



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:19 PM UTC

PDB ID : 8ZLY / pdb_00008zly
Title : Crystal structure of Streptococcus pneumoniae pyruvate kinase in complex with oxalate and fructose 1,6-bisphosphate and UDP
Authors : Nakashima, R.; Taguchi, A.
Deposited on : 2024-05-21
Resolution : 1.89 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

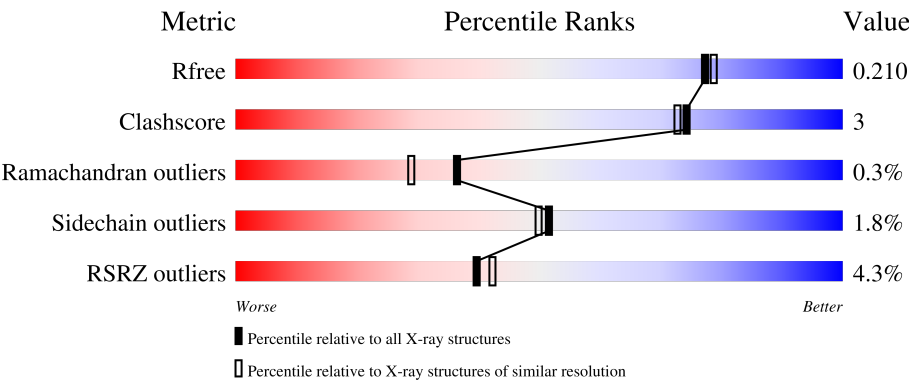
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



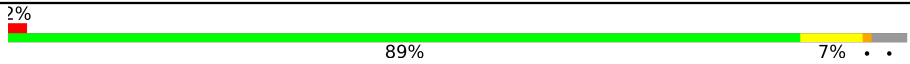
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	521	90%6% . .
1	B	521	12% 85%10% . .
1	C	521	% 90%5% . .
1	D	521	8% 85%10% . .
1	E	521	% 90%6% . .

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Mol	Chain	Length	Quality of chain
1	F	521	
1	G	521	
1	H	521	

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
6	OXL	A	606	-	X	-	-
6	OXL	B	606	-	X	-	-
6	OXL	D	606	-	X	-	-
6	OXL	H	604	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 34975 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			3840	2399	664	760	17			
1	B	501	Total	C	N	O	S	0	0	0
			3840	2399	664	760	17			
1	C	501	Total	C	N	O	S	0	0	0
			3840	2399	664	760	17			
1	D	501	Total	C	N	O	S	0	0	0
			3840	2399	664	760	17			
1	E	501	Total	C	N	O	S	0	0	0
			3840	2399	664	760	17			
1	F	501	Total	C	N	O	S	0	0	0
			3840	2399	664	760	17			
1	G	501	Total	C	N	O	S	0	0	0
			3840	2399	664	760	17			
1	H	501	Total	C	N	O	S	0	0	0
			3840	2399	664	760	17			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q8DQ84
A	-18	GLY	-	expression tag	UNP Q8DQ84
A	-17	SER	-	expression tag	UNP Q8DQ84
A	-16	SER	-	expression tag	UNP Q8DQ84
A	-15	HIS	-	expression tag	UNP Q8DQ84
A	-14	HIS	-	expression tag	UNP Q8DQ84
A	-13	HIS	-	expression tag	UNP Q8DQ84
A	-12	HIS	-	expression tag	UNP Q8DQ84
A	-11	HIS	-	expression tag	UNP Q8DQ84
A	-10	HIS	-	expression tag	UNP Q8DQ84
A	-9	SER	-	expression tag	UNP Q8DQ84
A	-8	SER	-	expression tag	UNP Q8DQ84
A	-7	GLY	-	expression tag	UNP Q8DQ84

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP Q8DQ84
A	-5	VAL	-	expression tag	UNP Q8DQ84
A	-4	PRO	-	expression tag	UNP Q8DQ84
A	-3	ARG	-	expression tag	UNP Q8DQ84
A	-2	GLY	-	expression tag	UNP Q8DQ84
A	-1	SER	-	expression tag	UNP Q8DQ84
A	0	HIS	-	expression tag	UNP Q8DQ84
B	-19	MET	-	initiating methionine	UNP Q8DQ84
B	-18	GLY	-	expression tag	UNP Q8DQ84
B	-17	SER	-	expression tag	UNP Q8DQ84
B	-16	SER	-	expression tag	UNP Q8DQ84
B	-15	HIS	-	expression tag	UNP Q8DQ84
B	-14	HIS	-	expression tag	UNP Q8DQ84
B	-13	HIS	-	expression tag	UNP Q8DQ84
B	-12	HIS	-	expression tag	UNP Q8DQ84
B	-11	HIS	-	expression tag	UNP Q8DQ84
B	-10	HIS	-	expression tag	UNP Q8DQ84
B	-9	SER	-	expression tag	UNP Q8DQ84
B	-8	SER	-	expression tag	UNP Q8DQ84
B	-7	GLY	-	expression tag	UNP Q8DQ84
B	-6	LEU	-	expression tag	UNP Q8DQ84
B	-5	VAL	-	expression tag	UNP Q8DQ84
B	-4	PRO	-	expression tag	UNP Q8DQ84
B	-3	ARG	-	expression tag	UNP Q8DQ84
B	-2	GLY	-	expression tag	UNP Q8DQ84
B	-1	SER	-	expression tag	UNP Q8DQ84
B	0	HIS	-	expression tag	UNP Q8DQ84
C	-19	MET	-	initiating methionine	UNP Q8DQ84
C	-18	GLY	-	expression tag	UNP Q8DQ84
C	-17	SER	-	expression tag	UNP Q8DQ84
C	-16	SER	-	expression tag	UNP Q8DQ84
C	-15	HIS	-	expression tag	UNP Q8DQ84
C	-14	HIS	-	expression tag	UNP Q8DQ84
C	-13	HIS	-	expression tag	UNP Q8DQ84
C	-12	HIS	-	expression tag	UNP Q8DQ84
C	-11	HIS	-	expression tag	UNP Q8DQ84
C	-10	HIS	-	expression tag	UNP Q8DQ84
C	-9	SER	-	expression tag	UNP Q8DQ84
C	-8	SER	-	expression tag	UNP Q8DQ84
C	-7	GLY	-	expression tag	UNP Q8DQ84
C	-6	LEU	-	expression tag	UNP Q8DQ84
C	-5	VAL	-	expression tag	UNP Q8DQ84

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP Q8DQ84
C	-3	ARG	-	expression tag	UNP Q8DQ84
C	-2	GLY	-	expression tag	UNP Q8DQ84
C	-1	SER	-	expression tag	UNP Q8DQ84
C	0	HIS	-	expression tag	UNP Q8DQ84
D	-19	MET	-	initiating methionine	UNP Q8DQ84
D	-18	GLY	-	expression tag	UNP Q8DQ84
D	-17	SER	-	expression tag	UNP Q8DQ84
D	-16	SER	-	expression tag	UNP Q8DQ84
D	-15	HIS	-	expression tag	UNP Q8DQ84
D	-14	HIS	-	expression tag	UNP Q8DQ84
D	-13	HIS	-	expression tag	UNP Q8DQ84
D	-12	HIS	-	expression tag	UNP Q8DQ84
D	-11	HIS	-	expression tag	UNP Q8DQ84
D	-10	HIS	-	expression tag	UNP Q8DQ84
D	-9	SER	-	expression tag	UNP Q8DQ84
D	-8	SER	-	expression tag	UNP Q8DQ84
D	-7	GLY	-	expression tag	UNP Q8DQ84
D	-6	LEU	-	expression tag	UNP Q8DQ84
D	-5	VAL	-	expression tag	UNP Q8DQ84
D	-4	PRO	-	expression tag	UNP Q8DQ84
D	-3	ARG	-	expression tag	UNP Q8DQ84
D	-2	GLY	-	expression tag	UNP Q8DQ84
D	-1	SER	-	expression tag	UNP Q8DQ84
D	0	HIS	-	expression tag	UNP Q8DQ84
E	-19	MET	-	initiating methionine	UNP Q8DQ84
E	-18	GLY	-	expression tag	UNP Q8DQ84
E	-17	SER	-	expression tag	UNP Q8DQ84
E	-16	SER	-	expression tag	UNP Q8DQ84
E	-15	HIS	-	expression tag	UNP Q8DQ84
E	-14	HIS	-	expression tag	UNP Q8DQ84
E	-13	HIS	-	expression tag	UNP Q8DQ84
E	-12	HIS	-	expression tag	UNP Q8DQ84
E	-11	HIS	-	expression tag	UNP Q8DQ84
E	-10	HIS	-	expression tag	UNP Q8DQ84
E	-9	SER	-	expression tag	UNP Q8DQ84
E	-8	SER	-	expression tag	UNP Q8DQ84
E	-7	GLY	-	expression tag	UNP Q8DQ84
E	-6	LEU	-	expression tag	UNP Q8DQ84
E	-5	VAL	-	expression tag	UNP Q8DQ84
E	-4	PRO	-	expression tag	UNP Q8DQ84
E	-3	ARG	-	expression tag	UNP Q8DQ84

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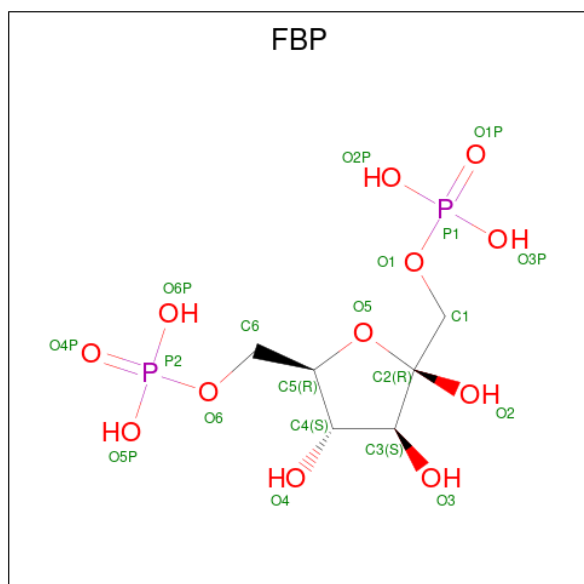
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP Q8DQ84
E	-1	SER	-	expression tag	UNP Q8DQ84
E	0	HIS	-	expression tag	UNP Q8DQ84
F	-19	MET	-	initiating methionine	UNP Q8DQ84
F	-18	GLY	-	expression tag	UNP Q8DQ84
F	-17	SER	-	expression tag	UNP Q8DQ84
F	-16	SER	-	expression tag	UNP Q8DQ84
F	-15	HIS	-	expression tag	UNP Q8DQ84
F	-14	HIS	-	expression tag	UNP Q8DQ84
F	-13	HIS	-	expression tag	UNP Q8DQ84
F	-12	HIS	-	expression tag	UNP Q8DQ84
F	-11	HIS	-	expression tag	UNP Q8DQ84
F	-10	HIS	-	expression tag	UNP Q8DQ84
F	-9	SER	-	expression tag	UNP Q8DQ84
F	-8	SER	-	expression tag	UNP Q8DQ84
F	-7	GLY	-	expression tag	UNP Q8DQ84
F	-6	LEU	-	expression tag	UNP Q8DQ84
F	-5	VAL	-	expression tag	UNP Q8DQ84
F	-4	PRO	-	expression tag	UNP Q8DQ84
F	-3	ARG	-	expression tag	UNP Q8DQ84
F	-2	GLY	-	expression tag	UNP Q8DQ84
F	-1	SER	-	expression tag	UNP Q8DQ84
F	0	HIS	-	expression tag	UNP Q8DQ84
G	-19	MET	-	initiating methionine	UNP Q8DQ84
G	-18	GLY	-	expression tag	UNP Q8DQ84
G	-17	SER	-	expression tag	UNP Q8DQ84
G	-16	SER	-	expression tag	UNP Q8DQ84
G	-15	HIS	-	expression tag	UNP Q8DQ84
G	-14	HIS	-	expression tag	UNP Q8DQ84
G	-13	HIS	-	expression tag	UNP Q8DQ84
G	-12	HIS	-	expression tag	UNP Q8DQ84
G	-11	HIS	-	expression tag	UNP Q8DQ84
G	-10	HIS	-	expression tag	UNP Q8DQ84
G	-9	SER	-	expression tag	UNP Q8DQ84
G	-8	SER	-	expression tag	UNP Q8DQ84
G	-7	GLY	-	expression tag	UNP Q8DQ84
G	-6	LEU	-	expression tag	UNP Q8DQ84
G	-5	VAL	-	expression tag	UNP Q8DQ84
G	-4	PRO	-	expression tag	UNP Q8DQ84
G	-3	ARG	-	expression tag	UNP Q8DQ84
G	-2	GLY	-	expression tag	UNP Q8DQ84
G	-1	SER	-	expression tag	UNP Q8DQ84

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP Q8DQ84
H	-19	MET	-	initiating methionine	UNP Q8DQ84
H	-18	GLY	-	expression tag	UNP Q8DQ84
H	-17	SER	-	expression tag	UNP Q8DQ84
H	-16	SER	-	expression tag	UNP Q8DQ84
H	-15	HIS	-	expression tag	UNP Q8DQ84
H	-14	HIS	-	expression tag	UNP Q8DQ84
H	-13	HIS	-	expression tag	UNP Q8DQ84
H	-12	HIS	-	expression tag	UNP Q8DQ84
H	-11	HIS	-	expression tag	UNP Q8DQ84
H	-10	HIS	-	expression tag	UNP Q8DQ84
H	-9	SER	-	expression tag	UNP Q8DQ84
H	-8	SER	-	expression tag	UNP Q8DQ84
H	-7	GLY	-	expression tag	UNP Q8DQ84
H	-6	LEU	-	expression tag	UNP Q8DQ84
H	-5	VAL	-	expression tag	UNP Q8DQ84
H	-4	PRO	-	expression tag	UNP Q8DQ84
H	-3	ARG	-	expression tag	UNP Q8DQ84
H	-2	GLY	-	expression tag	UNP Q8DQ84
H	-1	SER	-	expression tag	UNP Q8DQ84
H	0	HIS	-	expression tag	UNP Q8DQ84

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

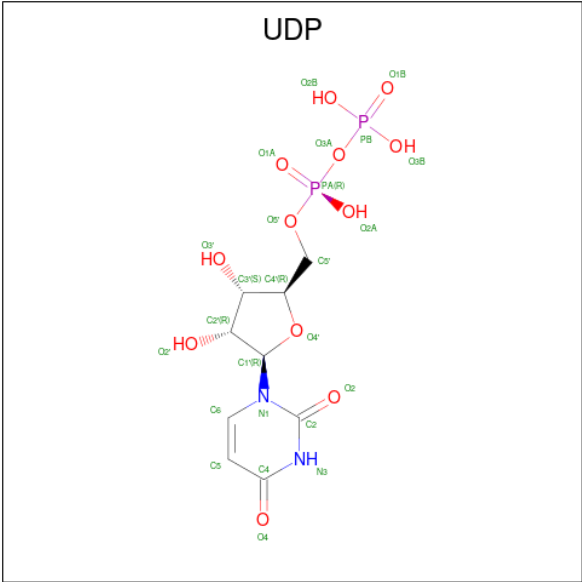


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O P 20 6 12 2	0	0
2	B	1	Total C O P 20 6 12 2	0	0
2	C	1	Total C O P 20 6 12 2	0	0
2	D	1	Total C O P 20 6 12 2	0	0
2	E	1	Total C O P 20 6 12 2	0	0
2	F	1	Total C O P 20 6 12 2	0	0
2	G	1	Total C O P 20 6 12 2	0	0
2	H	1	Total C O P 20 6 12 2	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: C₉H₁₄N₂O₁₂P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
4	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
4	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
4	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
4	E	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
4	F	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
4	G	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

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

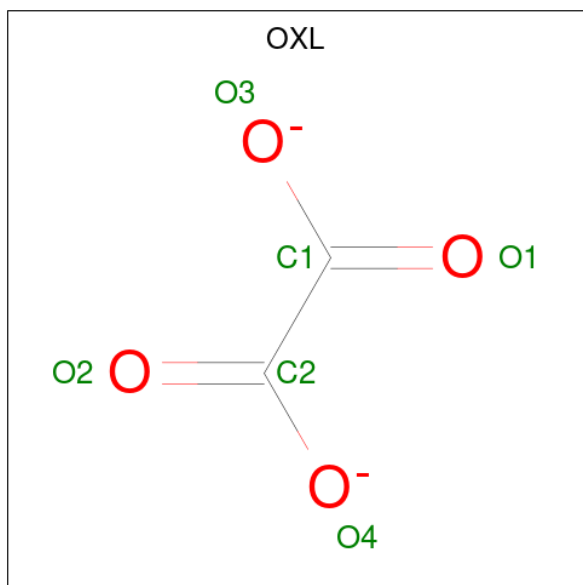
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	K	0	0
			1	1		
5	B	1	Total	K	0	0
			1	1		
5	C	1	Total	K	0	0
			1	1		
5	D	1	Total	K	0	0
			1	1		
5	E	1	Total	K	0	0
			1	1		

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

- Molecule 6 is OXALATE ION (CCD ID: OXL) (formula: C_2O_4).



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

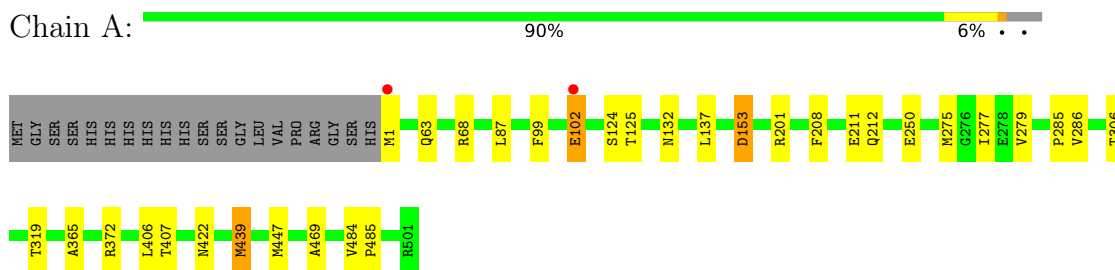
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	487	Total 487	O 487	0	0
7	B	358	Total 358	O 358	0	0
7	C	613	Total 613	O 613	0	0
7	D	468	Total 468	O 468	0	0
7	E	530	Total 530	O 530	0	0
7	F	433	Total 433	O 433	0	0
7	G	573	Total 573	O 573	0	0
7	H	387	Total 387	O 387	0	0

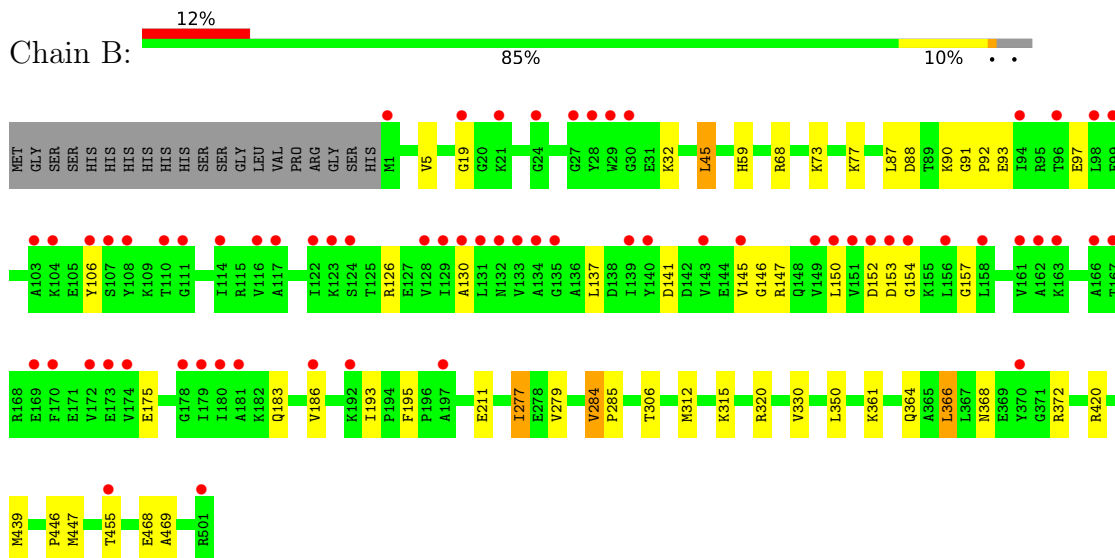
3 Residue-property plots [i](#)

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.

