



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:38 PM UTC

PDB ID : 8TBU / pdb_00008tbu
Title : Structure of human erythrocyte pyruvate kinase in complex with an allosteric activator Compound 12
Authors : Jin, L.; Padyana, A.
Deposited on : 2023-06-29
Resolution : 2.35 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

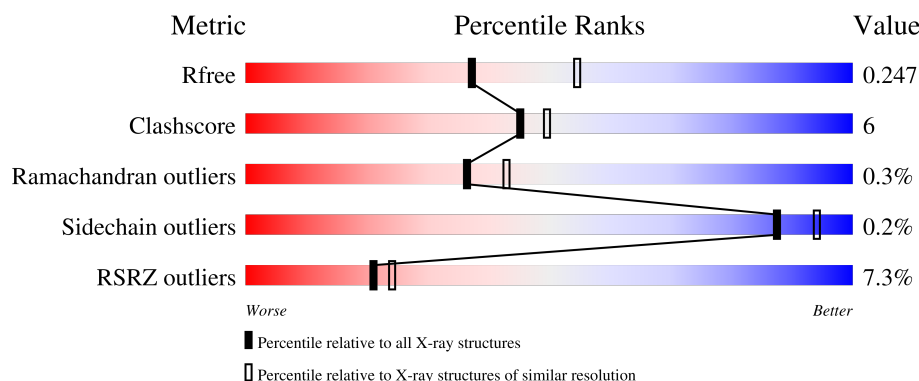
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	544	13% 78% 15% 6%
1	B	544	8% 75% 11% 14%
1	C	544	6% 73% 9% 18%
1	D	544	5% 85% 10% 5%
1	E	544	8% 63% 15% 21%

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Mol	Chain	Length	Quality of chain
1	F	544	 3% 85% 10% 5%
1	G	544	 5% 65% 13% 22%
1	H	544	 3% 84% 11% 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 30849 atoms, of which 0 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	509	Total	C	N	O	S	0	1	0
			3851	2420	696	717	18			
1	B	468	Total	C	N	O	S	0	0	0
			3546	2228	641	659	18			
1	C	446	Total	C	N	O	S	0	1	0
			3392	2133	611	630	18			
1	D	515	Total	C	N	O	S	0	0	0
			3895	2448	703	726	18			
1	E	429	Total	C	N	O	S	0	0	0
			3260	2048	592	602	18			
1	F	518	Total	C	N	O	S	0	0	0
			3912	2457	707	730	18			
1	G	426	Total	C	N	O	S	0	0	0
			3239	2035	586	600	18			
1	H	518	Total	C	N	O	S	0	0	0
			3912	2457	707	730	18			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	MET	-	initiating methionine	UNP P30613
A	32	GLY	-	expression tag	UNP P30613
A	33	SER	-	expression tag	UNP P30613
A	34	SER	-	expression tag	UNP P30613
A	35	HIS	-	expression tag	UNP P30613
A	36	HIS	-	expression tag	UNP P30613
A	37	HIS	-	expression tag	UNP P30613
A	38	HIS	-	expression tag	UNP P30613
A	39	HIS	-	expression tag	UNP P30613
A	40	HIS	-	expression tag	UNP P30613
A	41	SER	-	expression tag	UNP P30613
A	42	SER	-	expression tag	UNP P30613
A	43	GLY	-	expression tag	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
A	44	LEU	-	expression tag	UNP P30613
A	45	VAL	-	expression tag	UNP P30613
A	46	PRO	-	expression tag	UNP P30613
A	47	ARG	-	expression tag	UNP P30613
A	48	GLY	-	expression tag	UNP P30613
A	49	SER	-	expression tag	UNP P30613
B	31	MET	-	initiating methionine	UNP P30613
B	32	GLY	-	expression tag	UNP P30613
B	33	SER	-	expression tag	UNP P30613
B	34	SER	-	expression tag	UNP P30613
B	35	HIS	-	expression tag	UNP P30613
B	36	HIS	-	expression tag	UNP P30613
B	37	HIS	-	expression tag	UNP P30613
B	38	HIS	-	expression tag	UNP P30613
B	39	HIS	-	expression tag	UNP P30613
B	40	HIS	-	expression tag	UNP P30613
B	41	SER	-	expression tag	UNP P30613
B	42	SER	-	expression tag	UNP P30613
B	43	GLY	-	expression tag	UNP P30613
B	44	LEU	-	expression tag	UNP P30613
B	45	VAL	-	expression tag	UNP P30613
B	46	PRO	-	expression tag	UNP P30613
B	47	ARG	-	expression tag	UNP P30613
B	48	GLY	-	expression tag	UNP P30613
B	49	SER	-	expression tag	UNP P30613
C	31	MET	-	initiating methionine	UNP P30613
C	32	GLY	-	expression tag	UNP P30613
C	33	SER	-	expression tag	UNP P30613
C	34	SER	-	expression tag	UNP P30613
C	35	HIS	-	expression tag	UNP P30613
C	36	HIS	-	expression tag	UNP P30613
C	37	HIS	-	expression tag	UNP P30613
C	38	HIS	-	expression tag	UNP P30613
C	39	HIS	-	expression tag	UNP P30613
C	40	HIS	-	expression tag	UNP P30613
C	41	SER	-	expression tag	UNP P30613
C	42	SER	-	expression tag	UNP P30613
C	43	GLY	-	expression tag	UNP P30613
C	44	LEU	-	expression tag	UNP P30613
C	45	VAL	-	expression tag	UNP P30613
C	46	PRO	-	expression tag	UNP P30613
C	47	ARG	-	expression tag	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
C	48	GLY	-	expression tag	UNP P30613
C	49	SER	-	expression tag	UNP P30613
D	31	MET	-	initiating methionine	UNP P30613
D	32	GLY	-	expression tag	UNP P30613
D	33	SER	-	expression tag	UNP P30613
D	34	SER	-	expression tag	UNP P30613
D	35	HIS	-	expression tag	UNP P30613
D	36	HIS	-	expression tag	UNP P30613
D	37	HIS	-	expression tag	UNP P30613
D	38	HIS	-	expression tag	UNP P30613
D	39	HIS	-	expression tag	UNP P30613
D	40	HIS	-	expression tag	UNP P30613
D	41	SER	-	expression tag	UNP P30613
D	42	SER	-	expression tag	UNP P30613
D	43	GLY	-	expression tag	UNP P30613
D	44	LEU	-	expression tag	UNP P30613
D	45	VAL	-	expression tag	UNP P30613
D	46	PRO	-	expression tag	UNP P30613
D	47	ARG	-	expression tag	UNP P30613
D	48	GLY	-	expression tag	UNP P30613
D	49	SER	-	expression tag	UNP P30613
E	31	MET	-	initiating methionine	UNP P30613
E	32	GLY	-	expression tag	UNP P30613
E	33	SER	-	expression tag	UNP P30613
E	34	SER	-	expression tag	UNP P30613
E	35	HIS	-	expression tag	UNP P30613
E	36	HIS	-	expression tag	UNP P30613
E	37	HIS	-	expression tag	UNP P30613
E	38	HIS	-	expression tag	UNP P30613
E	39	HIS	-	expression tag	UNP P30613
E	40	HIS	-	expression tag	UNP P30613
E	41	SER	-	expression tag	UNP P30613
E	42	SER	-	expression tag	UNP P30613
E	43	GLY	-	expression tag	UNP P30613
E	44	LEU	-	expression tag	UNP P30613
E	45	VAL	-	expression tag	UNP P30613
E	46	PRO	-	expression tag	UNP P30613
E	47	ARG	-	expression tag	UNP P30613
E	48	GLY	-	expression tag	UNP P30613
E	49	SER	-	expression tag	UNP P30613
F	31	MET	-	initiating methionine	UNP P30613
F	32	GLY	-	expression tag	UNP P30613

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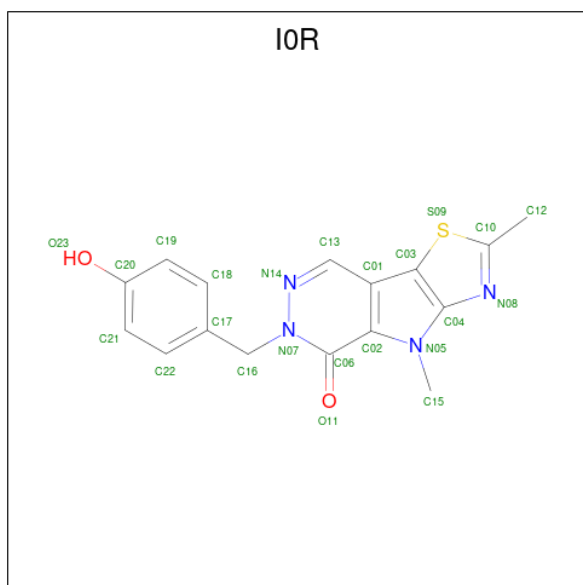
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F	34	SER	-	expression tag	UNP P30613
F	35	HIS	-	expression tag	UNP P30613
F	36	HIS	-	expression tag	UNP P30613
F	37	HIS	-	expression tag	UNP P30613
F	38	HIS	-	expression tag	UNP P30613
F	39	HIS	-	expression tag	UNP P30613
F	40	HIS	-	expression tag	UNP P30613
F	41	SER	-	expression tag	UNP P30613
F	42	SER	-	expression tag	UNP P30613
F	43	GLY	-	expression tag	UNP P30613
F	44	LEU	-	expression tag	UNP P30613
F	45	VAL	-	expression tag	UNP P30613
F	46	PRO	-	expression tag	UNP P30613
F	47	ARG	-	expression tag	UNP P30613
F	48	GLY	-	expression tag	UNP P30613
F	49	SER	-	expression tag	UNP P30613
G	31	MET	-	initiating methionine	UNP P30613
G	32	GLY	-	expression tag	UNP P30613
G	33	SER	-	expression tag	UNP P30613
G	34	SER	-	expression tag	UNP P30613
G	35	HIS	-	expression tag	UNP P30613
G	36	HIS	-	expression tag	UNP P30613
G	37	HIS	-	expression tag	UNP P30613
G	38	HIS	-	expression tag	UNP P30613
G	39	HIS	-	expression tag	UNP P30613
G	40	HIS	-	expression tag	UNP P30613
G	41	SER	-	expression tag	UNP P30613
G	42	SER	-	expression tag	UNP P30613
G	43	GLY	-	expression tag	UNP P30613
G	44	LEU	-	expression tag	UNP P30613
G	45	VAL	-	expression tag	UNP P30613
G	46	PRO	-	expression tag	UNP P30613
G	47	ARG	-	expression tag	UNP P30613
G	48	GLY	-	expression tag	UNP P30613
G	49	SER	-	expression tag	UNP P30613
H	31	MET	-	initiating methionine	UNP P30613
H	32	GLY	-	expression tag	UNP P30613
H	33	SER	-	expression tag	UNP P30613
H	34	SER	-	expression tag	UNP P30613
H	35	HIS	-	expression tag	UNP P30613
H	36	HIS	-	expression tag	UNP P30613

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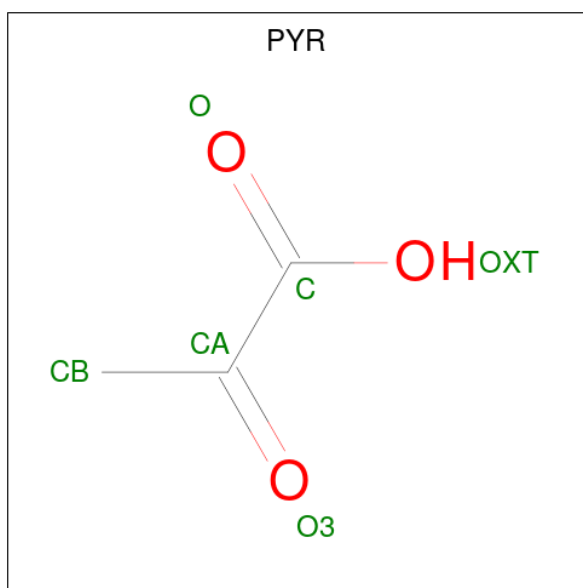
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H	37	HIS	-	expression tag	UNP P30613
H	38	HIS	-	expression tag	UNP P30613
H	39	HIS	-	expression tag	UNP P30613
H	40	HIS	-	expression tag	UNP P30613
H	41	SER	-	expression tag	UNP P30613
H	42	SER	-	expression tag	UNP P30613
H	43	GLY	-	expression tag	UNP P30613
H	44	LEU	-	expression tag	UNP P30613
H	45	VAL	-	expression tag	UNP P30613
H	46	PRO	-	expression tag	UNP P30613
H	47	ARG	-	expression tag	UNP P30613
H	48	GLY	-	expression tag	UNP P30613
H	49	SER	-	expression tag	UNP P30613

- Molecule 2 is 6-[(4-hydroxyphenyl)methyl]-2,4-dimethyl-4,6-dihydro-5H-[1,3]thiazolo[5',4':4,5]pyrrolo[2,3-d]pyridazin-5-one (CCD ID: I0R) (formula: C₁₆H₁₄N₄O₂S) (labeled as "Ligand of Interest" by depositor).



