



wwPDB X-ray Structure Validation Summary Report i

Dec 21, 2023 – 04:17 PM EST

PDB ID : 8TBS
Title : Structure of human erythrocyte pyruvate kinase in complex with an allosteric activator AG-946
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 i 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](#) i) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

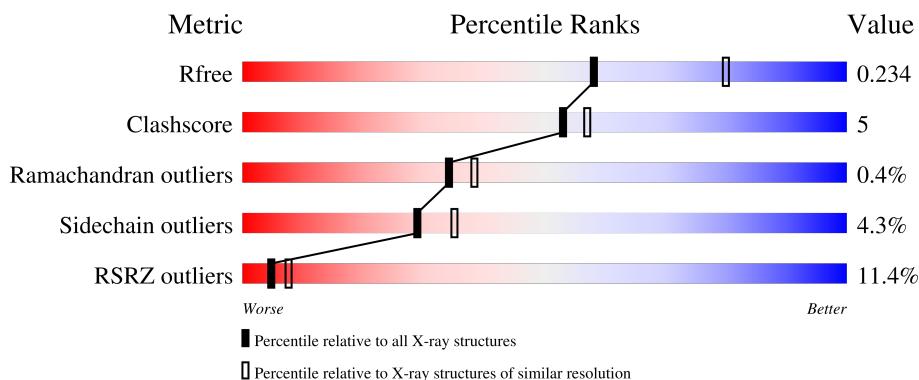
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

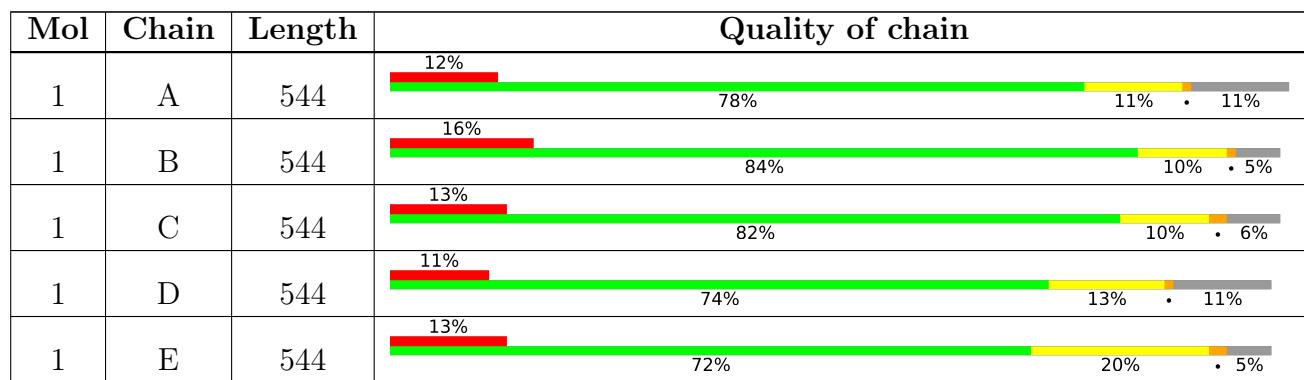
The reported resolution of this entry is 2.35 Å.

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.



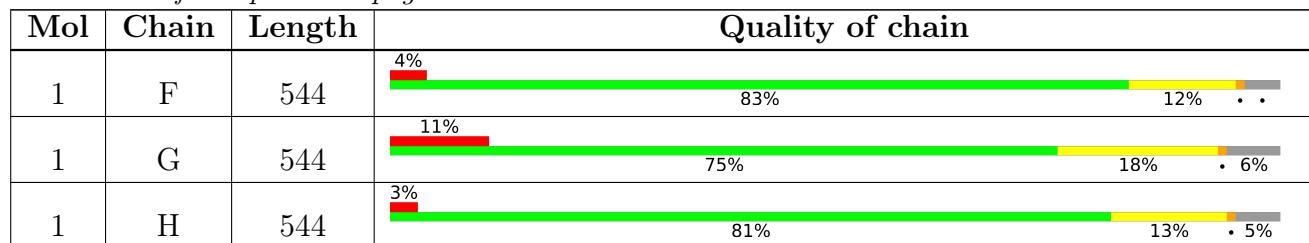
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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.



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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MN	H	603	-	-	-	X
5	PYR	E	604	-	X	-	-
5	PYR	H	604	-	X	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 31741 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	485	Total	C 3693	N 2322	O 670	S 683	18	0	1	0
1	B	517	Total	C 3922	N 2468	O 708	S 728	18	0	0	0
1	C	512	Total	C 3895	N 2450	O 705	S 722	18	0	2	0
1	D	483	Total	C 3661	N 2303	O 664	S 676	18	0	0	0
1	E	515	Total	C 3908	N 2459	O 709	S 722	18	0	1	0
1	F	520	Total	C 3941	N 2479	O 712	S 732	18	0	0	0
1	G	509	Total	C 3901	N 2449	O 709	S 725	18	0	6	0
1	H	519	Total	C 3943	N 2480	O 712	S 733	18	0	1	0

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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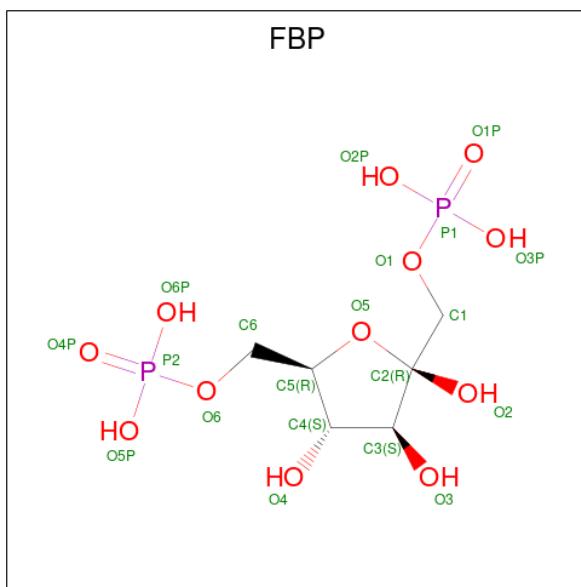
Chain	Residue	Modelled	Actual	Comment	Reference
F	33	SER	-	expression tag	UNP P30613
F	34	SER	-	expression tag	UNP P30613
F	35	HIS	-	expression tag	UNP P30613
F	36	HIS	-	expression tag	UNP P30613
F	37	HIS	-	expression tag	UNP P30613
F	38	HIS	-	expression tag	UNP P30613
F	39	HIS	-	expression tag	UNP P30613
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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Chain	Residue	Modelled	Actual	Comment	Reference
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 1,6-di-O-phosphono-beta-D-fructofuranose (three-letter code: FBP) (formula: C₆H₁₄O₁₂P₂).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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 MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

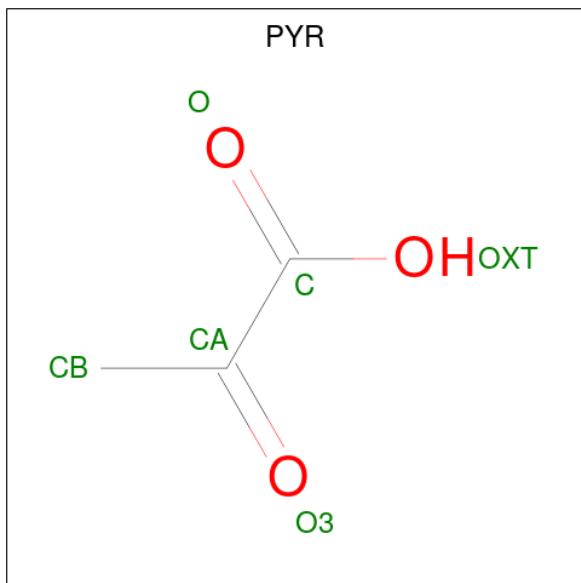
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0
4	C	1	Total K 1 1	0	0
4	E	1	Total K 1 1	0	0
4	F	1	Total K 1 1	0	0

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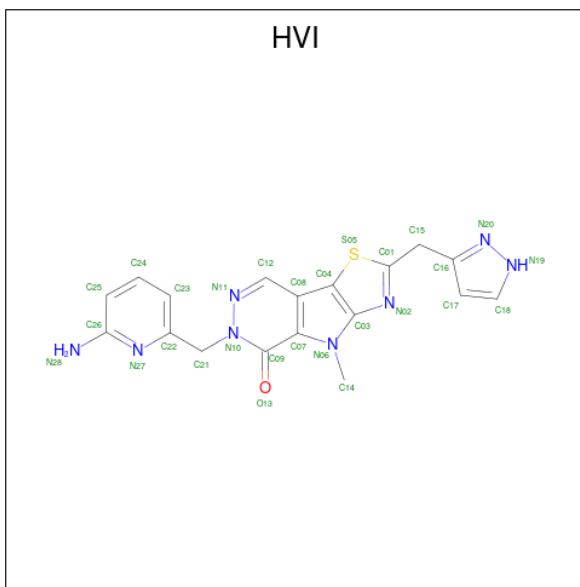
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total K 1 1	0	0

- Molecule 5 is PYRUVIC ACID (three-letter code: PYR) (formula: C₃H₄O₃).