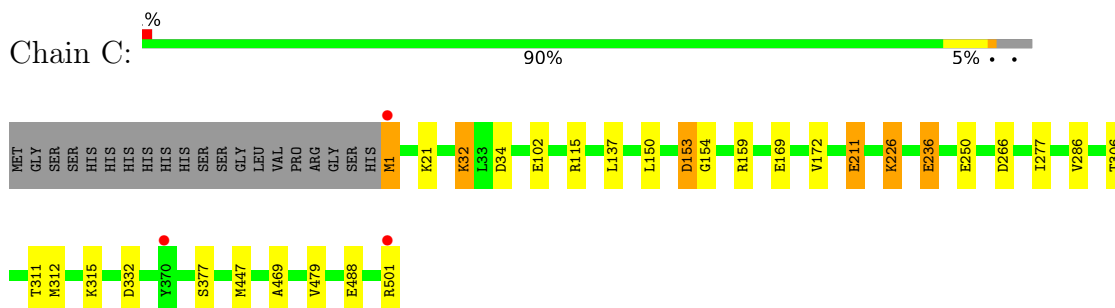
• Molecule 1: Pyruvate kinase



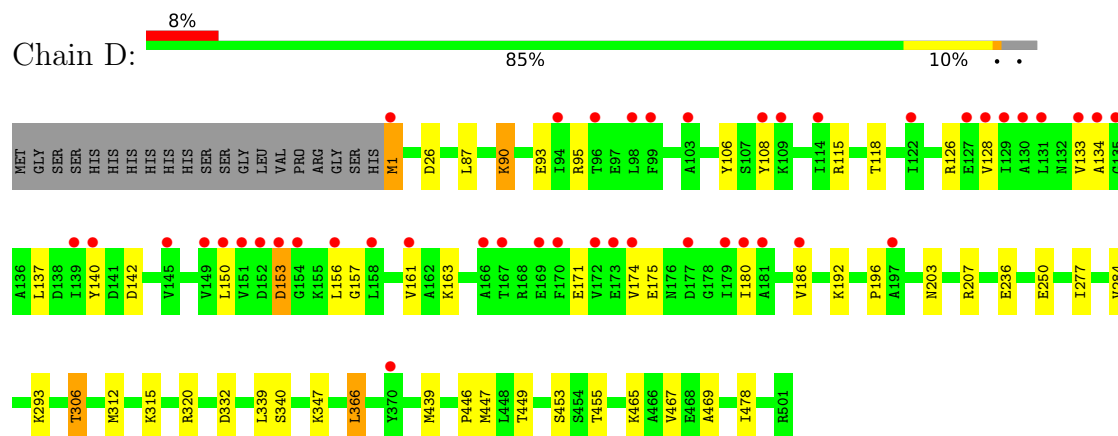
• Molecule 1: Pyruvate kinase



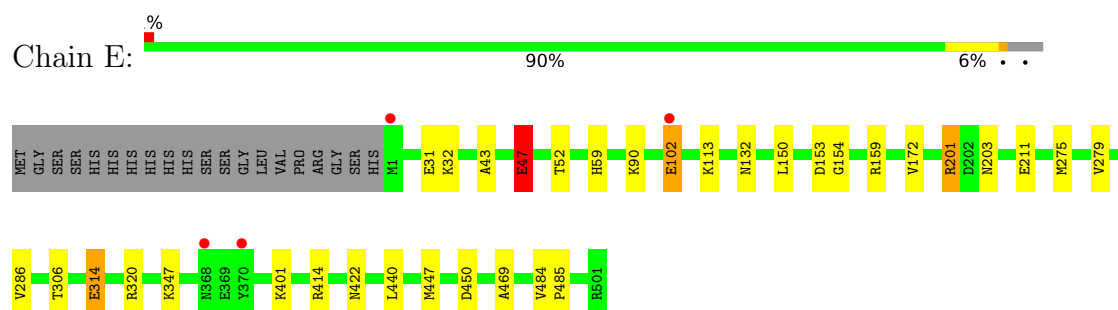
• Molecule 1: Pyruvate kinase



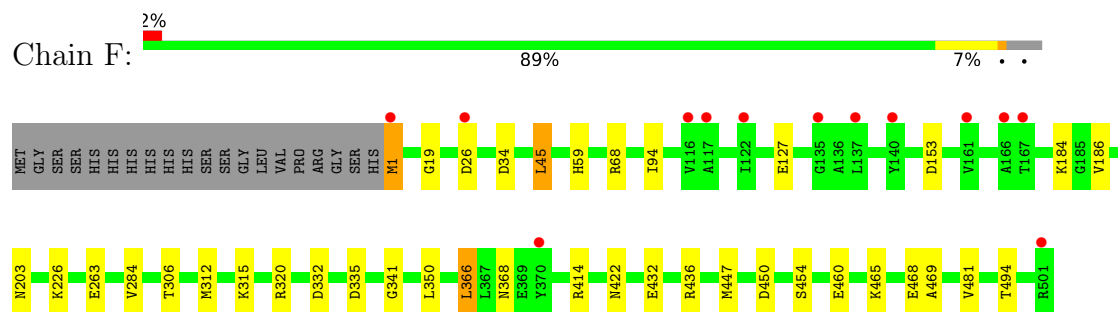
- Molecule 1: Pyruvate kinase



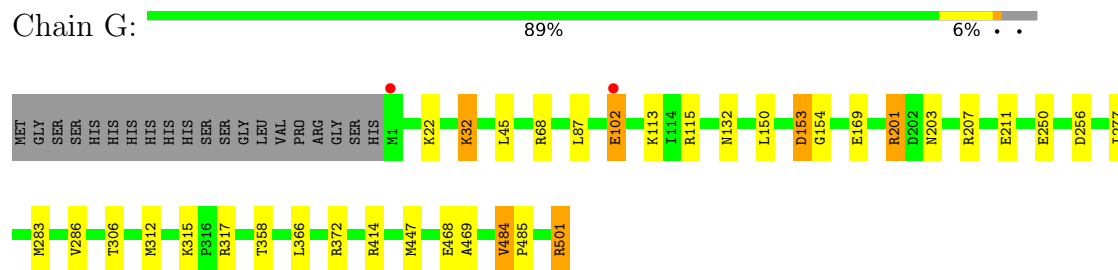
- Molecule 1: Pyruvate kinase



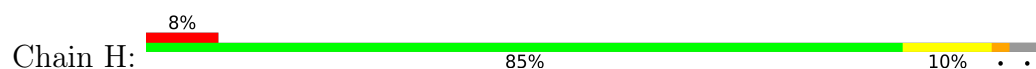
- Molecule 1: Pyruvate kinase

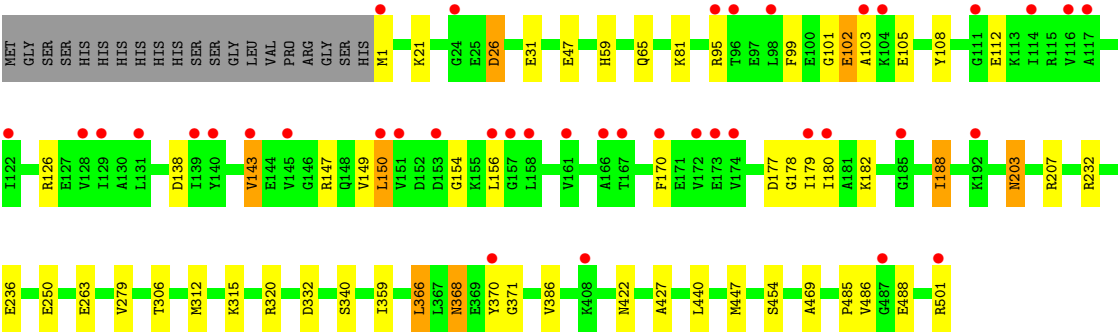


- Molecule 1: Pyruvate kinase



- Molecule 1: Pyruvate kinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	115.81Å 403.20Å 113.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.16 – 1.89 48.16 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.16-1.89) 100.0 (48.16-1.89)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.165 , 0.205 (Not available) , 0.210	Depositor DCC
R_{free} test set	21187 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	34975	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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 44.55 % 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 1.5015e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.07	1/3885 (0.0%)	1.35	3/5238 (0.1%)
1	B	1.13	1/3885 (0.0%)	1.41	5/5238 (0.1%)
1	C	1.08	1/3885 (0.0%)	1.30	7/5238 (0.1%)
1	D	1.14	2/3885 (0.1%)	1.36	9/5238 (0.2%)
1	E	1.06	0/3885	1.35	6/5238 (0.1%)
1	F	1.07	0/3885	1.36	9/5238 (0.2%)
1	G	1.04	0/3885	1.32	7/5238 (0.1%)
1	H	1.10	4/3885 (0.1%)	1.38	5/5238 (0.1%)
All	All	1.09	9/31080 (0.0%)	1.36	51/41904 (0.1%)

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	A	0	1
1	E	0	1
1	G	0	1
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	420	ARG	C-O	-6.30	1.21	1.23
1	H	440	LEU	C-O	6.29	1.32	1.24
1	D	478	ILE	C-O	6.03	1.29	1.24
1	C	479	VAL	C-O	5.67	1.30	1.24
1	A	285	PRO	C-O	-5.41	1.17	1.24
1	H	386	VAL	C-O	5.34	1.30	1.24
1	H	427	ALA	C-O	5.31	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	359	ILE	C-O	5.30	1.30	1.24
1	D	339	LEU	C-O	5.21	1.30	1.24

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	153	ASP	CA-CB-CG	7.35	119.95	112.60
1	B	141	ASP	CA-CB-CG	7.22	119.82	112.60
1	H	340	SER	CA-C-O	-6.76	115.92	119.77
1	C	153	ASP	CA-CB-CG	6.67	119.27	112.60
1	B	152	ASP	CA-CB-CG	6.48	119.08	112.60
1	H	332	ASP	CA-CB-CG	6.39	118.99	112.60
1	F	335	ASP	CA-CB-CG	6.34	118.94	112.60
1	B	284	VAL	N-CA-CB	6.26	114.45	110.50
1	E	47	GLU	CB-CG-CD	6.21	123.16	112.60
1	D	196	PRO	CA-C-N	6.12	128.73	120.65
1	D	196	PRO	C-N-CA	6.12	128.73	120.65
1	C	236	GLU	CB-CG-CD	6.04	122.88	112.60
1	C	311	THR	CA-CB-OG1	-5.99	100.61	109.60
1	F	153	ASP	CA-CB-CG	5.88	118.48	112.60
1	E	31	GLU	CA-C-N	5.87	132.11	122.07
1	E	31	GLU	C-N-CA	5.87	132.11	122.07
1	F	26	ASP	CB-CA-C	5.86	118.60	110.16
1	H	177	ASP	CB-CA-C	5.83	119.95	109.64
1	G	283	MET	CA-C-N	-5.82	116.57	120.24
1	G	283	MET	C-N-CA	-5.82	116.57	120.24
1	A	407	THR	CB-CA-C	5.81	119.44	110.14
1	F	414	ARG	CG-CD-NE	-5.78	99.29	112.00
1	D	340	SER	CA-C-O	-5.74	116.50	119.77
1	D	153	ASP	CA-CB-CG	5.73	118.33	112.60
1	G	358	THR	CA-CB-OG1	-5.64	101.14	109.60
1	G	153	ASP	CA-CB-CG	5.57	118.17	112.60
1	D	306	THR	CA-CB-OG1	-5.48	101.38	109.60
1	G	414	ARG	CG-CD-NE	-5.43	100.05	112.00
1	A	153	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	277	ILE	N-CA-C	-5.40	107.56	112.96
1	C	102	GLU	CB-CG-CD	5.39	121.76	112.60
1	F	450	ASP	CA-C-O	-5.36	115.29	121.19
1	C	266	ASP	N-CA-C	-5.32	106.84	113.38
1	H	340	SER	O-C-N	5.30	124.75	120.83
1	G	113	LYS	CB-CA-C	5.29	118.87	110.19
1	F	332	ASP	CA-CB-CG	5.28	117.88	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	332	ASP	CA-CB-CG	5.27	117.87	112.60
1	E	450	ASP	CA-C-O	-5.25	115.28	121.16
1	B	88	ASP	CA-CB-CG	5.24	117.84	112.60
1	C	34	ASP	CA-CB-CG	5.22	117.82	112.60
1	G	256	ASP	CA-CB-CG	5.19	117.79	112.60
1	D	332	ASP	CA-CB-CG	5.18	117.78	112.60
1	E	414	ARG	CG-CD-NE	-5.16	100.64	112.00
1	F	184	LYS	CA-C-N	5.15	124.86	119.92
1	F	184	LYS	C-N-CA	5.15	124.86	119.92
1	A	319	THR	CA-CB-OG1	-5.09	101.96	109.60
1	F	284	VAL	N-CA-CB	5.09	113.71	110.50
1	H	371	GLY	CA-C-O	-5.07	116.94	121.41
1	D	467	VAL	CA-C-O	-5.06	115.43	121.05
1	D	284	VAL	N-CA-CB	5.03	113.67	110.50
1	D	26	ASP	CA-CB-CG	5.03	117.63	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	GLU	Peptide
1	E	102	GLU	Peptide
1	G	102	GLU	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	3840	0	3887	22	0
1	B	3840	0	3887	31	0
1	C	3840	0	3887	15	0
1	D	3840	0	3887	30	0
1	E	3840	0	3887	23	0
1	F	3840	0	3887	29	0
1	G	3840	0	3887	21	0
1	H	3840	0	3887	32	0
2	A	20	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	20	0	10	0	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
2	E	20	0	10	0	0
2	F	20	0	10	0	0
2	G	20	0	10	0	0
2	H	20	0	10	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	1	0	0	0	0
4	A	25	0	11	0	0
4	B	25	0	11	0	0
4	C	25	0	11	0	0
4	D	25	0	11	0	0
4	E	25	0	11	1	0
4	F	25	0	11	1	0
4	G	25	0	11	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	6	0	0	0	0
6	B	6	0	0	0	0
6	C	6	0	0	0	0
6	D	6	0	0	0	0
6	E	6	0	0	0	0
6	F	6	0	0	0	0
6	G	6	0	0	0	0
6	H	6	0	0	0	0
7	A	487	0	0	4	0
7	B	358	0	0	8	0
7	C	613	0	0	7	0
7	D	468	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	530	0	0	6	0
7	F	433	0	0	17	0
7	G	573	0	0	9	0
7	H	387	0	0	5	0
All	All	34975	0	31253	192	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 3.