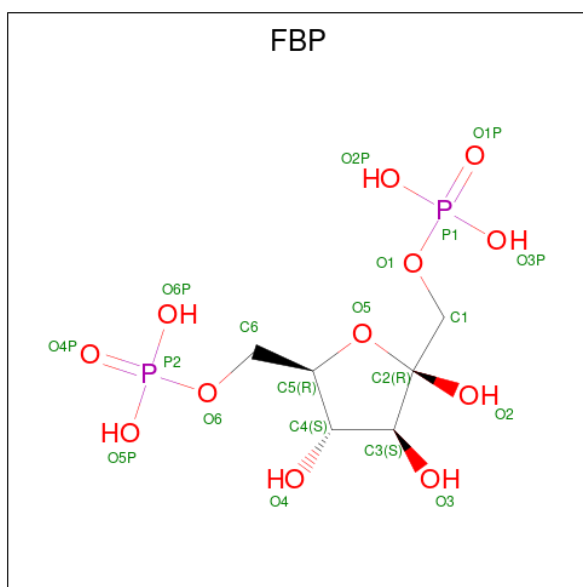
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			23	16	4	2	1		
2	D	1	Total	C	N	O	S	0	0
			23	16	4	2	1		
2	F	1	Total	C	N	O	S	0	0
			23	16	4	2	1		
2	H	1	Total	C	N	O	S	0	0
			23	16	4	2	1		

- Molecule 3 is PYRUVIC ACID (CCD ID: PYR) (formula: $C_3H_4O_3$).



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

- Molecule 4 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
4	A	1	Total	C	O	P	0	0
			20	6	12	2		
4	B	1	Total	C	O	P	0	0
			20	6	12	2		
4	C	1	Total	C	O	P	0	0
			20	6	12	2		
4	D	1	Total	C	O	P	0	0
			20	6	12	2		
4	E	1	Total	C	O	P	0	0
			20	6	12	2		
4	F	1	Total	C	O	P	0	0
			20	6	12	2		
4	G	1	Total	C	O	P	0	0
			20	6	12	2		
4	H	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mn	0	0
			1	1		
5	B	1	Total	Mn	0	0
			1	1		
5	C	1	Total	Mn	0	0
			1	1		
5	D	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	1	Total 1	Mn 1	0	0
5	F	1	Total 1	Mn 1	0	0
5	G	1	Total 1	Mn 1	0	0
5	H	1	Total 1	Mn 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	K 1	0	0
6	D	1	Total 1	K 1	0	0

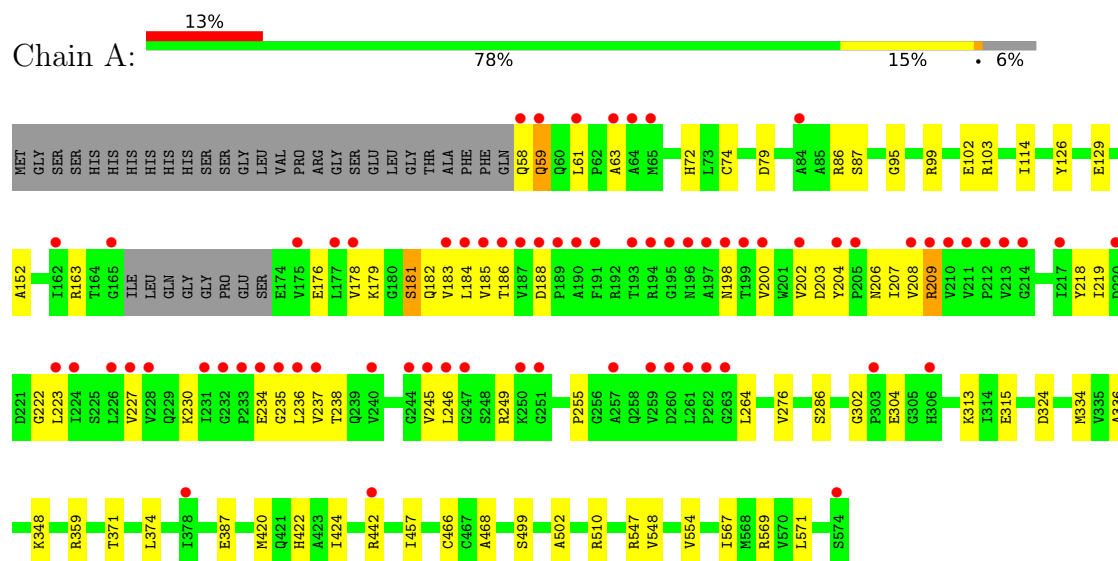
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	208	Total 208	O 208	0	0
7	B	191	Total 191	O 191	0	0
7	C	189	Total 189	O 189	0	0
7	D	252	Total 252	O 252	0	0
7	E	93	Total 93	O 93	0	0
7	F	244	Total 244	O 244	0	0
7	G	109	Total 109	O 109	0	0
7	H	258	Total 258	O 258	0	0

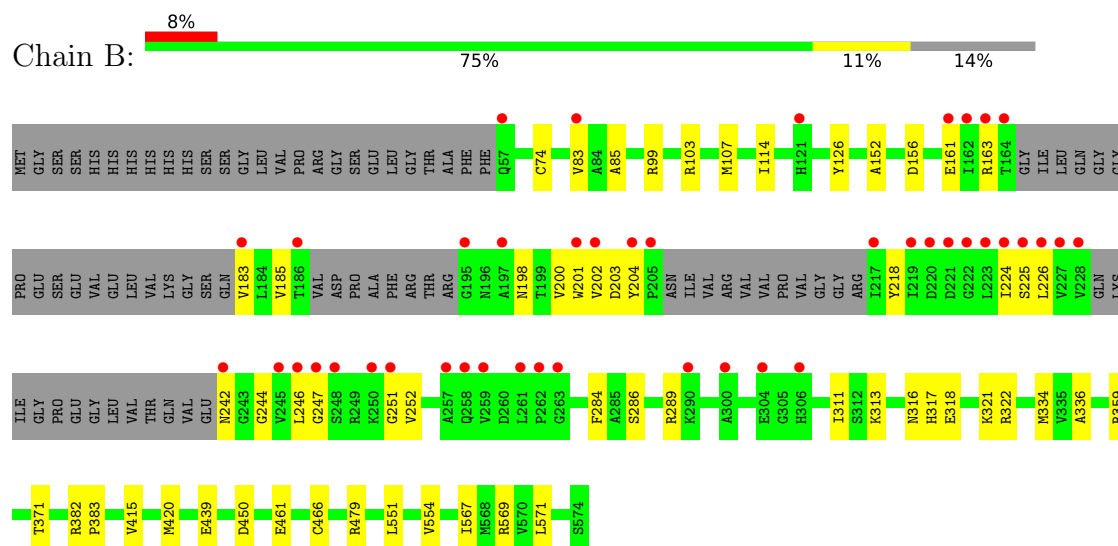
3 Residue-property plots

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

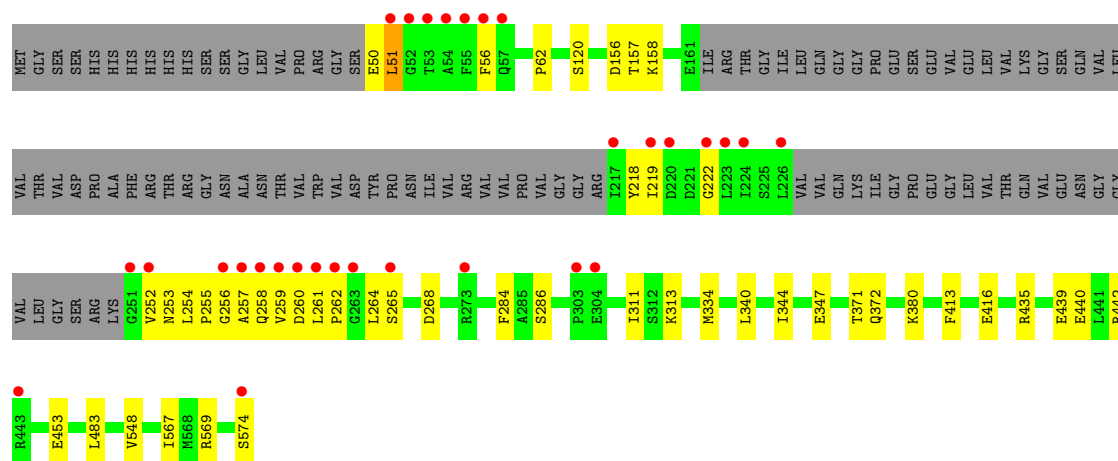


• Molecule 1: Pyruvate kinase PKLR

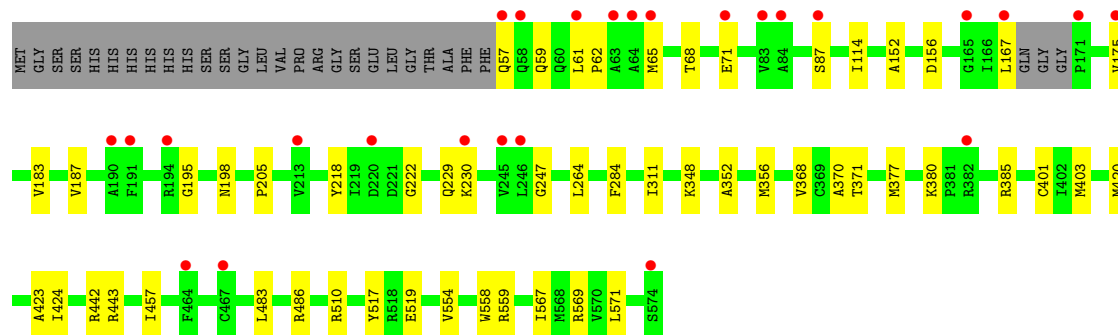
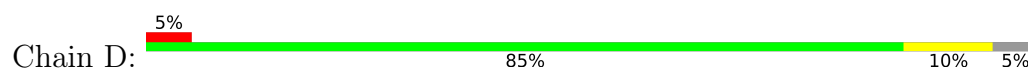


• Molecule 1: Pyruvate kinase PKLR

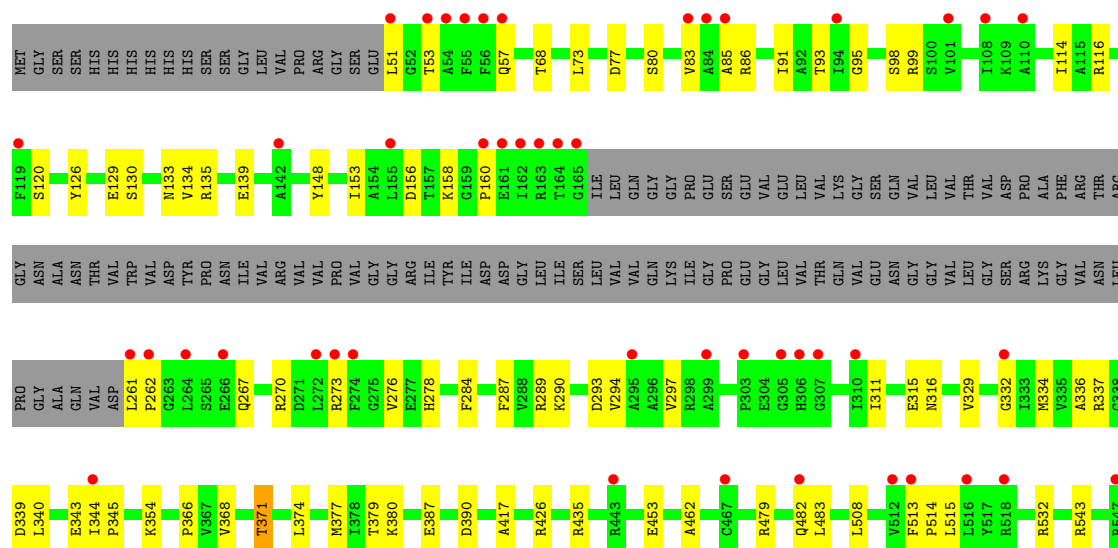




• Molecule 1: Pyruvate kinase PKLR

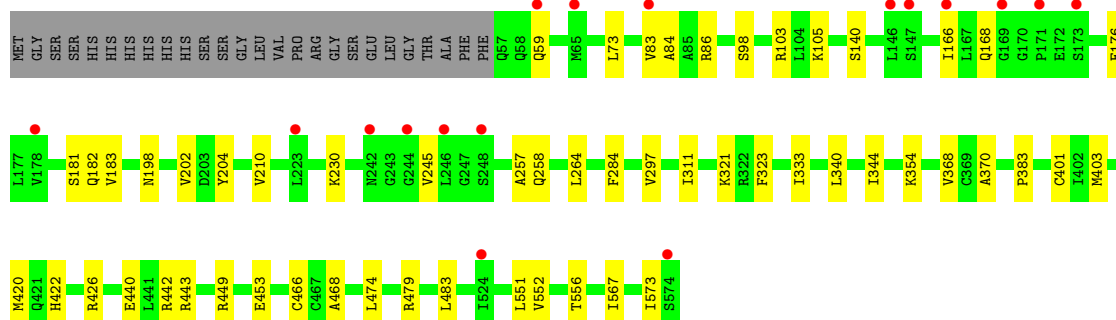
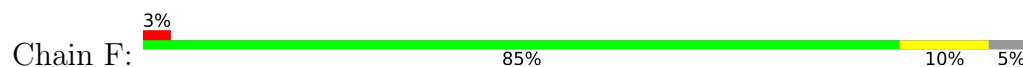