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

- Molecule 6 is 6-[(6-aminopyridin-2-yl)methyl]-4-methyl-2-[(1H-pyrazol-3-yl)methyl]-4,6-dihydro-5H-[1,3]thiazolo[5',4':4,5]pyrrolo[2,3-d]pyridazin-5-one (three-letter code: HVI) (formula: C₁₈H₁₆N₈OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	B	1	28	18	8	1	1	0	0
6	D	1	28	18	8	1	1	0	0
6	F	1	28	18	8	1	1	0	0
6	H	1	28	18	8	1	1	0	0

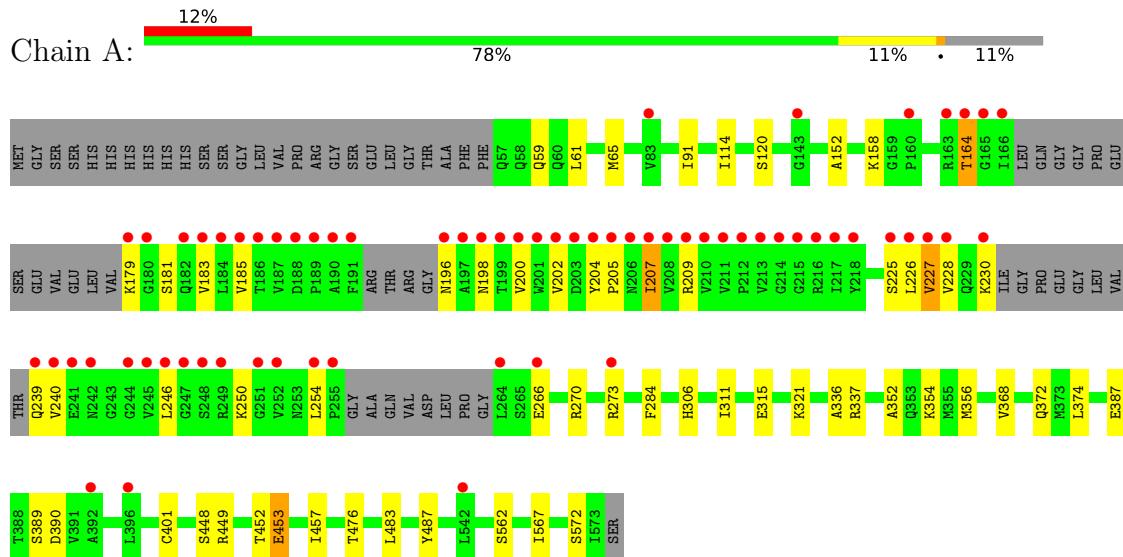
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	73	Total O 73 73		0	0
7	B	64	Total O 64 64		0	0
7	C	62	Total O 62 62		0	0
7	D	55	Total O 55 55		0	0
7	E	41	Total O 41 41		0	0
7	F	91	Total O 91 91		0	0
7	G	48	Total O 48 48		0	0
7	H	109	Total O 109 109		0	0

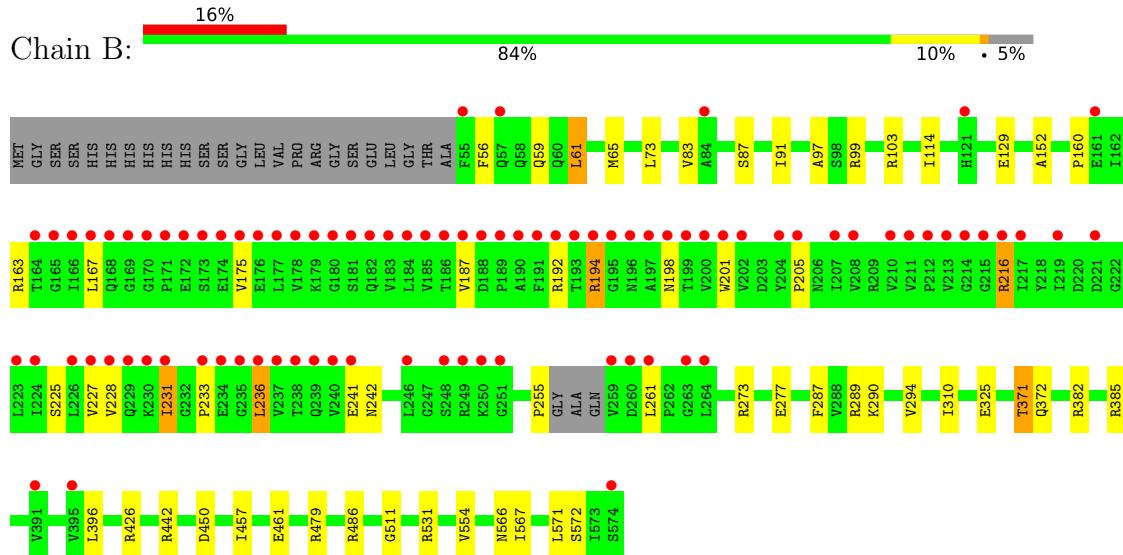
3 Residue-property plots [\(i\)](#)

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

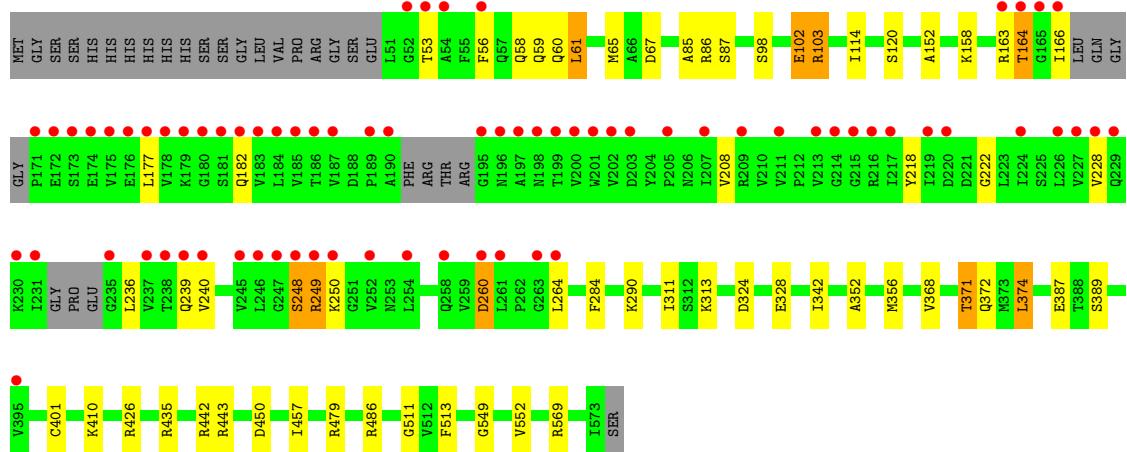
- Molecule 1: Pyruvate kinase PKLR



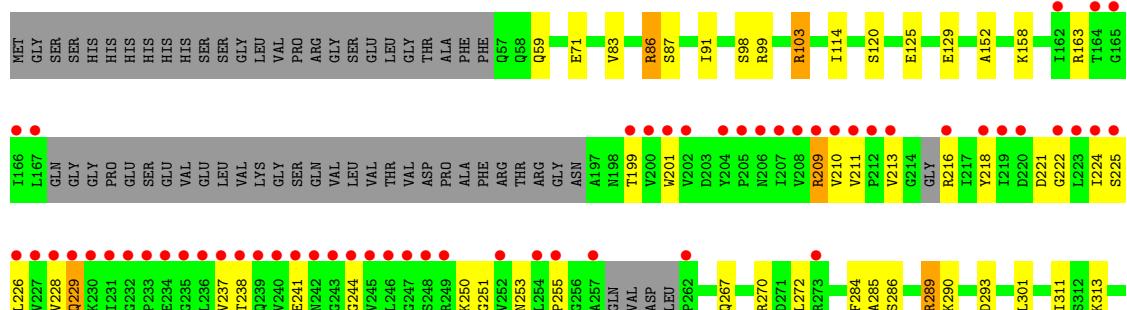
- Molecule 1: Pyruvate kinase PKLR



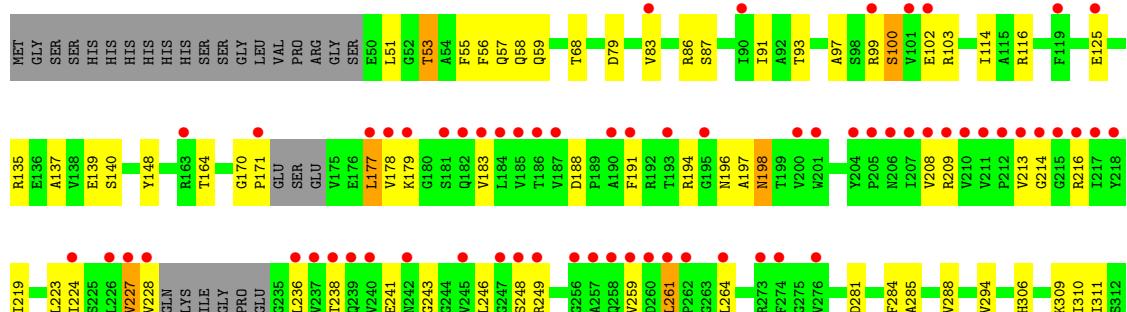
- Molecule 1: Pyruvate kinase PKLR



- Molecule 1: Pyruvate kinase PKLR



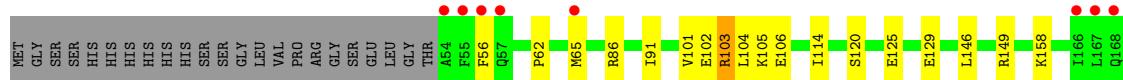
- Molecule 1: Pyruvate kinase PKLR





- Molecule 1: Pyruvate kinase PKLR

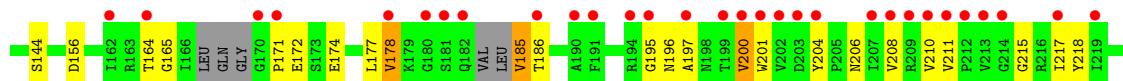
Category	Percentage
Red	4%
Green	83%
Yellow	12%
Black	1%



- Molecule 1: Pyruvate kinase PKLR

A horizontal bar chart illustrating the distribution of Chain G across various categories. The total length of the bar is 100%.

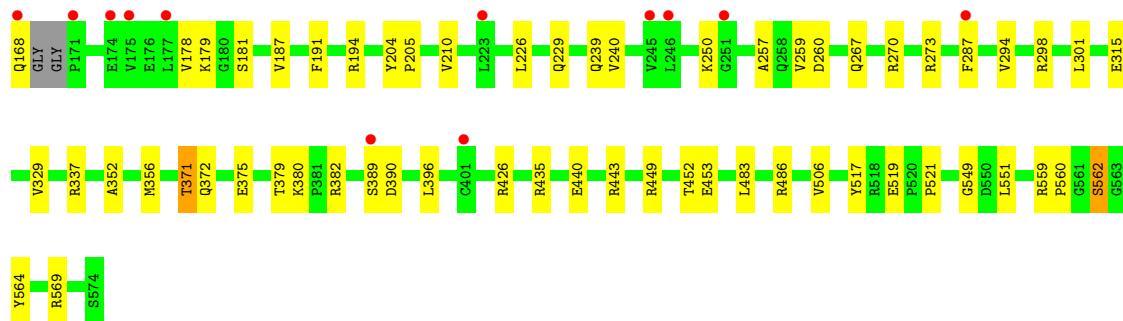
Category	Percentage
Chain G	11%
Other	75%
Category A	18%
Category B	6%



- Molecule 1: Pyruvate kinase PKLR

A horizontal bar chart titled "Chain H:" at the top left. The bar is divided into four segments: a red segment at the far left labeled "3%", a long green segment labeled "81%", a yellow segment labeled "13%", and an orange segment at the far right labeled "5%".