All (192) 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:F:1:MET:HB3	7:F:1010:HOH:O	1.50	1.08
1:E:447:MET:HE1	1:E:469:ALA:HB2	1.41	1.00
1:E:422:ASN:HB2	7:E:709:HOH:O	1.62	1.00
1:H:203:ASN:HD21	1:H:207:ARG:HE	1.16	0.94
1:F:1:MET:SD	7:F:1010:HOH:O	2.28	0.91
1:A:102:GLU:HG2	1:E:102:GLU:HG2	1.51	0.91
1:H:447:MET:HE1	1:H:469:ALA:HB2	1.50	0.91
1:A:211:GLU:HG3	7:A:1126:HOH:O	1.70	0.89
1:D:203:ASN:HD21	1:D:207:ARG:HE	1.21	0.84
1:C:447:MET:HE1	1:C:469:ALA:HB2	1.62	0.82
1:D:447:MET:HE1	1:D:469:ALA:HB2	1.63	0.80
1:G:447:MET:HE1	1:G:469:ALA:HB2	1.65	0.79
1:A:102:GLU:HG2	1:E:102:GLU:CG	2.15	0.77
1:F:1:MET:CG	7:F:1010:HOH:O	2.36	0.74
1:E:59:HIS:HD2	7:E:1026:HOH:O	1.72	0.72
1:G:203:ASN:HD21	1:G:207:ARG:HE	1.37	0.72
1:F:127:GLU:HG2	7:F:1069:HOH:O	1.91	0.70
1:G:317:ARG:HD2	1:H:154:GLY:O	1.92	0.69
1:F:447:MET:HE1	1:F:469:ALA:HB2	1.74	0.69
1:B:90:LYS:HG3	1:B:93:GLU:OE1	1.92	0.69
1:H:99:PHE:HB2	1:H:103:ALA:O	1.94	0.67
1:B:447:MET:HE1	1:B:469:ALA:HB2	1.77	0.65
1:G:501:ARG:HD2	7:G:1117:HOH:O	1.98	0.63
1:G:115:ARG:HD3	1:G:169:GLU:OE2	1.99	0.62
1:D:153:ASP:C	1:D:277:ILE:HD11	2.25	0.62
1:H:447:MET:HE1	1:H:469:ALA:CB	2.27	0.61
1:E:447:MET:HE1	1:E:469:ALA:CB	2.24	0.61
1:F:34:ASP:HB3	7:F:984:HOH:O	2.00	0.61
1:H:26:ASP:OD1	1:H:26:ASP:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:VAL:HG22	1:F:366:LEU:HD13	1.82	0.61
1:A:447:MET:HE1	1:A:469:ALA:HB2	1.81	0.61
1:C:447:MET:HE1	1:C:469:ALA:CB	2.30	0.61
1:F:368:ASN:HD21	1:F:422:ASN:HD22	1.47	0.60
1:A:132:ASN:HD21	1:A:201:ARG:HH12	1.51	0.59
1:E:43:ALA:O	1:E:47:GLU:HG2	2.03	0.59
1:E:90:LYS:HE2	1:E:201:ARG:CZ	2.32	0.58
1:B:106:TYR:CG	1:B:126:ARG:HG3	2.39	0.58
1:D:453:SER:OG	1:D:455:THR:HG22	2.03	0.58
1:A:447:MET:HE1	1:A:469:ALA:CB	2.35	0.57
1:F:422:ASN:HB3	7:F:1044:HOH:O	2.03	0.57
1:D:157:GLY:HA3	1:D:175:GLU:OE1	2.05	0.55
1:D:106:TYR:CG	1:D:126:ARG:HG3	2.41	0.55
1:F:1:MET:HE2	7:F:972:HOH:O	2.06	0.55
1:G:447:MET:HE3	7:G:1261:HOH:O	2.05	0.55
1:E:314:GLU:HA	1:E:347:LYS:HE3	1.87	0.55
1:H:312:MET:HA	1:H:315:LYS:O	2.07	0.55
1:H:47:GLU:HG2	7:H:764:HOH:O	2.08	0.54
1:F:432:GLU:CD	1:F:436:ARG:HE	2.14	0.54
1:D:108:TYR:CE2	1:D:180:ILE:HD12	2.43	0.54
1:F:1:MET:CB	7:F:1010:HOH:O	2.21	0.54
1:F:465:LYS:NZ	7:F:715:HOH:O	2.40	0.54
1:D:140:TYR:OH	1:D:163:LYS:HB3	2.08	0.54
1:A:1:MET:CE	1:A:365:ALA:HB2	2.38	0.54
1:B:147:ARG:HD3	7:B:714:HOH:O	2.07	0.54
1:D:161:VAL:HG22	1:D:171:GLU:O	2.07	0.53
1:A:102:GLU:N	1:A:102:GLU:CD	2.66	0.53
1:H:368:ASN:ND2	1:H:422:ASN:OD1	2.41	0.53
1:B:157:GLY:HA3	1:B:175:GLU:OE1	2.08	0.53
1:A:372:ARG:NH2	1:B:372:ARG:NH2	2.57	0.53
1:H:203:ASN:HD21	1:H:207:ARG:NE	1.97	0.52
1:H:203:ASN:ND2	1:H:207:ARG:HE	1.97	0.52
1:G:22:LYS:HE2	7:G:1172:HOH:O	2.08	0.52
1:G:132:ASN:HD21	1:G:201:ARG:HH12	1.57	0.52
1:C:226:LYS:HG2	7:C:1097:HOH:O	2.10	0.52
1:D:447:MET:HE1	1:D:469:ALA:CB	2.39	0.52
1:F:59:HIS:HD2	7:F:812:HOH:O	1.92	0.52
1:G:32:LYS:HE2	7:G:962:HOH:O	2.09	0.52
1:A:68:ARG:HD2	7:A:702:HOH:O	2.09	0.52
1:D:156:LEU:HD11	1:D:174:VAL:HG13	1.93	0.51
1:F:312:MET:HA	1:F:315:LYS:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:ASN:HD21	1:E:201:ARG:HH11	1.58	0.51
1:H:143:VAL:HG22	1:H:170:PHE:CE1	2.45	0.51
1:D:312:MET:HA	1:D:315:LYS:O	2.10	0.51
1:C:286:VAL:HG22	1:D:366:LEU:HD13	1.93	0.51
1:D:90:LYS:HE2	1:D:95:ARG:HG3	1.92	0.51
1:D:115:ARG:HB2	1:D:128:VAL:HG22	1.93	0.50
1:B:153:ASP:C	1:B:277:ILE:HD11	2.37	0.50
1:F:68:ARG:HD2	7:F:707:HOH:O	2.11	0.50
1:H:178:GLY:HA2	7:H:1034:HOH:O	2.12	0.50
1:E:150:LEU:HB3	1:E:154:GLY:HA2	1.94	0.50
1:H:138:ASP:HA	7:H:781:HOH:O	2.11	0.50
1:E:275:MET:O	1:E:279:VAL:HG22	2.12	0.50
1:F:320:ARG:HD3	7:F:965:HOH:O	2.12	0.49
1:H:59:HIS:O	1:H:65:GLN:NE2	2.46	0.49
1:H:101:GLY:O	1:H:103:ALA:N	2.44	0.49
1:E:203:ASN:ND2	7:E:710:HOH:O	2.41	0.49
1:F:263:GLU:HG3	7:F:1025:HOH:O	2.13	0.49
1:D:320:ARG:HD3	7:D:968:HOH:O	2.13	0.49
1:A:153:ASP:C	1:A:277:ILE:HD11	2.38	0.48
1:A:208:PHE:O	1:A:212:GLN:HG2	2.14	0.48
1:B:447:MET:HE1	1:B:469:ALA:CB	2.42	0.48
1:E:201:ARG:HG3	7:E:768:HOH:O	2.13	0.48
1:G:468:GLU:HG3	7:G:905:HOH:O	2.14	0.48
1:D:203:ASN:HD21	1:D:207:ARG:NE	2.02	0.48
1:C:32:LYS:NZ	7:C:714:HOH:O	2.42	0.47
1:D:1:MET:HE2	7:D:1046:HOH:O	2.13	0.47
1:E:401:LYS:HE3	7:E:730:HOH:O	2.14	0.47
1:H:149:VAL:HG22	1:H:188:ILE:HD12	1.96	0.47
1:D:203:ASN:ND2	1:D:207:ARG:HE	2.01	0.47
1:B:59:HIS:CE1	1:B:183:GLN:O	2.68	0.47
1:B:91:GLY:O	1:B:93:GLU:N	2.48	0.47
1:B:361:LYS:O	1:B:364:GLN:HG2	2.15	0.47
1:H:150:LEU:HB3	1:H:154:GLY:HA2	1.97	0.47
1:C:159:ARG:O	1:C:172:VAL:HA	2.14	0.47
1:E:286:VAL:HG22	1:F:366:LEU:CD1	2.44	0.46
1:B:150:LEU:O	1:B:186:VAL:HA	2.15	0.46
1:G:211:GLU:HG3	7:G:1229:HOH:O	2.14	0.46
1:H:108:TYR:OH	1:H:126:ARG:O	2.25	0.46
1:B:97:GLU:HB2	1:B:130:ALA:HB3	1.98	0.46
1:B:146:GLY:HA3	7:B:701:HOH:O	2.16	0.46
1:D:87:LEU:C	1:D:87:LEU:HD23	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:368:ASN:HD21	1:F:422:ASN:ND2	2.12	0.45
1:C:1:MET:HE2	7:C:1110:HOH:O	2.16	0.45
1:D:90:LYS:HE2	1:D:93:GLU:OE1	2.16	0.45
1:G:286:VAL:HG22	1:H:366:LEU:HD13	1.99	0.45
1:D:133:VAL:O	1:D:134:ALA:C	2.59	0.45
1:B:87:LEU:C	1:B:87:LEU:HD23	2.42	0.45
1:G:68:ARG:HD2	7:G:738:HOH:O	2.17	0.45
1:F:341:GLY:HA3	7:F:806:HOH:O	2.16	0.45
1:H:485:PRO:HG2	1:H:488:GLU:HB3	1.98	0.44
1:A:286:VAL:HG22	1:B:366:LEU:HD13	1.98	0.44
1:H:81:LYS:NZ	7:H:723:HOH:O	2.49	0.44
1:F:94:ILE:HG22	1:F:186:VAL:HB	2.00	0.44
1:H:454:SER:HA	1:H:486:VAL:HG22	1.99	0.44
1:B:150:LEU:HB3	1:B:154:GLY:HA2	1.99	0.44
1:D:439:MET:HG3	1:D:446:PRO:HG2	1.99	0.44
1:H:21:LYS:HE2	1:H:31:GLU:OE2	2.18	0.44
1:C:153:ASP:C	1:C:277:ILE:HD11	2.43	0.44
1:D:150:LEU:O	1:D:186:VAL:HA	2.18	0.44
1:B:145:VAL:O	7:B:701:HOH:O	2.20	0.44
1:G:87:LEU:C	1:G:87:LEU:HD23	2.43	0.44
1:C:236:GLU:HG2	7:C:1099:HOH:O	2.18	0.44
1:D:118:THR:HG21	1:D:140:TYR:HB2	2.00	0.44
1:A:125:THR:HG21	1:E:32:LYS:HB2	1.99	0.43
1:B:68:ARG:HD2	7:B:755:HOH:O	2.17	0.43
1:C:211:GLU:HG3	7:C:1221:HOH:O	2.19	0.43
1:A:439:MET:HG2	7:A:1065:HOH:O	2.18	0.43
1:B:320:ARG:HD3	7:B:966:HOH:O	2.16	0.43
1:G:201:ARG:HG3	7:G:778:HOH:O	2.17	0.43
1:B:73:LYS:O	1:B:77:LYS:HD2	2.18	0.43
1:D:293:LYS:NZ	7:D:725:HOH:O	2.49	0.43
1:B:439:MET:HG3	1:B:446:PRO:HG2	2.00	0.43
1:D:347:LYS:HE2	7:D:945:HOH:O	2.18	0.43
1:E:320:ARG:HD3	7:E:1092:HOH:O	2.19	0.43
1:B:5:VAL:HG21	1:B:330:VAL:HG22	2.01	0.42
1:D:93:GLU:CD	1:D:95:ARG:HE	2.26	0.42
1:A:1:MET:HE1	1:A:365:ALA:HB2	2.01	0.42
1:C:312:MET:HA	1:C:315:LYS:O	2.20	0.42
1:D:142:ASP:OD1	7:D:701:HOH:O	2.21	0.42
1:G:312:MET:HA	1:G:315:LYS:O	2.19	0.42
1:F:454:SER:HA	7:F:720:HOH:O	2.19	0.42
1:G:372:ARG:NH2	1:H:370:TYR:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ASN:ND2	7:A:735:HOH:O	2.52	0.42
1:F:203:ASN:ND2	7:F:706:HOH:O	2.35	0.42
1:A:132:ASN:HD21	1:A:201:ARG:NH1	2.13	0.42
1:E:159:ARG:O	1:E:172:VAL:HA	2.20	0.42
1:C:21:LYS:HE2	7:C:801:HOH:O	2.19	0.42
1:F:481:VAL:HA	1:F:494:THR:O	2.20	0.42
1:A:275:MET:O	1:A:279:VAL:HG22	2.20	0.42
1:B:147:ARG:NH1	7:B:714:HOH:O	2.45	0.42
1:G:153:ASP:C	1:G:277:ILE:HD11	2.45	0.42
1:H:320:ARG:HD3	7:H:954:HOH:O	2.18	0.42
1:B:106:TYR:CB	1:B:126:ARG:HG3	2.50	0.41
1:B:368:ASN:HB2	7:B:836:HOH:O	2.19	0.41
1:F:45:LEU:HD22	1:F:350:LEU:HA	2.01	0.41
1:G:447:MET:CE	7:G:1261:HOH:O	2.66	0.41
1:H:112:GLU:CD	1:H:126:ARG:HH12	2.28	0.41
1:A:99:PHE:CD1	1:A:124:SER:HB2	2.55	0.41
1:A:87:LEU:C	1:A:87:LEU:HD23	2.46	0.41
1:F:454:SER:CA	7:F:720:HOH:O	2.68	0.41
1:H:501:ARG:HE	1:H:501:ARG:HB2	1.57	0.41
1:F:447:MET:HE1	1:F:469:ALA:CB	2.48	0.41
1:G:150:LEU:HB3	1:G:154:GLY:HA2	2.01	0.41
1:C:115:ARG:HD3	1:C:169:GLU:OE2	2.21	0.41
1:B:45:LEU:CD2	1:B:350:LEU:HA	2.51	0.41
1:C:150:LEU:HB3	1:C:154:GLY:HA2	2.02	0.41
1:D:449:THR:OG1	1:D:465:LYS:HE3	2.20	0.41
1:H:156:LEU:HD22	1:H:180:ILE:CG1	2.51	0.41
1:B:193:ILE:HB	1:B:195:PHE:CE2	2.55	0.41
1:B:312:MET:HA	1:B:315:LYS:O	2.21	0.41
1:E:59:HIS:HE1	4:E:604:UDP:O2B	2.04	0.41
1:B:92:PRO:HB3	7:B:935:HOH:O	2.20	0.40
1:H:105:GLU:OE1	1:H:179:ILE:HD13	2.21	0.40
1:E:52:THR:HB	1:E:440:LEU:HD21	2.04	0.40
1:E:484:VAL:HA	1:E:485:PRO:HA	1.84	0.40
1:H:147:ARG:HD3	1:H:147:ARG:HA	1.88	0.40
1:A:484:VAL:HA	1:A:485:PRO:HA	1.87	0.40
1:C:377:SER:OG	7:C:702:HOH:O	2.22	0.40
1:G:484:VAL:HA	1:G:485:PRO:HA	1.83	0.40
1:H:232:ARG:O	1:H:236:GLU:HG2	2.21	0.40
1:B:284:VAL:N	1:B:285:PRO:CD	2.84	0.40
1:F:59:HIS:HE1	4:F:604:UDP:O1B	2.04	0.40

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	499/521 (96%)	487 (98%)	11 (2%)	1 (0%)	43	36
1	B	499/521 (96%)	485 (97%)	12 (2%)	2 (0%)	30	22
1	C	499/521 (96%)	491 (98%)	7 (1%)	1 (0%)	43	36
1	D	499/521 (96%)	486 (97%)	12 (2%)	1 (0%)	43	36
1	E	499/521 (96%)	491 (98%)	7 (1%)	1 (0%)	43	36
1	F	499/521 (96%)	486 (97%)	11 (2%)	2 (0%)	30	22
1	G	499/521 (96%)	490 (98%)	7 (1%)	2 (0%)	30	22
1	H	499/521 (96%)	482 (97%)	15 (3%)	2 (0%)	30	22
All	All	3992/4168 (96%)	3898 (98%)	82 (2%)	12 (0%)	36	29

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	102	GLU
1	G	102	GLU
1	B	306	THR
1	C	306	THR
1	D	306	THR
1	E	306	THR
1	F	306	THR
1	H	306	THR
1	A	306	THR
1	G	306	THR
1	F	19	GLY
1	B	19	GLY

5.3.2 Protein sidechains [i](#)

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	411/428 (96%)	406 (99%)	5 (1%)	63	63
1	B	411/428 (96%)	403 (98%)	8 (2%)	50	47
1	C	411/428 (96%)	403 (98%)	8 (2%)	50	47
1	D	411/428 (96%)	404 (98%)	7 (2%)	53	52
1	E	411/428 (96%)	406 (99%)	5 (1%)	63	63
1	F	411/428 (96%)	405 (98%)	6 (2%)	57	56
1	G	411/428 (96%)	404 (98%)	7 (2%)	53	52
1	H	411/428 (96%)	397 (97%)	14 (3%)	32	25
All	All	3288/3424 (96%)	3228 (98%)	60 (2%)	51	50

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	137	LEU
1	A	250	GLU
1	A	406	LEU
1	A	439	MET
1	B	32	LYS
1	B	45	LEU
1	B	137	LEU
1	B	211	GLU
1	B	279	VAL
1	B	366	LEU
1	B	455	THR
1	B	468	GLU
1	C	1	MET
1	C	32	LYS
1	C	137	LEU
1	C	211	GLU
1	C	226	LYS
1	C	250	GLU
1	C	488	GLU
1	C	501	ARG
1	D	1	MET
1	D	90	LYS

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Mol	Chain	Res	Type
1	D	137	LEU
1	D	192	LYS
1	D	236	GLU
1	D	250	GLU
1	D	366	LEU
1	E	47	GLU
1	E	113	LYS
1	E	201	ARG
1	E	211	GLU
1	E	314	GLU
1	F	1	MET
1	F	45	LEU
1	F	226	LYS
1	F	366	LEU
1	F	460	GLU
1	F	468	GLU
1	G	32	LYS
1	G	45	LEU
1	G	201	ARG
1	G	250	GLU
1	G	366	LEU
1	G	484	VAL
1	G	501	ARG
1	H	1	MET
1	H	26	ASP
1	H	95	ARG
1	H	102	GLU
1	H	143	VAL
1	H	150	LEU
1	H	182	LYS
1	H	188	ILE
1	H	203	ASN
1	H	250	GLU
1	H	263	GLU
1	H	279	VAL
1	H	366	LEU
1	H	368	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	ASN

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Mol	Chain	Res	Type
1	A	368	ASN
1	A	422	ASN
1	B	253	GLN
1	C	368	ASN
1	D	203	ASN
1	D	253	GLN
1	D	368	ASN
1	E	59	HIS
1	E	132	ASN
1	E	187	ASN
1	E	190	ASN
1	E	422	ASN
1	F	2	ASN
1	F	422	ASN
1	G	203	ASN
1	G	252	GLN
1	G	381	ASN
1	H	183	GLN
1	H	203	ASN
1	H	252	GLN
1	H	368	ASN
1	H	422	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 46 ligands modelled in this entry, 23 are monoatomic - leaving 23 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
6	OXL	E	606	3	5,5,5	1.60	1 (20%)	6,6,6	1.33	0
2	FBP	C	601	-	18,20,20	1.18	1 (5%)	21,32,32	1.29	5 (23%)
4	UDP	E	604	3	25,26,26	1.30	3 (12%)	38,40,40	1.86	7 (18%)
4	UDP	D	604	3	25,26,26	1.29	4 (16%)	38,40,40	1.74	10 (26%)
6	OXL	D	606	3	5,5,5	2.32	3 (60%)	6,6,6	1.35	1 (16%)
4	UDP	F	604	3	25,26,26	1.10	1 (4%)	38,40,40	2.00	7 (18%)
2	FBP	E	601	-	18,20,20	1.08	2 (11%)	21,32,32	1.18	3 (14%)
6	OXL	F	606	3	5,5,5	1.88	1 (20%)	6,6,6	1.01	0
2	FBP	H	601	-	18,20,20	1.16	1 (5%)	21,32,32	1.44	4 (19%)
6	OXL	A	606	3	5,5,5	1.68	2 (40%)	6,6,6	1.37	0
6	OXL	G	606	3	5,5,5	1.96	1 (20%)	6,6,6	0.87	0
2	FBP	G	601	-	18,20,20	0.96	0	21,32,32	1.19	3 (14%)
6	OXL	C	606	3	5,5,5	1.40	1 (20%)	6,6,6	1.32	0
4	UDP	C	604	3	25,26,26	1.12	1 (4%)	38,40,40	1.80	6 (15%)
6	OXL	B	606	3	5,5,5	1.86	1 (20%)	6,6,6	1.73	2 (33%)
4	UDP	A	604	3	25,26,26	2.15	3 (12%)	38,40,40	1.81	9 (23%)
2	FBP	B	601	-	18,20,20	1.04	2 (11%)	21,32,32	1.11	2 (9%)
6	OXL	H	604	3	5,5,5	1.90	2 (40%)	6,6,6	1.42	1 (16%)
2	FBP	D	601	-	18,20,20	1.01	1 (5%)	21,32,32	1.58	5 (23%)
2	FBP	A	601	-	18,20,20	1.13	2 (11%)	21,32,32	1.03	1 (4%)
2	FBP	F	601	-	18,20,20	0.87	0	21,32,32	1.16	1 (4%)
4	UDP	G	604	3	25,26,26	1.54	4 (16%)	38,40,40	2.04	10 (26%)
4	UDP	B	604	3	25,26,26	1.36	3 (12%)	38,40,40	1.80	9 (23%)

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
6	OXL	E	606	3	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	C	601	-	-	3/13/32/32	0/1/1/1
4	UDP	E	604	3	-	2/16/32/32	0/2/2/2
4	UDP	D	604	3	-	1/16/32/32	0/2/2/2
6	OXL	D	606	3	-	4/4/4/4	-
4	UDP	F	604	3	-	1/16/32/32	0/2/2/2
2	FBP	E	601	-	-	3/13/32/32	0/1/1/1
6	OXL	F	606	3	-	4/4/4/4	-
2	FBP	H	601	-	-	4/13/32/32	0/1/1/1
6	OXL	A	606	3	-	4/4/4/4	-
6	OXL	G	606	3	-	4/4/4/4	-
2	FBP	G	601	-	-	2/13/32/32	0/1/1/1
6	OXL	C	606	3	-	4/4/4/4	-
4	UDP	C	604	3	-	0/16/32/32	0/2/2/2
6	OXL	B	606	3	-	4/4/4/4	-
4	UDP	A	604	3	-	2/16/32/32	0/2/2/2
2	FBP	B	601	-	-	1/13/32/32	0/1/1/1
6	OXL	H	604	3	-	4/4/4/4	-
2	FBP	D	601	-	-	0/13/32/32	0/1/1/1
2	FBP	A	601	-	-	1/13/32/32	0/1/1/1
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
4	UDP	G	604	3	-	0/16/32/32	0/2/2/2
4	UDP	B	604	3	-	1/16/32/32	0/2/2/2

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604	UDP	PA-O3A	6.13	1.66	1.59
4	A	604	UDP	C4-N3	-5.95	1.28	1.38
4	G	604	UDP	C4-N3	-4.27	1.31	1.38
4	A	604	UDP	C2-N3	-3.89	1.31	1.38
4	B	604	UDP	PA-O3A	3.86	1.63	1.59
6	D	606	OXL	O4-C2	-3.80	1.20	1.30
4	C	604	UDP	C4-N3	-3.51	1.32	1.38
6	G	606	OXL	O4-C2	-3.44	1.21	1.30
4	E	604	UDP	C4-N3	-3.32	1.32	1.38
4	D	604	UDP	C2-N3	-3.31	1.32	1.38
6	H	604	OXL	O1-C1	3.27	1.30	1.22
6	F	606	OXL	O4-C2	-3.23	1.21	1.30
6	B	606	OXL	O4-C2	-3.13	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	606	OXL	O4-C2	-3.03	1.22	1.30
4	G	604	UDP	PA-O3A	2.95	1.62	1.59
4	B	604	UDP	C2-N3	-2.91	1.32	1.38
4	D	604	UDP	PA-O3A	2.88	1.62	1.59
2	C	601	FBP	O5-C2	-2.82	1.39	1.43
4	G	604	UDP	C2-N3	-2.75	1.33	1.38
2	E	601	FBP	P1-O3P	-2.52	1.45	1.54
2	A	601	FBP	O3-C3	-2.46	1.37	1.42
6	D	606	OXL	O1-C1	2.44	1.28	1.22
4	E	604	UDP	PA-O3A	2.43	1.62	1.59
4	D	604	UDP	O2-C2	2.35	1.27	1.23
6	A	606	OXL	O1-C1	2.34	1.28	1.22
2	B	601	FBP	P2-O6P	-2.32	1.46	1.54
2	D	601	FBP	P1-O3P	-2.31	1.46	1.54
6	A	606	OXL	O4-C2	-2.26	1.24	1.30
2	H	601	FBP	P2-O6P	-2.20	1.46	1.54
2	E	601	FBP	P2-O5P	-2.19	1.46	1.54
6	H	604	OXL	O4-C2	-2.19	1.24	1.30
6	C	606	OXL	O4-C2	-2.14	1.24	1.30
2	A	601	FBP	P1-O3P	-2.09	1.47	1.54
4	B	604	UDP	C5-C4	-2.09	1.39	1.43
6	D	606	OXL	C2-C1	2.08	1.58	1.54
2	B	601	FBP	O5-C2	-2.08	1.40	1.43
4	F	604	UDP	C2-N3	-2.07	1.34	1.38
4	E	604	UDP	C2-N3	-2.07	1.34	1.38
4	D	604	UDP	C5-C4	-2.02	1.39	1.43
4	G	604	UDP	PB-O1B	2.01	1.56	1.50

