU
1	G	412	ARG
1	G	443	LEU
1	G	475	VAL
1	H	68	ARG
1	H	273	GLU
1	H	395	ARG
1	H	412	ARG
1	H	511	LEU
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	405	GLN
1	B	27	GLN
1	B	405	GLN
1	C	275	HIS
1	C	405	GLN
1	D	405	GLN
1	D	535	ASN
1	E	405	GLN
1	F	405	GLN
1	G	275	HIS
1	G	405	GLN
1	H	405	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [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$
4	I7N	F	602	6	41,41,41	0.34	0	60,62,62	0.67	1 (1%)
2	FBP	G	601	-	18,20,20	0.72	1 (5%)	21,32,32	0.76	0
3	OXL	C	603	5	5,5,5	1.87	2 (40%)	6,6,6	1.85	1 (16%)
3	OXL	E	602	5	5,5,5	2.33	2 (40%)	6,6,6	1.83	2 (33%)
2	FBP	F	601	-	18,20,20	0.52	0	21,32,32	0.53	0
4	I7N	A	603	-	41,41,41	0.31	0	60,62,62	0.56	1 (1%)
3	OXL	H	602	5	5,5,5	2.35	3 (60%)	6,6,6	1.84	1 (16%)
3	OXL	A	602	5	5,5,5	2.34	3 (60%)	6,6,6	2.13	3 (50%)
2	FBP	A	601	-	18,20,20	0.53	0	21,32,32	0.61	0
2	FBP	E	601	-	18,20,20	0.73	0	21,32,32	0.71	1 (4%)
2	FBP	H	601	-	18,20,20	0.97	1 (5%)	21,32,32	0.79	0
2	FBP	C	601	-	18,20,20	0.98	2 (11%)	21,32,32	0.78	0
4	I7N	E	603	-	41,41,41	0.31	0	60,62,62	0.53	1 (1%)
3	OXL	B	602	5	5,5,5	2.37	2 (40%)	6,6,6	1.70	2 (33%)
3	OXL	D	602	5	5,5,5	2.43	3 (60%)	6,6,6	2.18	2 (33%)
3	OXL	F	603	5	5,5,5	3.10	4 (80%)	6,6,6	2.36	3 (50%)
2	FBP	B	601	-	18,20,20	0.79	1 (5%)	21,32,32	0.74	1 (4%)
4	I7N	C	602	-	41,41,41	0.30	0	60,62,62	0.79	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FBP	D	601	-	18,20,20	0.67	0	21,32,32	0.87	1 (4%)
3	OXL	G	602	5	5,5,5	2.20	2 (40%)	6,6,6	2.00	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
4	I7N	F	602	6	-	6/28/54/54	0/4/4/4
2	FBP	G	601	-	-	2/13/32/32	0/1/1/1
3	OXL	C	603	5	-	4/4/4/4	-
3	OXL	E	602	5	-	4/4/4/4	-
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
4	I7N	A	603	-	-	7/28/54/54	0/4/4/4
3	OXL	H	602	5	-	4/4/4/4	-
3	OXL	A	602	5	-	4/4/4/4	-
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
2	FBP	E	601	-	-	2/13/32/32	0/1/1/1
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
4	I7N	E	603	-	-	11/28/54/54	0/4/4/4
3	OXL	B	602	5	-	4/4/4/4	-
3	OXL	D	602	5	-	4/4/4/4	-
3	OXL	F	603	5	-	4/4/4/4	-
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
4	I7N	C	602	-	-	14/28/54/54	1/4/4/4
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
3	OXL	G	602	5	-	4/4/4/4	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	OXL	O1-C1	4.69	1.34	1.22
3	A	602	OXL	O2-C2	4.13	1.32	1.22
3	B	602	OXL	O2-C2	4.09	1.32	1.22
3	F	603	OXL	O2-C2	3.79	1.31	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	602	OXL	O3-C1	-3.52	1.21	1.30
3	F	603	OXL	O1-C1	3.45	1.31	1.22
3	F	603	OXL	O3-C1	-3.43	1.21	1.30
3	D	602	OXL	O2-C2	3.26	1.30	1.22
3	H	602	OXL	C2-C1	3.20	1.60	1.54
3	D	602	OXL	O4-C2	-3.20	1.21	1.30
3	B	602	OXL	O4-C2	-2.73	1.23	1.30
3	H	602	OXL	O4-C2	-2.73	1.23	1.30
3	C	603	OXL	O3-C1	-2.72	1.23	1.30
3	H	602	OXL	O2-C2	2.62	1.29	1.22
3	C	603	OXL	O1-C1	2.58	1.28	1.22
2	B	601	FBP	P2-O5P	-2.57	1.45	1.54
3	F	603	OXL	C2-C1	2.57	1.59	1.54
3	G	602	OXL	O1-C1	2.52	1.28	1.22
2	C	601	FBP	P1-O3P	-2.44	1.45	1.54
2	G	601	FBP	P2-O6P	-2.38	1.46	1.54
3	A	602	OXL	C2-C1	2.36	1.58	1.54
2	C	601	FBP	P2-O6P	-2.20	1.46	1.54
3	E	602	OXL	O3-C1	-2.17	1.24	1.30
3	A	602	OXL	O4-C2	-2.16	1.24	1.30
3	D	602	OXL	C2-C1	2.15	1.58	1.54
2	H	601	FBP	P1-O3P	-2.11	1.46	1.54

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	602	I7N	C23-C17-C18	4.66	118.82	110.07
3	F	603	OXL	O4-C2-C1	4.11	120.80	112.83
3	H	602	OXL	O4-C2-C1	3.97	120.53	112.83
3	C	603	OXL	O3-C1-C2	3.91	120.42	112.83
3	A	602	OXL	O4-C2-C1	3.75	120.11	112.83
4	F	602	I7N	C16-C17-C18	3.69	118.57	110.79
3	G	602	OXL	O3-C1-C2	3.50	119.63	112.83
3	D	602	OXL	O4-C2-C1	3.49	119.59	112.83
3	D	602	OXL	O3-C1-C2	3.17	118.99	112.83
3	F	603	OXL	O3-C1-C2	3.04	118.72	112.83
3	E	602	OXL	O4-C2-C1	2.88	118.42	112.83
3	B	602	OXL	O3-C1-C2	2.83	118.31	112.83
3	A	602	OXL	O3-C1-C2	2.82	118.30	112.83
3	E	602	OXL	O3-C1-C2	2.75	118.16	112.83
3	B	602	OXL	O4-C2-C1	2.74	118.15	112.83
4	A	603	I7N	C23-C17-C18	2.74	115.21	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	602	OXL	O4-C2-C1	2.68	118.03	112.83
2	E	601	FBP	O3P-P1-O2P	2.62	117.62	107.80
3	F	603	OXL	O2-C2-C1	-2.50	115.42	120.63
2	D	601	FBP	O5P-P2-O6	2.41	112.95	106.67
2	B	601	FBP	O3P-P1-O2P	2.40	116.78	107.80
4	C	602	I7N	C3-C-C1	-2.30	118.53	121.10
3	A	602	OXL	O2-C2-C1	-2.07	116.31	120.63
4	E	603	I7N	C-S-N	-2.07	102.86	106.69

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	I7N	C20-C19-C21-C22
4	A	603	I7N	C1-C-S-O10
4	A	603	I7N	C1-C-S-O
4	C	602	I7N	C23-N-S-C
4	C	602	I7N	C1-C-S-O10
4	C	602	I7N	C1-C-S-O
4	C	602	I7N	C23-C17-C18-N1
4	C	602	I7N	C17-C18-N1-C19
4	C	602	I7N	O9-C18-N1-C19
4	C	602	I7N	C14-N-S-O10
4	C	602	I7N	C14-N-S-O
4	C	602	I7N	C23-N-S-O10
2	H	601	FBP	C4-C5-C6-O6
4	E	603	I7N	C14-N-S-O
4	C	602	I7N	C14-N-S-C
4	A	603	I7N	C23-N-S-O10
4	F	602	I7N	C14-N-S-O10
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
4	E	603	I7N	C14-N-S-C
4	F	602	I7N	C16-C17-C18-N1
4	A	603	I7N	C23-N-S-C
4	F	602	I7N	C14-N-S-C
4	C	602	I7N	C23-C17-C18-O9

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Mol	Chain	Res	Type	Atoms
4	A	603	I7N	N1-C19-C21-C22
4	F	602	I7N	C16-C17-C18-O9
2	A	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
2	B	601	FBP	O5-C5-C6-O6
4	E	603	I7N	C19-C21-C22-O8
4	E	603	I7N	N1-C19-C21-C22
4	E	603	I7N	C19-C21-C22-O7
4	C	602	I7N	C19-C21-C22-O8
4	C	602	I7N	C19-C21-C22-O7
4	C	602	I7N	C23-N-S-O
3	B	602	OXL	O3-C1-C2-O4
3	C	603	OXL	O3-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O4
3	F	603	OXL	O3-C1-C2-O4
3	G	602	OXL	O3-C1-C2-O4
3	D	602	OXL	O3-C1-C2-O4
3	H	602	OXL	O3-C1-C2-O4
3	B	602	OXL	O1-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O2
3	F	603	OXL	O1-C1-C2-O2
3	G	602	OXL	O1-C1-C2-O2
3	A	602	OXL	O3-C1-C2-O4
4	A	603	I7N	C21-C19-N1-C18
4	E	603	I7N	C20-C19-C21-C22
3	A	602	OXL	O1-C1-C2-O2
3	C	603	OXL	O1-C1-C2-O2
3	E	602	OXL	O1-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O2
4	F	602	I7N	C19-C21-C22-O8
4	F	602	I7N	C19-C21-C22-O7
4	E	603	I7N	N1-C19-C20-O6
4	E	603	I7N	N1-C19-C20-O5
3	B	602	OXL	O3-C1-C2-O2
3	D	602	OXL	O3-C1-C2-O2
3	F	603	OXL	O3-C1-C2-O2
3	B	602	OXL	O1-C1-C2-O4

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Mol	Chain	Res	Type	Atoms
3	C	603	OXL	O1-C1-C2-O4
3	C	603	OXL	O3-C1-C2-O2
3	E	602	OXL	O1-C1-C2-O4
3	F	603	OXL	O1-C1-C2-O4
3	G	602	OXL	O1-C1-C2-O4
3	G	602	OXL	O3-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O4
4	E	603	I7N	C21-C19-C20-O6
3	A	602	OXL	O3-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O2
3	A	602	OXL	O1-C1-C2-O4
3	H	602	OXL	O3-C1-C2-O2
4	E	603	I7N	C3-C-S-O10
4	E	603	I7N	C21-C19-C20-O5