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.32Å 122.60Å 378.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.44 – 2.35 49.86 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.44-2.35) 99.5 (49.86-2.35)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	4.02 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R , R_{free}	0.193 , 0.234 0.193 , 0.234	Depositor DCC
R_{free} test set	10643 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.1	EDS
L-test for twinning ²	$< L > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	31741	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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 66.22 % 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 6.2563e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $< |L| >$, $< L^2 >$ 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, HVI, FBP, K, PYR

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	0.27	0/3750	0.53	0/5076
1	B	0.28	0/3987	0.55	1/5403 (0.0%)
1	C	0.28	0/3956	0.56	2/5357 (0.0%)
1	D	0.27	0/3719	0.53	0/5035
1	E	0.28	0/3971	0.54	0/5380
1	F	0.29	0/4006	0.54	0/5428
1	G	0.27	0/3975	0.54	0/5381
1	H	0.29	0/4008	0.55	0/5431
All	All	0.28	0/31372	0.54	3/42491 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	61	LEU	CB-CG-CD2	7.79	124.24	111.00
1	C	61	LEU	CA-CB-CG	7.75	133.12	115.30
1	B	261	LEU	CA-CB-CG	6.28	129.74	115.30

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	3693	0	3766	32	0
1	B	3922	0	3998	32	0
1	C	3895	0	3974	40	0
1	D	3661	0	3741	48	0
1	E	3908	0	3987	73	0
1	F	3941	0	4016	37	0
1	G	3901	0	3971	53	1
1	H	3943	0	4018	45	0
2	A	20	0	9	0	0
2	B	20	0	9	0	0
2	C	20	0	9	0	0
2	D	20	0	9	0	0
2	E	20	0	9	0	0
2	F	20	0	9	0	0
2	G	20	0	9	0	0
2	H	20	0	9	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
5	A	6	0	0	0	0
5	B	6	0	0	0	0
5	C	6	0	0	0	0
5	D	6	0	0	0	0
5	E	6	0	0	0	0
5	F	6	0	0	0	0
5	G	6	0	0	1	0
5	H	6	0	0	0	0
6	B	28	0	0	0	0
6	D	28	0	0	0	0
6	F	28	0	0	0	0
6	H	28	0	0	0	0
7	A	73	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	64	0	0	0	0
7	C	62	0	0	2	0
7	D	55	0	0	0	0
7	E	41	0	0	3	0
7	F	91	0	0	6	0
7	G	48	0	0	1	0
7	H	109	0	0	0	0
All	All	31741	0	31543	337	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 337 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:E:179:LYS:HB2	1:E:243:GLY:HA3	1.55	0.87
1:G:99:ARG:NH2	1:G:126:TYR:O	2.12	0.82
1:E:59:GLN:O	1:E:490[A]:ARG:NH2	2.10	0.82
1:F:486:ARG:NH1	7:F:701:HOH:O	2.11	0.79
1:G:185:VAL:N	1:G:200:VAL:O	2.18	0.77

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:53:THR:OG1	1:G:304:GLU:OE1[4_544]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	476/544 (88%)	458 (96%)	16 (3%)	2 (0%)	34 38
1	B	513/544 (94%)	498 (97%)	13 (2%)	2 (0%)	34 38
1	C	506/544 (93%)	489 (97%)	12 (2%)	5 (1%)	15 15
1	D	475/544 (87%)	460 (97%)	14 (3%)	1 (0%)	47 56
1	E	510/544 (94%)	491 (96%)	17 (3%)	2 (0%)	34 38
1	F	516/544 (95%)	505 (98%)	10 (2%)	1 (0%)	47 56
1	G	507/544 (93%)	485 (96%)	18 (4%)	4 (1%)	19 20
1	H	516/544 (95%)	507 (98%)	8 (2%)	1 (0%)	47 56
All	All	4019/4352 (92%)	3893 (97%)	108 (3%)	18 (0%)	34 38

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	59	GLN
1	G	178	VAL
1	E	227	VAL
1	G	196	ASN
1	C	164	THR

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	391/436 (90%)	376 (96%)	15 (4%)	33 41
1	B	416/436 (95%)	400 (96%)	16 (4%)	33 41
1	C	412/436 (94%)	401 (97%)	11 (3%)	44 55
1	D	386/436 (88%)	370 (96%)	16 (4%)	30 37
1	E	412/436 (94%)	388 (94%)	24 (6%)	20 22
1	F	417/436 (96%)	401 (96%)	16 (4%)	33 41
1	G	413/436 (95%)	387 (94%)	26 (6%)	18 19
1	H	418/436 (96%)	399 (96%)	19 (4%)	27 33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3265/3488 (94%)	3122 (96%)	143 (4%)	29 34

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	486	ARG
1	G	531[A]	ARG
1	H	259	VAL
1	D	229	GLN
1	D	221	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	239	GLN
1	H	267	GLN
1	E	58	GLN
1	E	482	GLN
1	F	198	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 monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

Of 34 ligands modelled in this entry, 14 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	PYR	G	604	3	5,5,5	2.88	3 (60%)	3,6,6	1.75	1 (33%)
6	HVI	B	601	-	25,32,32	2.47	8 (32%)	26,47,47	2.55	9 (34%)
6	HVI	F	601	-	25,32,32	2.35	7 (28%)	26,47,47	2.50	9 (34%)
6	HVI	D	601	-	25,32,32	2.40	7 (28%)	26,47,47	2.53	8 (30%)
2	FBP	E	601	-	18,20,20	3.40	6 (33%)	23,32,32	0.74	0
2	FBP	G	601	-	18,20,20	3.41	5 (27%)	23,32,32	0.79	0
5	PYR	A	604	3	5,5,5	2.88	3 (60%)	3,6,6	1.75	2 (66%)
5	PYR	F	605	-	5,5,5	2.93	3 (60%)	3,6,6	1.57	1 (33%)
2	FBP	F	602	-	18,20,20	3.38	5 (27%)	23,32,32	0.63	0
5	PYR	B	605	3	5,5,5	3.01	3 (60%)	3,6,6	1.34	0
2	FBP	A	601	-	18,20,20	3.42	5 (27%)	23,32,32	0.71	0
2	FBP	B	602	-	18,20,20	3.42	5 (27%)	23,32,32	0.74	0
2	FBP	H	602	-	18,20,20	3.43	6 (33%)	23,32,32	0.66	0
2	FBP	D	602	-	18,20,20	3.43	5 (27%)	23,32,32	0.82	1 (4%)
5	PYR	E	604	3	5,5,5	2.88	3 (60%)	3,6,6	1.81	2 (66%)
2	FBP	C	601	-	18,20,20	3.59	6 (33%)	23,32,32	1.53	6 (26%)
6	HVI	H	601	-	25,32,32	2.36	8 (32%)	26,47,47	2.55	10 (38%)
5	PYR	C	604	3	5,5,5	3.00	3 (60%)	3,6,6	1.43	1 (33%)
5	PYR	H	604	-	5,5,5	2.91	3 (60%)	3,6,6	1.49	1 (33%)
5	PYR	D	604	3	5,5,5	2.88	3 (60%)	3,6,6	1.85	1 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PYR	G	604	3	-	0/4/4/4	-
6	HVI	B	601	-	-	2/4/8/8	0/5/5/5
6	HVI	F	601	-	-	2/4/8/8	0/5/5/5
6	HVI	D	601	-	-	2/4/8/8	0/5/5/5
2	FBP	E	601	-	-	4/13/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	G	601	-	-	4/13/32/32	0/1/1/1
5	PYR	A	604	3	-	0/4/4/4	-
5	PYR	F	605	-	-	0/4/4/4	-
2	FBP	F	602	-	-	2/13/32/32	0/1/1/1
5	PYR	B	605	3	-	0/4/4/4	-
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
2	FBP	B	602	-	-	2/13/32/32	0/1/1/1
2	FBP	H	602	-	-	2/13/32/32	0/1/1/1
2	FBP	D	602	-	-	2/13/32/32	0/1/1/1
5	PYR	E	604	3	-	3/4/4/4	-
2	FBP	C	601	-	-	3/13/32/32	0/1/1/1
6	HVI	H	601	-	-	2/4/8/8	0/5/5/5
5	PYR	C	604	3	-	0/4/4/4	-
5	PYR	H	604	-	-	4/4/4/4	-
5	PYR	D	604	3	-	0/4/4/4	-

The worst 5 of 97 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	602	FBP	O5-C2	-8.83	1.29	1.43
2	C	601	FBP	O5-C5	8.71	1.62	1.43
2	C	601	FBP	O5-C2	-8.46	1.30	1.43
2	A	601	FBP	O5-C5	8.41	1.62	1.43
6	B	601	HVI	C03-N02	8.37	1.41	1.33

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	601	HVI	C12-N11-N10	6.75	122.55	117.12
6	F	601	HVI	C12-N11-N10	6.46	122.32	117.12
6	H	601	HVI	C12-N11-N10	6.46	122.32	117.12
6	B	601	HVI	C12-N11-N10	6.43	122.29	117.12
6	D	601	HVI	C08-C12-N11	-4.88	119.45	125.87

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

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

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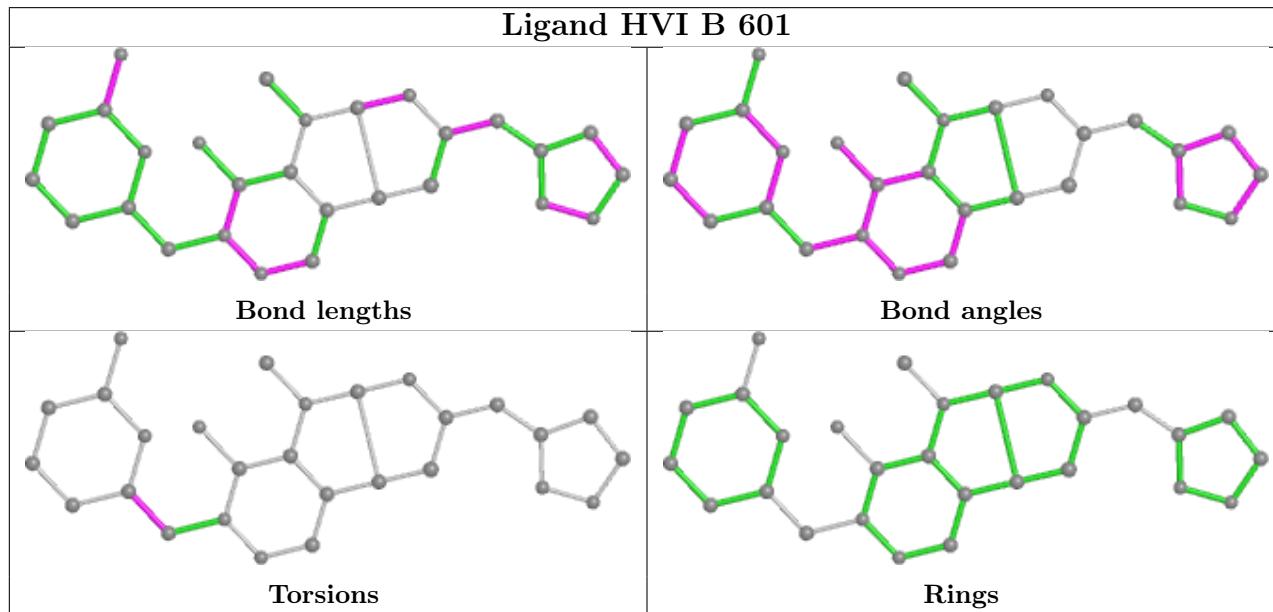
Mol	Chain	Res	Type	Atoms
2	C	601	FBP	C4-C5-C6-O6
2	C	601	FBP	O5-C5-C6-O6
2	E	601	FBP	O1-C1-C2-O2
2	E	601	FBP	O1-C1-C2-O5