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	604	UDP	N3-C2-N1	5.94	122.62	114.89
4	C	604	UDP	O2-C2-N1	-5.78	115.27	122.80
4	G	604	UDP	N3-C2-N1	5.55	122.11	114.89
4	F	604	UDP	C4-N3-C2	-5.36	119.96	126.61
4	F	604	UDP	O2-C2-N1	-5.10	116.16	122.80
4	A	604	UDP	N3-C2-N1	4.99	121.38	114.89
4	G	604	UDP	O2-C2-N1	-4.88	116.44	122.80
4	F	604	UDP	N3-C2-N1	4.85	121.20	114.89
4	B	604	UDP	C4-N3-C2	-4.83	120.62	126.61
4	D	604	UDP	C5-C4-N3	4.66	121.33	114.80
4	E	604	UDP	O2-C2-N1	-4.60	116.81	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	604	UDP	O4-C4-C5	-4.33	117.70	125.16
4	E	604	UDP	C4-N3-C2	-4.11	121.51	126.61
4	C	604	UDP	N3-C2-N1	4.03	120.13	114.89
4	G	604	UDP	O3A-PB-O1B	-3.99	90.03	111.04
4	B	604	UDP	C5-C4-N3	3.99	120.39	114.80
4	F	604	UDP	O4-C4-C5	-3.96	118.33	125.16
4	G	604	UDP	C6-N1-C2	-3.86	116.30	121.00
4	D	604	UDP	O4-C4-C5	-3.83	118.56	125.16
4	C	604	UDP	C5-C4-N3	3.78	120.09	114.80
4	A	604	UDP	O2-C2-N1	-3.74	117.93	122.80
4	F	604	UDP	C5-C4-N3	3.69	119.97	114.80
4	A	604	UDP	C4-N3-C2	-3.68	122.05	126.61
4	D	604	UDP	C4-N3-C2	-3.67	122.05	126.61
4	B	604	UDP	N3-C2-N1	3.61	119.60	114.89
4	C	604	UDP	C4-N3-C2	-3.45	122.32	126.61
4	D	604	UDP	O3B-PB-O2B	3.44	120.70	107.80
4	C	604	UDP	O4-C4-C5	-3.36	119.37	125.16
4	G	604	UDP	O3B-PB-O2B	3.19	119.77	107.80
4	E	604	UDP	C6-N1-C2	-3.12	117.20	121.00
2	H	601	FBP	O3P-P1-O1	3.04	114.59	106.67
2	G	601	FBP	O2-C2-O5	-3.02	103.53	109.33
4	A	604	UDP	C6-N1-C2	-2.99	117.35	121.00
2	D	601	FBP	O6-P2-O4P	-2.95	98.48	106.44
4	G	604	UDP	C4-N3-C2	-2.91	123.01	126.61
4	A	604	UDP	C5-C4-N3	2.90	118.86	114.80
4	C	604	UDP	C6-N1-C2	-2.86	117.52	121.00
2	D	601	FBP	O3P-P1-O1	2.83	114.05	106.67
2	F	601	FBP	O5P-P2-O6	-2.74	99.53	106.67
2	D	601	FBP	O6P-P2-O5P	2.71	117.98	107.80
2	D	601	FBP	O1-P1-O1P	-2.70	99.15	106.44
6	B	606	OXL	O4-C2-C1	2.67	118.01	112.83
4	B	604	UDP	O2-C2-N1	-2.66	119.33	122.80
4	G	604	UDP	O4-C4-C5	-2.65	120.59	125.16
2	H	601	FBP	O1-P1-O1P	-2.59	99.43	106.44
2	E	601	FBP	O2-C2-O5	-2.59	104.35	109.33
4	G	604	UDP	O4-C4-N3	2.59	123.03	119.27
4	A	604	UDP	O2B-PB-O3A	2.59	113.32	104.64
2	D	601	FBP	O5-C5-C6	-2.59	103.42	109.50
4	D	604	UDP	C2'-C3'-C4'	-2.57	97.64	102.61
2	C	601	FBP	O2-C2-O5	-2.56	104.41	109.33
6	B	606	OXL	O3-C1-C2	2.53	117.73	112.83
2	A	601	FBP	O6P-P2-O5P	2.53	117.28	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	601	FBP	O5P-P2-O6	-2.50	100.15	106.67
6	H	604	OXL	O4-C2-C1	2.35	117.38	112.83
4	D	604	UDP	O3A-PB-O1B	-2.34	98.73	111.04
2	C	601	FBP	O6P-P2-O5P	2.32	116.50	107.80
2	E	601	FBP	O6P-P2-O6	-2.31	100.65	106.67
2	C	601	FBP	O1-P1-O1P	-2.30	100.22	106.44
4	E	604	UDP	O3B-PB-O2B	2.30	116.43	107.80
2	H	601	FBP	O5P-P2-O6	-2.30	100.68	106.67
4	F	604	UDP	O3B-PB-O2B	2.24	116.19	107.80
4	A	604	UDP	O2A-PA-O1A	2.23	122.80	112.44
4	B	604	UDP	O3A-PB-O1B	-2.20	99.47	111.04
4	E	604	UDP	O2B-PB-O3A	-2.20	97.26	104.64
6	D	606	OXL	O4-C2-C1	2.18	117.06	112.83
4	G	604	UDP	O2'-C2'-C3'	-2.18	104.83	111.82
2	E	601	FBP	O6P-P2-O5P	2.17	115.94	107.80
4	E	604	UDP	O4-C4-C5	-2.16	121.44	125.16
4	B	604	UDP	O2B-PB-O1B	2.16	119.25	110.83
4	A	604	UDP	O4'-C1'-N1	2.12	113.17	108.36
2	H	601	FBP	O6P-P2-O6	2.12	112.20	106.67
4	D	604	UDP	C6-C5-C4	-2.12	116.83	119.53
4	D	604	UDP	O5'-PA-O1A	-2.12	100.54	108.94
2	B	601	FBP	O3P-P1-O1	2.11	112.16	106.67
4	B	604	UDP	O3'-C3'-C2'	2.09	118.52	111.82
4	G	604	UDP	C2'-C1'-N1	-2.09	107.44	113.25
4	F	604	UDP	O4'-C4'-C3'	-2.09	101.01	105.15
4	D	604	UDP	C3'-C2'-C1'	2.06	105.36	101.46
2	G	601	FBP	O6P-P2-O5P	2.06	115.51	107.80
4	A	604	UDP	O3'-C3'-C2'	2.05	118.39	111.82
4	D	604	UDP	O2-C2-N1	-2.05	120.13	122.80
4	B	604	UDP	O2A-PA-O1A	2.04	121.95	112.44
2	B	601	FBP	O3P-P1-O2P	2.04	115.46	107.80
2	C	601	FBP	O2P-P1-O1P	2.02	118.70	110.83
2	C	601	FBP	O3P-P1-O2P	2.00	115.32	107.80

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	FBP	O1-C1-C2-C3
2	E	601	FBP	O1-C1-C2-C3
2	H	601	FBP	O1-C1-C2-C3
6	A	606	OXL	O3-C1-C2-O4

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Mol	Chain	Res	Type	Atoms
6	F	606	OXL	O3-C1-C2-O4
2	G	601	FBP	O1-C1-C2-C3
2	H	601	FBP	C1-O1-P1-O2P
6	A	606	OXL	O1-C1-C2-O2
6	C	606	OXL	O3-C1-C2-O4
6	D	606	OXL	O3-C1-C2-O4
6	E	606	OXL	O3-C1-C2-O4
6	H	604	OXL	O3-C1-C2-O4
6	B	606	OXL	O3-C1-C2-O4
6	G	606	OXL	O3-C1-C2-O4
2	C	601	FBP	O1-C1-C2-O2
2	E	601	FBP	O1-C1-C2-O2
2	H	601	FBP	O1-C1-C2-O2
6	C	606	OXL	O1-C1-C2-O2
6	D	606	OXL	O1-C1-C2-O2
6	E	606	OXL	O1-C1-C2-O2
6	F	606	OXL	O3-C1-C2-O2
6	H	604	OXL	O1-C1-C2-O2
6	B	606	OXL	O1-C1-C2-O2
6	F	606	OXL	O1-C1-C2-O2
6	G	606	OXL	O1-C1-C2-O2
2	H	601	FBP	C6-O6-P2-O4P
6	A	606	OXL	O1-C1-C2-O4
6	A	606	OXL	O3-C1-C2-O2
6	B	606	OXL	O3-C1-C2-O2
6	G	606	OXL	O1-C1-C2-O4
2	F	601	FBP	O1-C1-C2-C3
4	E	604	UDP	PB-O3A-PA-O1A
4	E	604	UDP	PB-O3A-PA-O2A
6	C	606	OXL	O1-C1-C2-O4
6	B	606	OXL	O1-C1-C2-O4
6	D	606	OXL	O1-C1-C2-O4
6	D	606	OXL	O3-C1-C2-O2
6	E	606	OXL	O3-C1-C2-O2
6	F	606	OXL	O1-C1-C2-O4
6	H	604	OXL	O1-C1-C2-O4
2	A	601	FBP	C1-O1-P1-O2P
2	B	601	FBP	C1-O1-P1-O2P
2	C	601	FBP	C1-O1-P1-O2P
2	E	601	FBP	C1-O1-P1-O2P
6	C	606	OXL	O3-C1-C2-O2
6	E	606	OXL	O1-C1-C2-O4

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Mol	Chain	Res	Type	Atoms
6	G	606	OXL	O3-C1-C2-O2
6	H	604	OXL	O3-C1-C2-O2
4	A	604	UDP	PB-O3A-PA-O1A
4	D	604	UDP	PB-O3A-PA-O2A
2	F	601	FBP	O1-C1-C2-O2
2	G	601	FBP	O1-C1-C2-O2
4	A	604	UDP	PB-O3A-PA-O2A
4	B	604	UDP	PB-O3A-PA-O2A
4	F	604	UDP	PB-O3A-PA-O1A

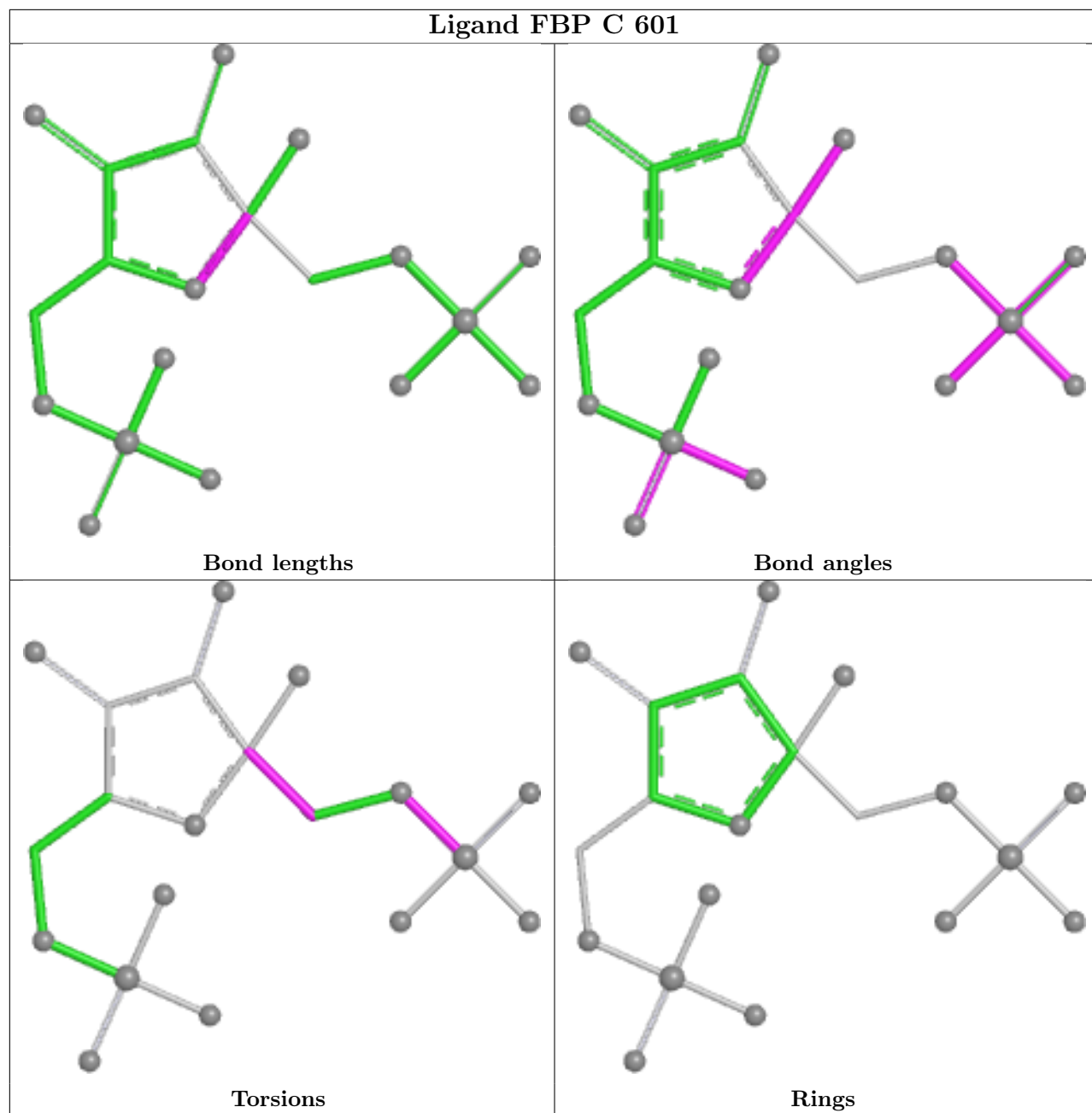
There are no ring outliers.

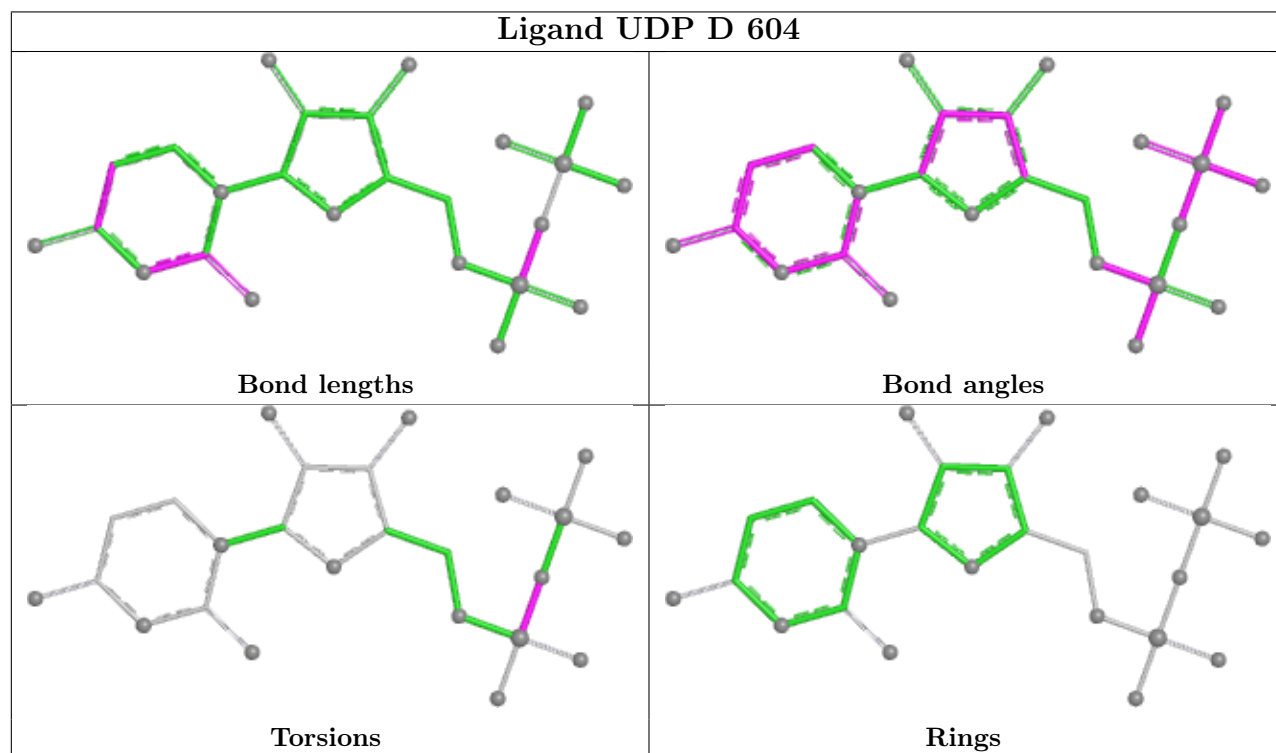
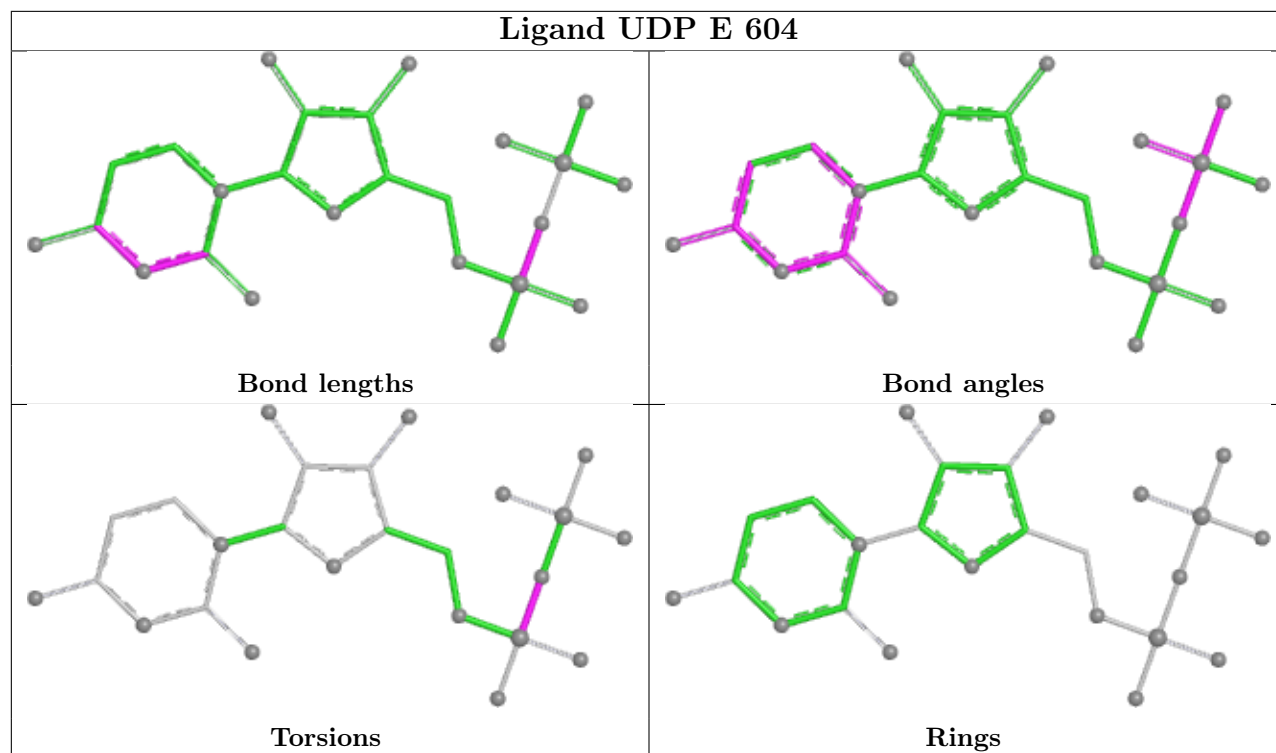
2 monomers are involved in 2 short contacts:

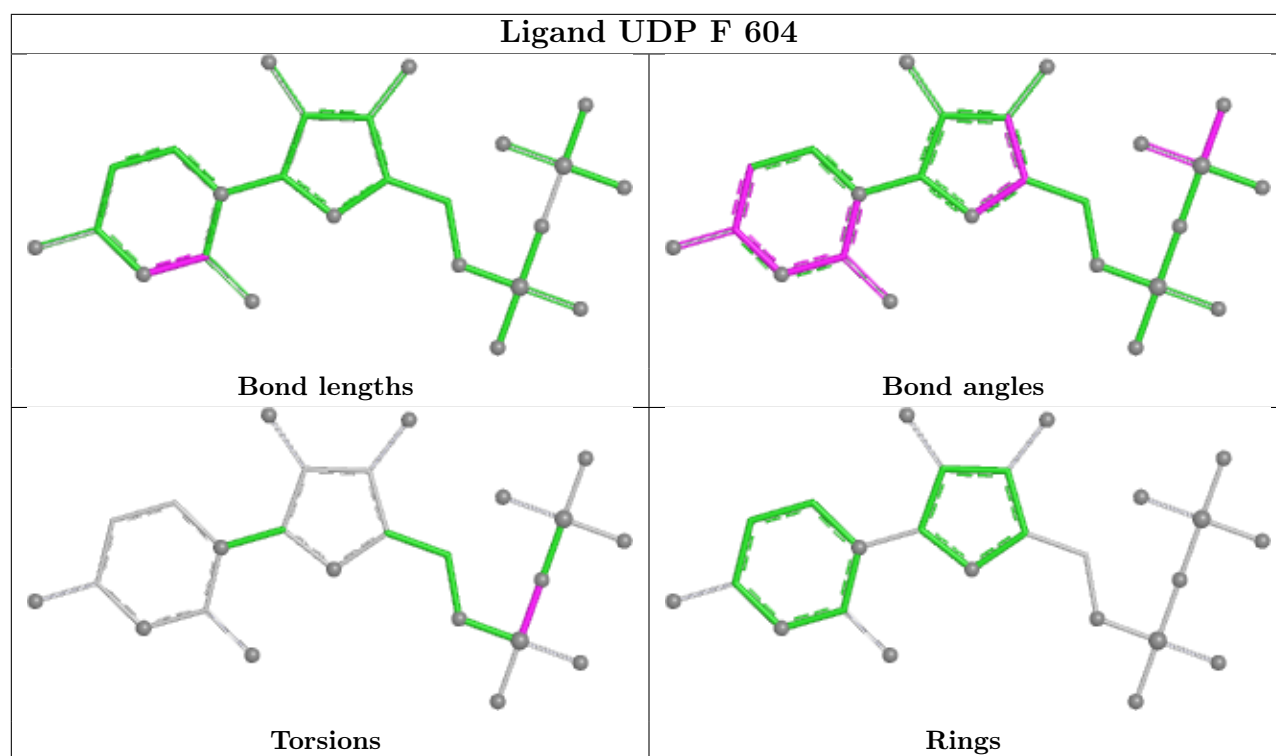
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	604	UDP	1	0
4	F	604	UDP	1	0

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.