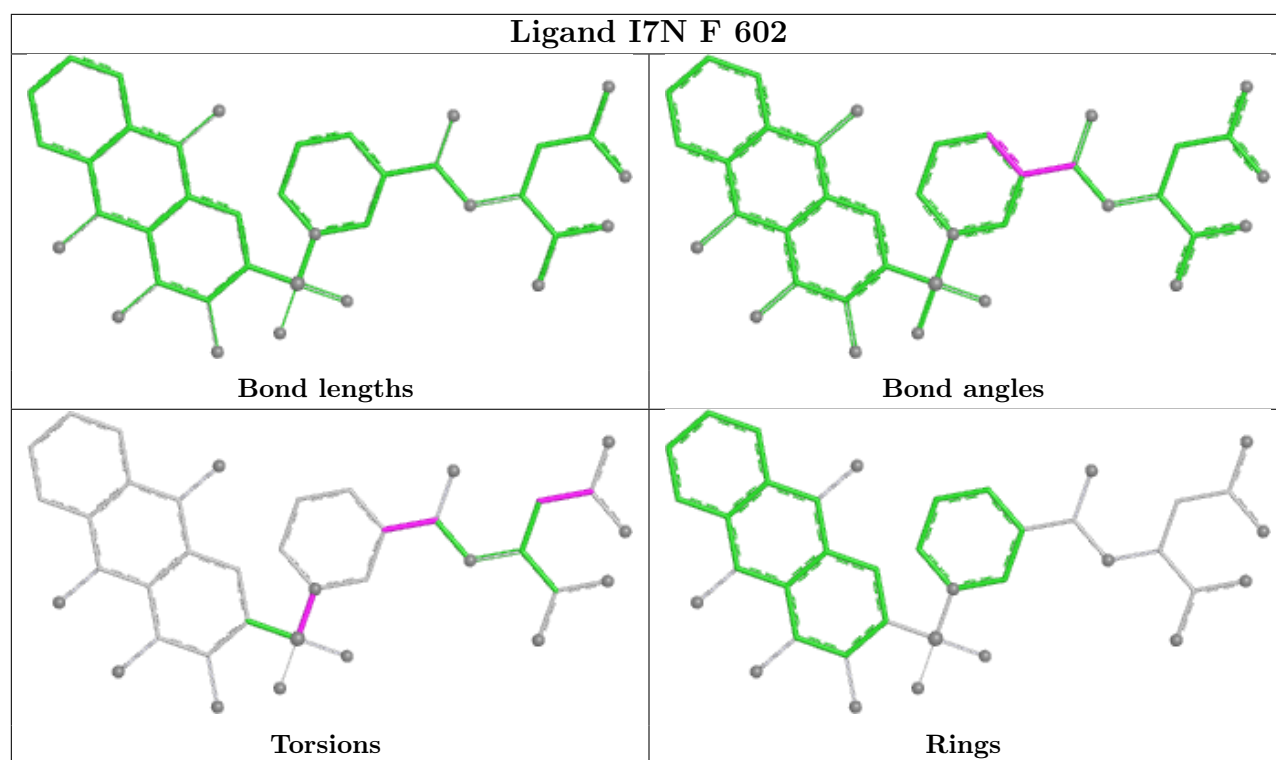
All (1) ring outliers are listed below:

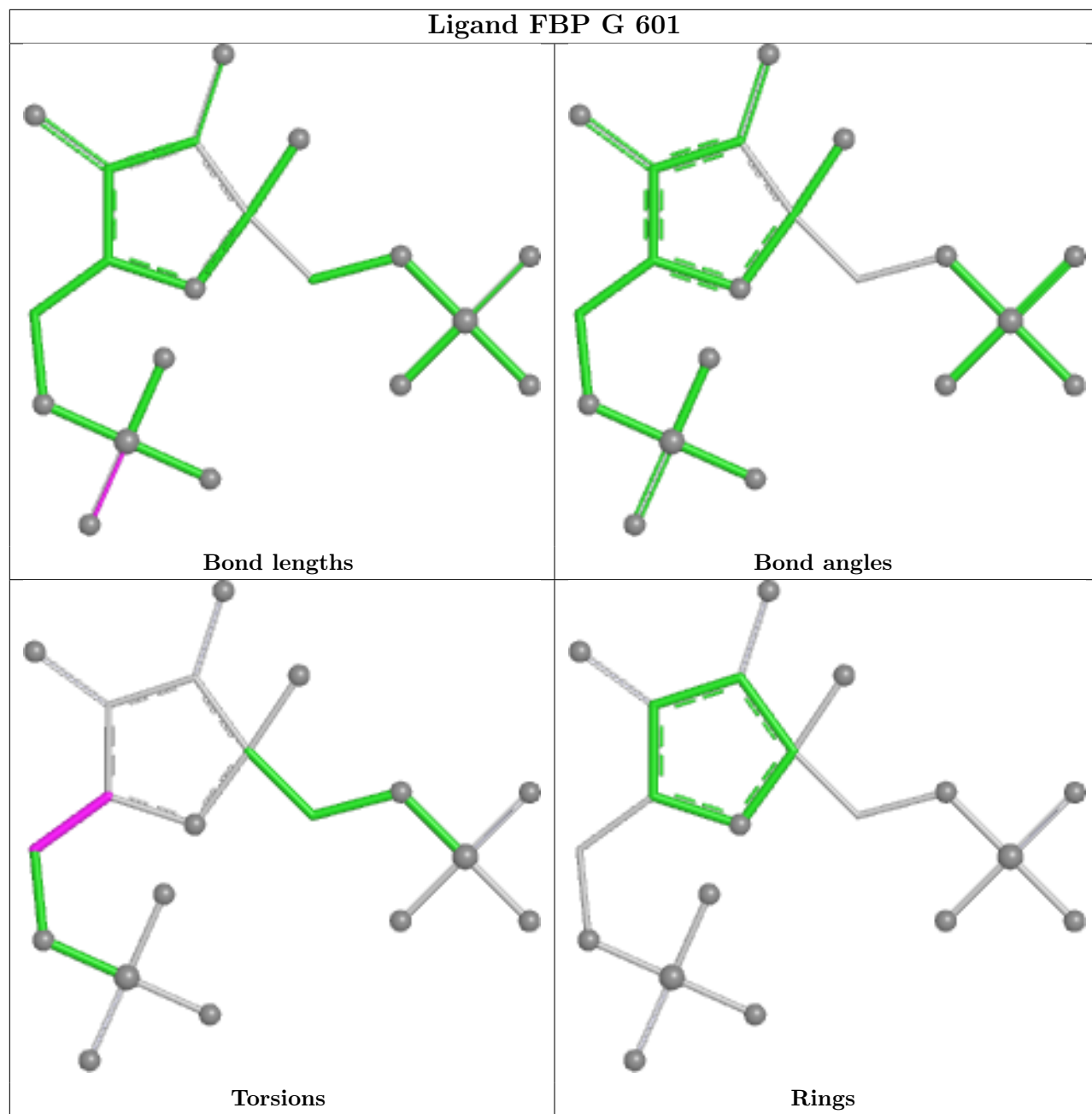
Mol	Chain	Res	Type	Atoms
4	C	602	I7N	C14-C15-C16-C17-C23-N

5 monomers are involved in 5 short contacts:

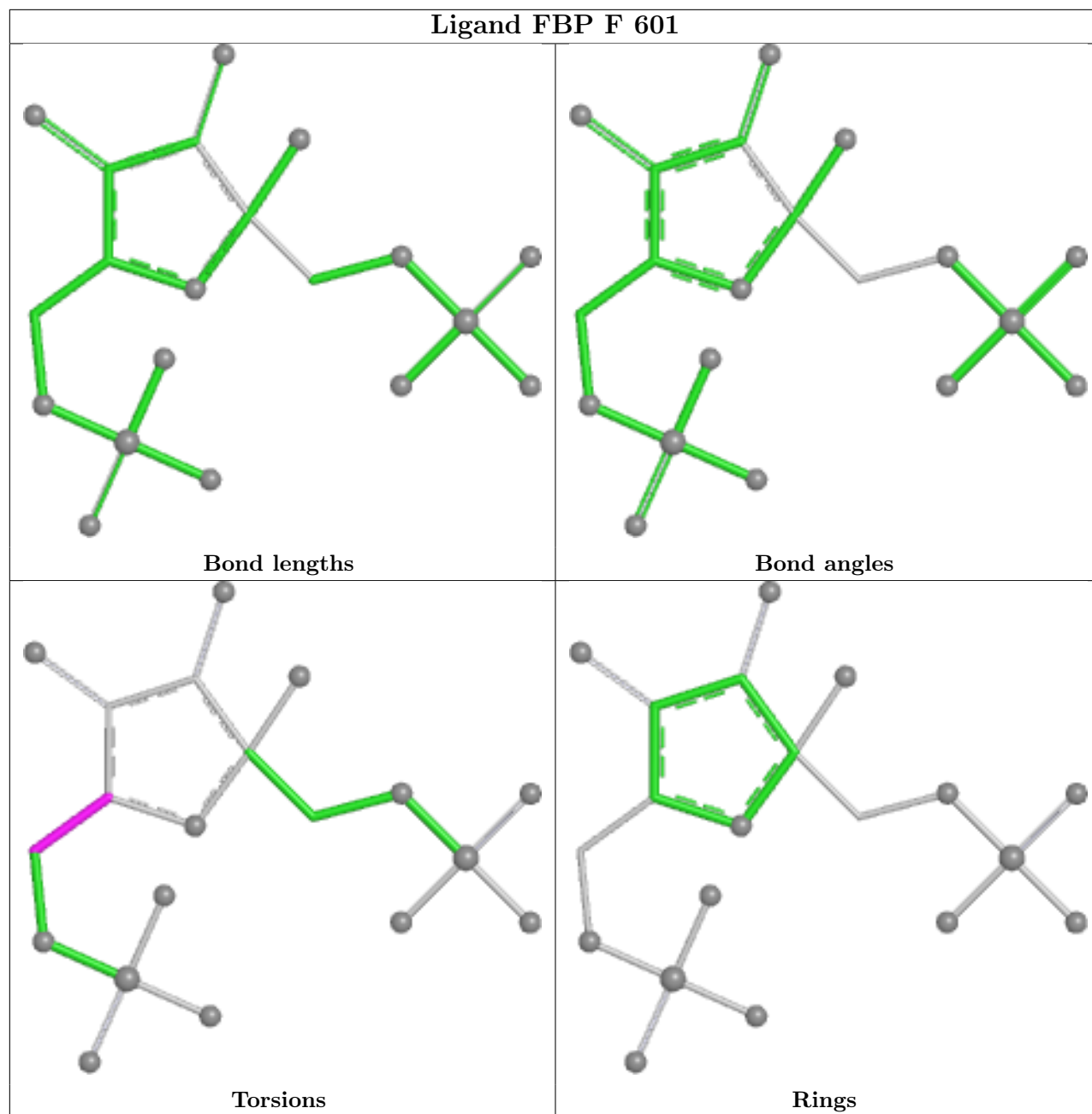
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	603	OXL	1	0
4	A	603	I7N	1	0
4	E	603	I7N	1	0
4	C	602	I7N	1	0
3	G	602	OXL	1	0