• Molecule 1: Pyruvate kinase PKLR

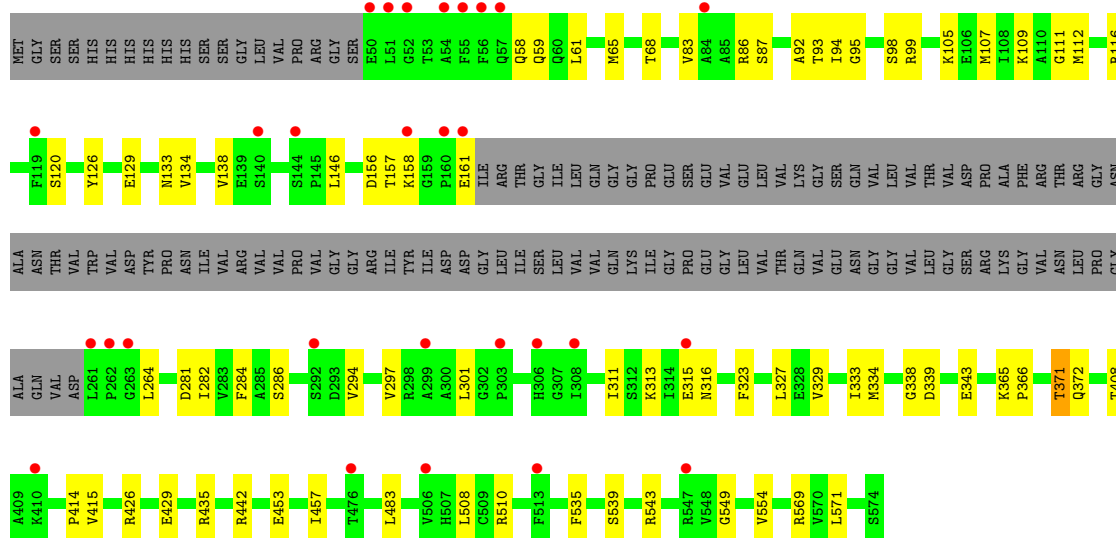




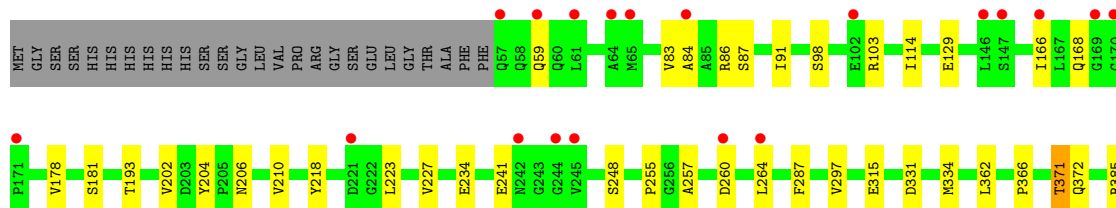
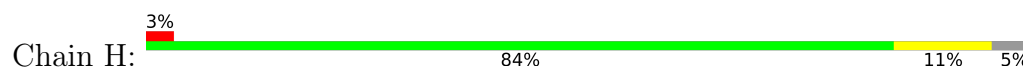
• Molecule 1: Pyruvate kinase PKLR



• Molecule 1: Pyruvate kinase PKLR



• Molecule 1: Pyruvate kinase PKLR





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.32Å 122.84Å 378.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.88 – 2.35 49.88 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.88-2.35) 99.6 (49.88-2.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.08 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.202 , 0.246 0.203 , 0.247	Depositor DCC
R_{free} test set	10680 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	30849	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 67.46 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1305e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, K, FBP, PYR, IOR

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	0.19	0/3916	0.42	0/5308
1	B	0.14	0/3601	0.35	0/4875
1	C	0.12	0/3450	0.34	0/4668
1	D	0.12	0/3958	0.34	0/5365
1	E	0.13	0/3314	0.35	0/4483
1	F	0.13	0/3976	0.35	0/5391
1	G	0.12	0/3293	0.35	0/4455
1	H	0.12	0/3976	0.35	0/5391
All	All	0.14	0/29484	0.36	0/39936

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3851	0	3928	64	0
1	B	3546	0	3606	39	0
1	C	3392	0	3445	35	0
1	D	3895	0	3972	38	0
1	E	3260	0	3316	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3912	0	3986	38	0
1	G	3239	0	3288	56	0
1	H	3912	0	3986	46	0
2	A	23	0	0	0	0
2	D	23	0	0	0	0
2	F	23	0	0	0	0
2	H	23	0	0	0	0
3	A	6	0	0	0	0
3	B	6	0	0	1	0
3	C	6	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0
3	G	6	0	0	2	0
4	A	20	0	10	0	0
4	B	20	0	10	0	0
4	C	20	0	10	0	0
4	D	20	0	10	0	0
4	E	20	0	10	1	0
4	F	20	0	10	0	0
4	G	20	0	10	0	0
4	H	20	0	10	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	D	1	0	0	0	0
7	A	208	0	0	4	0
7	B	191	0	0	1	0
7	C	189	0	0	1	0
7	D	252	0	0	4	0
7	E	93	0	0	1	0
7	F	244	0	0	3	0
7	G	109	0	0	0	0
7	H	258	0	0	6	0
All	All	30849	0	29607	347	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 347 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:229:GLN:O	1:D:230:LYS:HD2	1.69	0.93
1:A:182:GLN:O	1:A:198:ASN:ND2	2.01	0.92
1:A:230:LYS:HD3	1:A:237:VAL:HG21	1.55	0.86
1:C:380:LYS:NZ	7:C:701:HOH:O	2.07	0.86
1:A:185:VAL:HG12	1:A:200:VAL:HB	1.60	0.84

There are no symmetry-related clashes.

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	506/544 (93%)	491 (97%)	12 (2%)	3 (1%)	21	24
1	B	458/544 (84%)	446 (97%)	10 (2%)	2 (0%)	30	34
1	C	441/544 (81%)	428 (97%)	10 (2%)	3 (1%)	18	20
1	D	511/544 (94%)	498 (98%)	12 (2%)	1 (0%)	43	52
1	E	425/544 (78%)	414 (97%)	10 (2%)	1 (0%)	43	52
1	F	516/544 (95%)	504 (98%)	12 (2%)	0	100	100
1	G	422/544 (78%)	410 (97%)	11 (3%)	1 (0%)	43	52
1	H	516/544 (95%)	509 (99%)	5 (1%)	2 (0%)	30	34
All	All	3795/4352 (87%)	3700 (98%)	82 (2%)	13 (0%)	36	43

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	257	ALA
1	E	371	THR
1	A	181	SER

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Mol	Chain	Res	Type
1	A	59	GLN
1	G	371	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	408/436 (94%)	405 (99%)	3 (1%)	76	86
1	B	374/436 (86%)	374 (100%)	0	100	100
1	C	356/436 (82%)	356 (100%)	0	100	100
1	D	413/436 (95%)	412 (100%)	1 (0%)	87	94
1	E	341/436 (78%)	341 (100%)	0	100	100
1	F	414/436 (95%)	413 (100%)	1 (0%)	87	94
1	G	339/436 (78%)	339 (100%)	0	100	100
1	H	414/436 (95%)	414 (100%)	0	100	100
All	All	3059/3488 (88%)	3054 (100%)	5 (0%)	87	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	209	ARG
1	A	547	ARG
1	A	548	VAL
1	D	264	LEU
1	F	166	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	501	GLN
1	E	278	HIS
1	H	239	GLN

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Mol	Chain	Res	Type
1	E	353	GLN
1	G	372	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 10 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PYR	B	601	5	5,5,5	3.05	3 (60%)	3,6,6	1.63	1 (33%)
4	FBP	F	603	-	18,20,20	0.91	1 (5%)	21,32,32	0.71	0
4	FBP	H	602	-	18,20,20	0.92	1 (5%)	21,32,32	0.68	0
4	FBP	D	602	-	18,20,20	0.99	1 (5%)	21,32,32	0.59	0
3	PYR	C	601	5	5,5,5	3.02	3 (60%)	3,6,6	1.74	1 (33%)
4	FBP	B	602	-	18,20,20	0.92	1 (5%)	21,32,32	0.70	0
3	PYR	A	602	-	5,5,5	3.05	3 (60%)	3,6,6	1.66	1 (33%)
2	I0R	A	601	-	26,26,26	2.95	10 (38%)	28,39,39	3.17	9 (32%)
3	PYR	F	602	5	5,5,5	3.05	3 (60%)	3,6,6	1.65	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FBP	C	602	-	18,20,20	0.93	1 (5%)	21,32,32	0.70	0
4	FBP	E	602	-	18,20,20	0.90	1 (5%)	21,32,32	0.75	0
3	PYR	G	601	5	5,5,5	3.05	3 (60%)	3,6,6	1.71	1 (33%)
2	I0R	F	601	-	26,26,26	2.97	10 (38%)	28,39,39	3.17	9 (32%)
2	I0R	D	601	-	26,26,26	2.92	10 (38%)	28,39,39	3.10	9 (32%)
3	PYR	E	601	5	5,5,5	3.06	3 (60%)	3,6,6	1.67	1 (33%)
4	FBP	G	602	-	18,20,20	0.93	1 (5%)	21,32,32	0.70	0
4	FBP	A	603	-	18,20,20	0.90	1 (5%)	21,32,32	0.68	0
2	I0R	H	601	-	26,26,26	3.01	10 (38%)	28,39,39	3.28	10 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PYR	B	601	5	-	0/4/4/4	-
4	FBP	F	603	-	-	2/13/32/32	0/1/1/1
4	FBP	H	602	-	-	2/13/32/32	0/1/1/1
4	FBP	D	602	-	-	8/13/32/32	0/1/1/1
3	PYR	C	601	5	-	0/4/4/4	-
4	FBP	B	602	-	-	2/13/32/32	0/1/1/1
3	PYR	A	602	-	-	0/4/4/4	-
2	I0R	A	601	-	-	0/4/4/4	0/4/4/4
3	PYR	F	602	5	-	0/4/4/4	-
4	FBP	C	602	-	-	2/13/32/32	0/1/1/1
4	FBP	E	602	-	-	3/13/32/32	0/1/1/1
3	PYR	G	601	5	-	0/4/4/4	-
2	I0R	F	601	-	-	0/4/4/4	0/4/4/4
2	I0R	D	601	-	-	0/4/4/4	0/4/4/4
3	PYR	E	601	5	-	0/4/4/4	-
4	FBP	G	602	-	-	8/13/32/32	0/1/1/1
4	FBP	A	603	-	-	6/13/32/32	0/1/1/1
2	I0R	H	601	-	-	0/4/4/4	0/4/4/4

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	601	IOR	C13-N14	8.57	1.40	1.29
2	F	601	IOR	C13-N14	8.48	1.39	1.29
2	A	601	IOR	C13-N14	8.38	1.39	1.29
2	D	601	IOR	C13-N14	8.31	1.39	1.29
2	H	601	IOR	C16-C17	-6.61	1.39	1.51

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	601	IOR	C10-S09-C03	11.20	95.49	89.55
2	A	601	IOR	C10-S09-C03	10.64	95.19	89.55
2	F	601	IOR	C10-S09-C03	10.52	95.13	89.55
2	D	601	IOR	C10-S09-C03	10.13	94.92	89.55
2	A	601	IOR	S09-C10-N08	-7.54	109.44	114.64

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	FBP	C1-O1-P1-O2P
4	A	603	FBP	C1-O1-P1-O3P
4	D	602	FBP	C1-O1-P1-O2P
4	D	602	FBP	C1-O1-P1-O3P
4	D	602	FBP	O1-C1-C2-O2