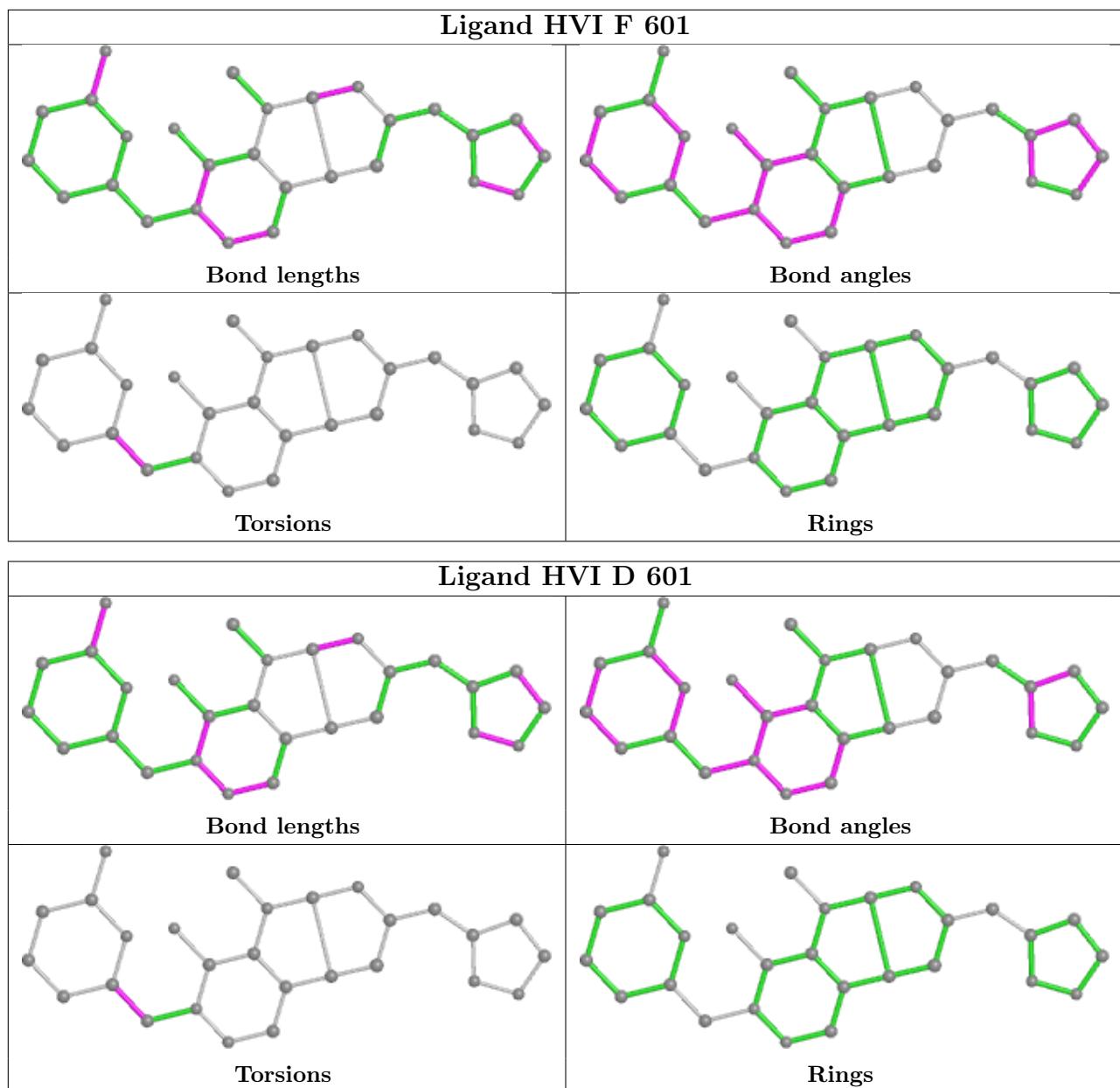
There are no ring outliers.

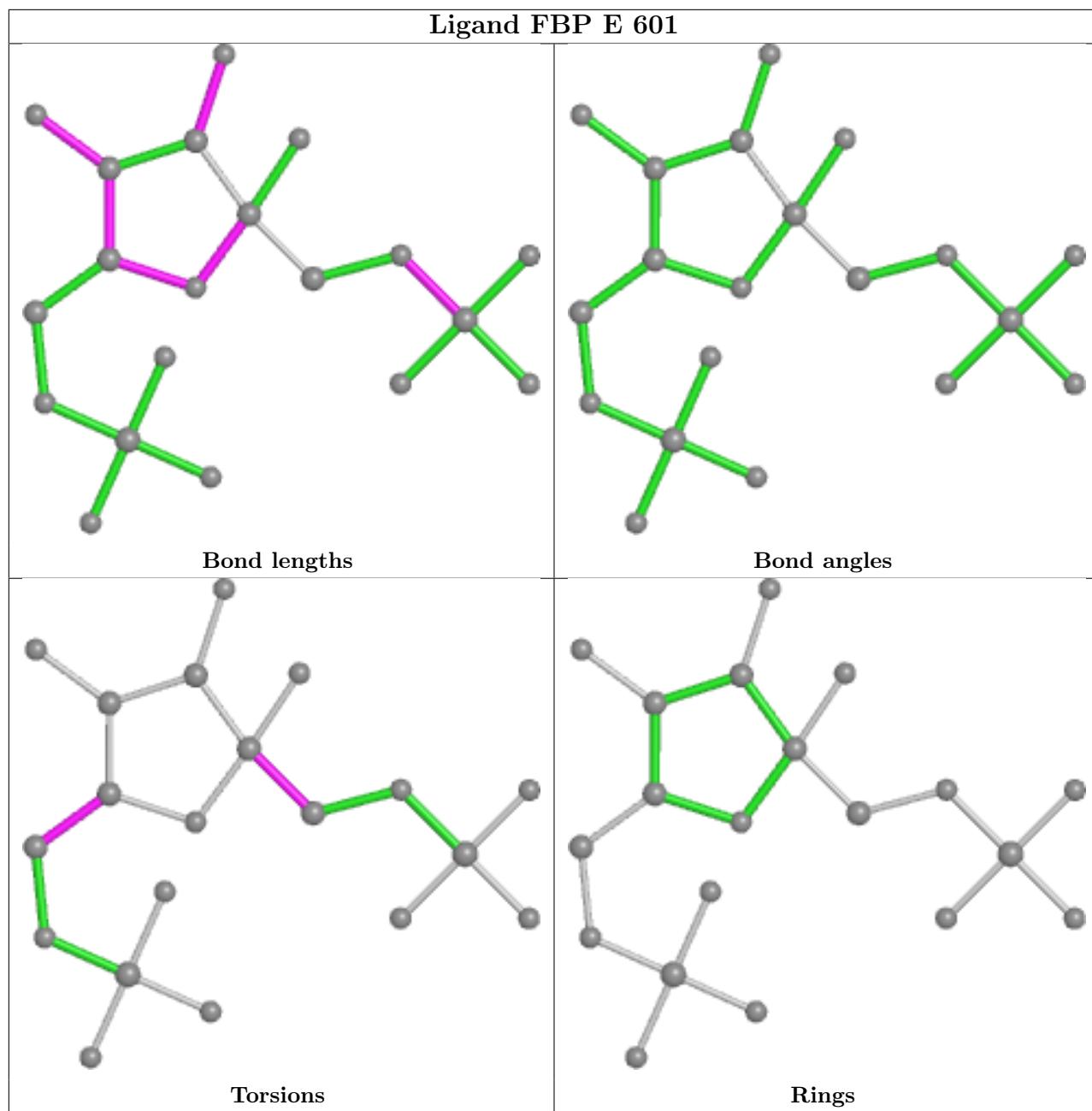
2 monomers are involved in 2 short contacts:

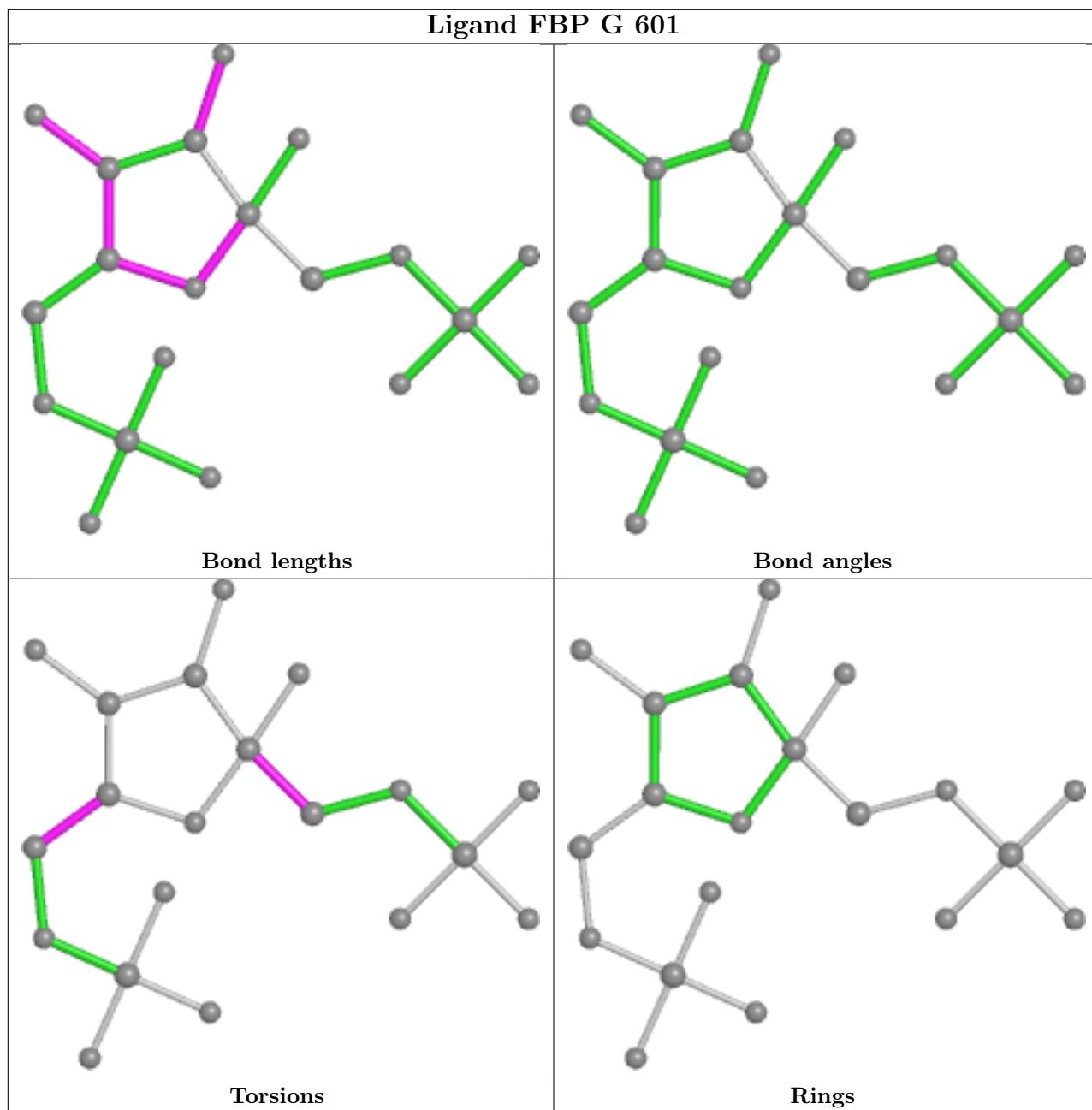
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	604	PYR	1	0
2	H	602	FBP	1	0

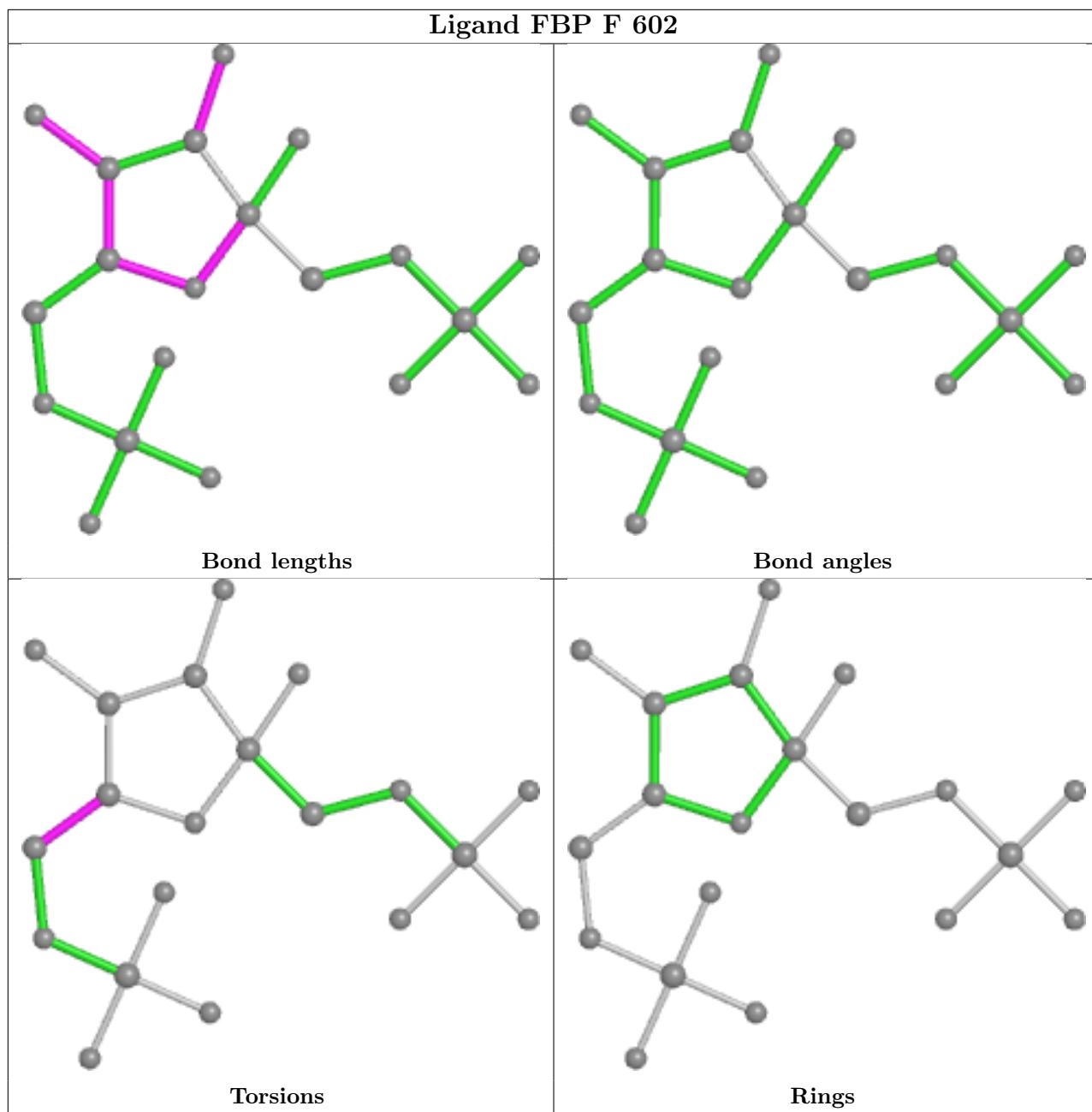
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