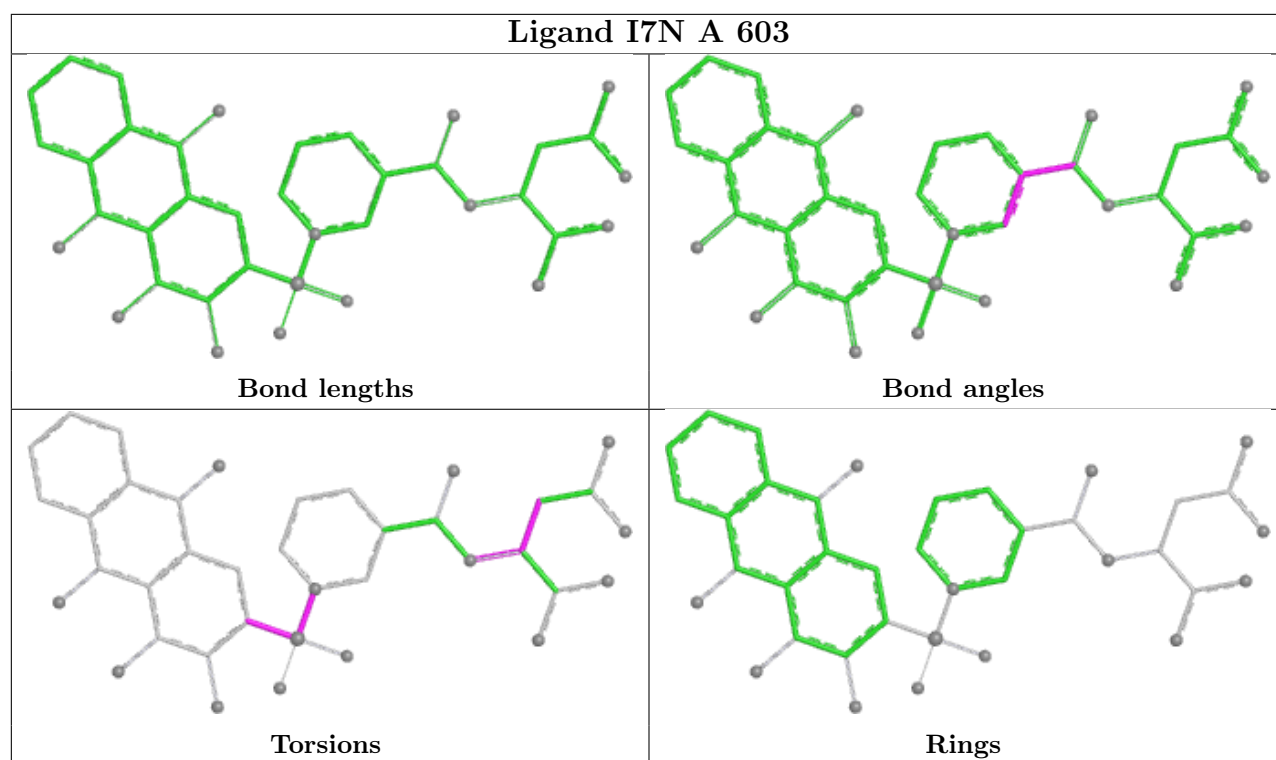
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