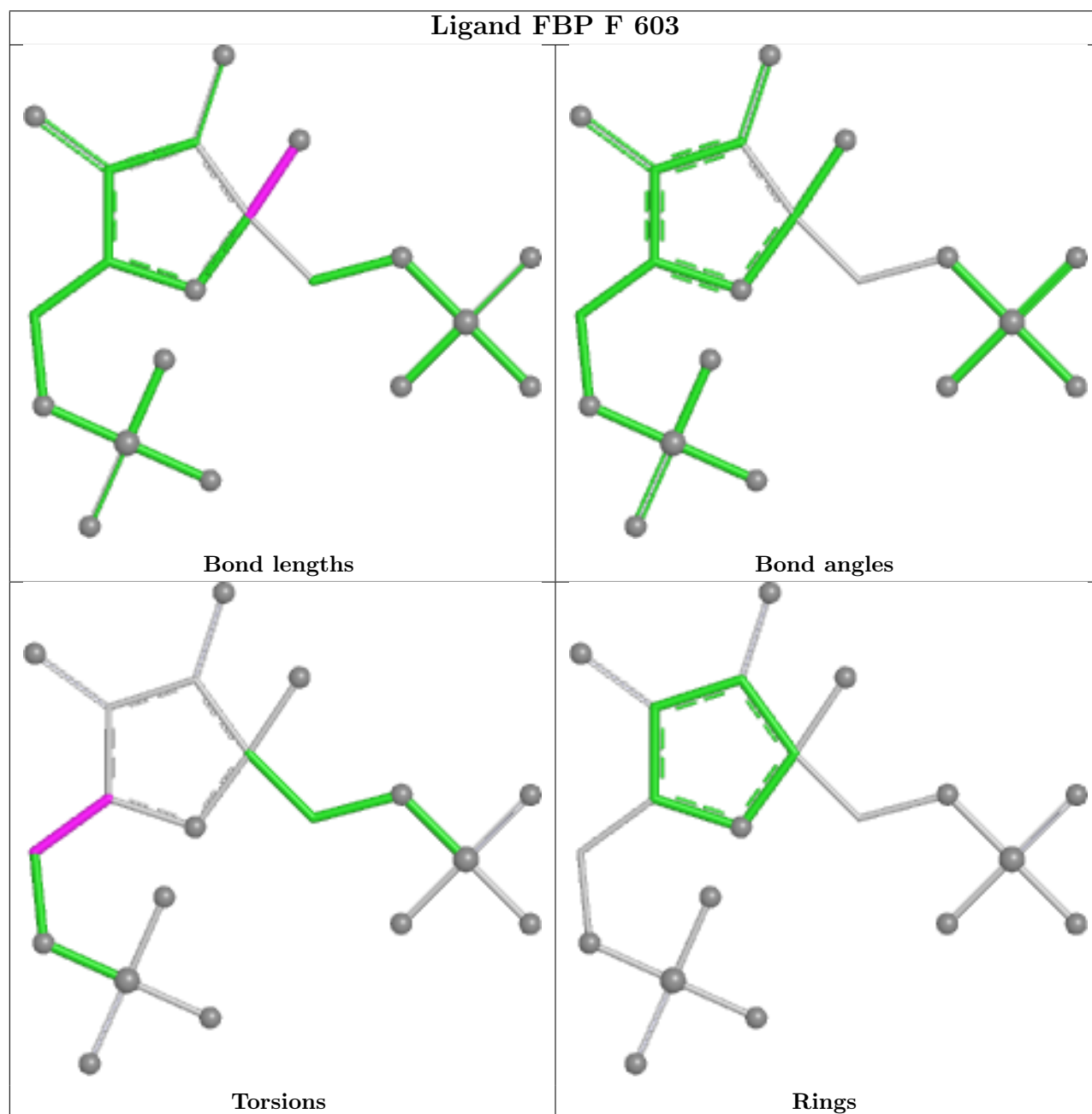
There are no ring outliers.

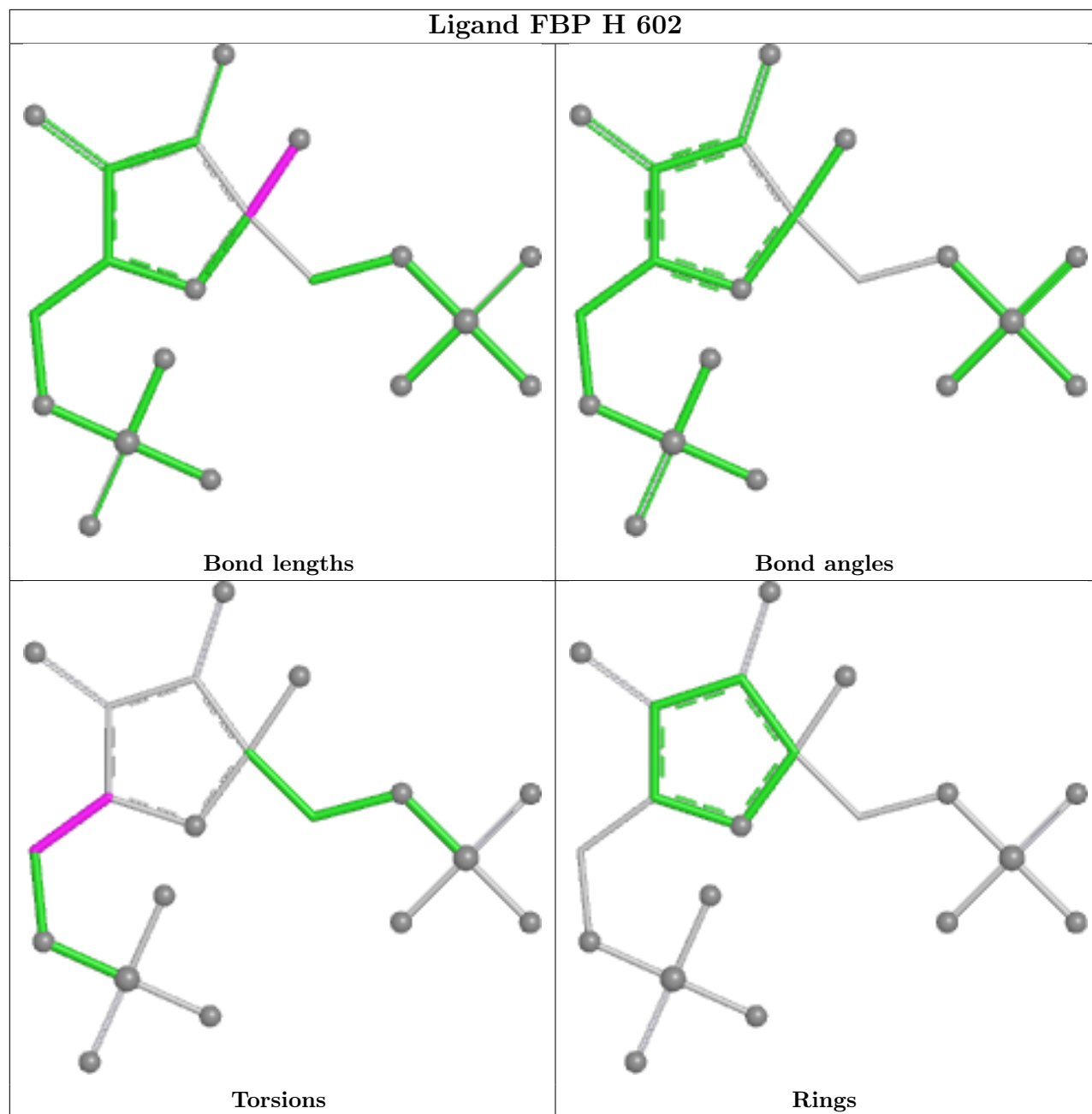
3 monomers are involved in 4 short contacts:

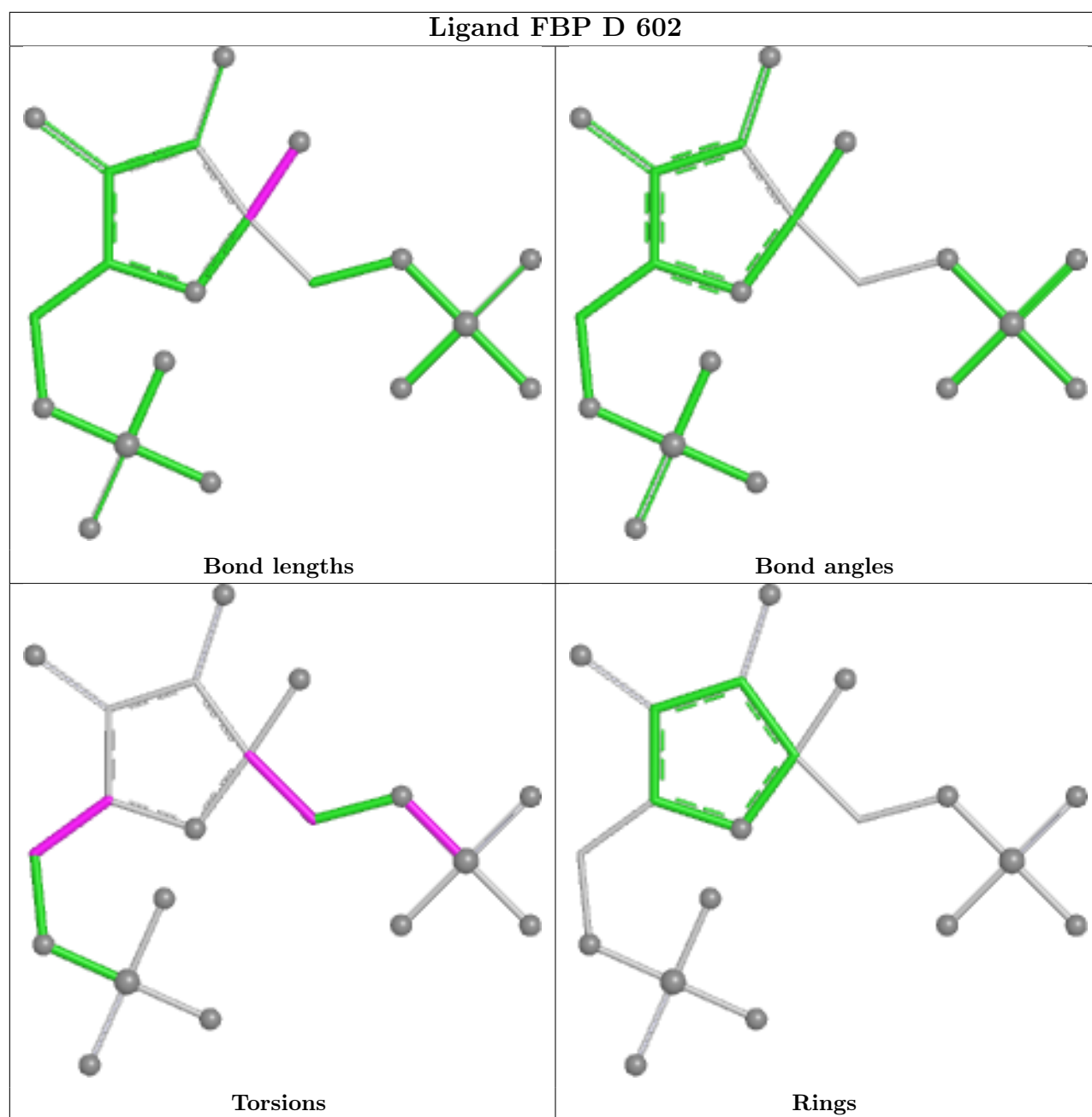
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	PYR	1	0
4	E	602	FBP	1	0
3	G	601	PYR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

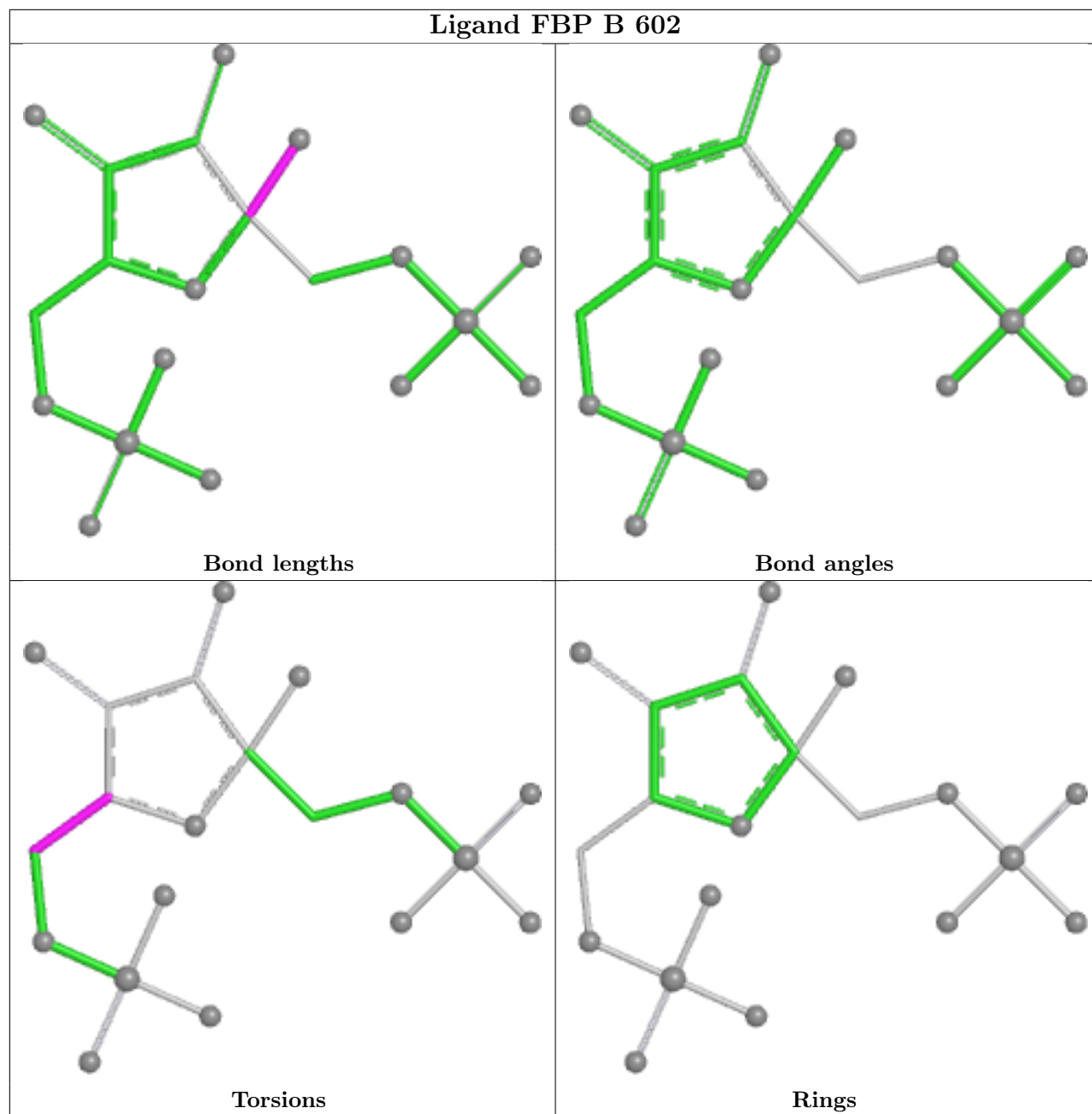
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