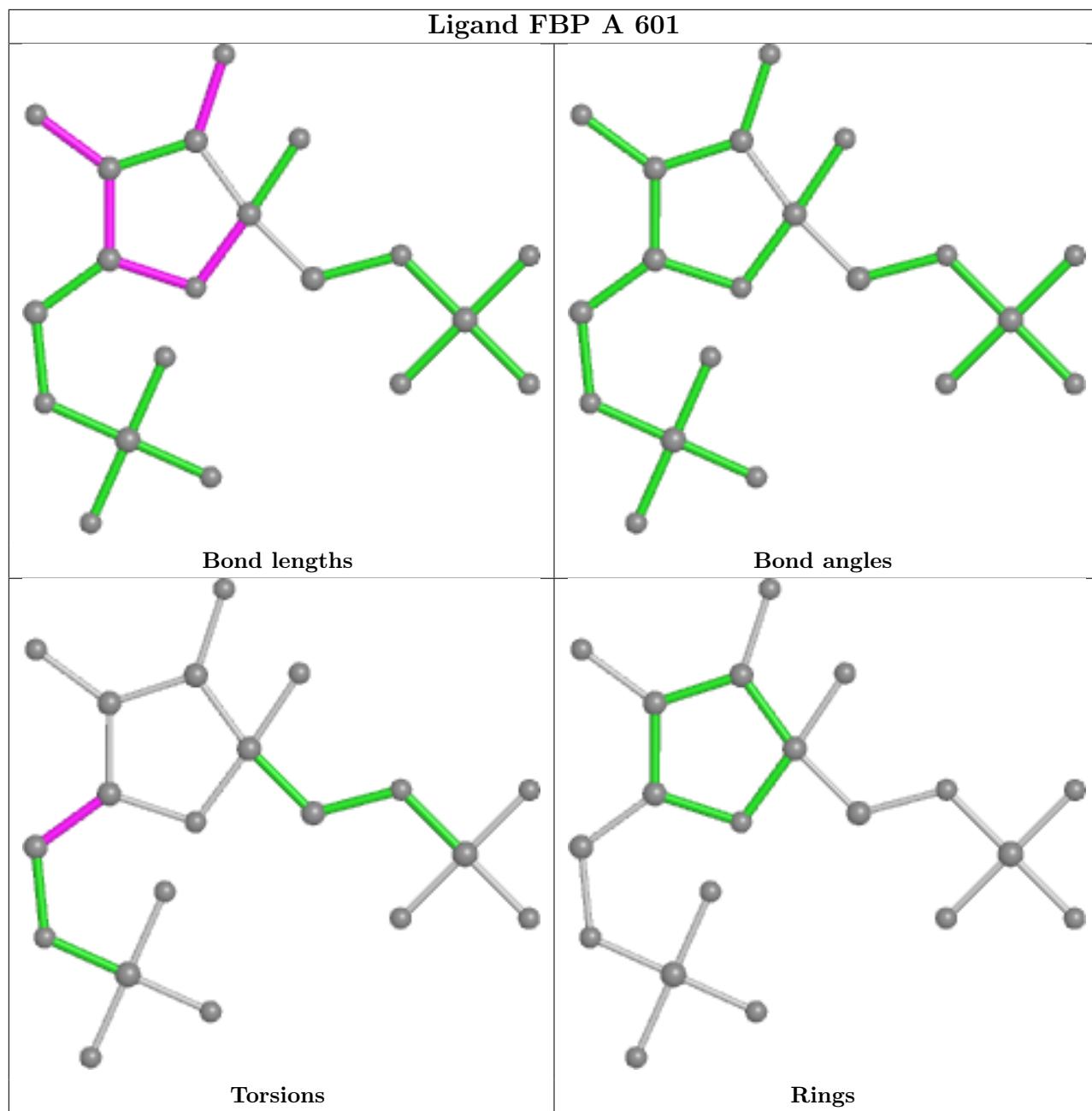


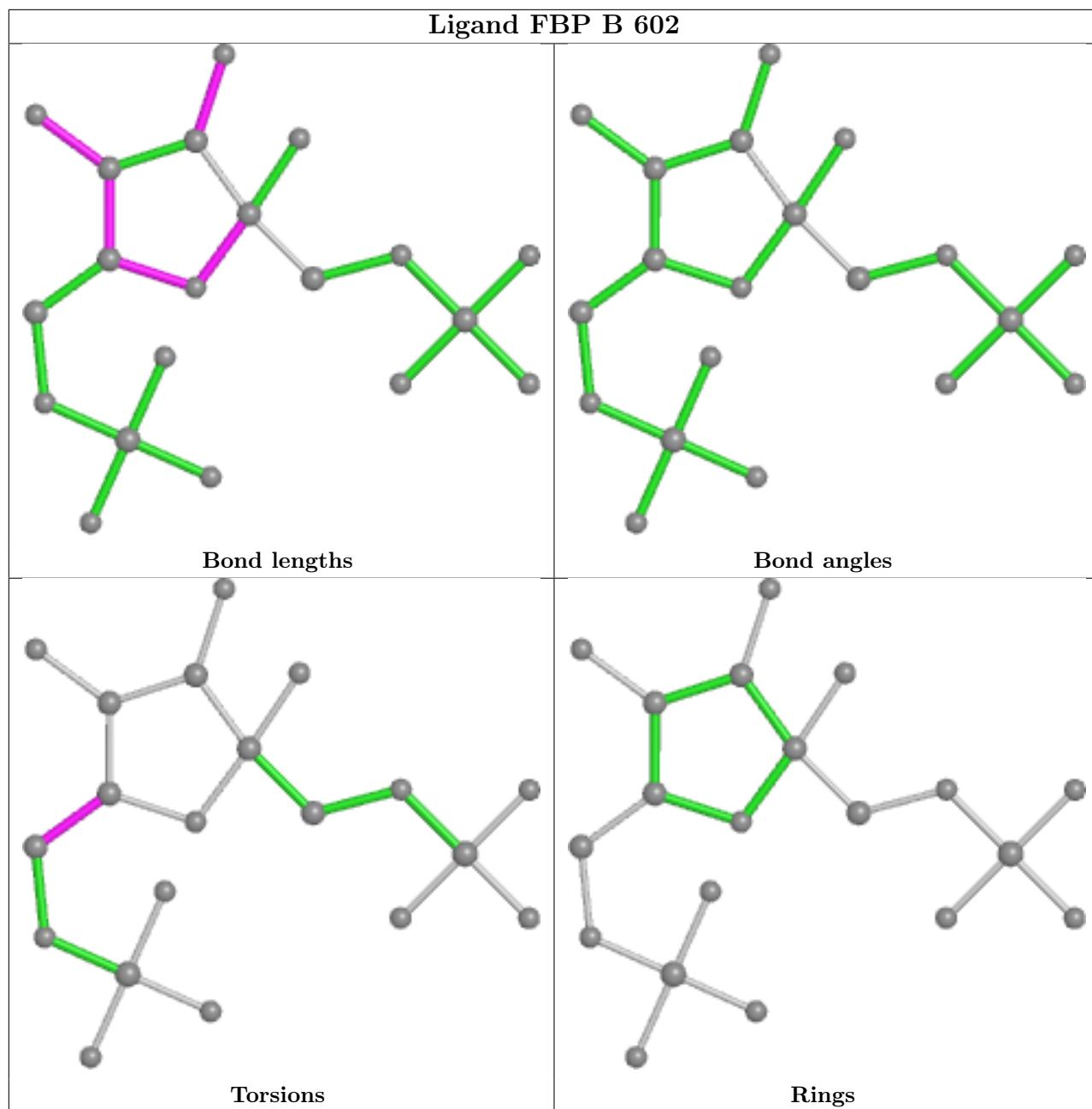


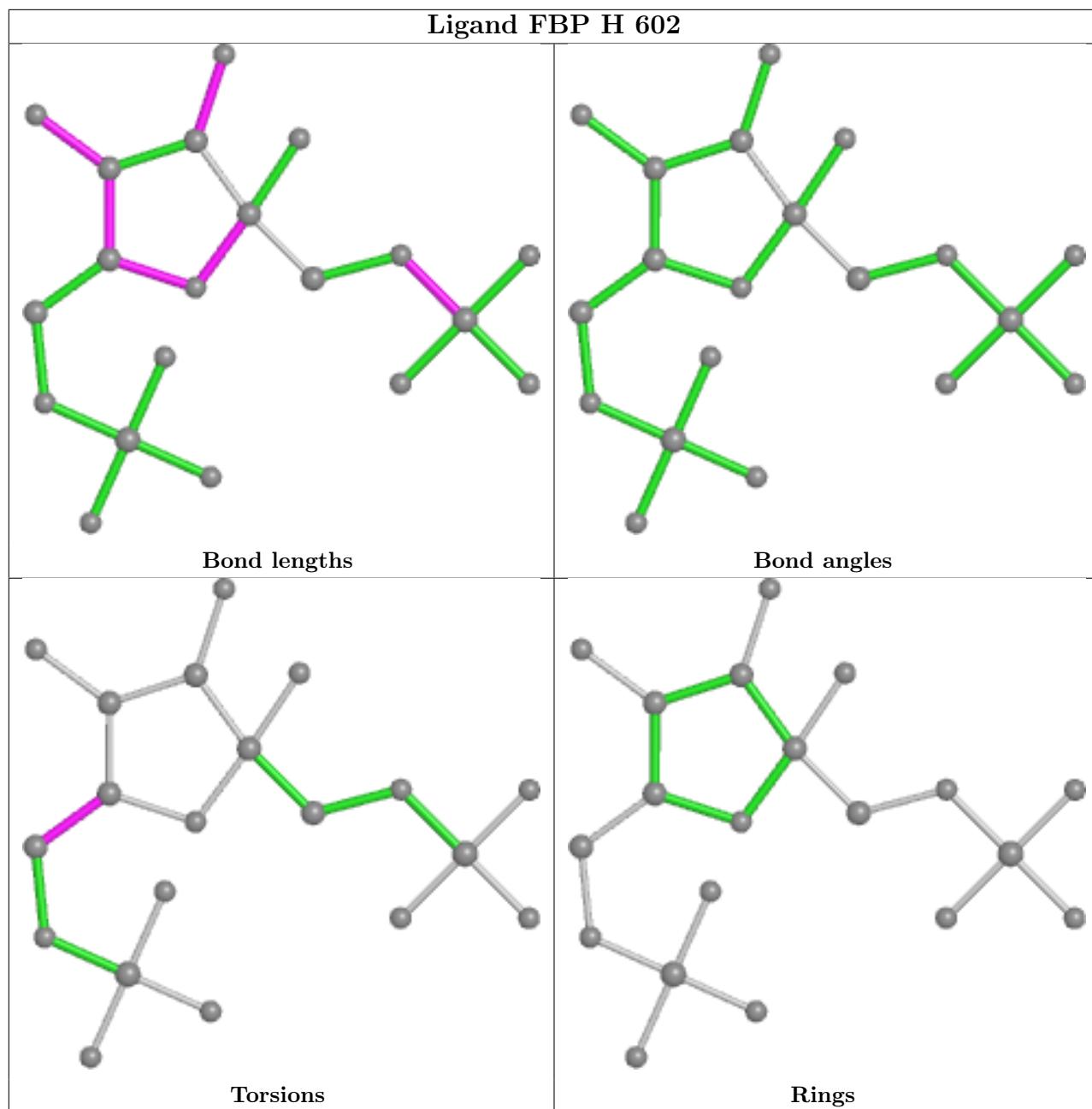


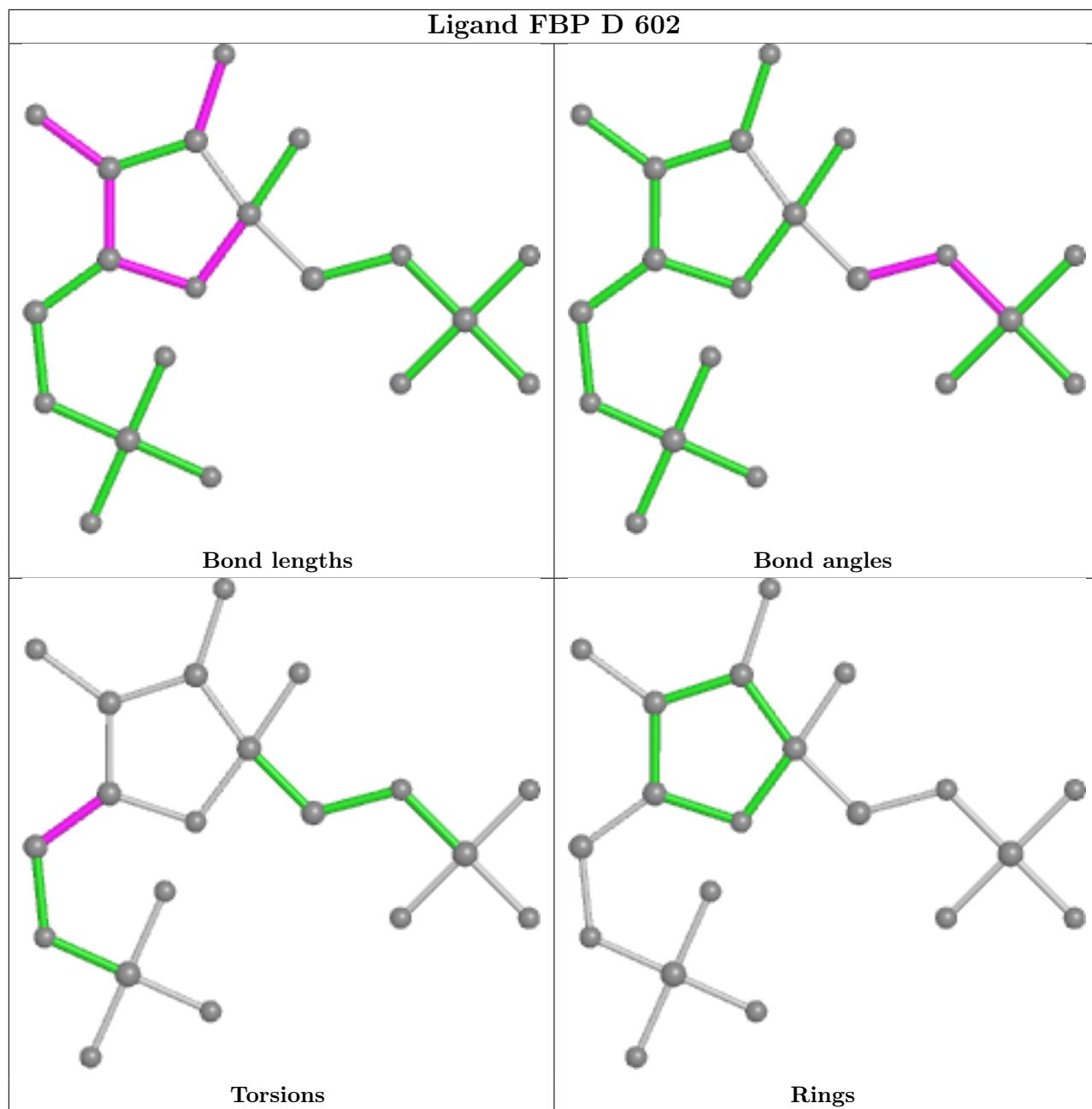


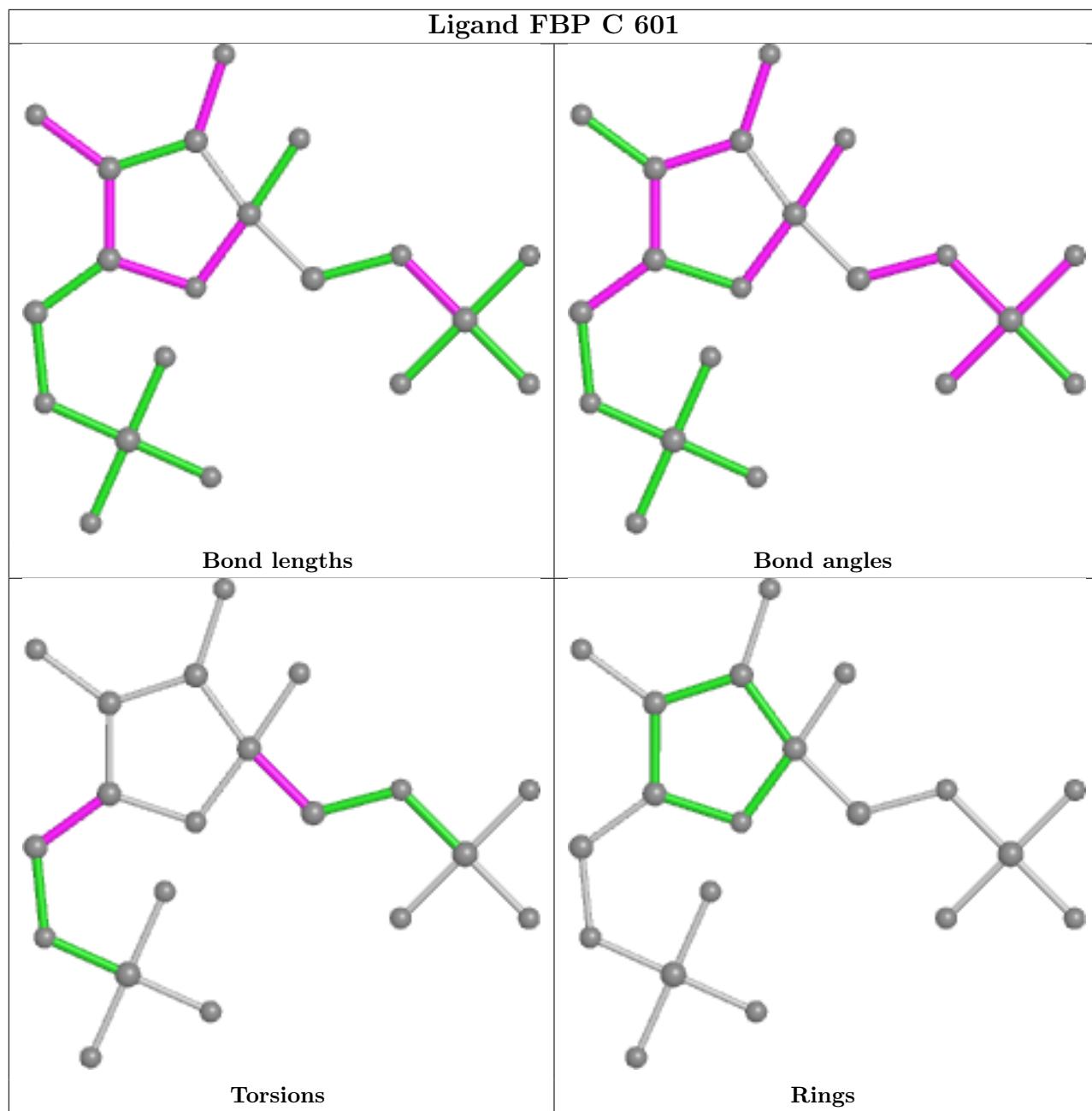


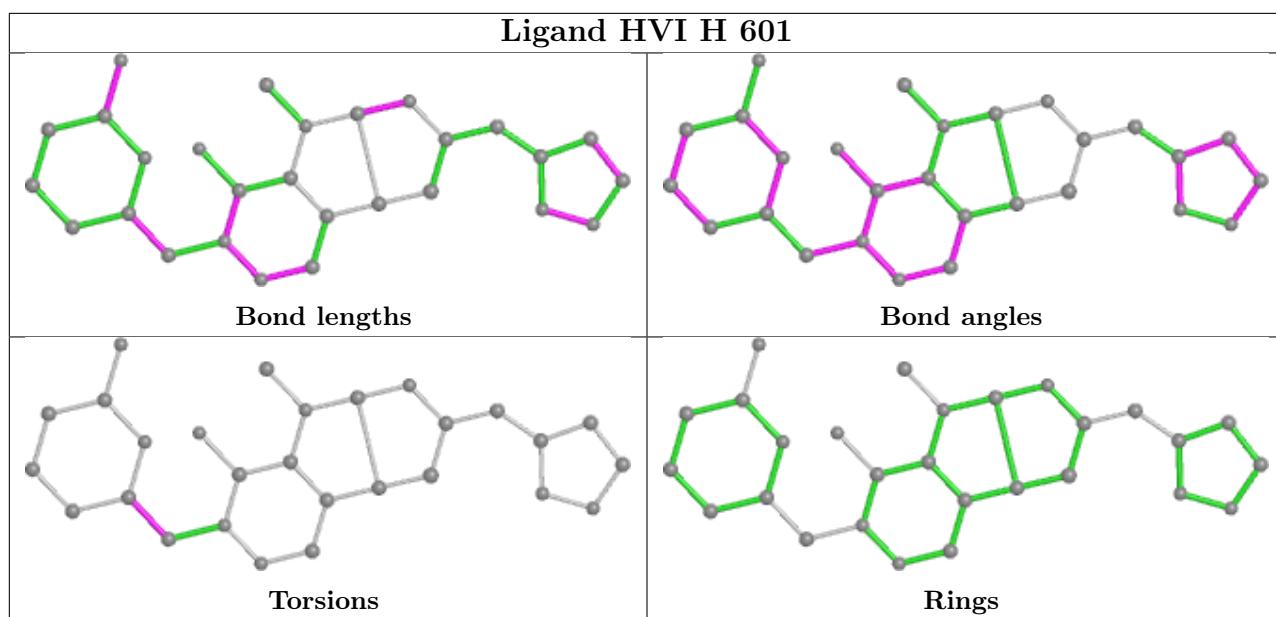












5.7 Other polymers [\(i\)](#)

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	485/544 (89%)	0.76	67 (13%) 2 4	36, 51, 124, 158	0
1	B	517/544 (95%)	0.88	88 (17%) 1 2	35, 51, 132, 162	0
1	C	512/544 (94%)	0.78	73 (14%) 2 4	33, 50, 135, 181	0
1	D	483/544 (88%)	0.63	58 (12%) 4 7	36, 50, 110, 153	0