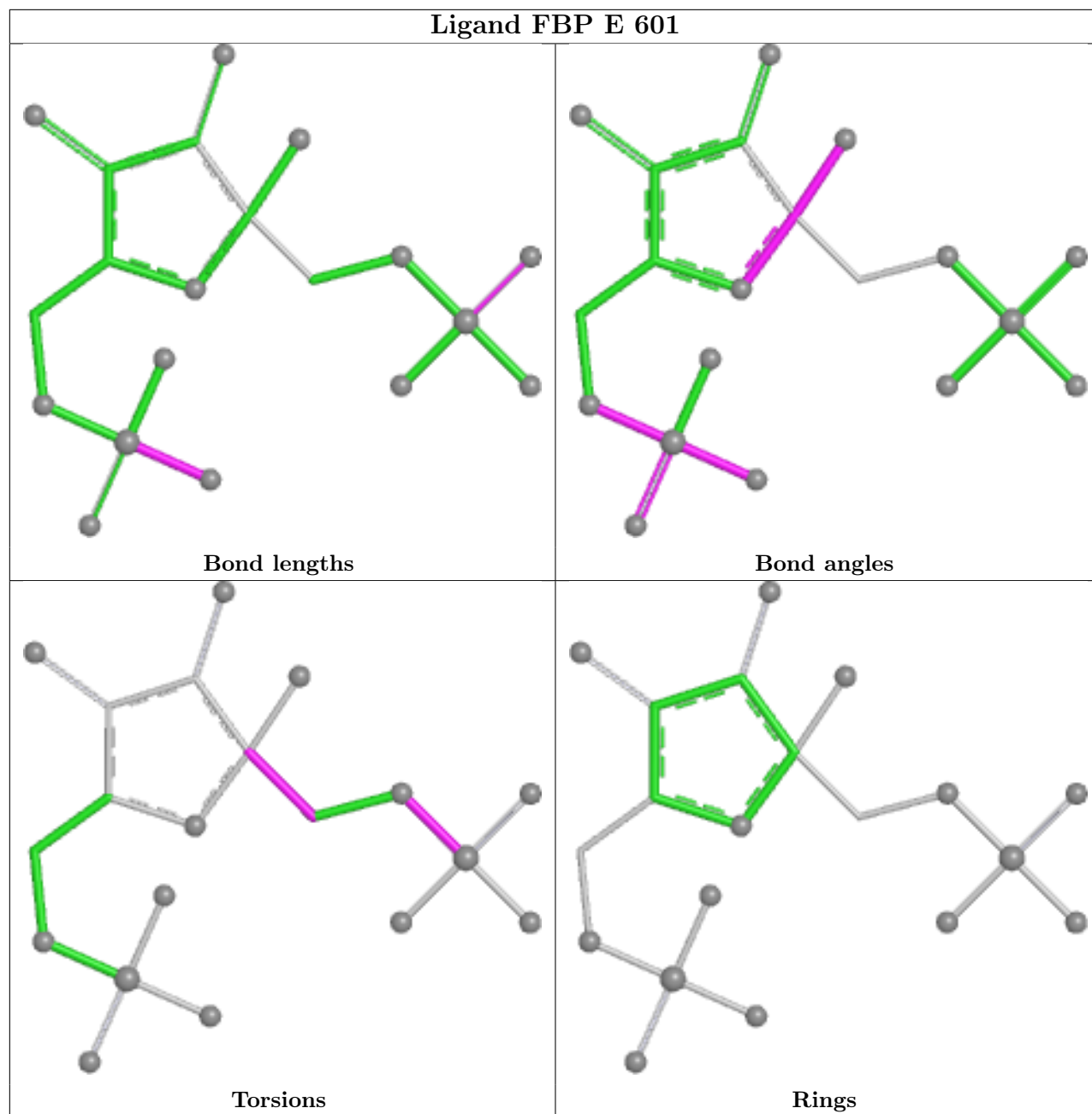
Ligand FBP C 601

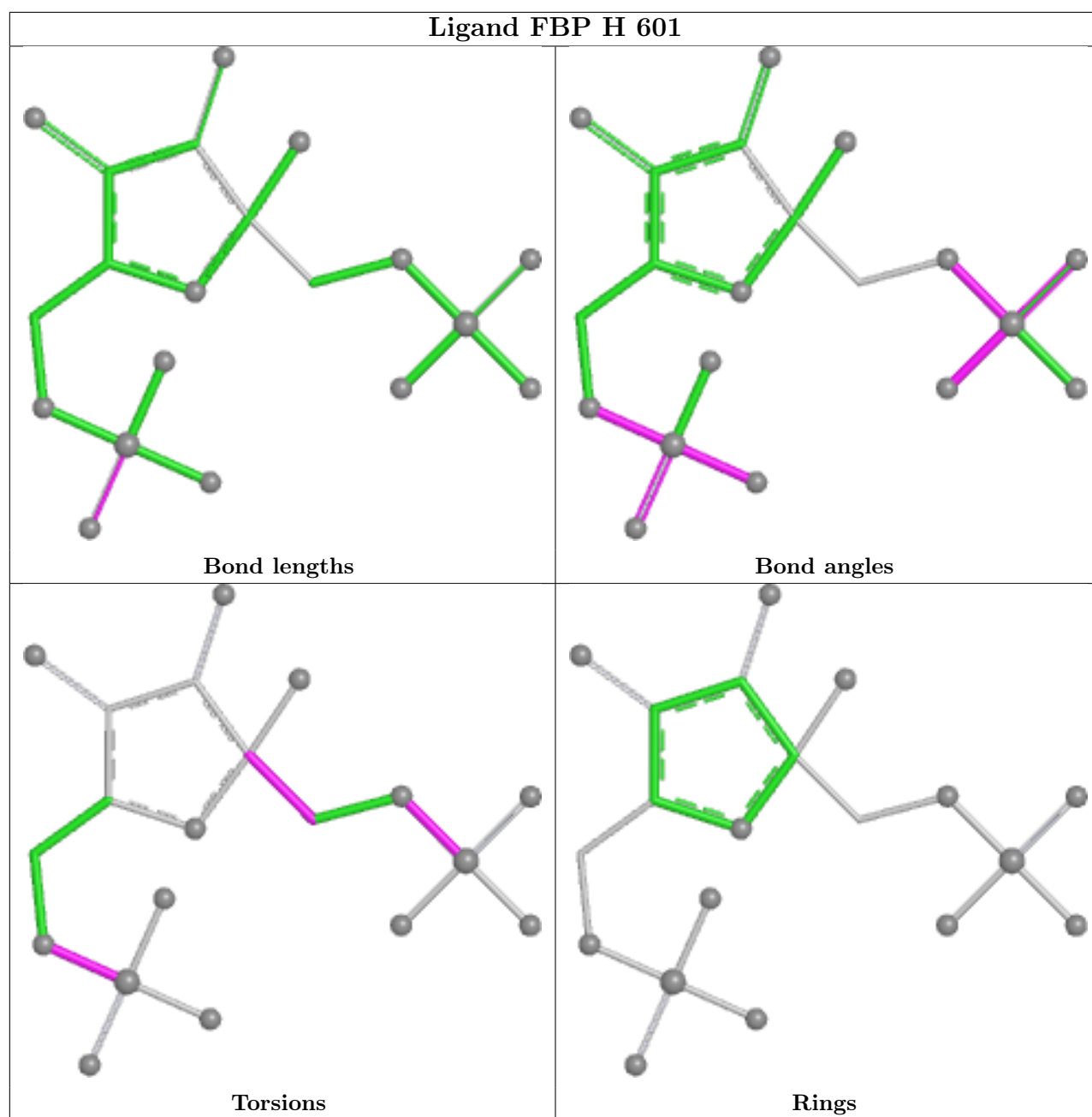


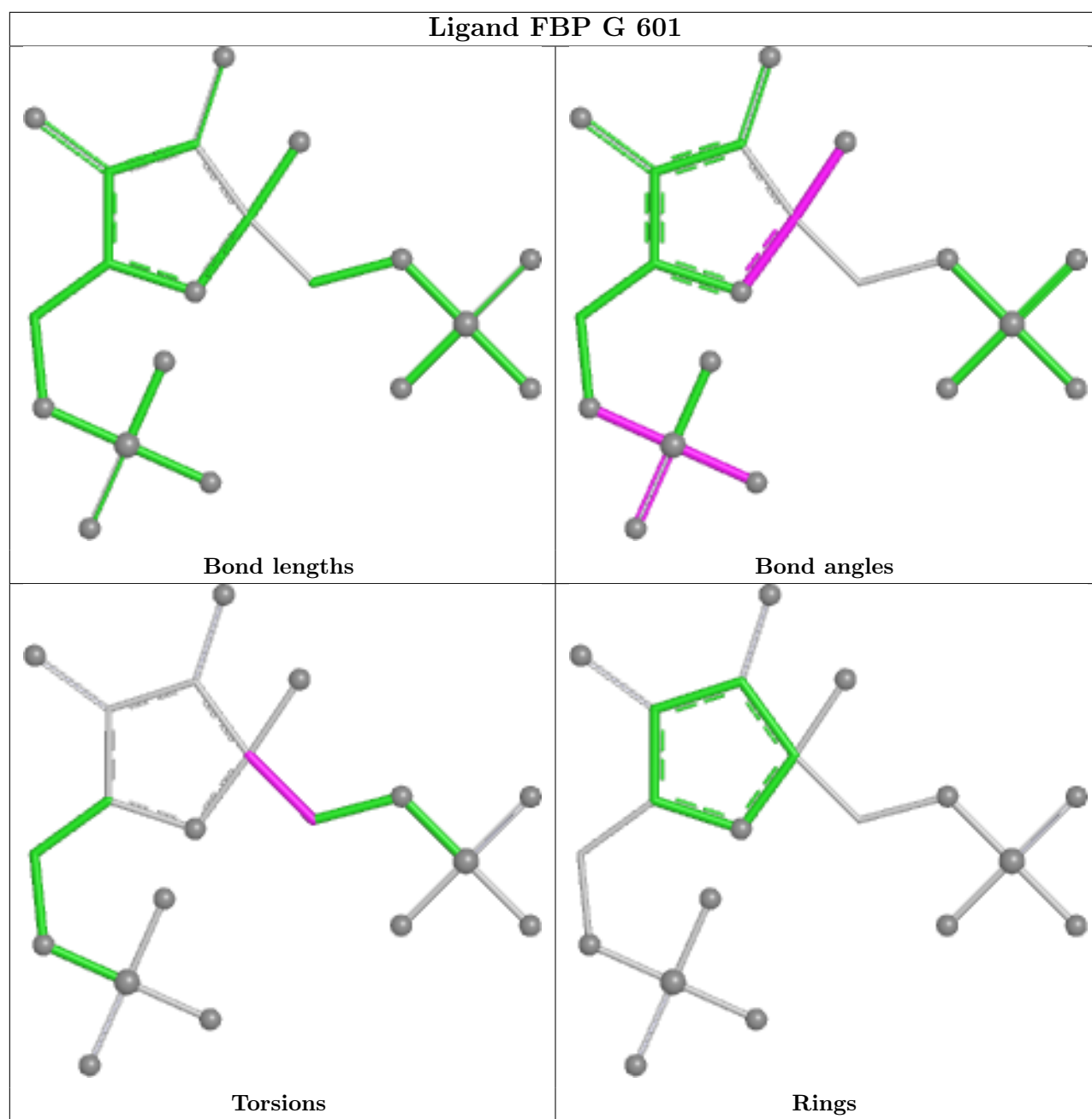


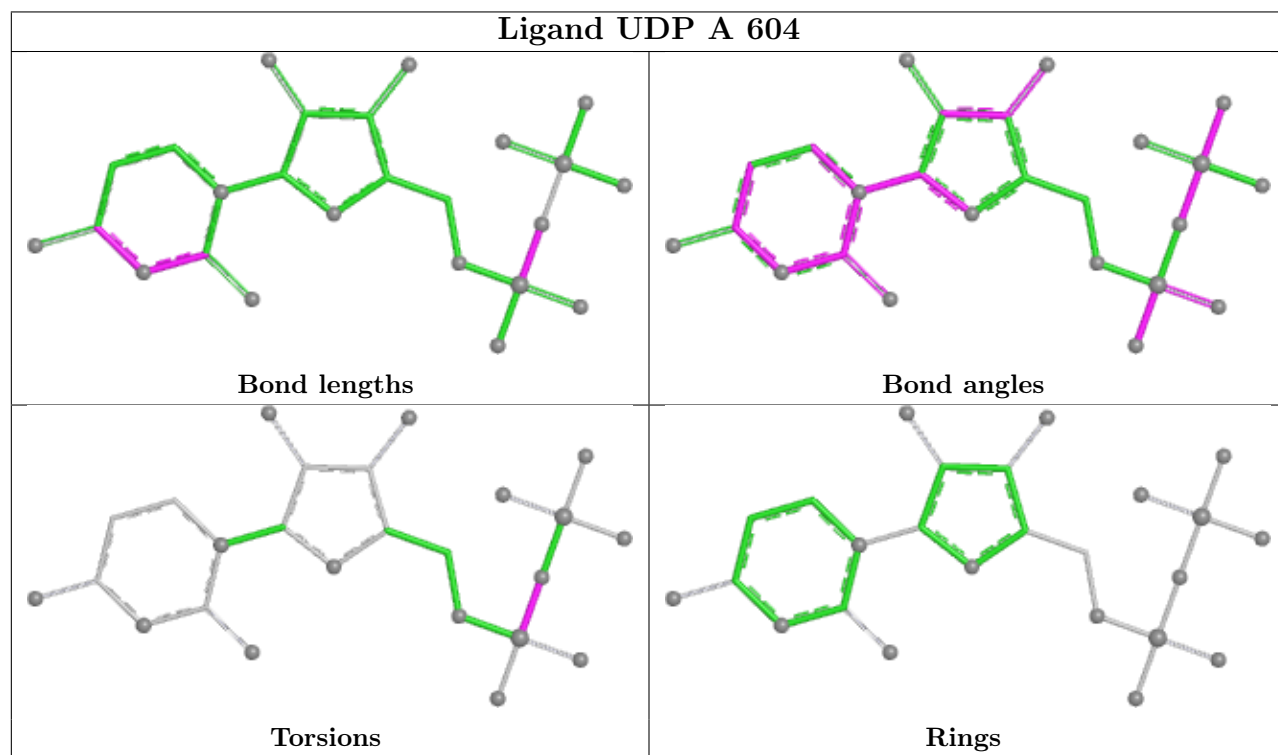
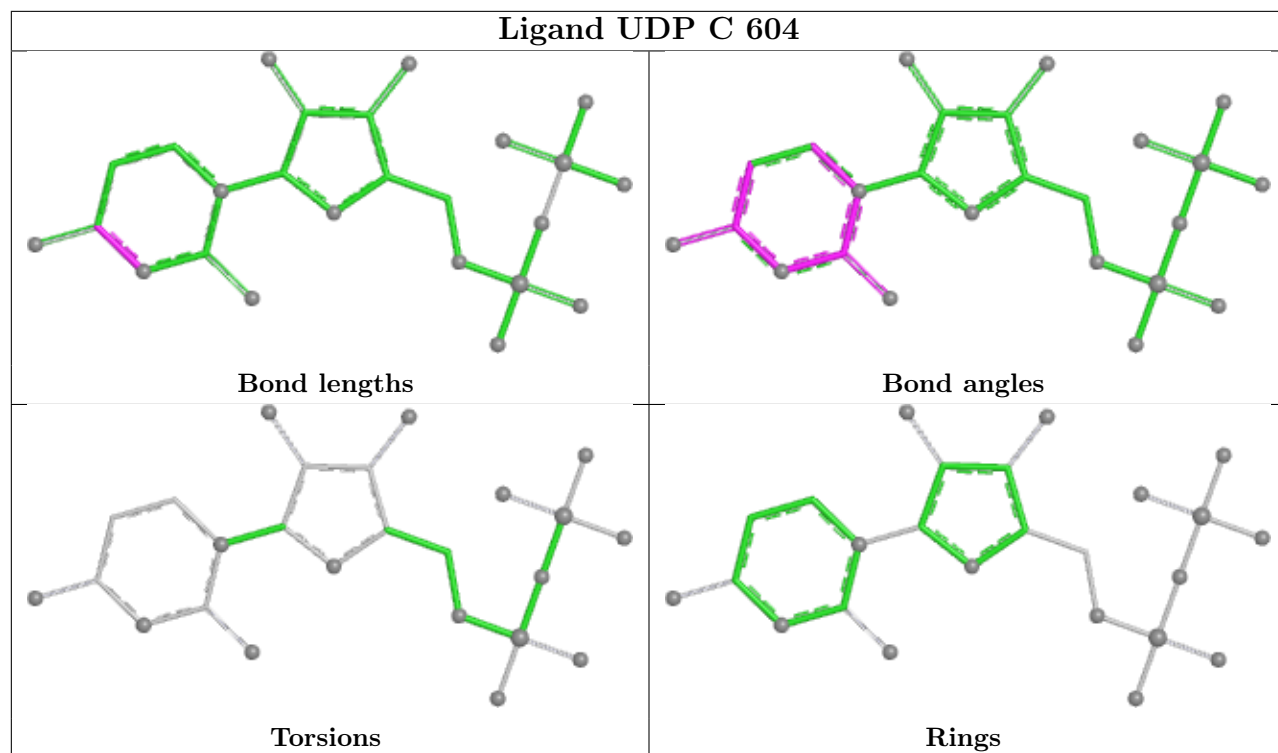