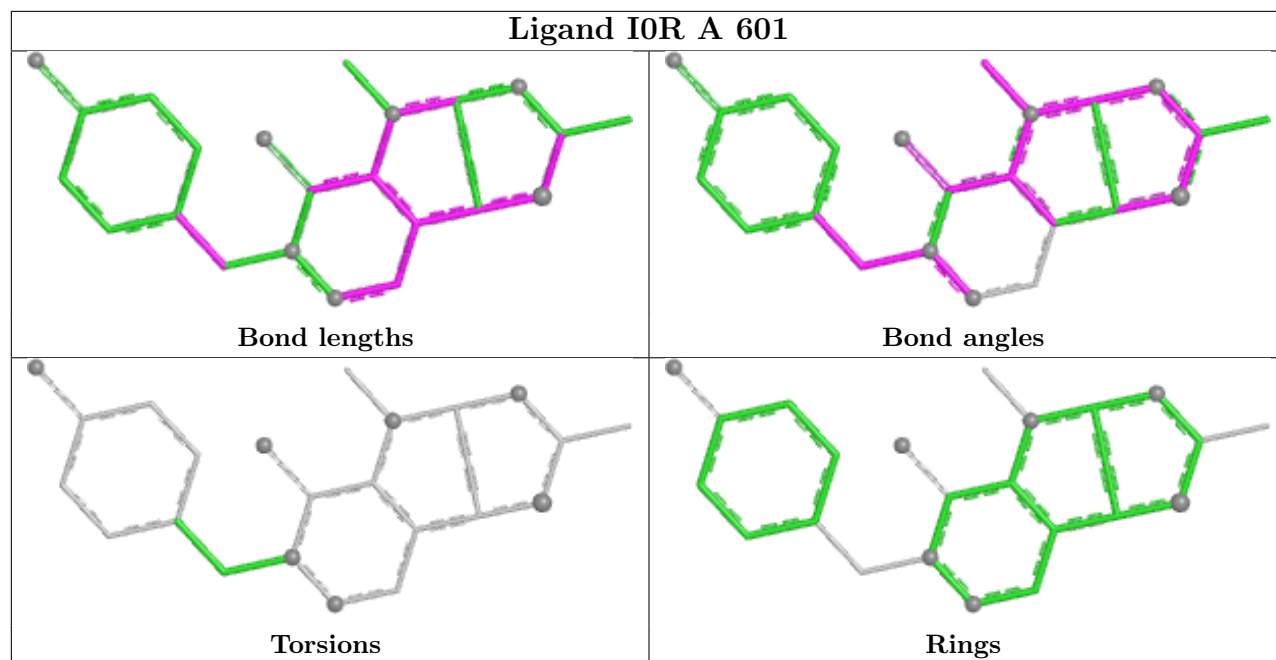




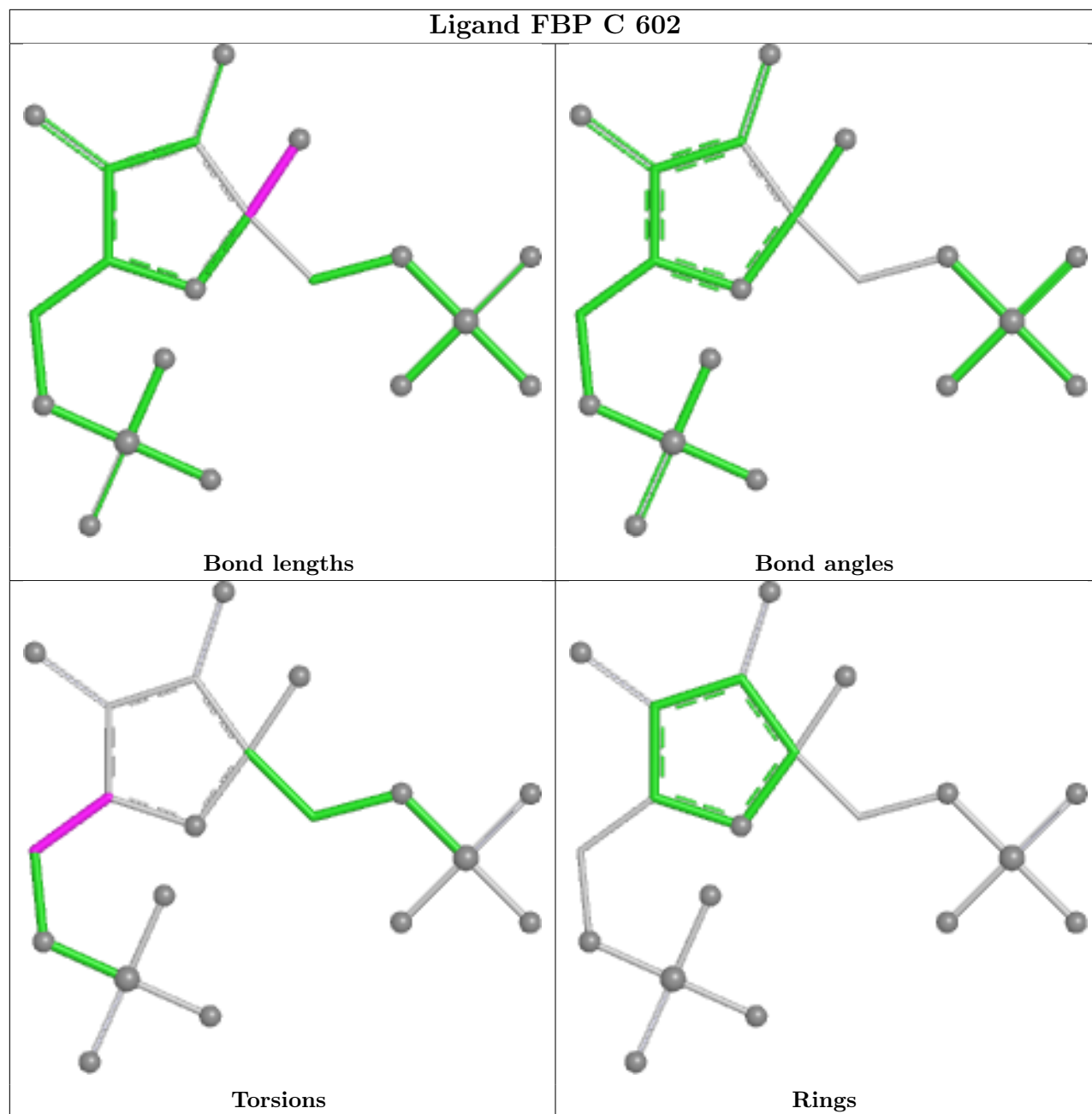


Ligand FBP B 602

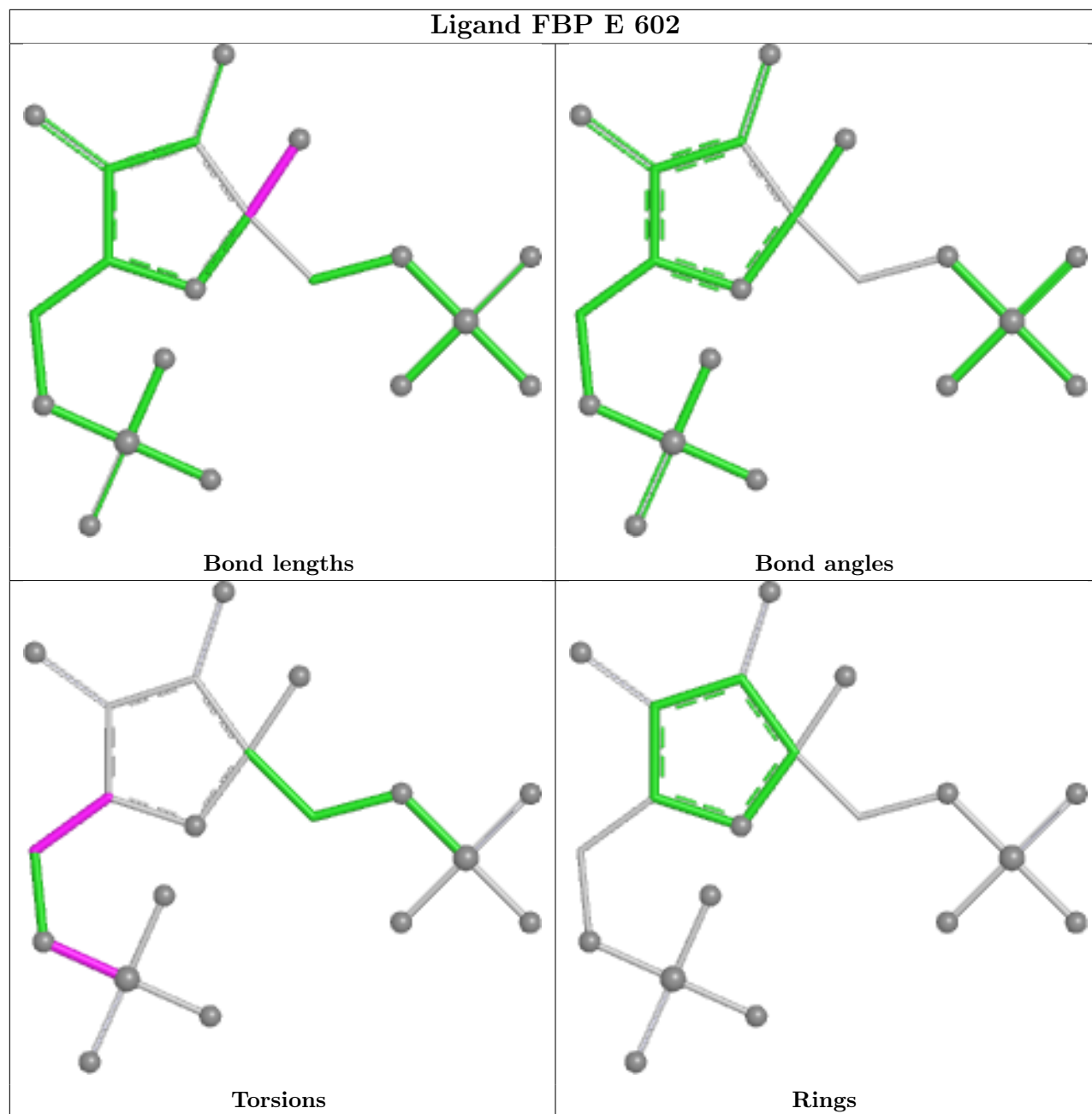




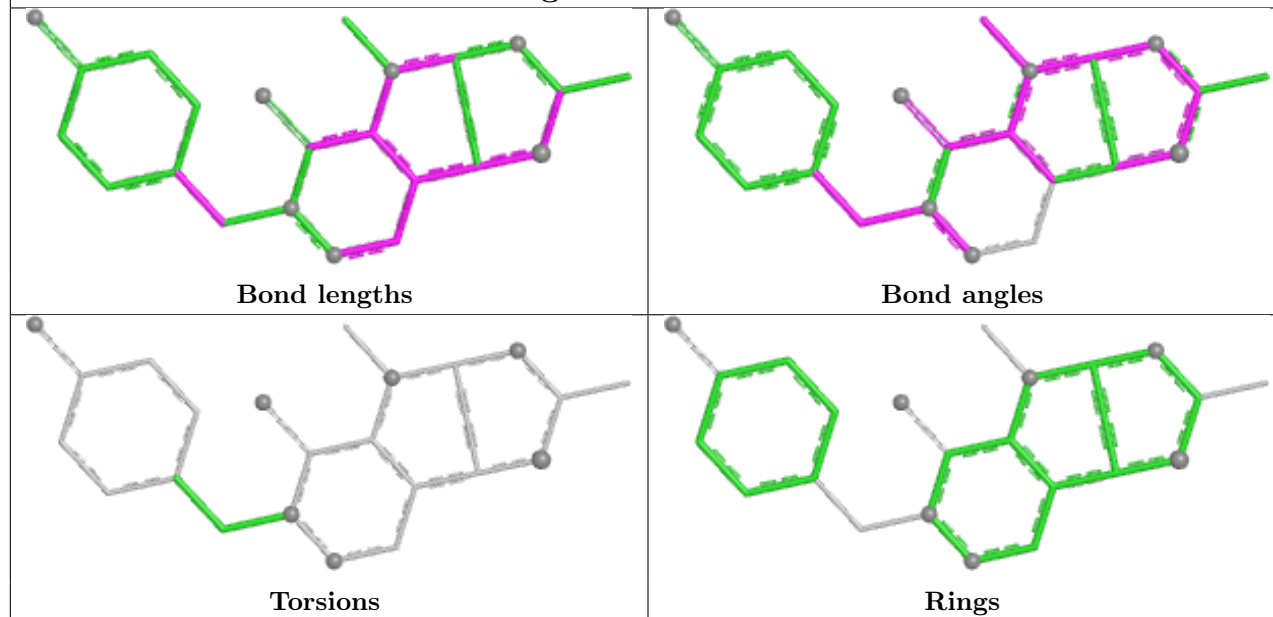
Ligand FBP C 602



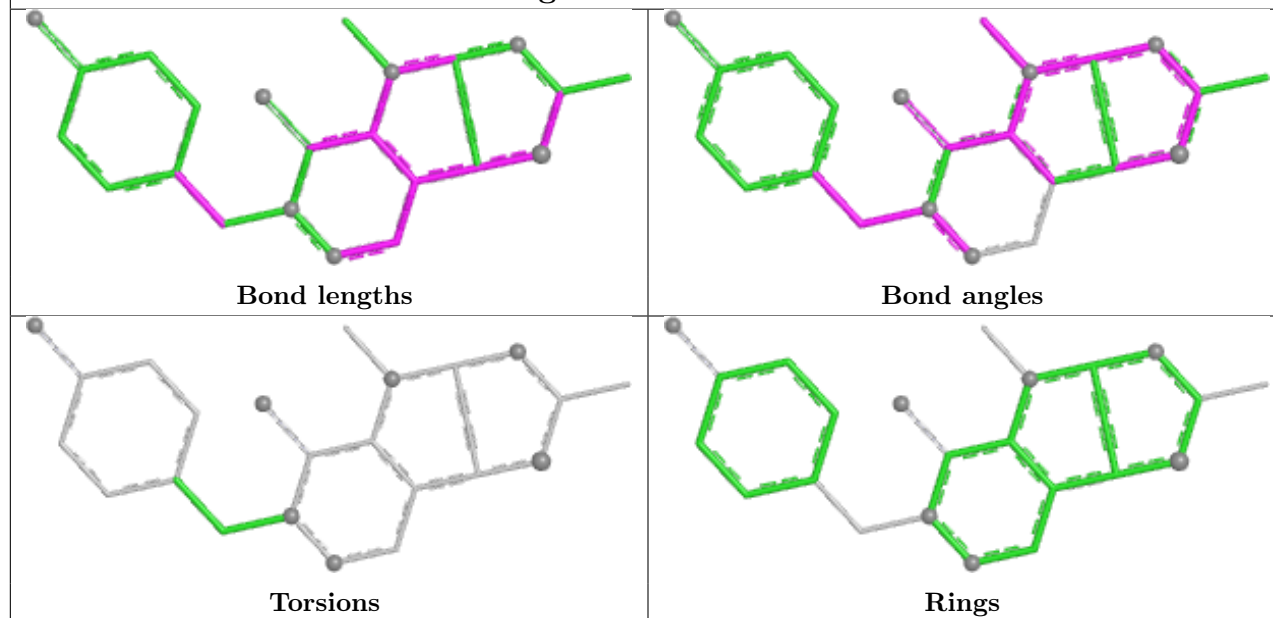
Ligand FBP E 602

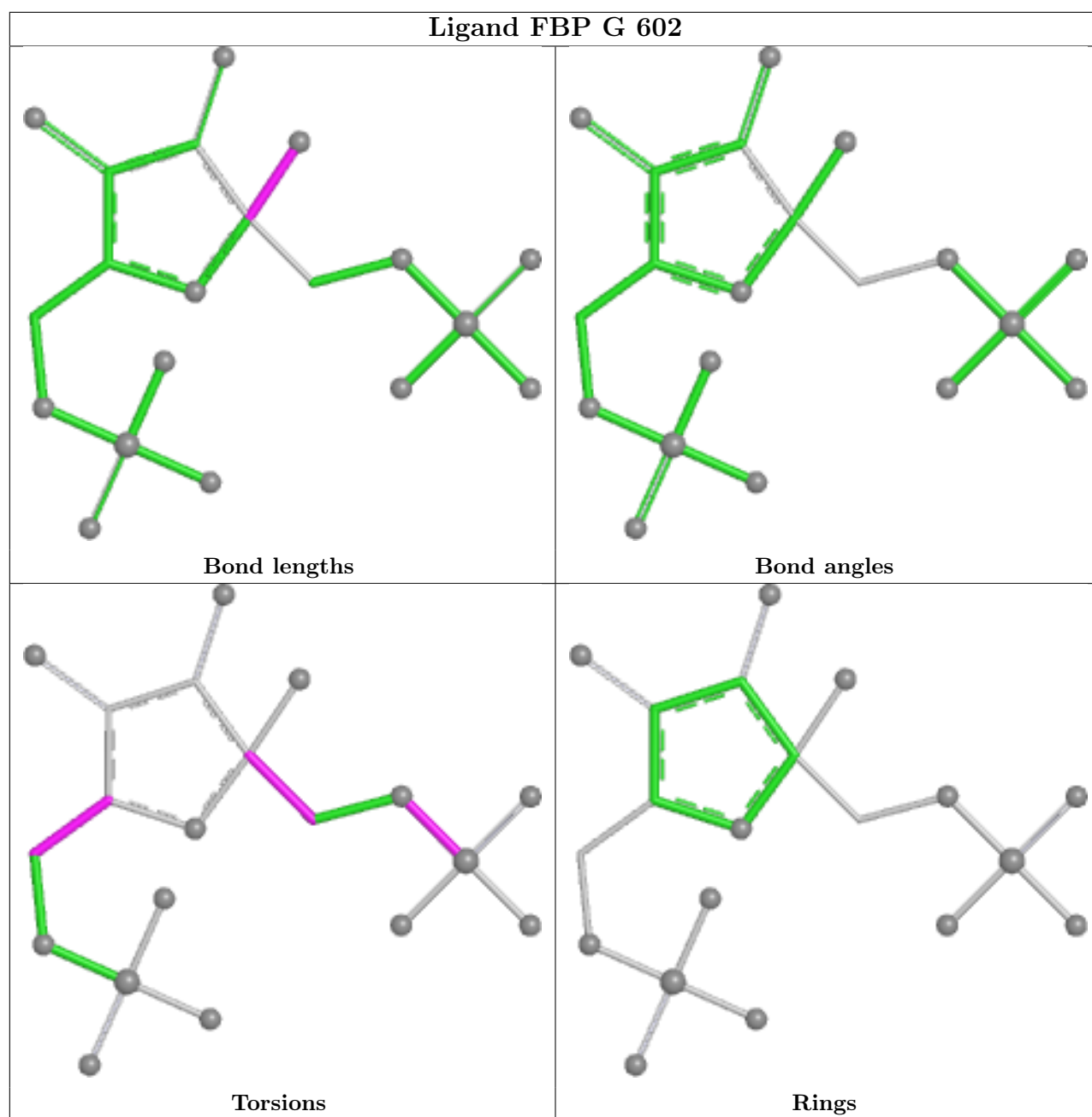


Ligand I0R F 601

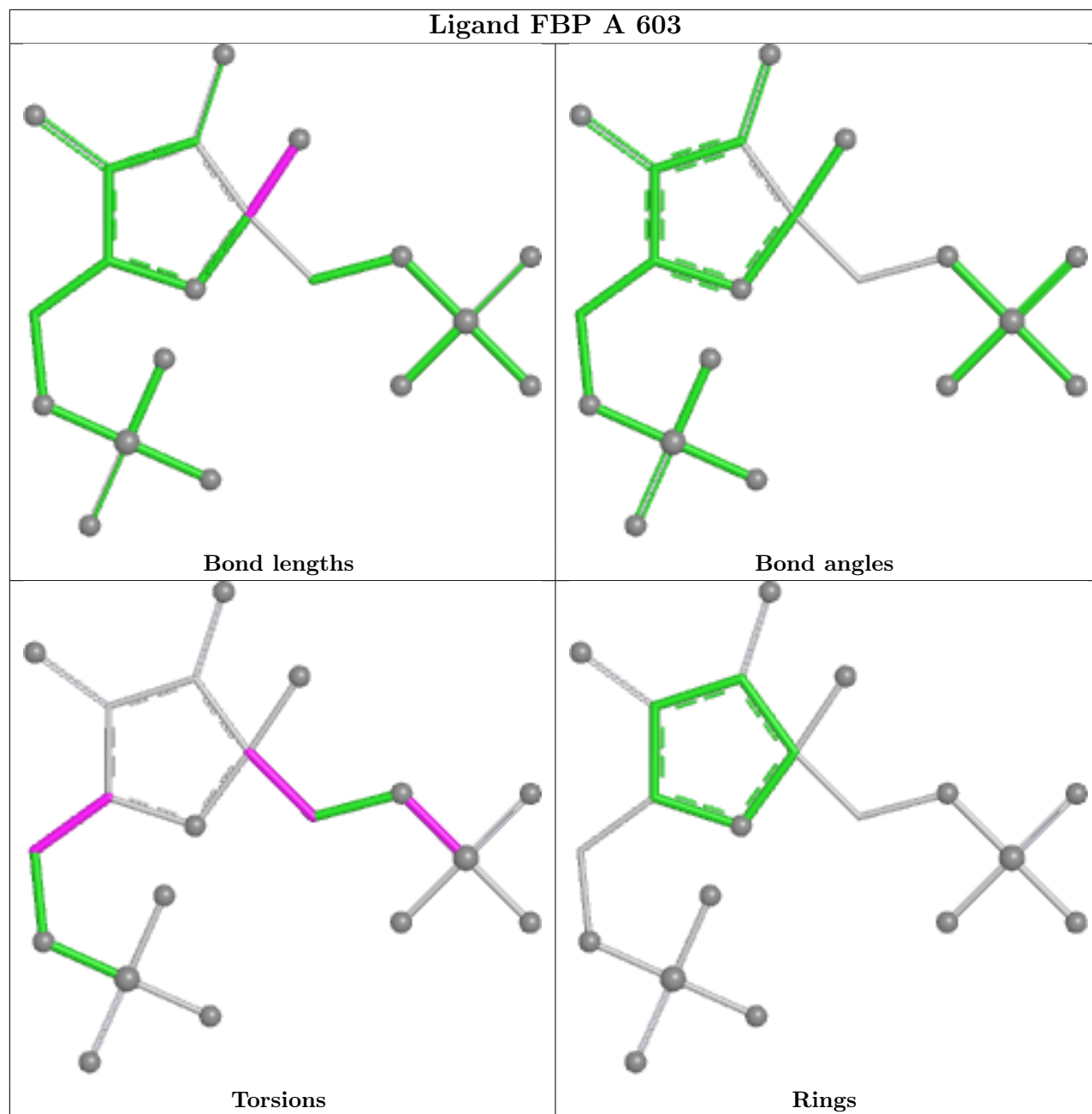


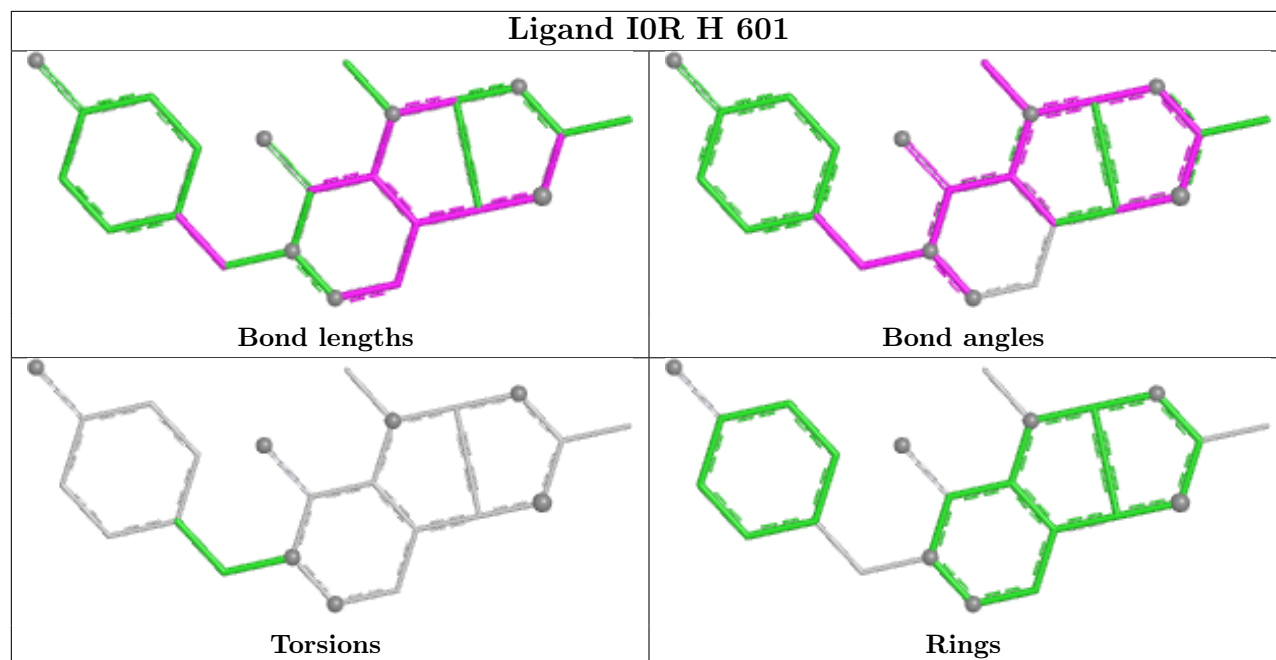
Ligand I0R D 601





Ligand FBP A 603





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	509/544 (93%)	0.54	71 (13%) 6 7	30, 47, 123, 156	1 (0%)
1	B	468/544 (86%)	0.28	43 (9%) 14 17	28, 44, 105, 126	0
1	C	446/544 (81%)	0.17	30 (6%) 24 27	20, 43, 87, 114	1 (0%)
1	D	515/544 (94%)	0.14	26 (5%) 34 40	29, 44, 86, 107	0
1	E	429/544 (78%)	0.79	46 (10%) 11 13	31, 69, 116, 159	0
1	F	518/544 (95%)	0.10	17 (3%) 49 56	27, 44, 80, 130	0
1	G	426/544 (78%)	0.49	28 (6%) 24 27	29, 58, 101, 136	0
1	H	518/544 (95%)	0.03	19 (3%) 45 51	25, 42, 71, 127	0
All	All	3829/4352 (87%)	0.31	280 (7%) 21 24	20, 47, 100, 159	2 (0%)