1	E	515/544 (94%)	0.75	73 (14%) 2 4	35, 62, 102, 155	0
1	F	520/544 (95%)	0.25	23 (4%) 34 46	31, 46, 75, 138	0
1	G	509/544 (93%)	0.74	60 (11%) 4 7	32, 61, 109, 155	0
1	H	519/544 (95%)	0.23	19 (3%) 41 54	29, 45, 73, 124	0
All	All	4060/4352 (93%)	0.63	461 (11%) 5 7	29, 51, 116, 181	0

The worst 5 of 461 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200	VAL	13.0
1	A	245	VAL	11.9
1	C	201	TRP	11.8
1	D	235	GLY	10.9
1	B	191	PHE	10.5

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 monosaccharides in this entry.

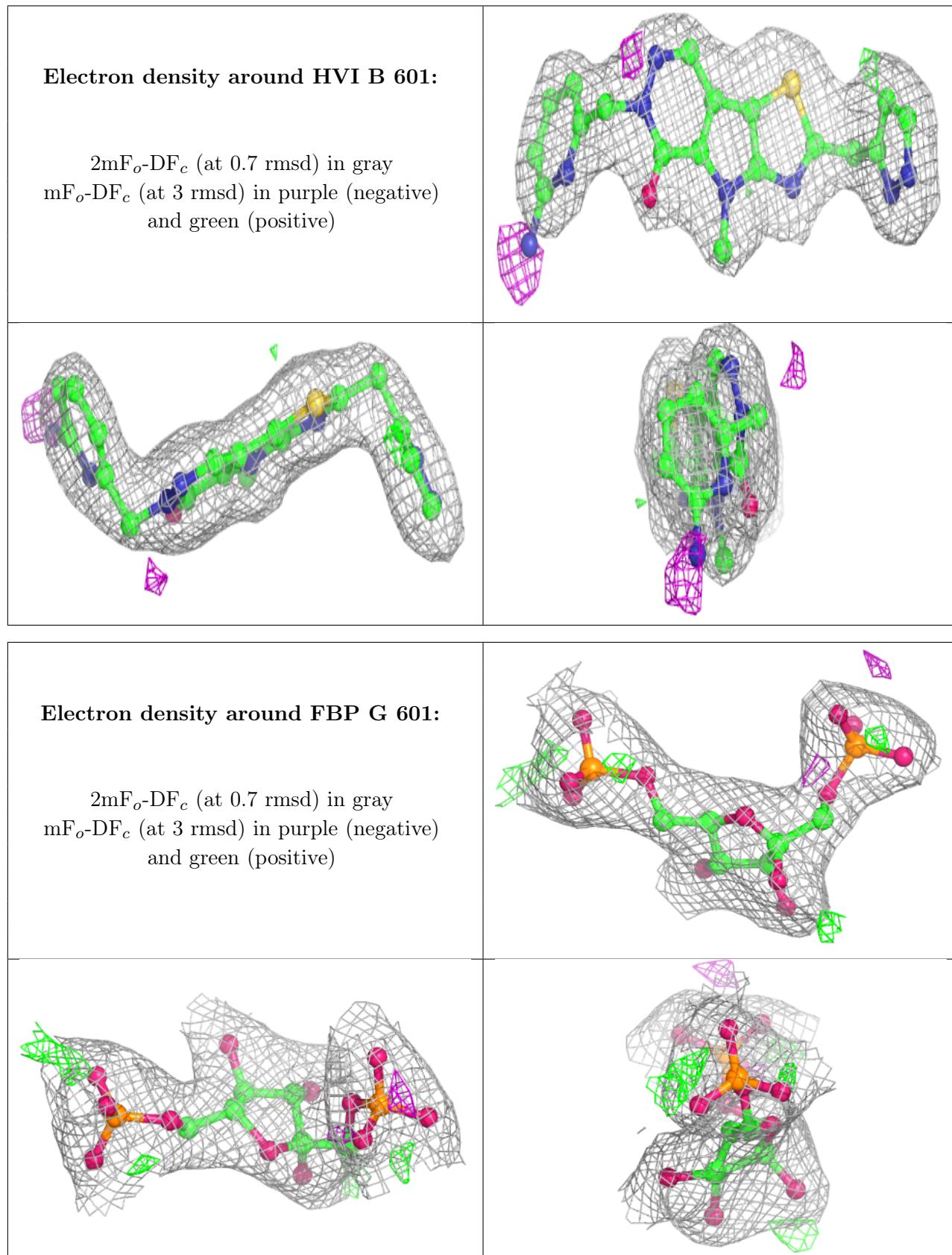
6.4 Ligands [\(i\)](#)