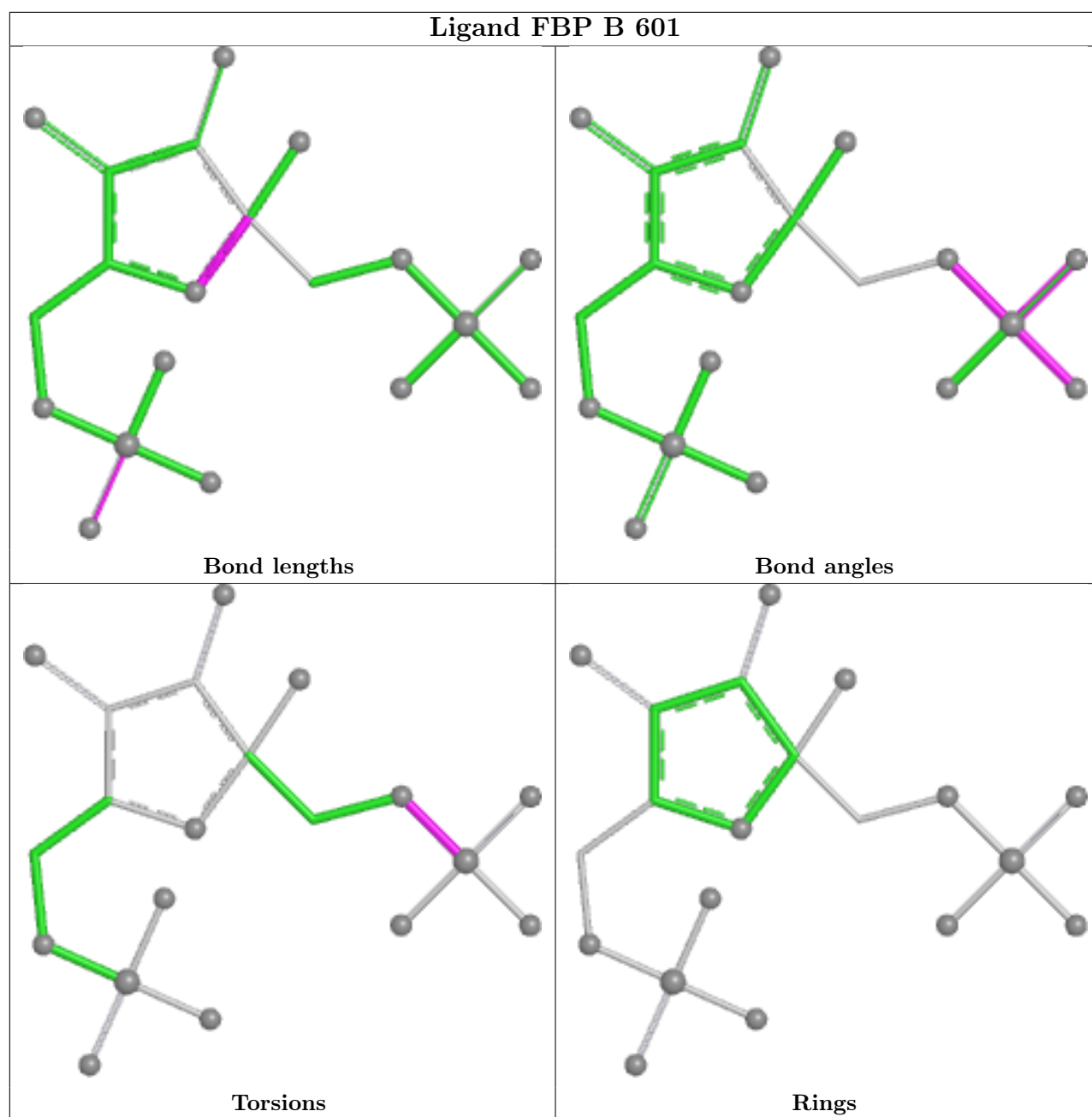
Ligand FBP E 601

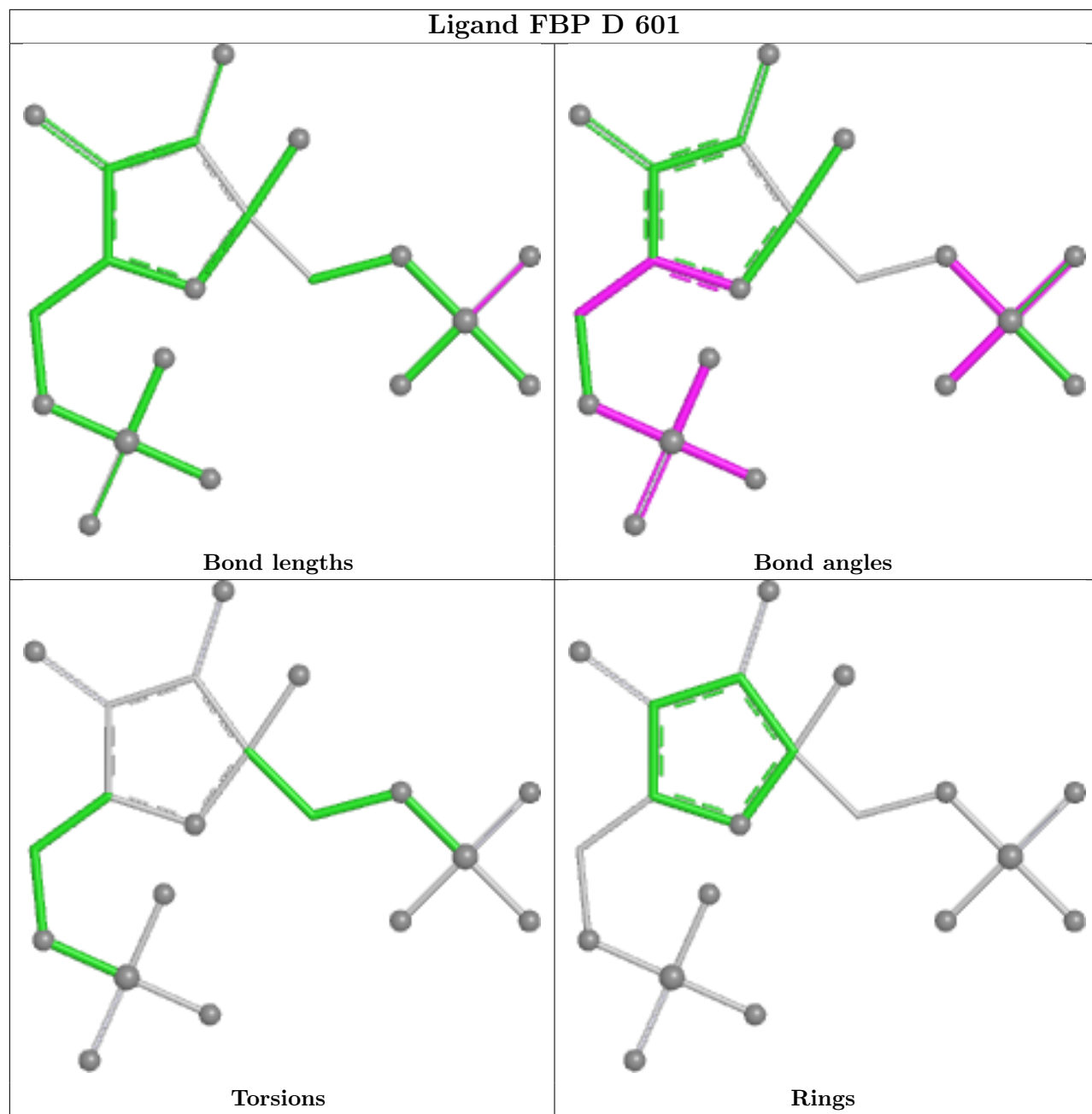


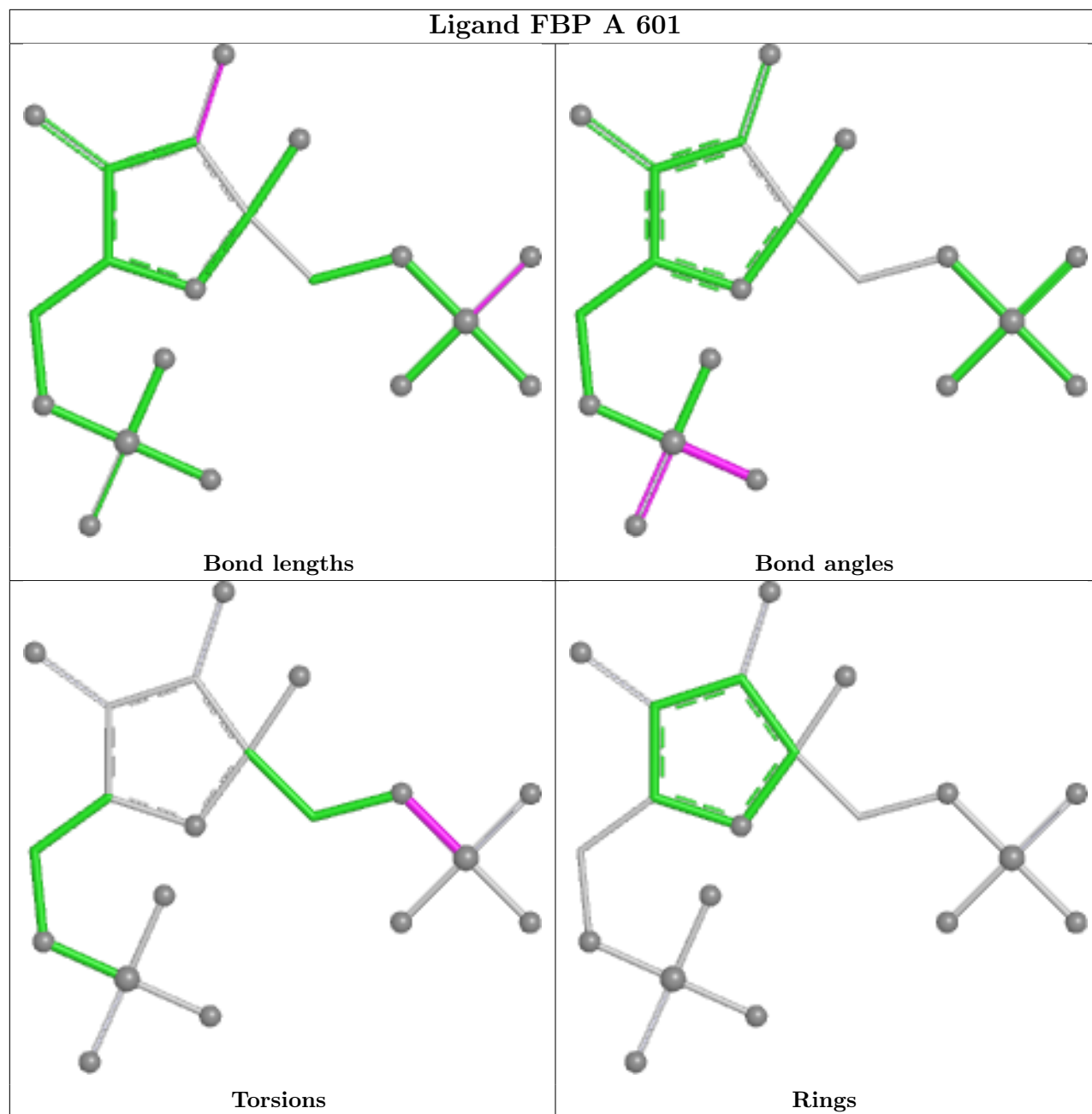




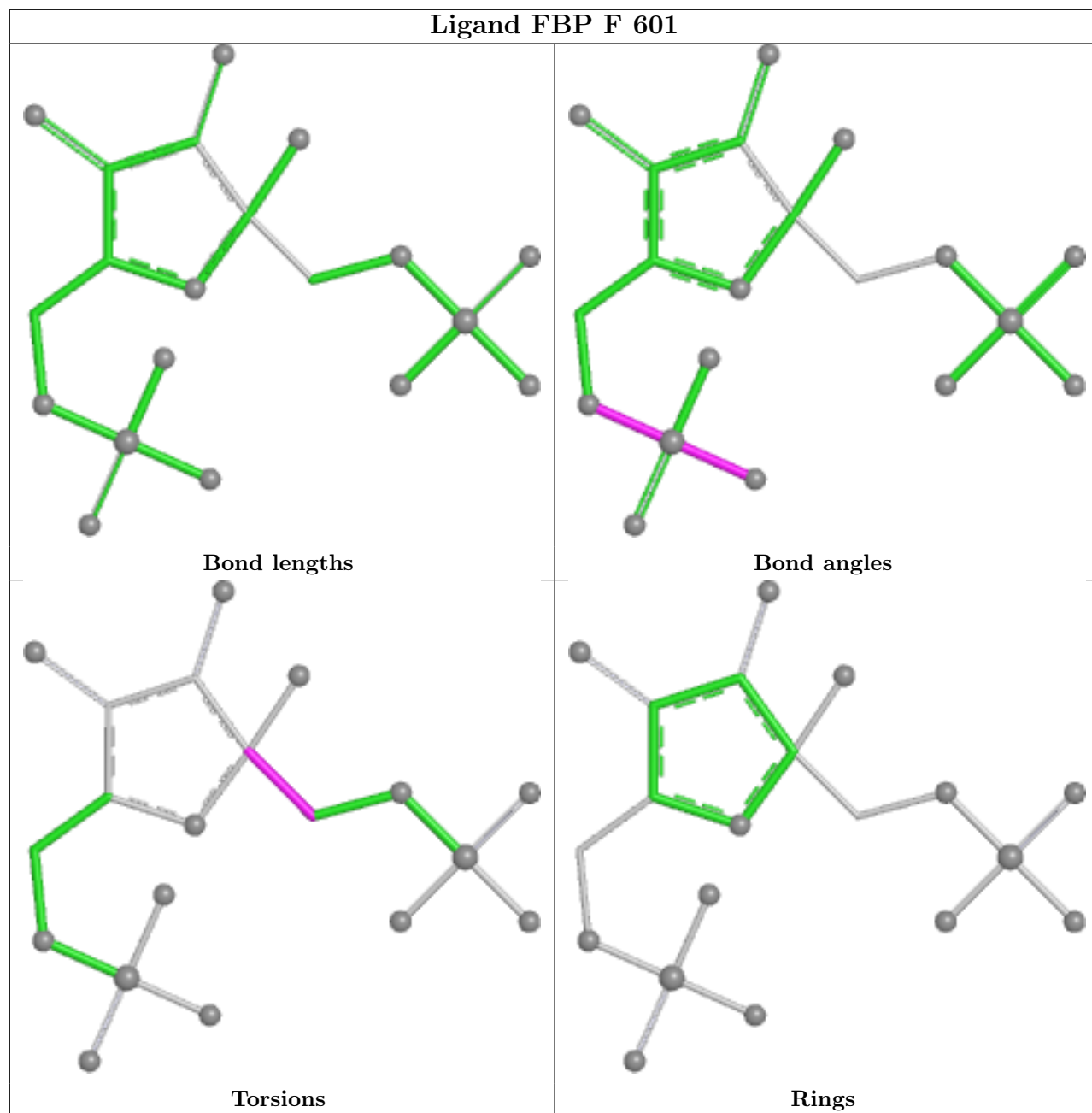


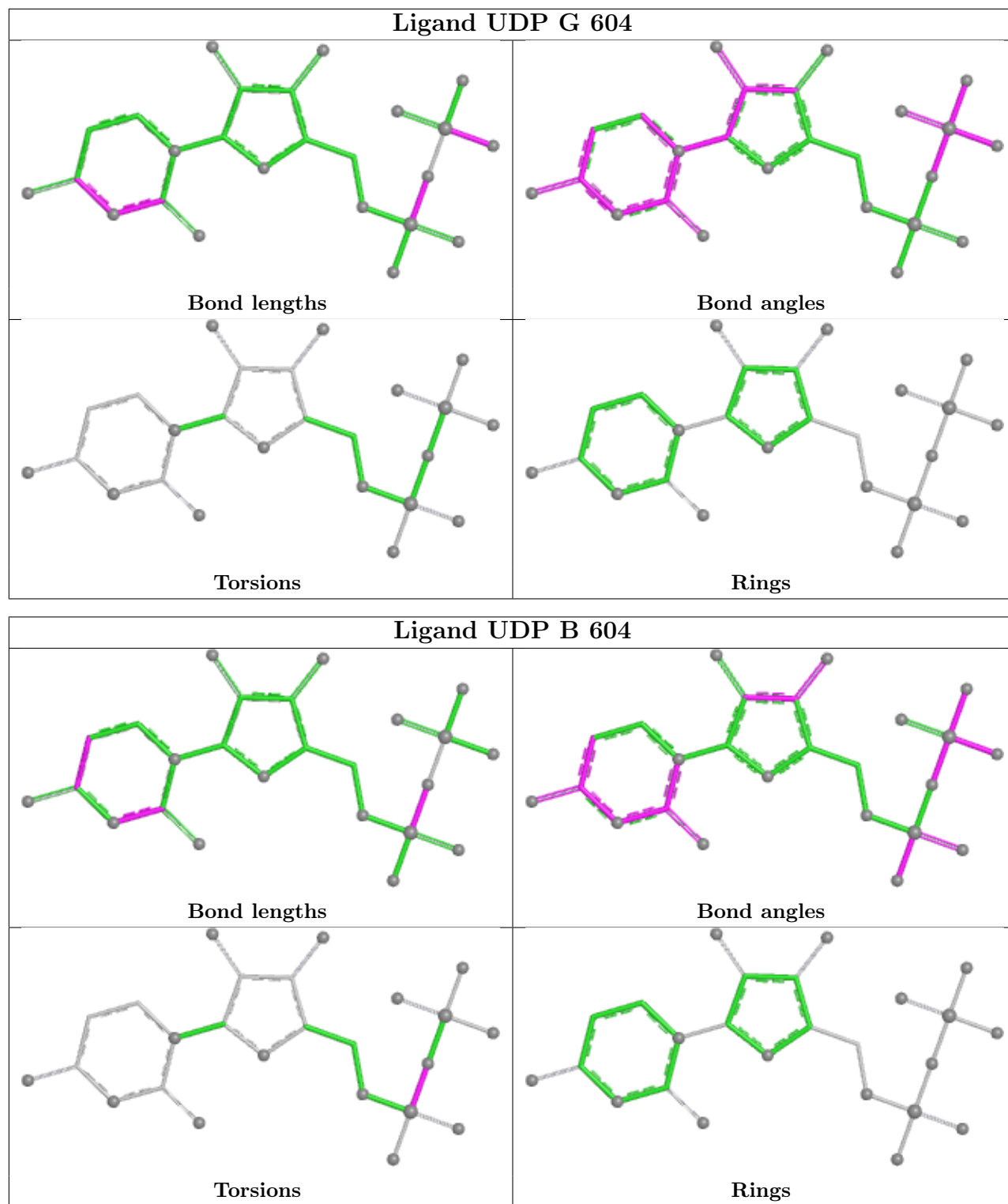






Ligand FBP F 601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	501/521 (96%)	-0.02	2 (0%) 88 90	25, 36, 55, 94	0
1	B	501/521 (96%)	0.53	65 (12%) 7 7	26, 40, 76, 117	0
1	C	501/521 (96%)	-0.29	3 (0%) 85 87	22, 30, 47, 83	0
1	D	501/521 (96%)	0.22	44 (8%) 15 16	23, 33, 59, 98	0
1	E	501/521 (96%)	-0.12	4 (0%) 82 85	24, 34, 51, 79	0
1	F	501/521 (96%)	0.15	13 (2%) 57 61	24, 37, 67, 109	0
1	G	501/521 (96%)	-0.23	2 (0%) 88 90	23, 32, 50, 83	0
1	H	501/521 (96%)	0.26	40 (7%) 18 19	24, 36, 79, 120	0
All	All	4008/4168 (96%)	0.06	173 (4%) 40 42	22, 34, 65, 120	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	129	ILE	5.1
1	B	180	ILE	4.7
1	B	128	VAL	4.6
1	B	172	VAL	4.4
1	D	103	ALA	4.4
1	D	172	VAL	4.4
1	B	122	ILE	4.2
1	H	103	ALA	4.2
1	B	145	VAL	4.1
1	D	174	VAL	4.0
1	B	174	VAL	4.0
1	B	131	LEU	3.8
1	D	131	LEU	3.7
1	B	114	ILE	3.6
1	B	151	VAL	3.5
1	H	156	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	167	THR	3.5
1	D	129	ILE	3.5
1	D	134	ALA	3.5
1	H	95	ARG	3.4
1	B	103	ALA	3.4
1	B	96	THR	3.4
1	D	180	ILE	3.4
1	B	134	ALA	3.3
1	B	117	ALA	3.2
1	C	501	ARG	3.2
1	D	108	TYR	3.2
1	D	114	ILE	3.2
1	D	130	ALA	3.2
1	D	167	THR	3.2
1	B	123	LYS	3.2
1	D	98	LEU	3.2
1	H	104	LYS	3.2
1	B	130	ALA	3.1
1	H	161	VAL	3.1
1	H	114	ILE	3.1
1	H	139	ILE	3.1
1	B	153	ASP	3.1
1	H	98	LEU	3.1
1	H	96	THR	3.1
1	H	24	GLY	3.1
1	B	94	ILE	3.0
1	D	158	LEU	3.0
1	C	1	MET	3.0
1	D	156	LEU	3.0
1	B	116	VAL	3.0
1	D	145	VAL	3.0
1	E	370	TYR	3.0
1	B	181	ALA	3.0
1	G	102	GLU	3.0
1	B	179	ILE	3.0
1	B	106	TYR	2.9
1	B	140	TYR	2.9
1	H	370	TYR	2.9
1	D	122	ILE	2.9
1	D	1	MET	2.9
1	F	135	GLY	2.9
1	A	1	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	27	GLY	2.9
1	B	161	VAL	2.8
1	H	174	VAL	2.8
1	D	197	ALA	2.8
1	D	135	GLY	2.8
1	H	111	GLY	2.8
1	D	94	ILE	2.8
1	F	1	MET	2.8
1	D	166	ALA	2.8
1	E	102	GLU	2.7
1	B	98	LEU	2.7
1	D	128	VAL	2.7
1	G	1	MET	2.7
1	B	192	LYS	2.7
1	F	166	ALA	2.7
1	B	455	THR	2.7
1	D	96	THR	2.7
1	H	180	ILE	2.7
1	H	128	VAL	2.7
1	D	170	PHE	2.6
1	H	172	VAL	2.6
1	B	166	ALA	2.6
1	B	111	GLY	2.6
1	D	181	ALA	2.6
1	F	117	ALA	2.6
1	B	99	PHE	2.6
1	B	170	PHE	2.6
1	D	370	TYR	2.5
1	H	501	ARG	2.5
1	D	173	GLU	2.5
1	B	152	ASP	2.5
1	H	150	LEU	2.5
1	H	158	LEU	2.5
1	H	179	ILE	2.5
1	F	501	ARG	2.5
1	A	102	GLU	2.5
1	D	151	VAL	2.5
1	B	150	LEU	2.5
1	H	157	GLY	2.5
1	H	117	ALA	2.5
1	H	143	VAL	2.5
1	B	30	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	197	ALA	2.4
1	B	133	VAL	2.4
1	B	1	MET	2.4
1	B	139	ILE	2.4
1	D	161	VAL	2.4
1	H	151	VAL	2.4
1	B	132	ASN	2.4
1	F	122	ILE	2.4
1	D	127	GLU	2.4
1	B	178	GLY	2.4
1	H	116	VAL	2.4
1	H	408	LYS	2.4
1	D	150	LEU	2.3
1	B	370	TYR	2.3
1	D	179	ILE	2.3
1	H	192	LYS	2.3
1	B	501	ARG	2.3
1	B	28	TYR	2.3
1	D	99	PHE	2.3
1	D	140	TYR	2.3
1	F	370	TYR	2.3
1	H	140	TYR	2.3
1	H	122	ILE	2.3
1	B	24	GLY	2.3
1	B	124	SER	2.3
1	F	116	VAL	2.3
1	H	153	ASP	2.3
1	B	156	LEU	2.3
1	B	162	ALA	2.2
1	D	169	GLU	2.2
1	H	173	GLU	2.2
1	B	143	VAL	2.2
1	D	186	VAL	2.2
1	H	145	VAL	2.2
1	B	104	LYS	2.2
1	H	1	MET	2.2
1	B	110	THR	2.2
1	D	149	VAL	2.2
1	D	153	ASP	2.2
1	H	487	GLY	2.2
1	C	370	TYR	2.2
1	H	170	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	21	LYS	2.2
1	E	1	MET	2.2
1	B	149	VAL	2.2
1	B	186	VAL	2.2
1	F	161	VAL	2.2
1	B	19	GLY	2.2
1	B	108	TYR	2.1
1	H	129	ILE	2.1
1	H	167	THR	2.1
1	B	135	GLY	2.1
1	B	158	LEU	2.1
1	D	139	ILE	2.1
1	F	167	THR	2.1
1	B	169	GLU	2.1
1	B	173	GLU	2.1
1	D	152	ASP	2.1
1	D	177	ASP	2.1
1	F	140	TYR	2.1
1	B	107	SER	2.1
1	B	29	TRP	2.1
1	H	131	LEU	2.1
1	H	166	ALA	2.1
1	F	26	ASP	2.1
1	B	163	LYS	2.0
1	B	154	GLY	2.0
1	H	185	GLY	2.0
1	F	137	LEU	2.0
1	D	109	LYS	2.0
1	D	154	GLY	2.0
1	E	368	ASN	2.0
1	D	133	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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.