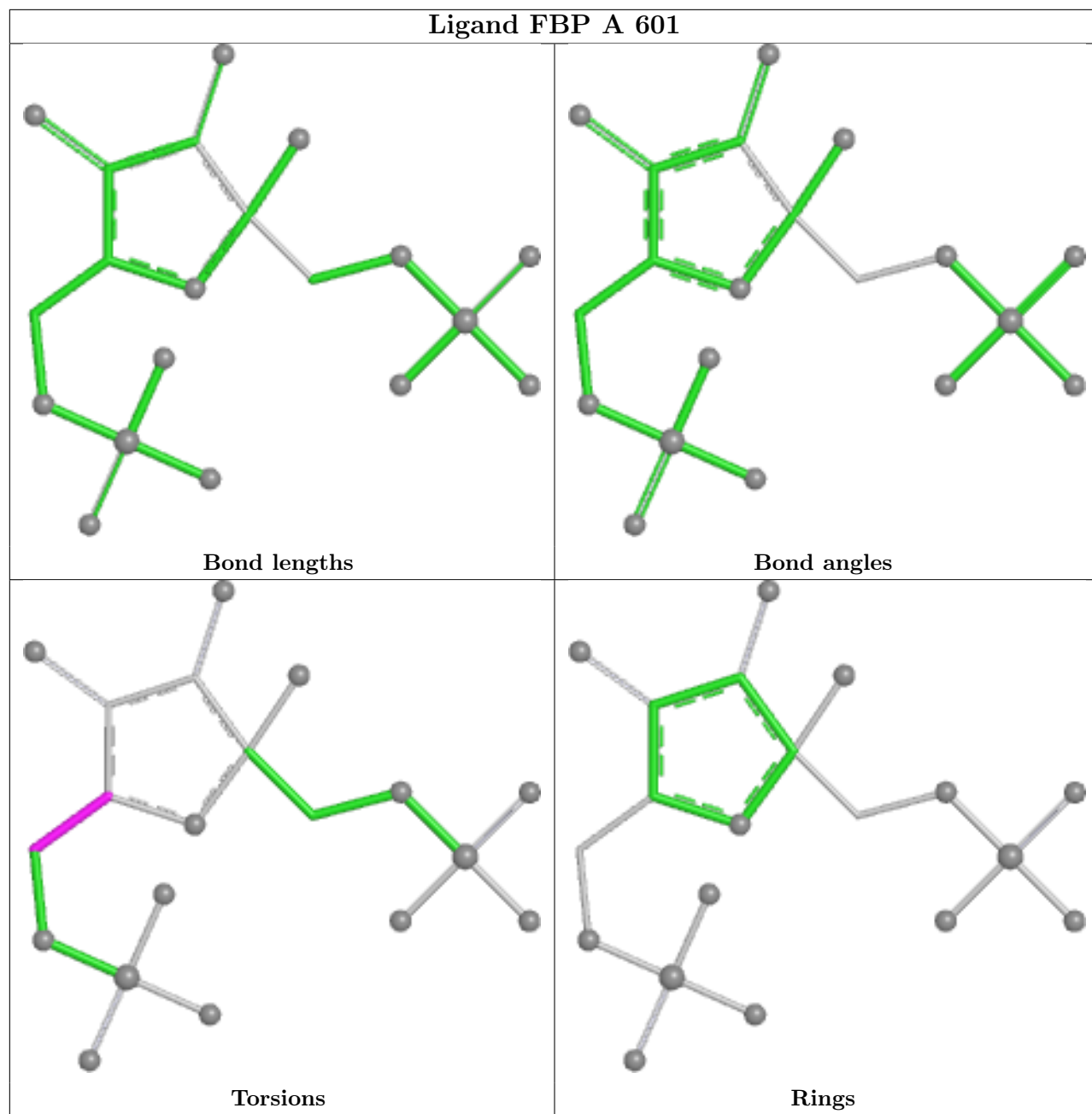




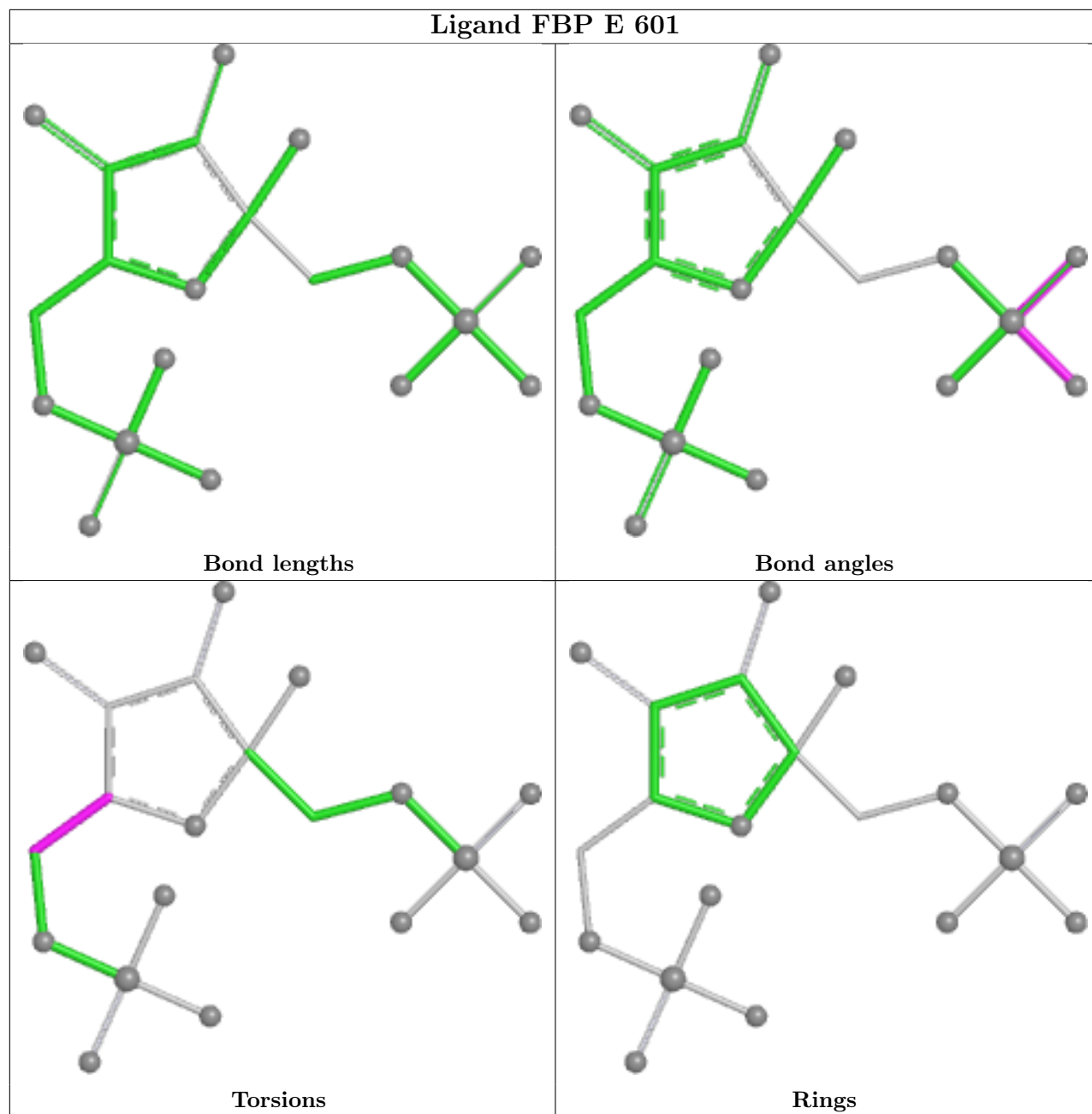
Ligand FBP F 601

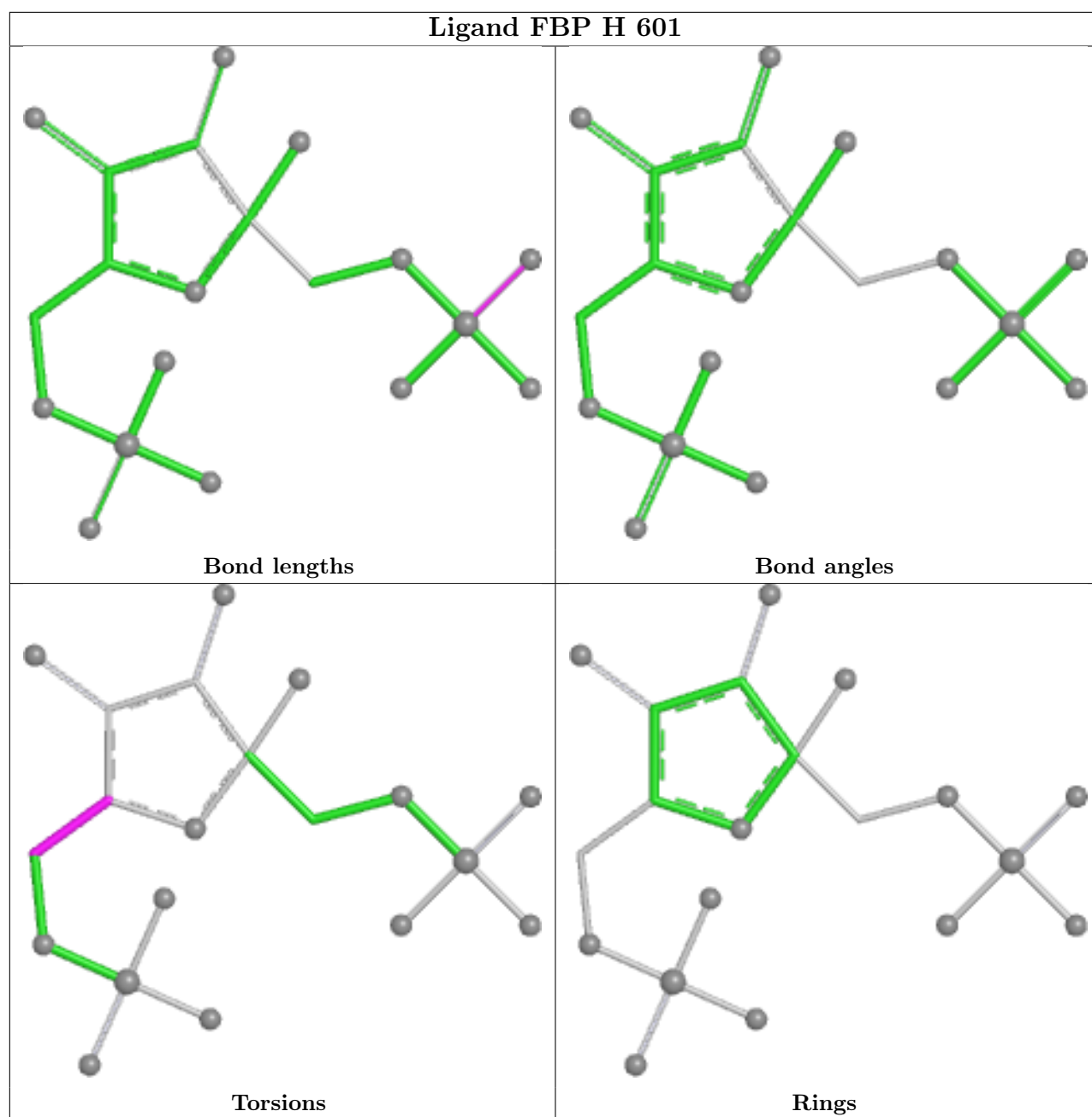


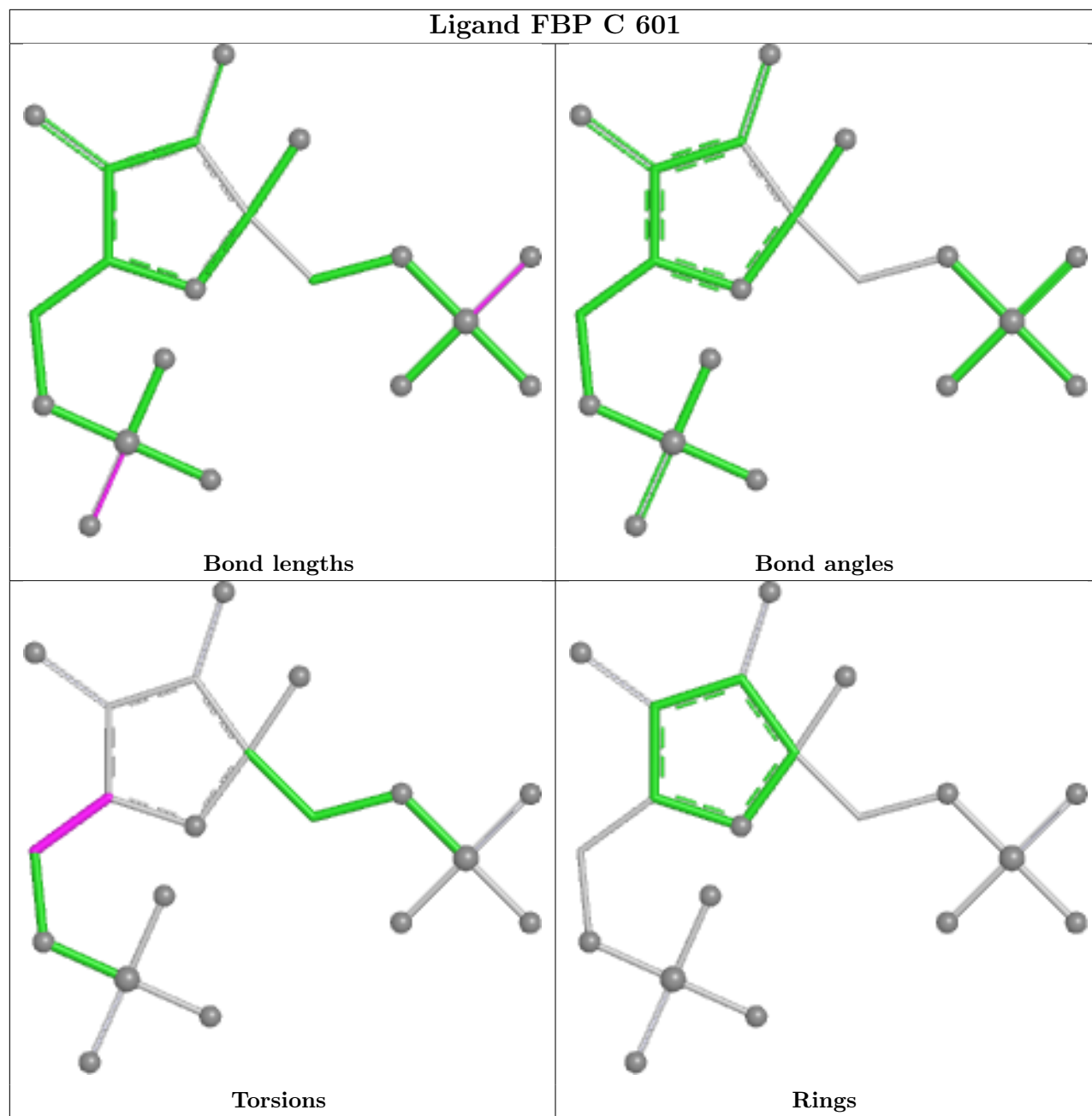


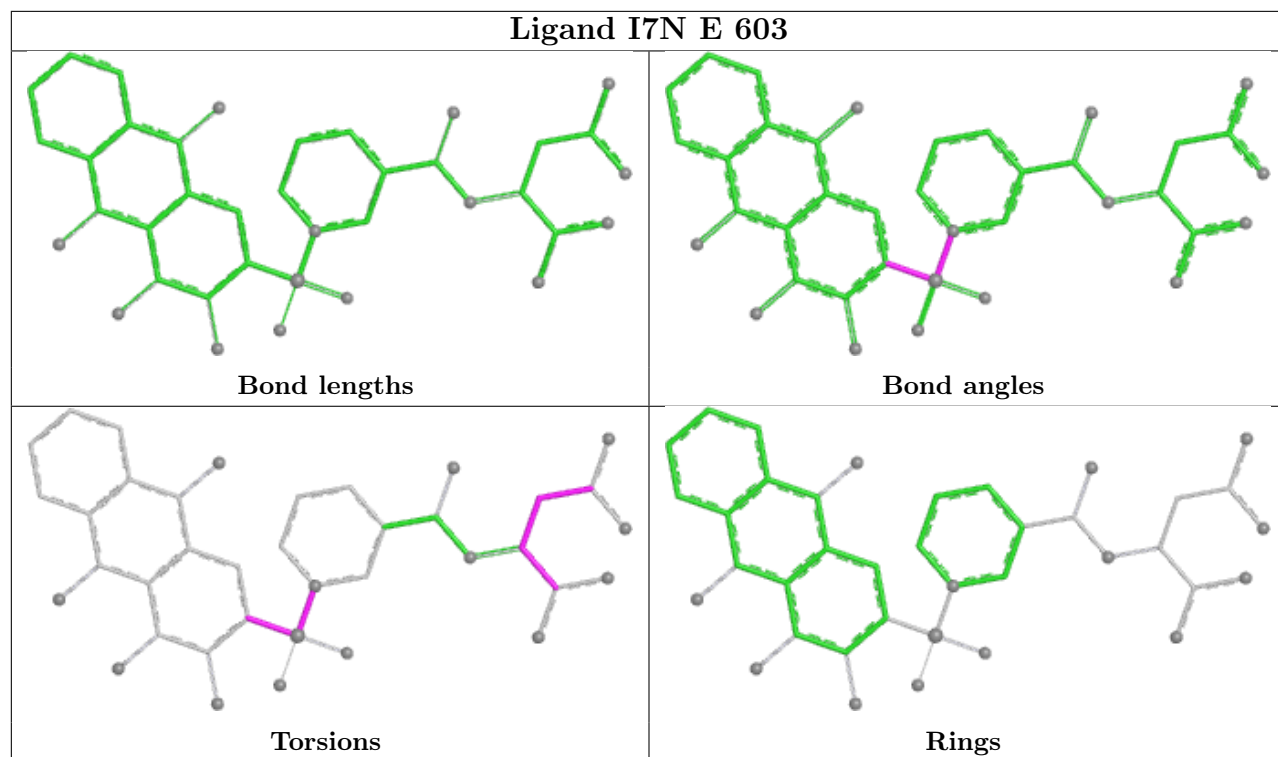


Ligand FBP E 601

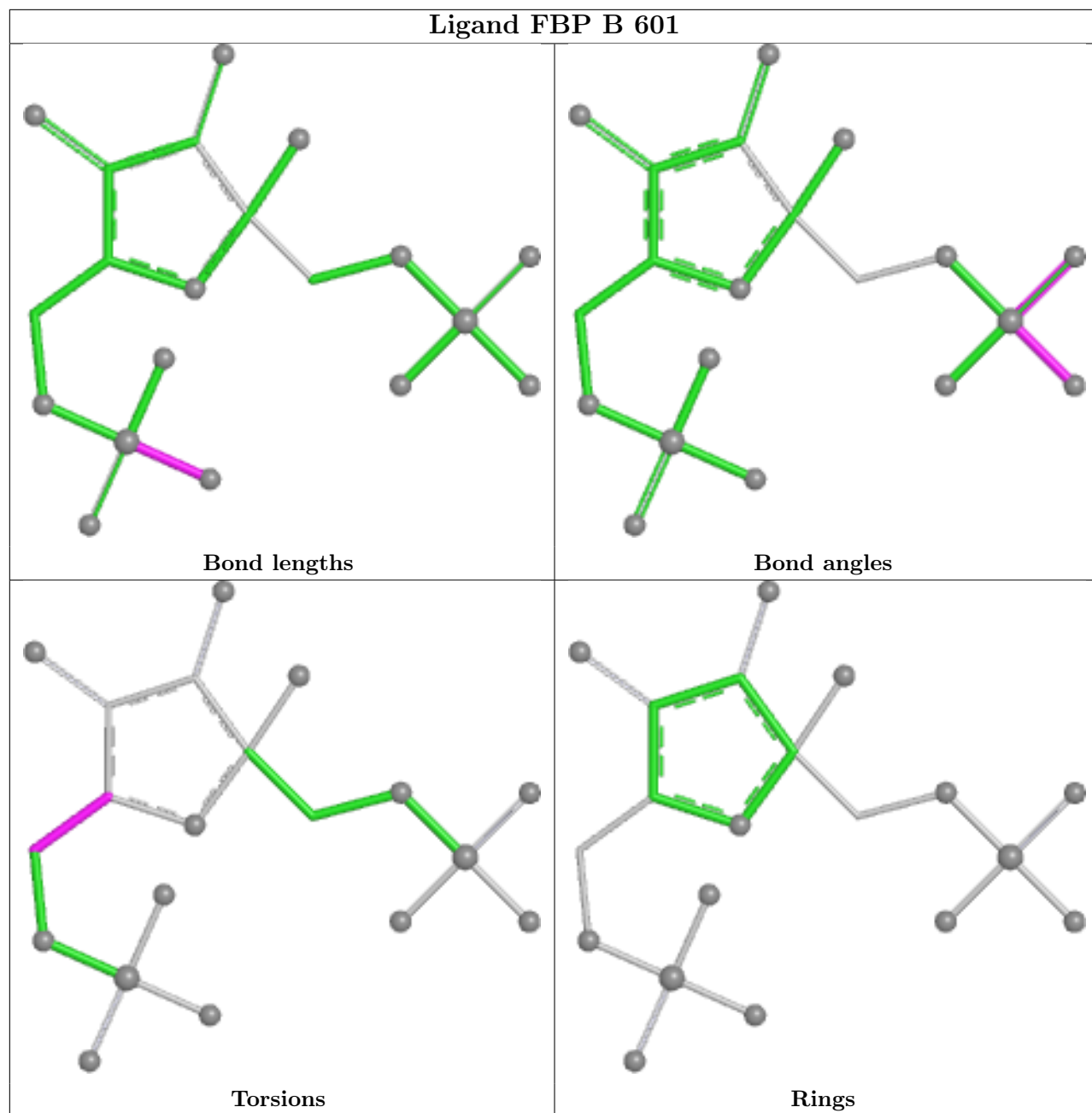


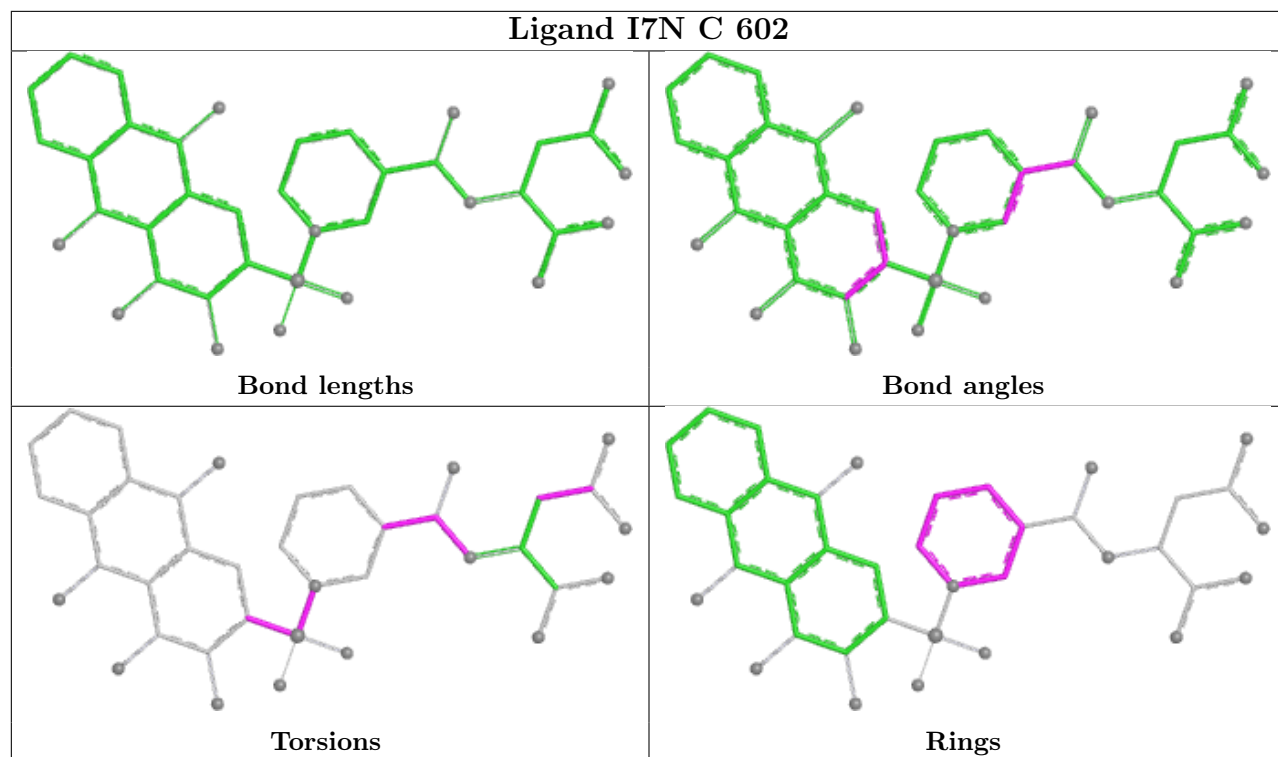


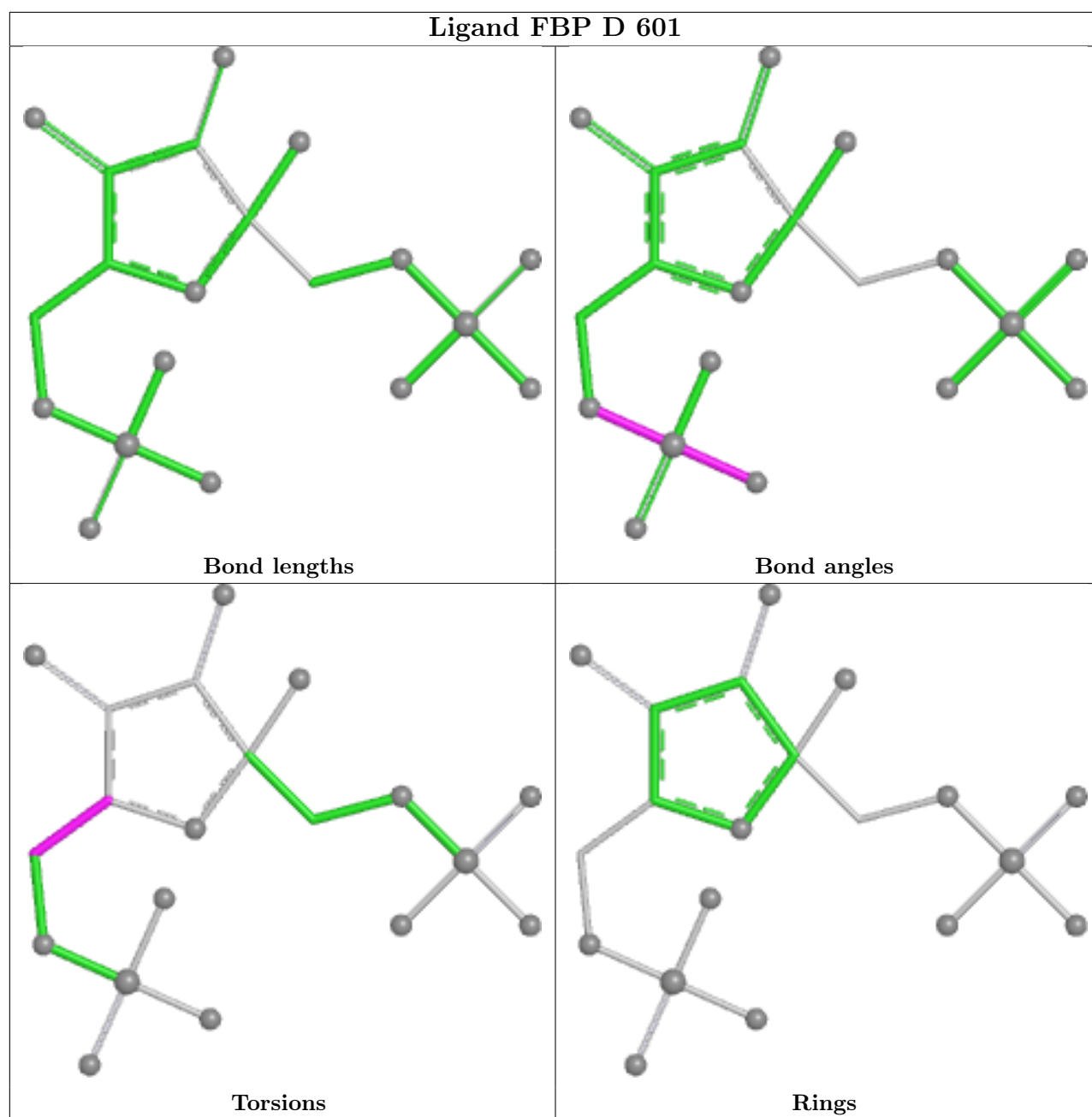




Ligand FBP B 601







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	419/447 (93%)	0.69	27 (6%) 25 29	21, 39, 61, 78	13 (3%)
1	B	436/447 (97%)	1.24	113 (25%) 1 2	20, 44, 75, 90	8 (1%)
1	C	424/447 (94%)	0.16	21 (4%) 34 38	20, 30, 51, 93	8 (1%)
1	D	425/447 (95%)	0.07	13 (3%) 51 56	14, 29, 51, 90	8 (1%)
1	E	419/447 (93%)	0.57	28 (6%) 24 28	20, 38, 62, 74	13 (3%)
1	F	432/447 (96%)	0.50	34 (7%) 18 22	20, 35, 59, 75	7 (1%)
1	G	423/447 (94%)	0.03	12 (2%) 55 61	16, 29, 44, 70	8 (1%)
1	H	425/447 (95%)	-0.06	14 (3%) 49 54	13, 27, 48, 70	9 (2%)
All	All	3403/3576 (95%)	0.40	262 (7%) 19 23	13, 34, 60, 93	74 (2%)