The worst 5 of 280 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	162	ILE	7.0
1	A	246	LEU	6.0
1	E	164	THR	5.9
1	B	222	GLY	5.7
1	E	165	GLY	5.6

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

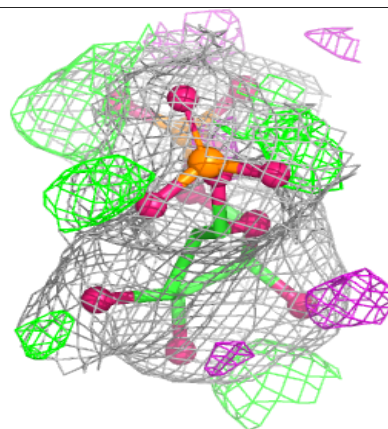
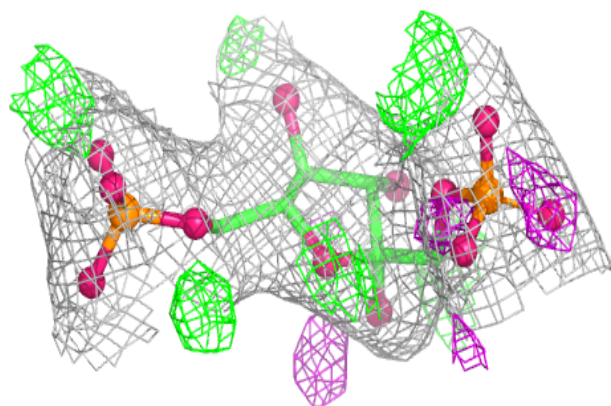
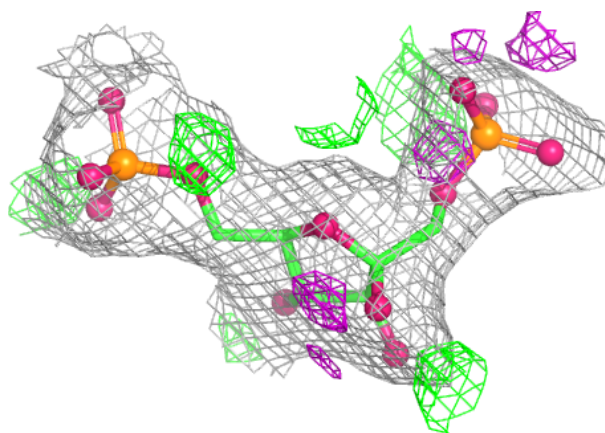
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PYR	E	601	6/6	0.64	0.21	99,101,102,102	0
6	K	D	604	1/1	0.69	0.25	138,138,138,138	0
3	PYR	G	601	6/6	0.73	0.24	95,97,99,100	0
5	MN	F	604	1/1	0.80	0.11	123,123,123,123	0
3	PYR	F	602	6/6	0.80	0.20	89,91,98,110	0
3	PYR	A	602	6/6	0.85	0.17	60,65,69,72	0
4	FBP	E	602	20/20	0.87	0.12	49,56,69,70	0
3	PYR	B	601	6/6	0.88	0.15	63,68,75,82	0
5	MN	G	603	1/1	0.88	0.10	101,101,101,101	0
5	MN	A	604	1/1	0.88	0.10	90,90,90,90	0
4	FBP	G	602	20/20	0.90	0.12	40,52,62,69	0
6	K	A	605	1/1	0.91	0.18	91,91,91,91	0
5	MN	H	603	1/1	0.91	0.22	94,94,94,94	0
5	MN	E	603	1/1	0.92	0.08	123,123,123,123	0
2	I0R	H	601	23/23	0.94	0.09	20,37,46,50	0
2	I0R	A	601	23/23	0.94	0.09	37,44,47,48	0
2	I0R	F	601	23/23	0.94	0.09	28,39,47,48	0
4	FBP	D	602	20/20	0.95	0.08	35,41,48,48	0
2	I0R	D	601	23/23	0.95	0.09	37,43,47,51	0
5	MN	B	603	1/1	0.95	0.07	73,73,73,73	0
4	FBP	A	603	20/20	0.96	0.07	39,43,50,53	0
3	PYR	C	601	6/6	0.96	0.10	67,70,77,86	0
4	FBP	H	602	20/20	0.98	0.05	34,40,45,47	0
4	FBP	C	602	20/20	0.98	0.05	33,36,40,40	0
4	FBP	F	603	20/20	0.98	0.06	31,37,40,41	0
5	MN	D	603	1/1	0.98	0.05	83,83,83,83	0
4	FBP	B	602	20/20	0.98	0.05	29,34,37,38	0
5	MN	C	603	1/1	0.99	0.03	61,61,61,61	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.

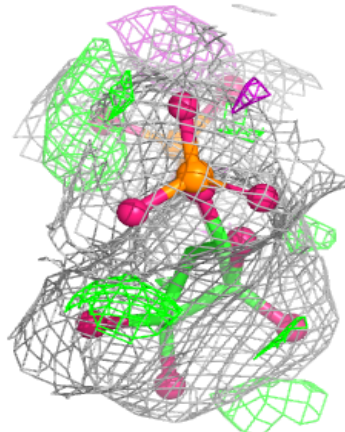
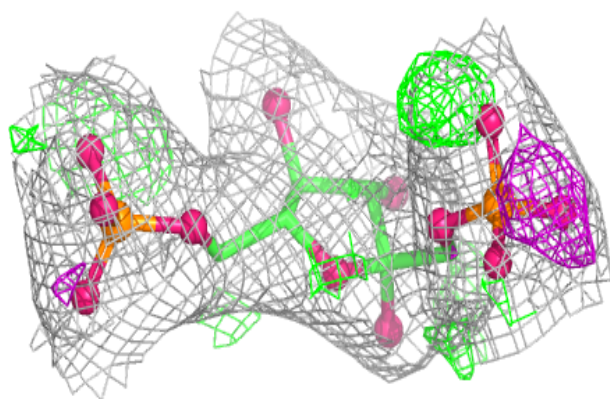
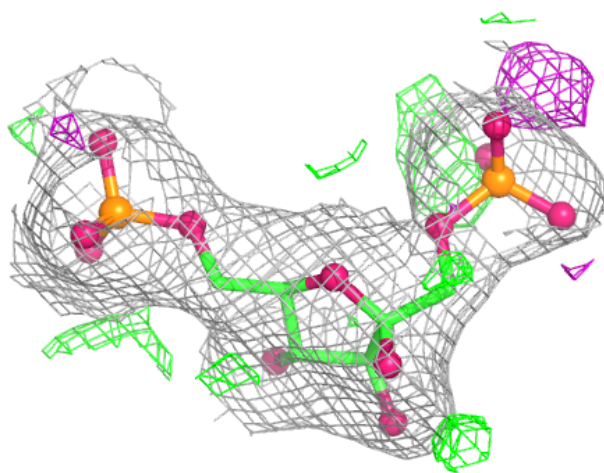
Electron density around FBP E 602:

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



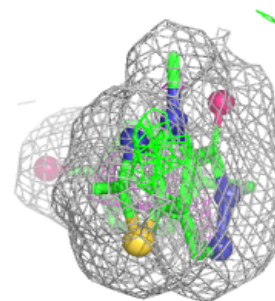
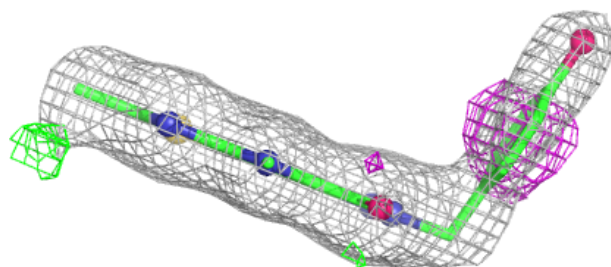
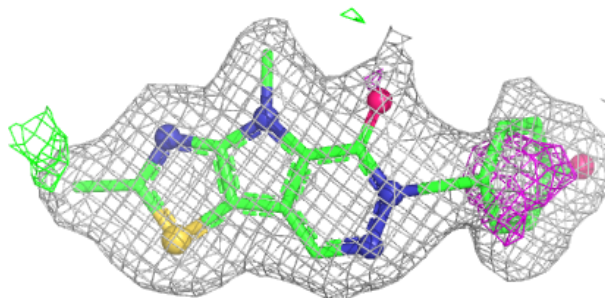
Electron density around FBP G 602:

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

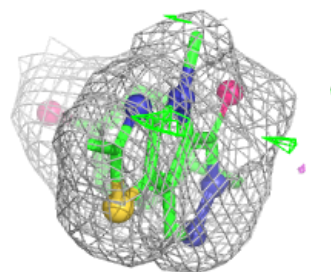
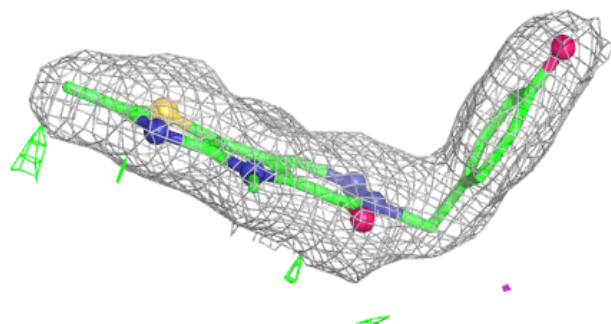
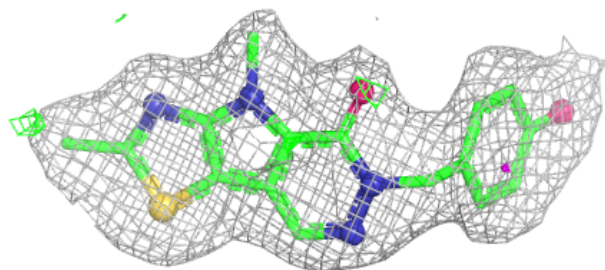


Electron density around I0R H 601:

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

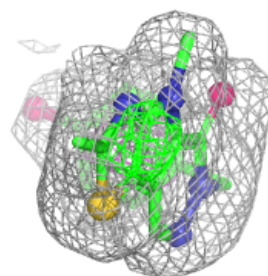
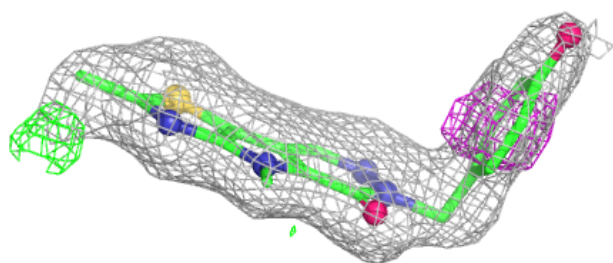
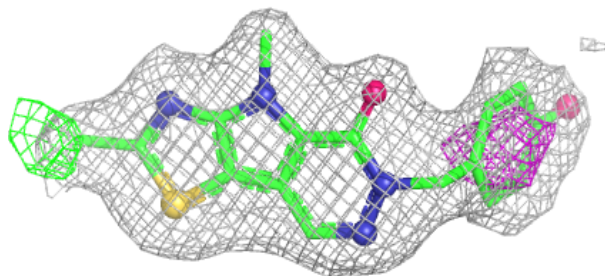
**Electron density around I0R A 601:**