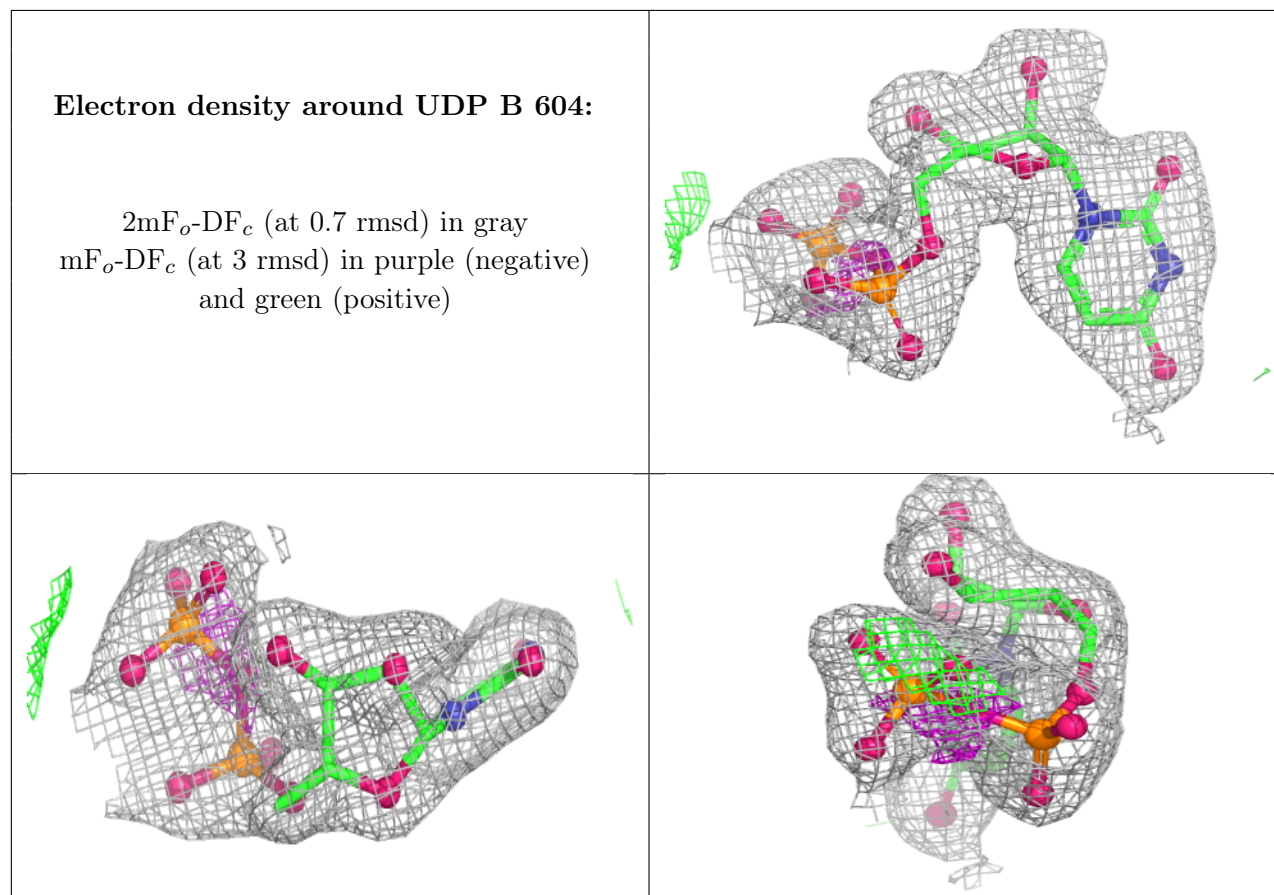
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	B	603	1/1	0.90	0.09	60,60,60,60	0
6	OXL	B	606	6/6	0.92	0.09	36,38,46,49	0
6	OXL	F	606	6/6	0.94	0.09	33,34,38,42	0
6	OXL	H	604	6/6	0.94	0.07	34,35,43,43	0
6	OXL	A	606	6/6	0.95	0.07	35,36,40,43	0
4	UDP	B	604	25/25	0.95	0.08	42,49,53,57	0
6	OXL	D	606	6/6	0.96	0.11	32,33,37,46	0
4	UDP	D	604	25/25	0.96	0.07	35,40,43,50	0
6	OXL	G	606	6/6	0.96	0.10	31,34,38,45	0
5	K	B	605	1/1	0.96	0.11	52,52,52,52	0
3	MG	D	603	1/1	0.97	0.16	50,50,50,50	0
5	K	A	605	1/1	0.97	0.08	41,41,41,41	0
6	OXL	C	606	6/6	0.97	0.07	28,31,32,38	0
2	FBP	E	601	20/20	0.97	0.06	30,34,40,43	0
6	OXL	E	606	6/6	0.97	0.06	33,40,42,47	0
5	K	D	605	1/1	0.97	0.09	42,42,42,42	0
5	K	E	605	1/1	0.97	0.09	45,45,45,45	0
5	K	F	605	1/1	0.97	0.09	44,44,44,44	0
2	FBP	C	601	20/20	0.98	0.04	27,30,34,41	0
4	UDP	A	604	25/25	0.98	0.05	30,33,36,38	0
5	K	G	605	1/1	0.98	0.09	40,40,40,40	0
2	FBP	D	601	20/20	0.98	0.05	25,32,38,44	0
2	FBP	A	601	20/20	0.98	0.05	27,35,37,50	0
4	UDP	E	604	25/25	0.98	0.05	29,32,35,35	0
4	UDP	F	604	25/25	0.98	0.05	31,35,40,40	0
2	FBP	F	601	20/20	0.98	0.06	28,34,42,46	0
2	FBP	H	601	20/20	0.98	0.05	29,34,39,45	0
5	K	C	605	1/1	0.98	0.07	37,37,37,37	0
2	FBP	B	601	20/20	0.98	0.05	29,36,41,49	0
3	MG	F	603	1/1	0.99	0.05	37,37,37,37	0
3	MG	G	602	1/1	0.99	0.04	36,36,36,36	0
3	MG	A	603	1/1	0.99	0.03	36,36,36,36	0
3	MG	B	602	1/1	0.99	0.02	38,38,38,38	0
5	K	H	603	1/1	0.99	0.06	43,43,43,43	0
4	UDP	C	604	25/25	0.99	0.04	24,27,30,30	0
2	FBP	G	601	20/20	0.99	0.04	30,36,38,48	0
3	MG	C	602	1/1	0.99	0.04	37,37,37,37	0

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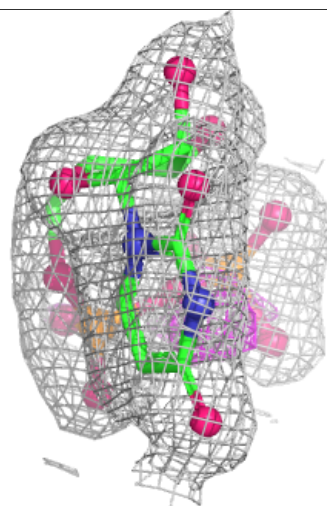
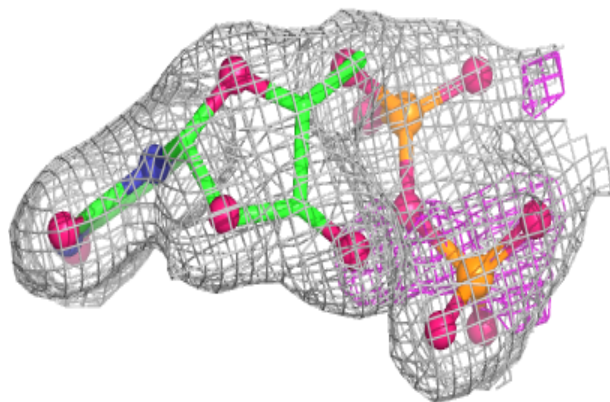
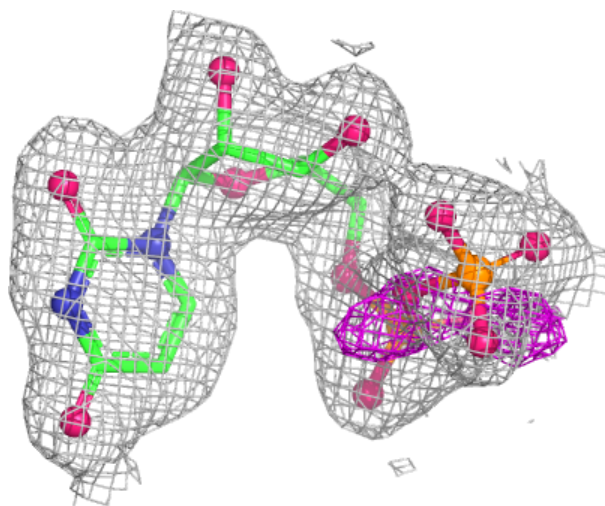
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	602	1/1	0.99	0.04	38,38,38,38	0
4	UDP	G	604	25/25	0.99	0.04	27,29,32,32	0
3	MG	E	602	1/1	0.99	0.07	37,37,37,37	0
3	MG	E	603	1/1	0.99	0.02	35,35,35,35	0
3	MG	F	602	1/1	0.99	0.05	43,43,43,43	0
3	MG	H	602	1/1	1.00	0.01	37,37,37,37	0
3	MG	C	603	1/1	1.00	0.02	28,28,28,28	0
3	MG	D	602	1/1	1.00	0.01	30,30,30,30	0
3	MG	G	603	1/1	1.00	0.04	33,33,33,33	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.



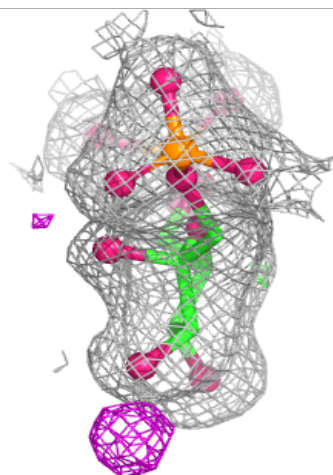
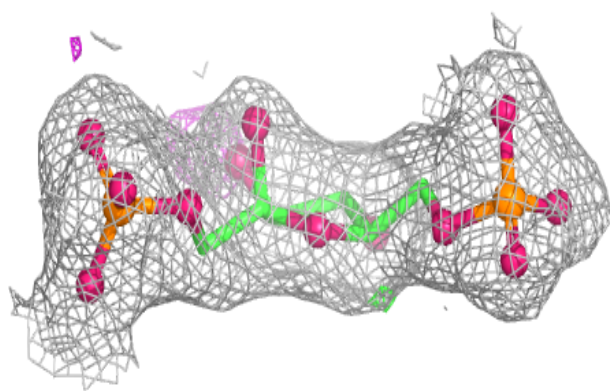
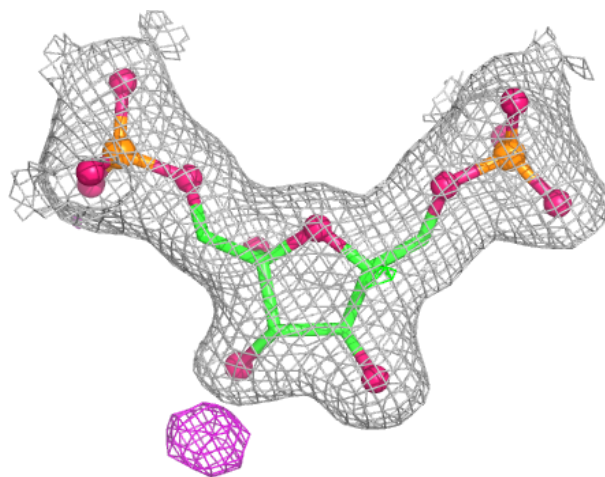
Electron density around UDP D 604:

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



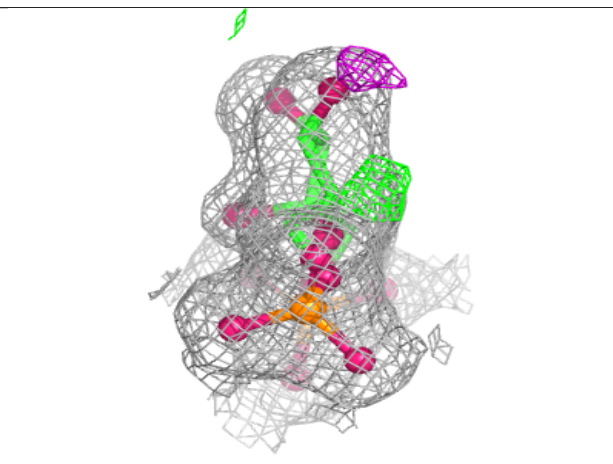
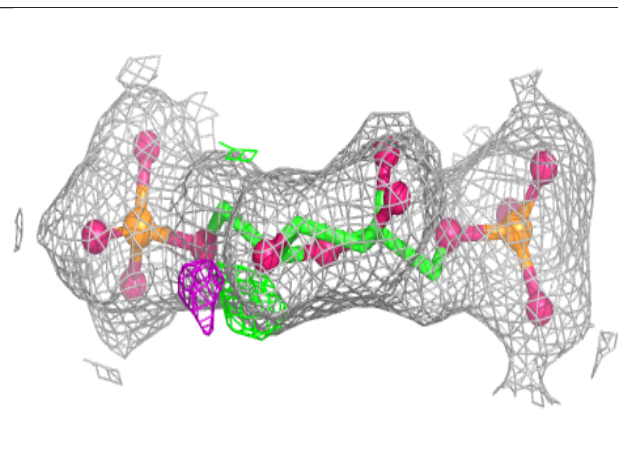
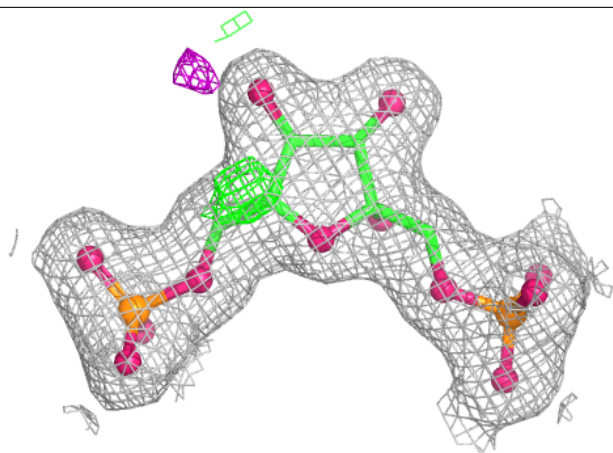
Electron density around FBP E 601:

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



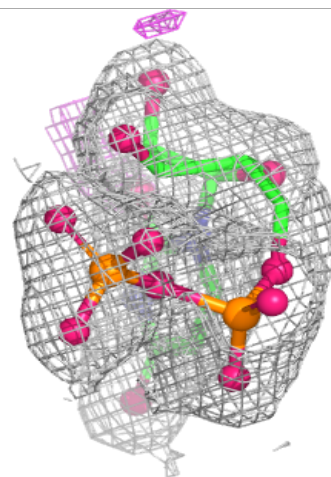
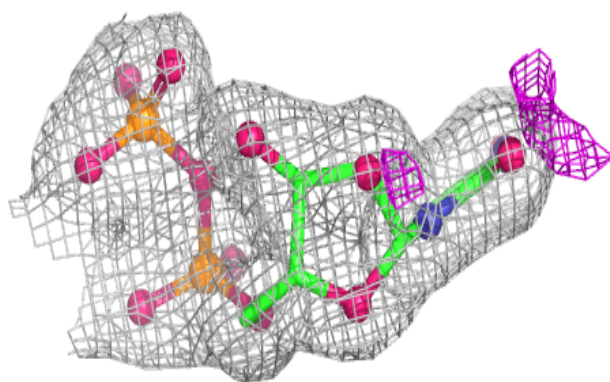
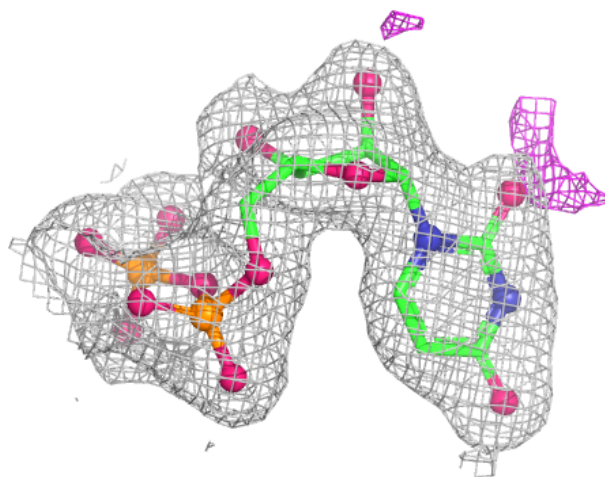
Electron density around FBP C 601:

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



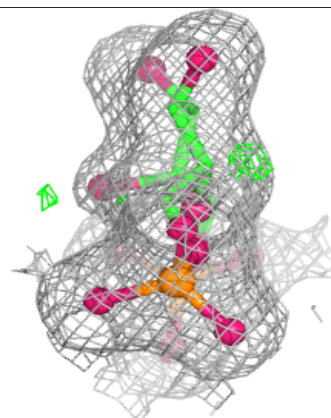
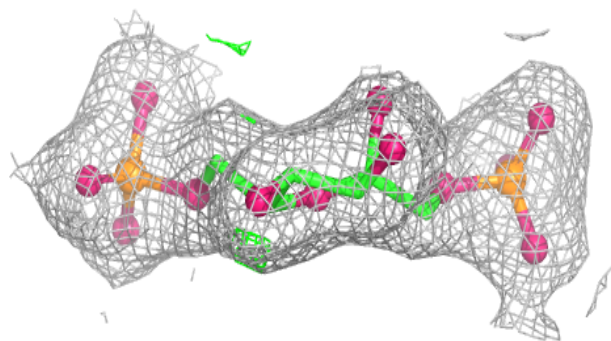
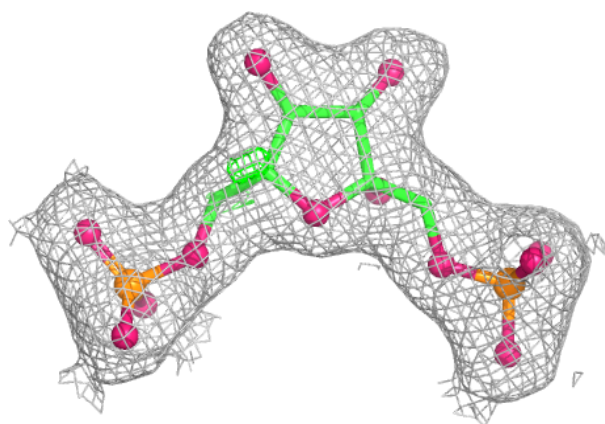
Electron density around UDP A 604:

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



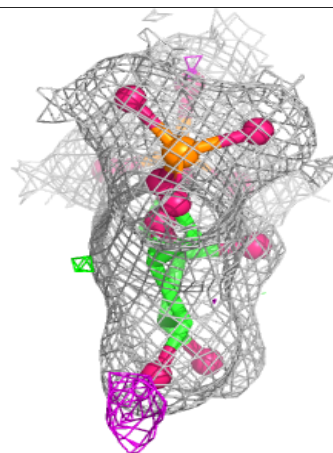
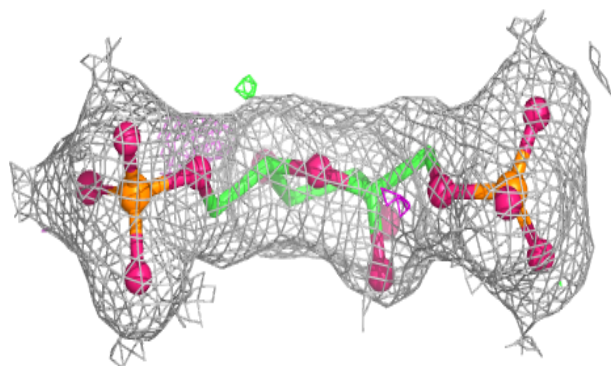
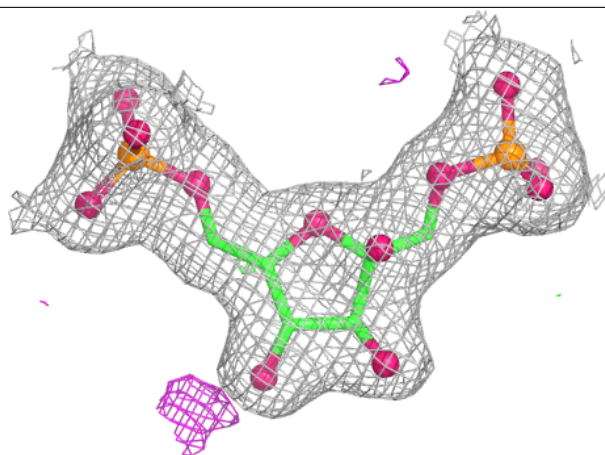
Electron density around FBP D 601:

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



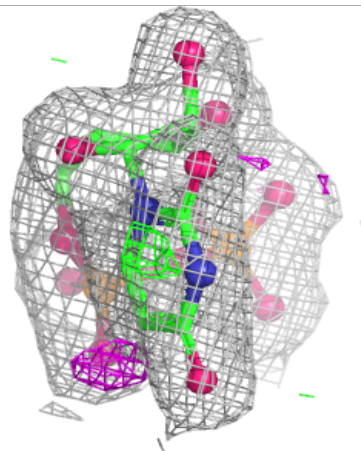
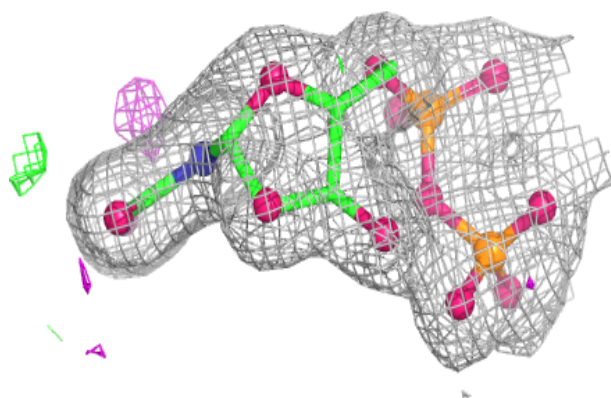
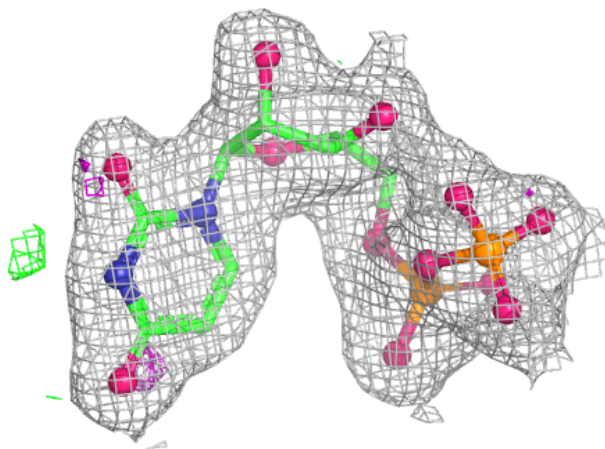
Electron density around FBP A 601:

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



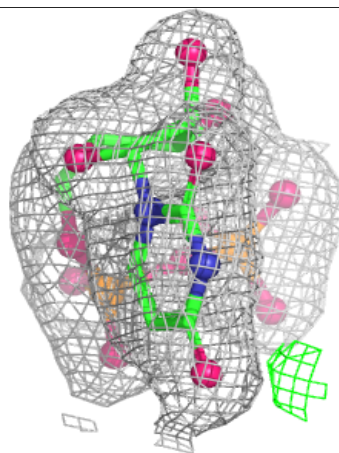
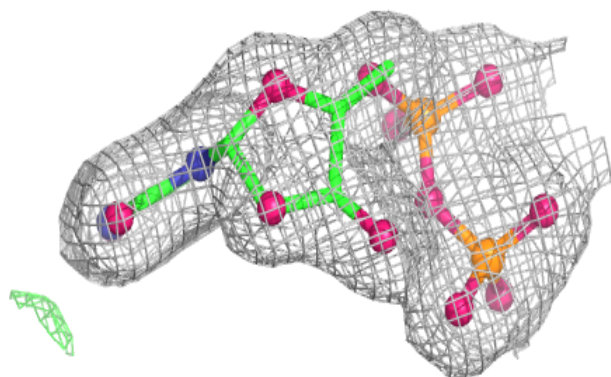
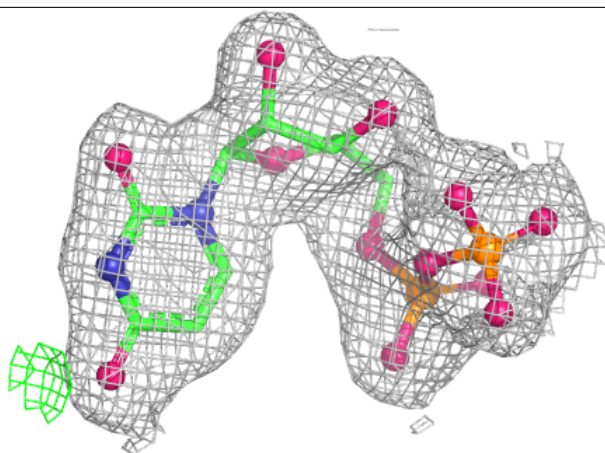
Electron density around UDP E 604:

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and green (positive)

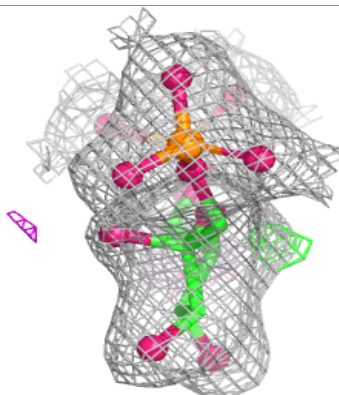
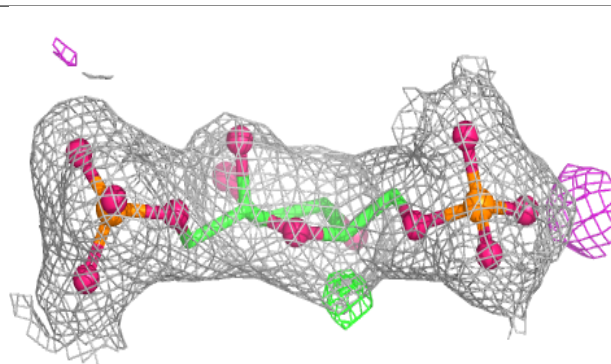
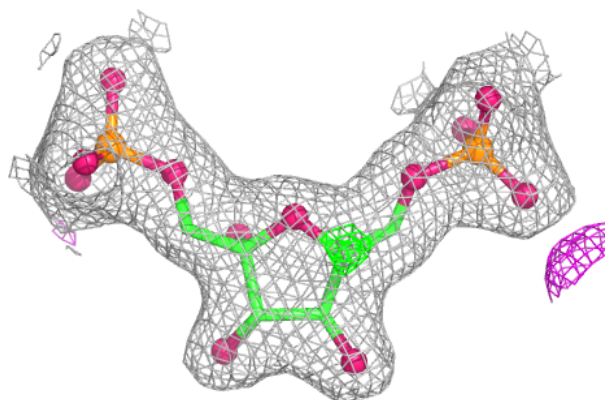


Electron density around UDP F 604:

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and green (positive)

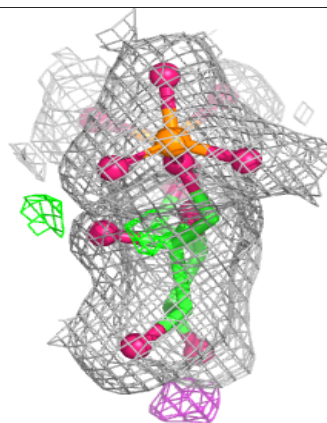
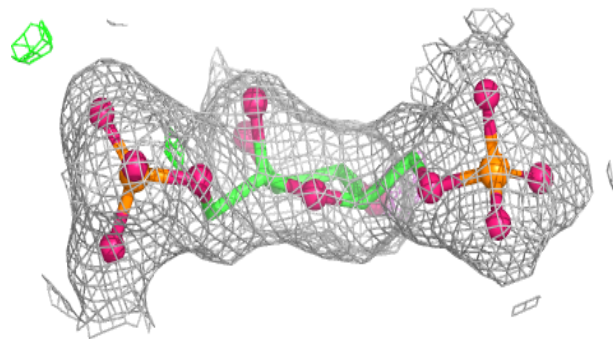
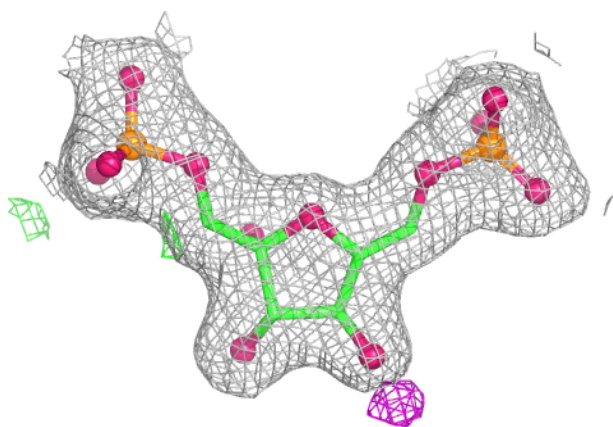
**Electron density around FBP F 601:**

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



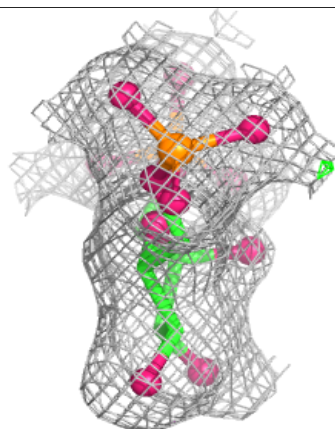
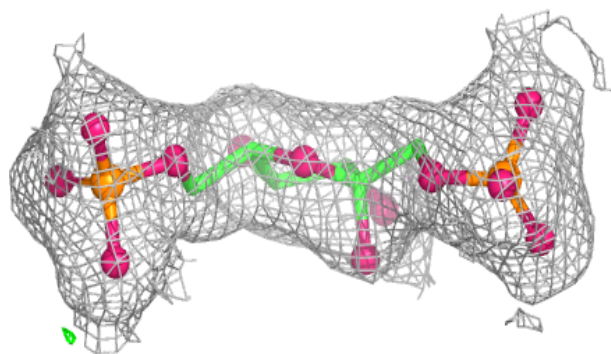
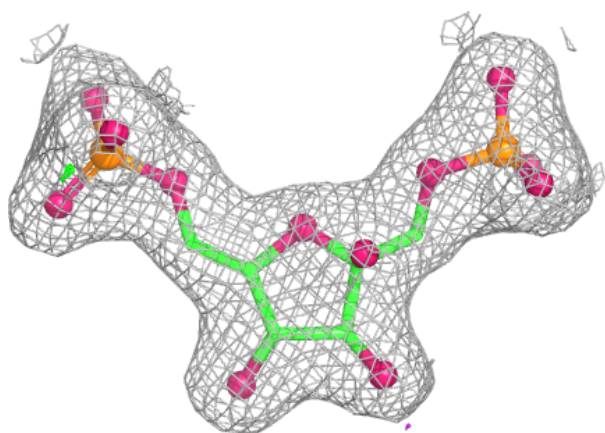
Electron density around FBP H 601:

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and green (positive)



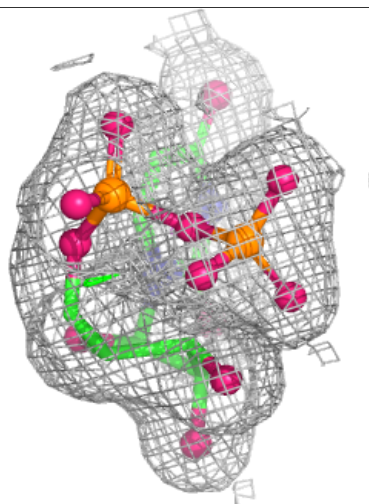
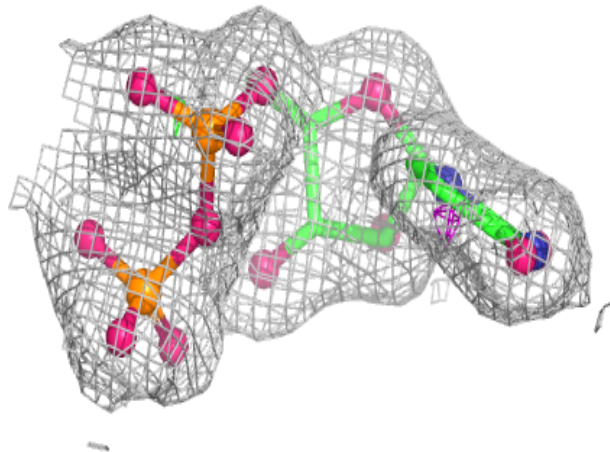
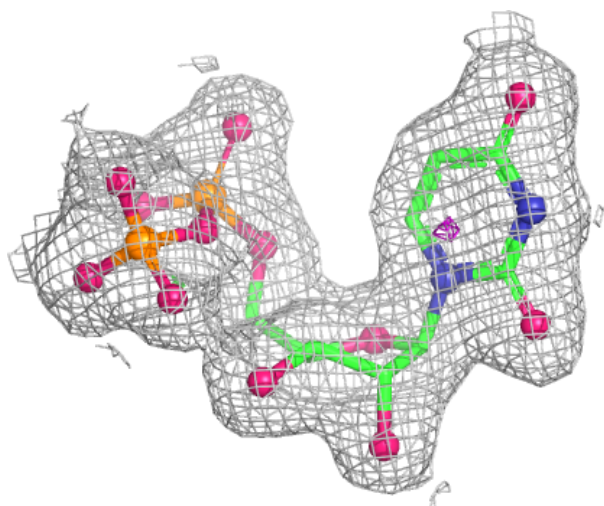
Electron density around FBP B 601:

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and green (positive)



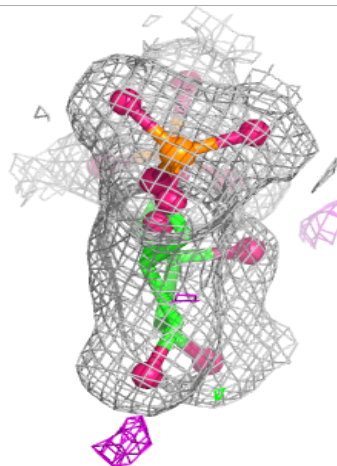
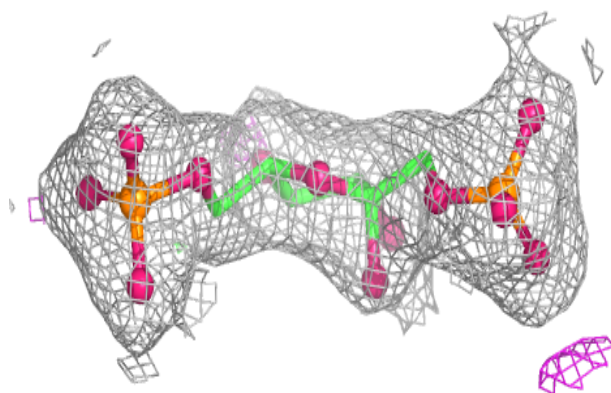
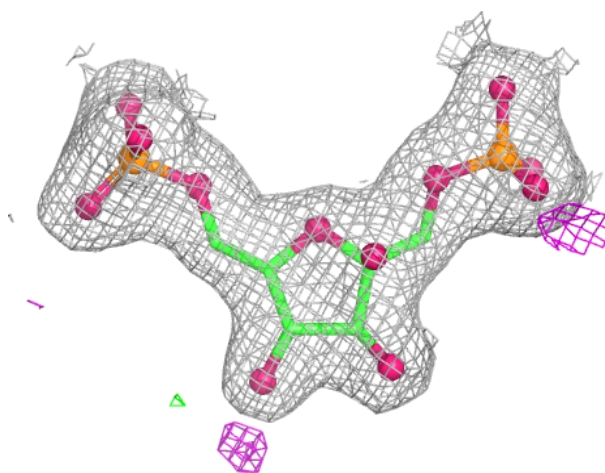
Electron density around UDP C 604:

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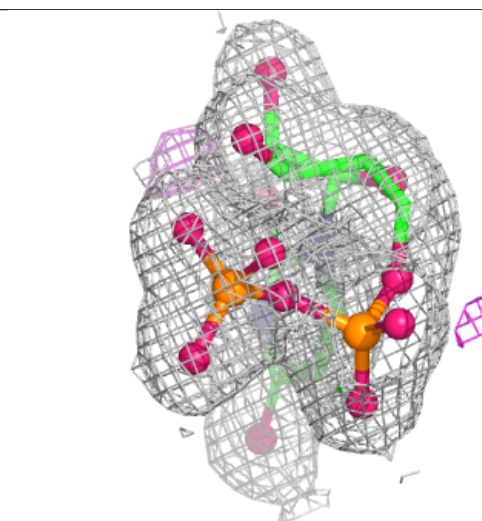
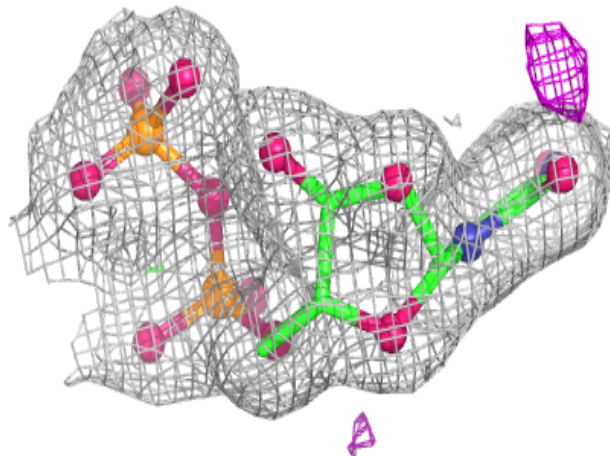
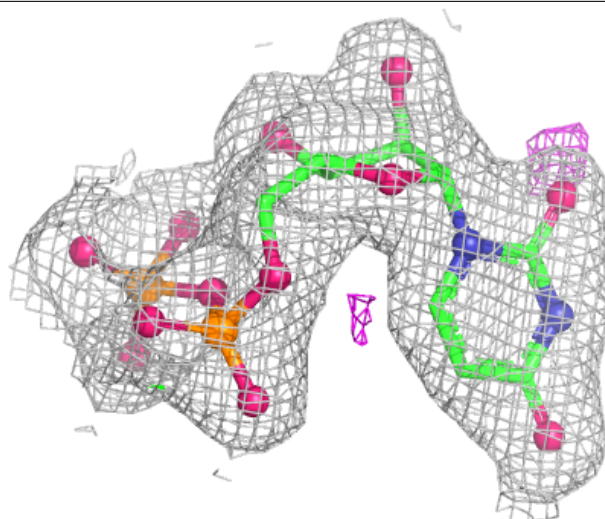
Electron density around FBP G 601:

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



Electron density around UDP G 604:

$2mF_o-DF_c$ (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.