All (262) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	115	LEU	11.4
1	B	511	LEU	9.6
1	G	271	GLY	6.7
1	A	543	SER	6.7
1	F	115	LEU	5.9
1	C	271	GLY	5.8
1	G	20	LEU	5.8
1	E	275[A]	HIS	5.6
1	G	231	PRO	5.5
1	B	116	SER	5.5
1	H	21	GLY	5.4
1	B	114	PRO	5.3
1	F	231	PRO	5.1
1	A	132	GLY	4.8
1	D	231	PRO	4.8
1	D	25	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	543	SER	4.7
1	B	267[A]	ARG	4.7
1	E	25	PHE	4.6
1	B	117	TYR	4.6
1	D	21	GLY	4.4
1	C	20	LEU	4.4
1	D	23	ALA	4.3
1	A	232	GLY	4.2
1	D	22	THR	4.2
1	B	238	VAL	4.0
1	B	231	PRO	4.0
1	C	21	GLY	4.0
1	E	232	GLY	4.0
1	B	348	THR	4.0
1	F	267[A]	ARG	3.9
1	B	118	ARG	3.9
1	B	512	ARG	3.9
1	H	22	THR	3.9
1	D	24	PHE	3.9
1	C	366	ASP	3.8
1	H	231	PRO	3.7
1	B	484	LEU	3.7
1	B	507	GLU	3.7
1	D	275[A]	HIS	3.7
1	B	90	HIS	3.6
1	B	268	ALA	3.6
1	A	500	ARG	3.6
1	F	543	SER	3.6
1	F	232	GLY	3.5
1	E	129	PRO	3.5
1	H	411	ARG	3.5
1	F	512	ARG	3.4
1	C	25	PHE	3.4
1	F	511	LEU	3.4
1	G	25	PHE	3.4
1	B	113	SER	3.4
1	B	233	LEU	3.4
1	A	311	ILE	3.4
1	E	543	SER	3.4
1	B	100	ILE	3.3
1	H	25	PHE	3.3
1	C	22	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	490	PRO	3.3
1	B	95	TYR	3.3
1	E	490	PRO	3.3
1	B	241	LEU	3.2
1	B	513	GLY	3.2
1	B	275	HIS	3.2
1	B	237	ASP	3.2
1	B	251	ILE	3.2
1	F	507	GLU	3.2
1	F	489	PRO	3.2
1	H	242[A]	ARG	3.2
1	E	23	ALA	3.1
1	A	34	MET	3.1
1	B	73	LEU	3.1
1	H	543	SER	3.1
1	C	543	SER	3.1
1	B	70	VAL	3.1
1	B	272	PRO	3.1
1	B	490	PRO	3.1
1	E	511	LEU	3.1
1	B	131	SER	3.1
1	G	21	GLY	3.0
1	B	84	ALA	3.0
1	A	238	VAL	3.0
1	B	489	PRO	3.0
1	C	231	PRO	3.0
1	F	516	ARG	3.0
1	B	347	ILE	3.0
1	C	24	PHE	2.9
1	B	416	LEU	2.9
1	E	269	ALA	2.9
1	E	492	ALA	2.9
1	D	232	GLY	2.9
1	C	23	ALA	2.9
1	E	233	LEU	2.9
1	B	132	GLY	2.9
1	C	232	GLY	2.9
1	B	379	LYS	2.8
1	B	111	ALA	2.8
1	B	67	SER	2.8
1	D	543	SER	2.8
1	B	97	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	11	ALA	2.8
1	F	484	LEU	2.8
1	B	266	VAL	2.8
1	B	106	ALA	2.8
1	B	265	ALA	2.8
1	B	128	GLY	2.8
1	F	233	LEU	2.8
1	E	493	ILE	2.8
1	B	119	PRO	2.8
1	A	111	ALA	2.7
1	C	111	ALA	2.7
1	B	510	LYS	2.7
1	B	232	GLY	2.7
1	B	244	GLY	2.7
1	A	30	LEU	2.7
1	B	410	LEU	2.7
1	F	416	LEU	2.7
1	A	366	ASP	2.7
1	B	122	ILE	2.7
1	A	514	PHE	2.7
1	B	88	PHE	2.7
1	F	113	SER	2.7
1	G	232	GLY	2.7
1	A	233	LEU	2.7
1	E	270	LEU	2.7
1	B	93	HIS	2.7
1	H	275[A]	HIS	2.7
1	B	378	ALA	2.6
1	A	26	GLN	2.6
1	B	485	LEU	2.6
1	B	380	GLY	2.6
1	F	112	GLY	2.6
1	B	123	ALA	2.6
1	B	258	ARG	2.6
1	B	71	GLU	2.6
1	G	543	SER	2.6
1	E	514	PHE	2.6
1	G	514	PHE	2.6
1	F	270	LEU	2.6
1	C	117	TYR	2.6
1	B	86	LEU	2.6
1	B	242	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	516	ARG	2.6
1	C	412	ARG	2.5
1	B	382	PHE	2.5
1	E	24	PHE	2.5
1	B	107	VAL	2.5
1	E	351	ARG	2.5
1	B	514	PHE	2.5
1	B	270	LEU	2.5
1	B	264	ALA	2.5
1	B	492	ALA	2.5
1	E	26	GLN	2.5
1	E	489	PRO	2.5
1	D	499	ASP	2.5
1	C	115	LEU	2.5
1	B	541	SER	2.5
1	A	488[A]	GLU	2.5
1	A	70	VAL	2.5
1	B	308	ASP	2.5
1	F	238	VAL	2.5
1	G	52	VAL	2.5
1	B	92	SER	2.4
1	C	113	SER	2.4
1	B	52	VAL	2.4
1	B	517	VAL	2.4
1	A	411	ARG	2.4
1	B	66	ALA	2.4
1	E	118	ARG	2.4
1	F	114	PRO	2.4
1	A	496	ASP	2.4
1	B	542	ILE	2.4
1	B	384	VAL	2.4
1	A	270	LEU	2.3
1	B	110	PHE	2.3
1	G	22	THR	2.3
1	E	128	GLY	2.3
1	B	109	SER	2.3
1	B	72	ARG	2.3
1	F	351	ARG	2.3
1	E	114	PRO	2.3
1	F	245	VAL	2.3
1	G	24	PHE	2.3
1	A	271	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	91	GLY	2.3
1	B	239	ARG	2.3
1	F	311	ILE	2.3
1	B	75[A]	GLU	2.3
1	A	95	TYR	2.2
1	B	65	PRO	2.2
1	B	243	PHE	2.2
1	B	408	GLU	2.2
1	C	19	GLU	2.2
1	B	245	VAL	2.2
1	A	118	ARG	2.2
1	A	459	ARG	2.2
1	G	412	ARG	2.2
1	B	383	PRO	2.2
1	E	272	PRO	2.2
1	B	269	ALA	2.2
1	F	12	ASP	2.2
1	H	366	ASP	2.2
1	B	103	VAL	2.2
1	B	125	ASP	2.2
1	E	541[A]	SER	2.2
1	C	272	PRO	2.2
1	D	413	ALA	2.2
1	B	280	ILE	2.2
1	B	74	LYS	2.2
1	B	411	ARG	2.2
1	B	487	ARG	2.2
1	C	34	MET	2.2
1	E	242	ARG	2.2
1	A	236	GLN	2.2
1	B	130	GLY	2.2
1	B	274	GLY	2.2
1	F	488	GLU	2.1
1	B	503	GLN	2.1
1	B	120	VAL	2.1
1	B	298	VAL	2.1
1	B	377	THR	2.1
1	A	242	ARG	2.1
1	B	68	ARG	2.1
1	B	124	LEU	2.1
1	B	373	LEU	2.1
1	C	410	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	504	PHE	2.1
1	B	493	ILE	2.1
1	D	311	ILE	2.1
1	B	498	VAL	2.1
1	C	411	ARG	2.1
1	E	491	GLU	2.1
1	F	71	GLU	2.1
1	A	511	LEU	2.1
1	B	236	GLN	2.1
1	B	260	ALA	2.1
1	E	412	ARG	2.1
1	F	411	ARG	2.1
1	H	273	GLU	2.1
1	A	112	GLY	2.1
1	B	112	GLY	2.1
1	F	275	HIS	2.1
1	B	252	VAL	2.1
1	E	111	ALA	2.1
1	F	487	ARG	2.1
1	B	63	ILE	2.0
1	H	489	PRO	2.0
1	F	241	LEU	2.0
1	F	118	ARG	2.0
1	F	412	ARG	2.0
1	H	23	ALA	2.0
1	E	366	ASP	2.0
1	F	499	ASP	2.0
1	B	94	GLU	2.0
1	B	508	SER	2.0
1	B	506	ILE	2.0
1	F	514	PHE	2.0
1	H	24	PHE	2.0
1	B	505	GLY	2.0
1	B	509	GLY	2.0
1	A	351	ARG	2.0
1	D	412	ARG	2.0

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

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

6.3 Carbohydrates [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
4	I7N	A	603	38/38	0.76	0.19	98,98,99,99	22
4	I7N	C	602	38/38	0.76	0.20	75,80,86,86	22
4	I7N	F	602	38/38	0.78	0.21	75,82,85,85	22
4	I7N	E	603	38/38	0.85	0.14	67,73,78,78	22
3	OXL	C	603	6/6	0.85	0.12	46,47,47,48	0
3	OXL	F	603	6/6	0.86	0.10	44,44,45,46	0
3	OXL	E	602	6/6	0.87	0.11	47,48,48,48	0
3	OXL	B	602	6/6	0.87	0.12	55,55,57,57	0
3	OXL	D	602	6/6	0.88	0.10	39,39,40,40	0
3	OXL	H	602	6/6	0.88	0.13	34,35,37,38	0
3	OXL	G	602	6/6	0.90	0.09	35,36,38,38	0
3	OXL	A	602	6/6	0.90	0.10	44,45,46,47	0
6	K	E	605	1/1	0.92	0.15	67,67,67,67	0
6	K	F	605	1/1	0.94	0.10	70,70,70,70	0
6	K	B	604	1/1	0.95	0.12	77,77,77,77	0
5	MG	A	604	1/1	0.95	0.06	50,50,50,50	0
6	K	A	605	1/1	0.95	0.10	64,64,64,64	0
2	FBP	B	601	20/20	0.96	0.07	36,37,40,40	0
6	K	C	605	1/1	0.96	0.14	50,50,50,50	0
5	MG	B	603	1/1	0.97	0.06	54,54,54,54	0
2	FBP	F	601	20/20	0.97	0.06	31,35,39,40	0
2	FBP	A	601	20/20	0.97	0.05	32,34,36,36	0
2	FBP	H	601	20/20	0.98	0.04	19,21,22,22	0
2	FBP	E	601	20/20	0.98	0.05	32,33,34,35	0
5	MG	F	604	1/1	0.99	0.05	37,37,37,37	0
5	MG	H	603	1/1	0.99	0.02	35,35,35,35	0
2	FBP	C	601	20/20	0.99	0.04	22,23,24,25	0
2	FBP	D	601	20/20	0.99	0.04	22,23,24,25	0
2	FBP	G	601	20/20	0.99	0.04	20,21,23,23	0
6	K	D	604	1/1	0.99	0.05	37,37,37,37	0
5	MG	D	603	1/1	0.99	0.02	33,33,33,33	0
5	MG	E	604	1/1	0.99	0.03	47,47,47,47	0

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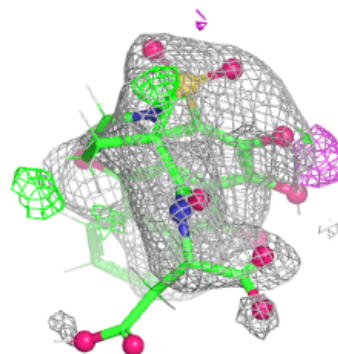
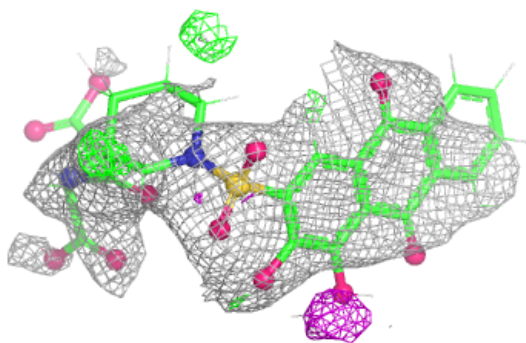
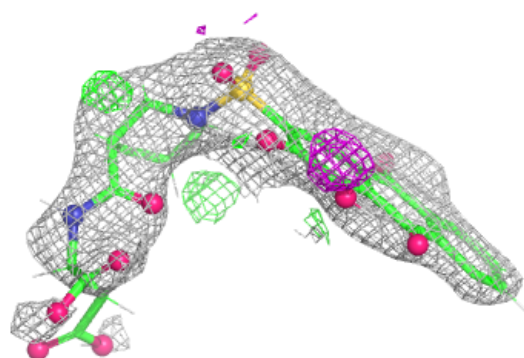
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	K	G	604	1/1	0.99	0.13	45,45,45,45	0
6	K	H	604	1/1	0.99	0.08	40,40,40,40	0
5	MG	G	603	1/1	1.00	0.03	34,34,34,34	0
5	MG	C	604	1/1	1.00	0.02	37,37,37,37	0

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.