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

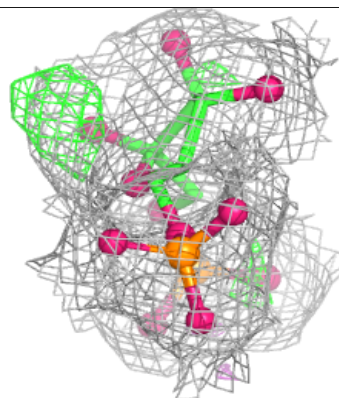
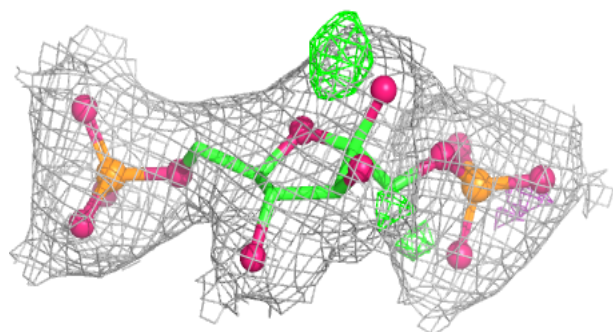
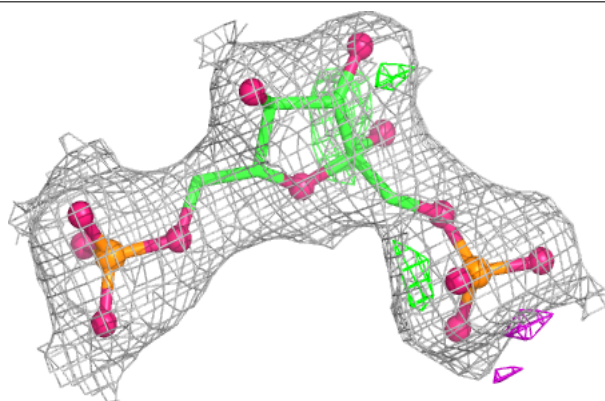


Electron density around I0R F 601:

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

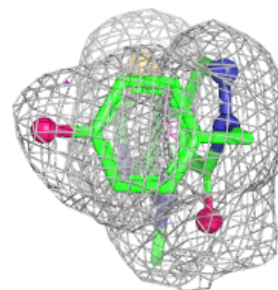
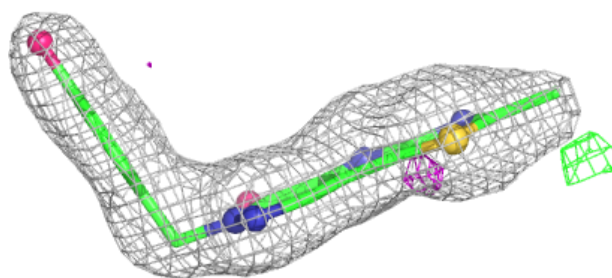
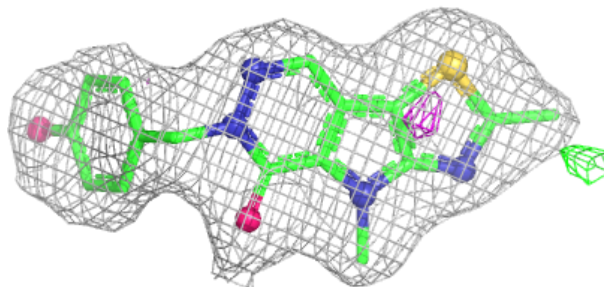
**Electron density around FBP D 602:**

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

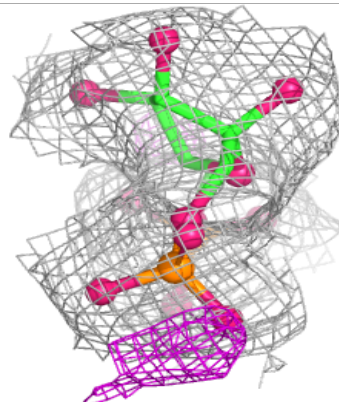
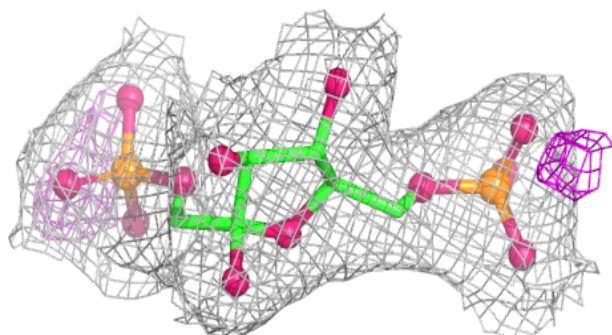
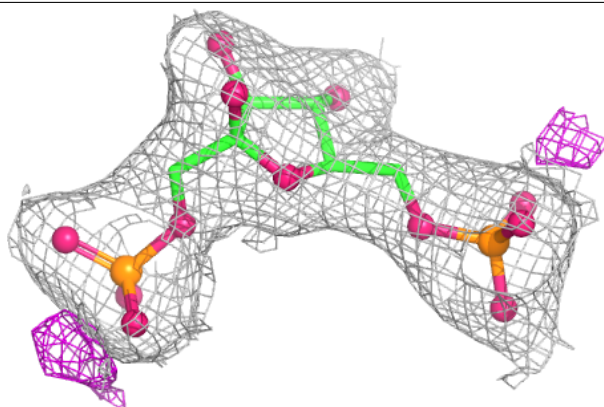


Electron density around IOR D 601:

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

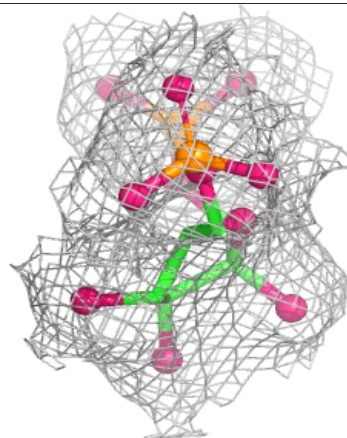
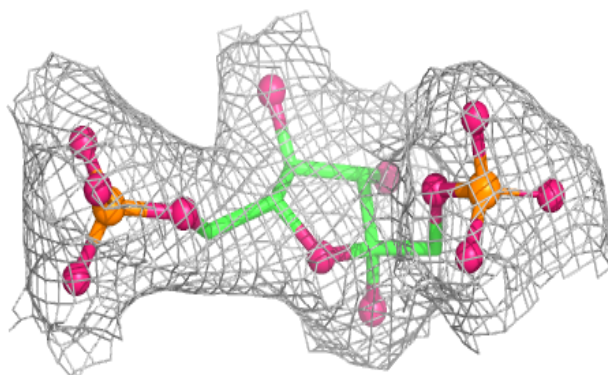
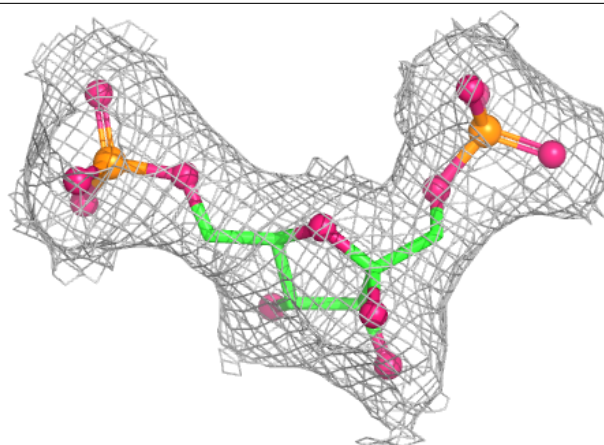
**Electron density around FBP A 603:**

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

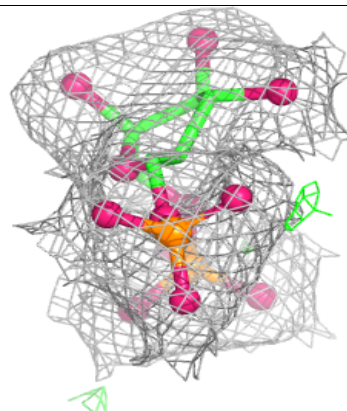
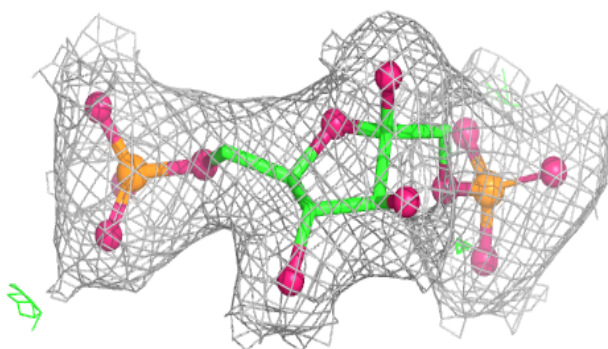
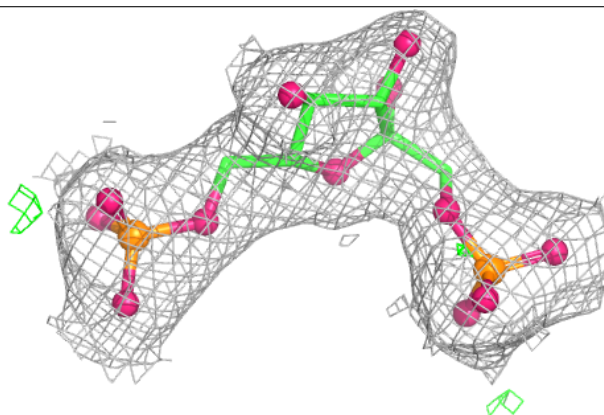


Electron density around FBP H 602:

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

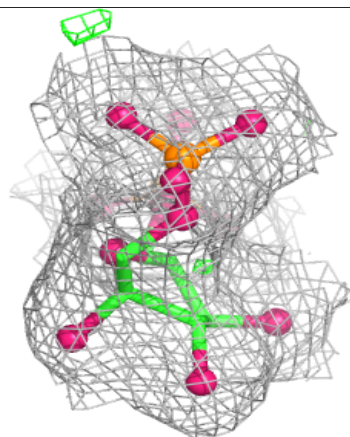
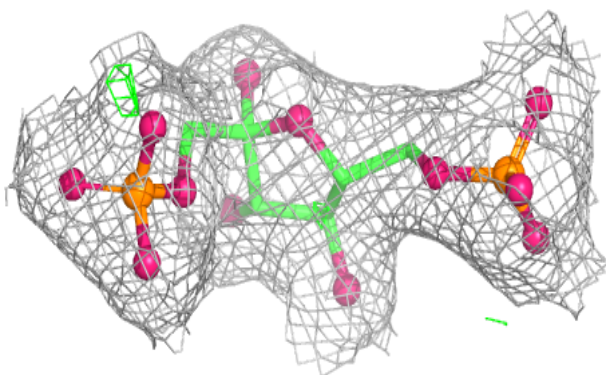
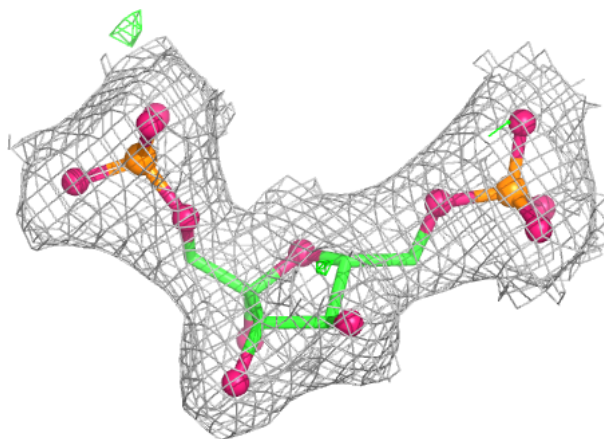
**Electron density around FBP C 602:**

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



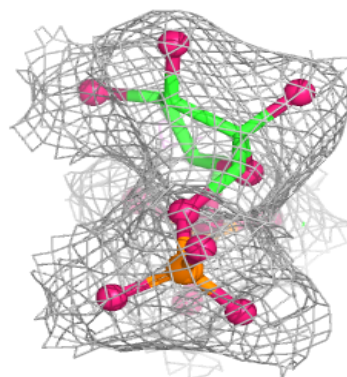
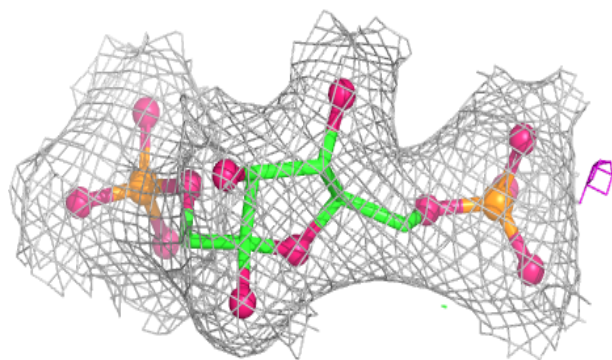
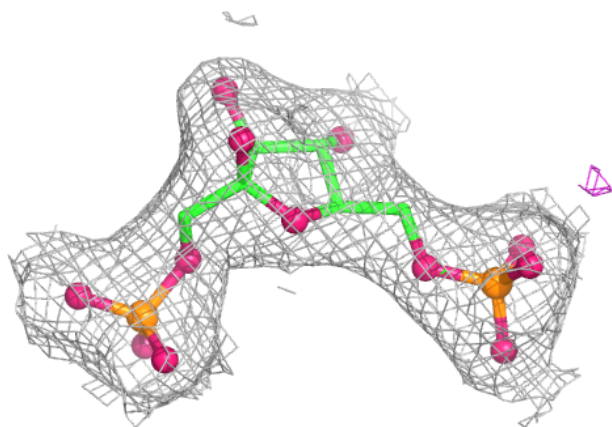
Electron density around FBP F 603:

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



Electron density around FBP B 602:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.