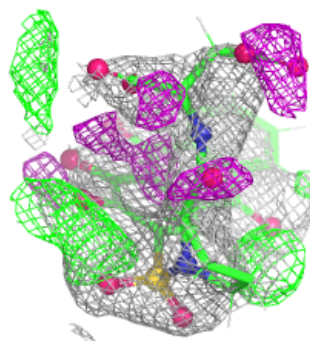
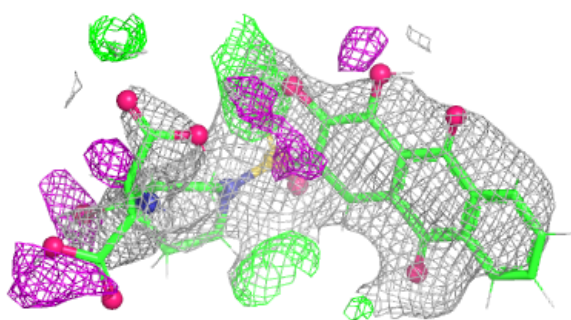
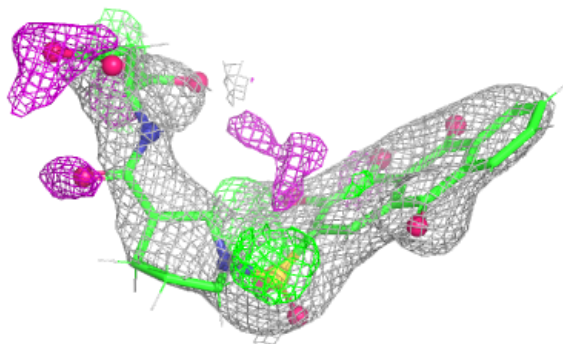
Electron density around I7N A 603:

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

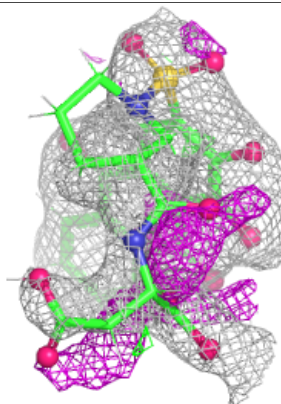
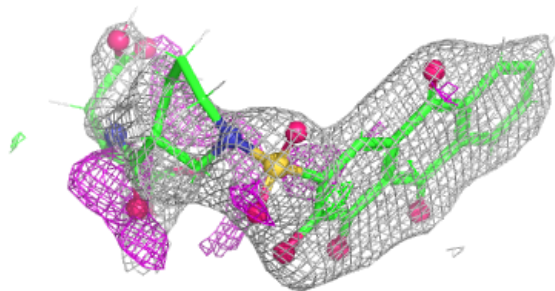
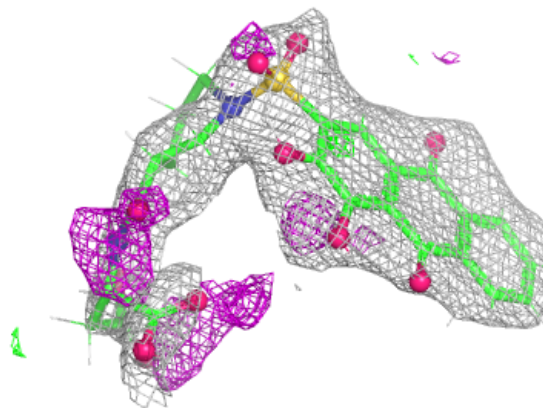


Electron density around I7N C 602:

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

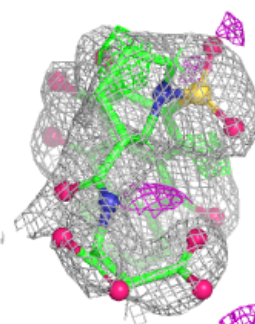
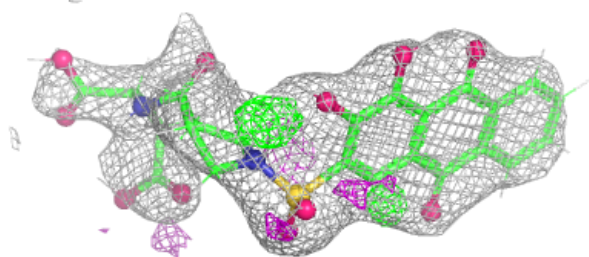
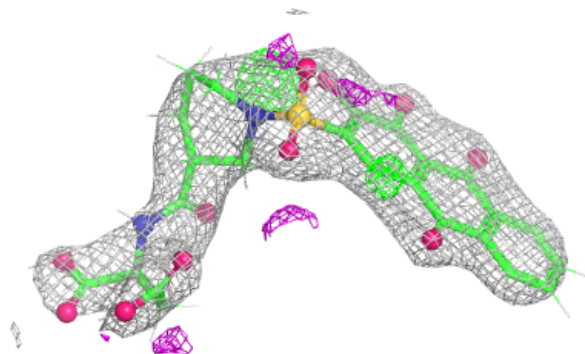
**Electron density around I7N F 602:**

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

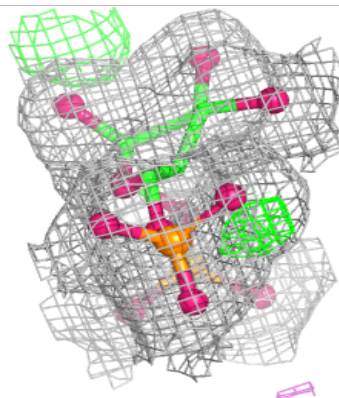
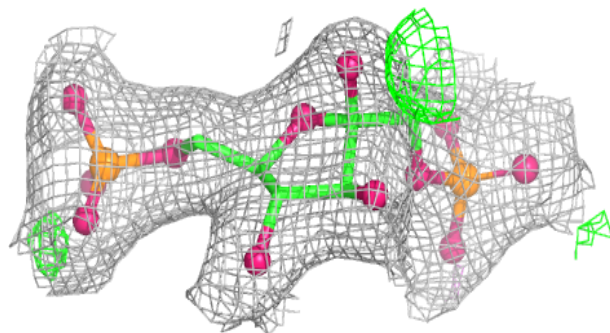
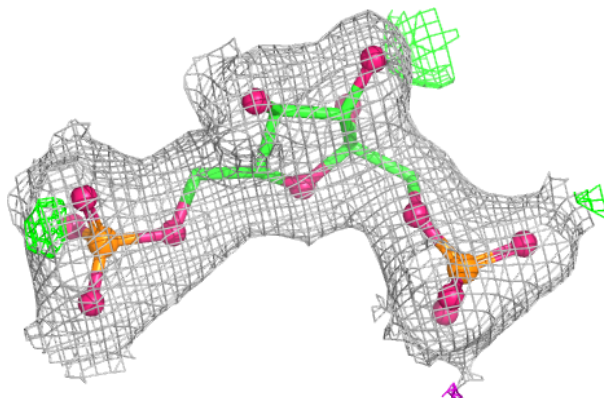


Electron density around I7N E 603:

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

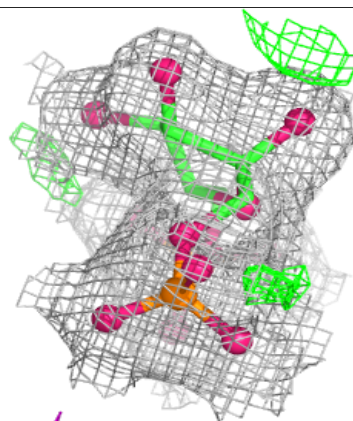
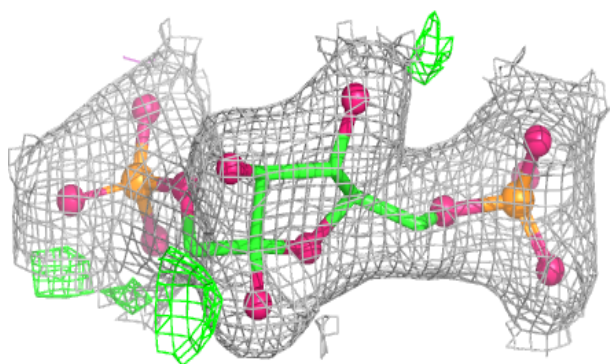
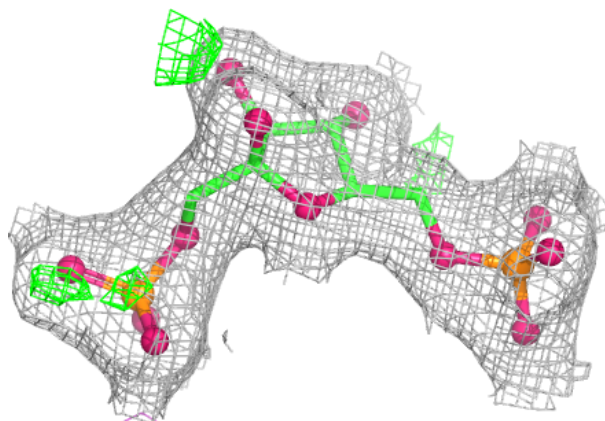
**Electron density around FBP B 601:**

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

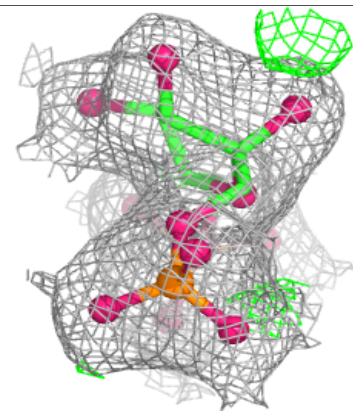
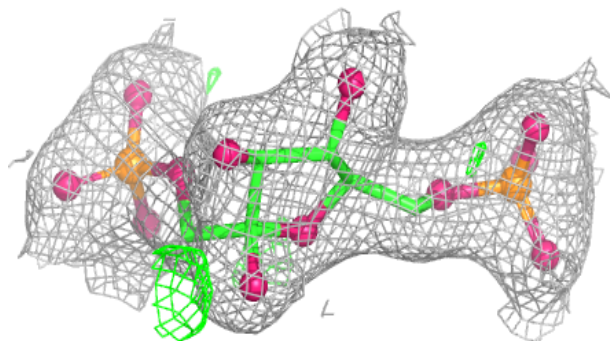
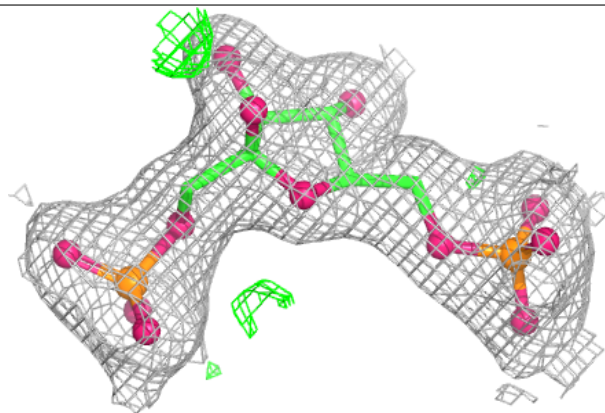


Electron density around FBP F 601:

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

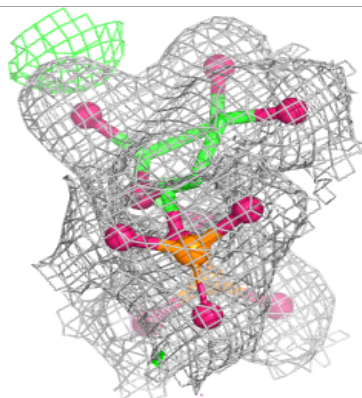
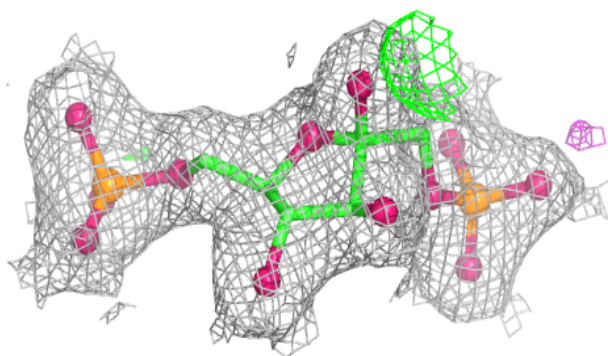
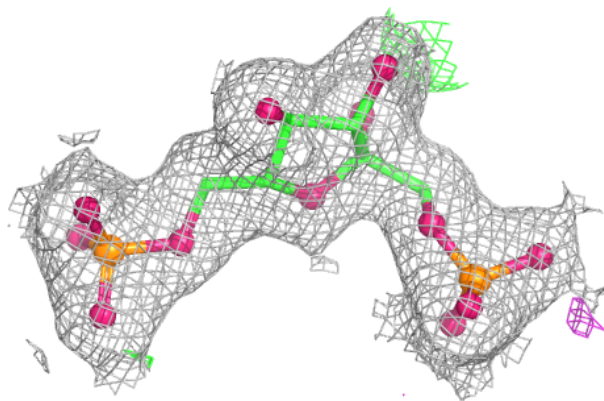
**Electron density around FBP A 601:**

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

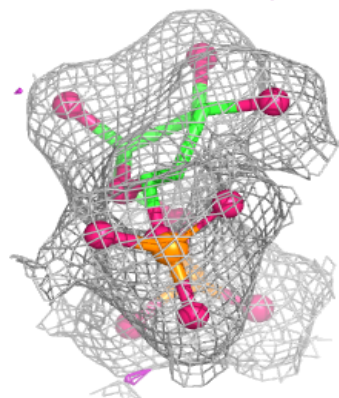
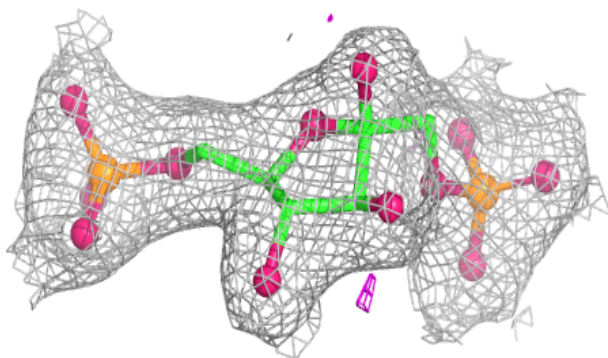
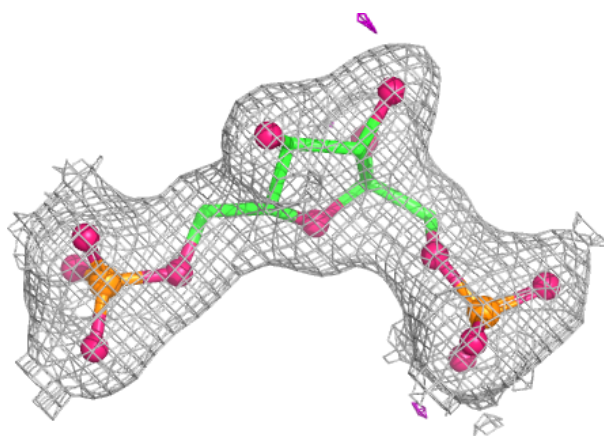


Electron density around FBP H 601:

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

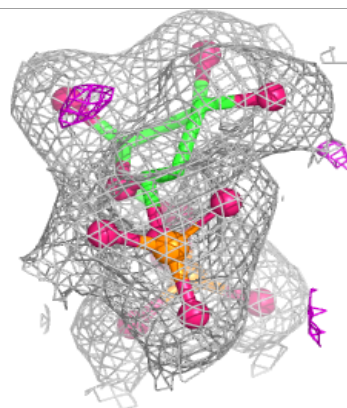
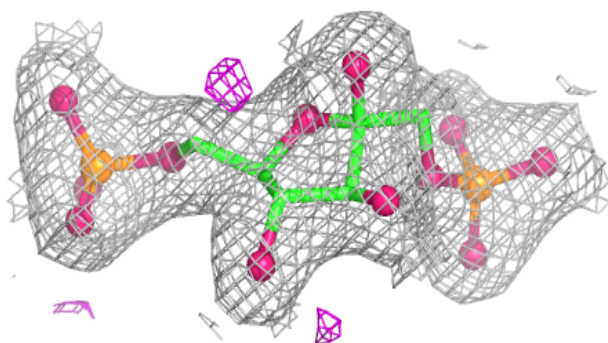
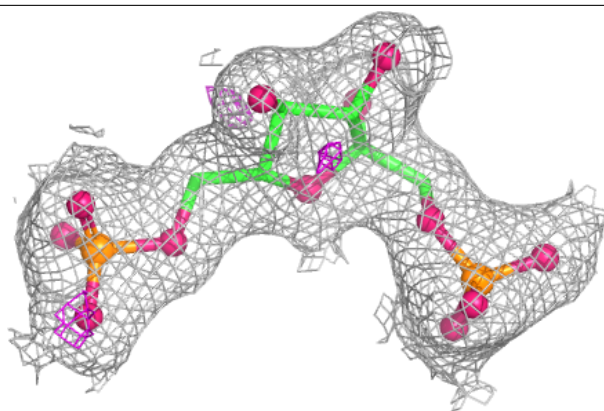
**Electron density around FBP E 601:**

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

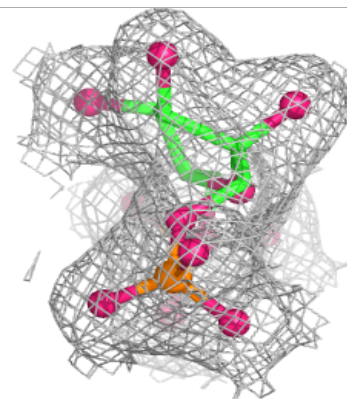
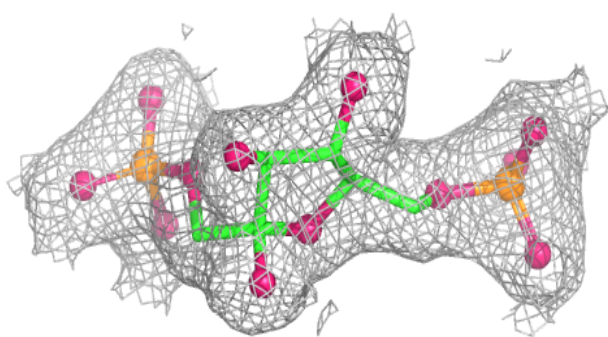
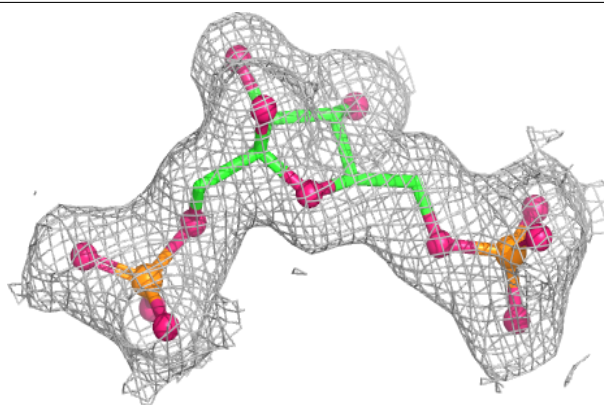


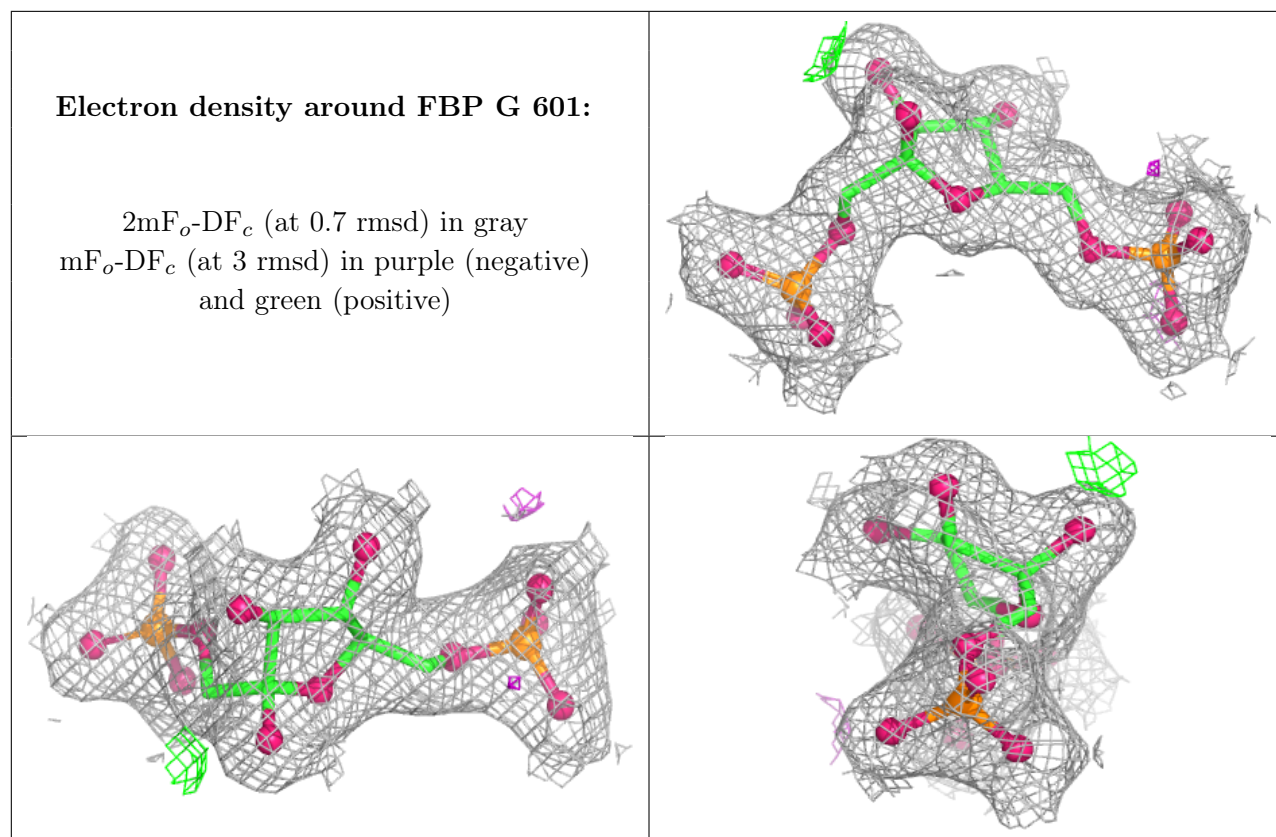
Electron density around FBP C 601:

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

**Electron density around FBP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.