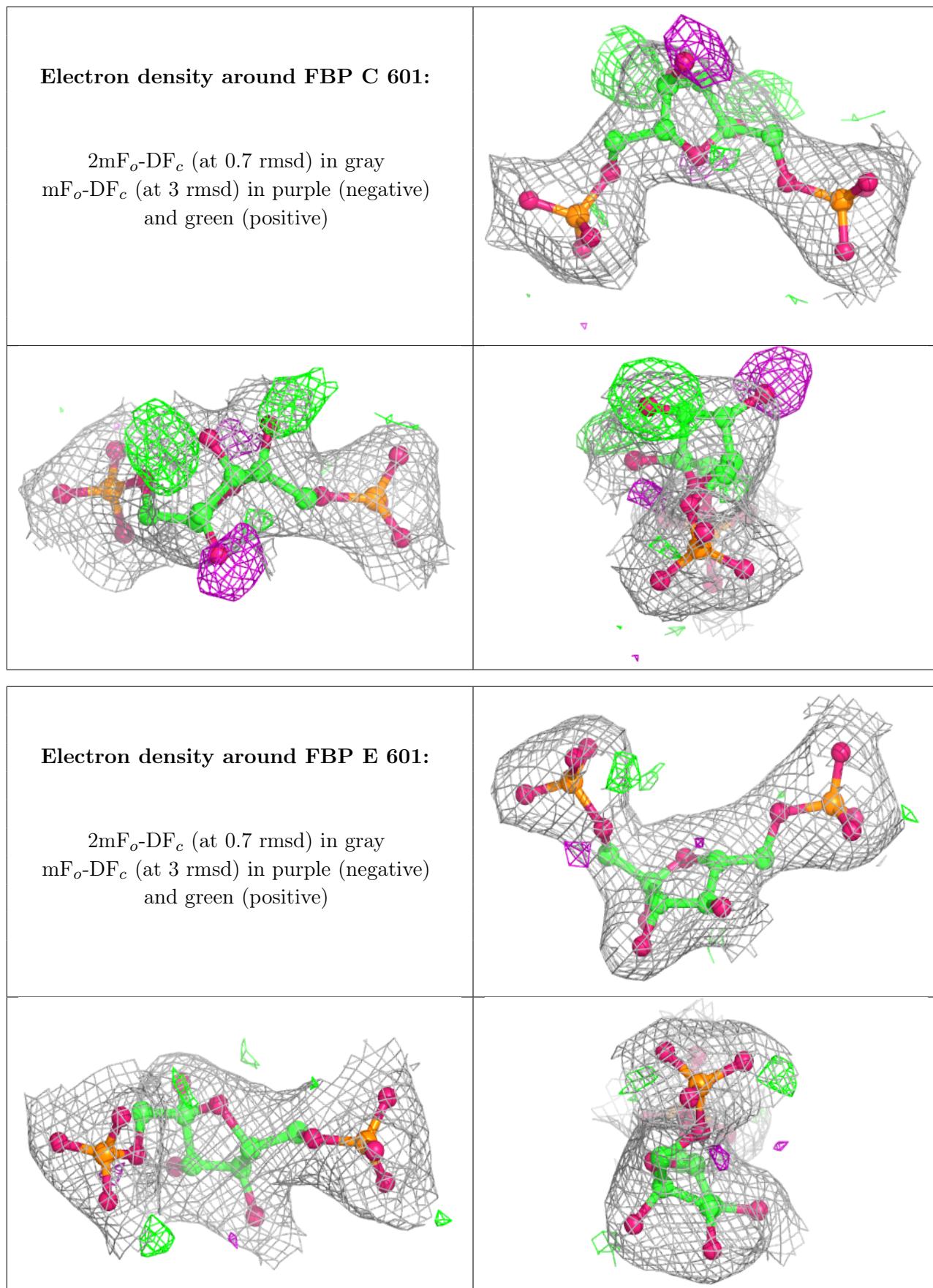
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

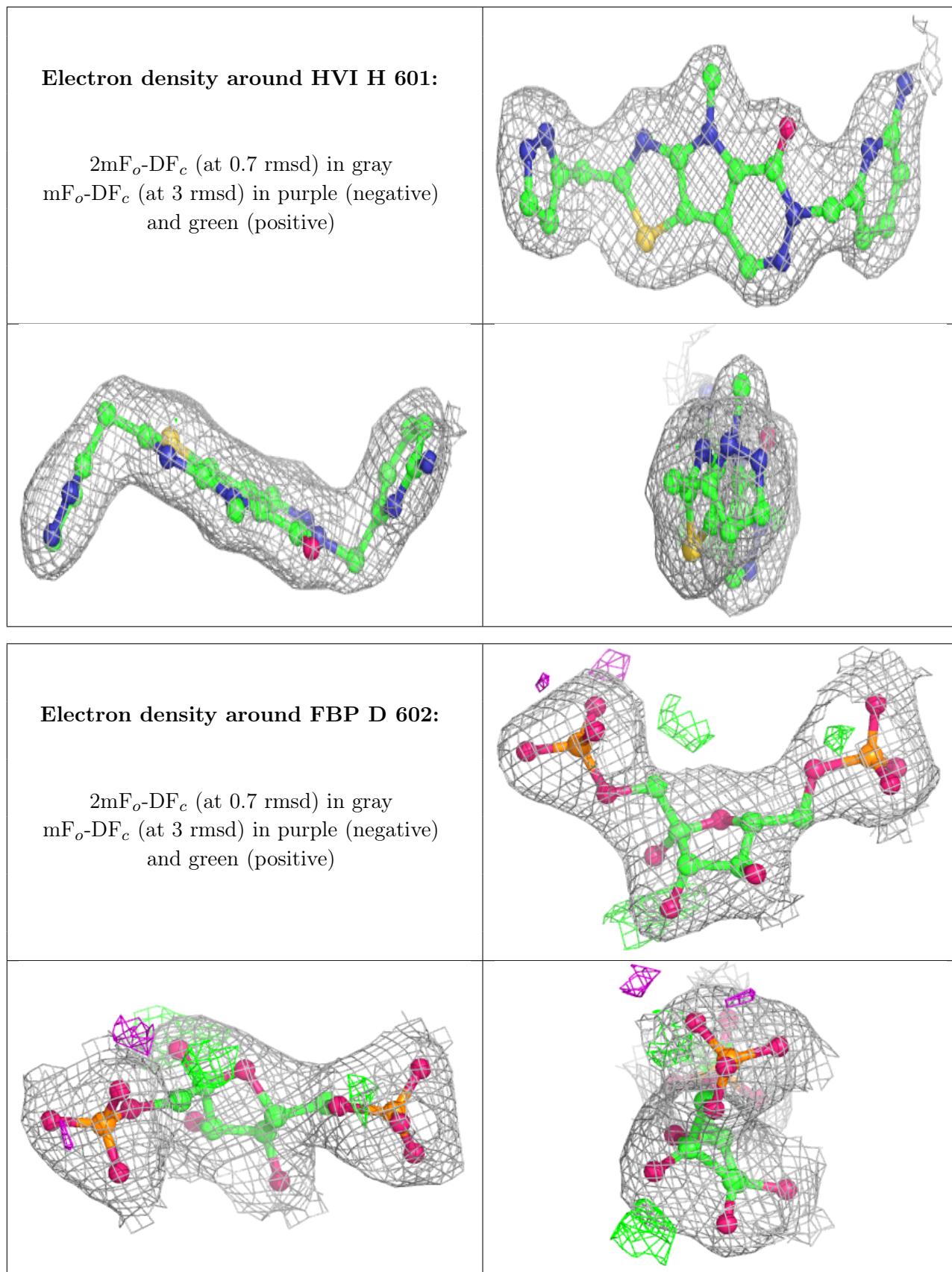
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MN	H	603	1/1	0.60	0.48	210,210,210,210	0
3	MN	F	603	1/1	0.69	0.34	160,160,160,160	0
4	K	E	603	1/1	0.73	0.29	140,140,140,140	0
4	K	C	603	1/1	0.75	0.15	102,102,102,102	0
4	K	B	604	1/1	0.79	0.21	98,98,98,98	0
5	PYR	F	605	6/6	0.81	0.14	74,75,85,90	0
4	K	G	603	1/1	0.84	0.10	119,119,119,119	0
5	PYR	D	604	6/6	0.89	0.19	58,68,78,84	0
4	K	A	603	1/1	0.89	0.17	90,90,90,90	0
5	PYR	E	604	6/6	0.90	0.16	61,75,77,84	0
3	MN	D	603	1/1	0.91	0.07	99,99,99,99	0
4	K	F	604	1/1	0.91	0.19	107,107,107,107	0
5	PYR	H	604	6/6	0.91	0.12	80,81,83,86	0
3	MN	G	602	1/1	0.93	0.23	133,133,133,133	0
5	PYR	G	604	6/6	0.94	0.10	63,70,75,78	0
5	PYR	B	605	6/6	0.94	0.15	51,72,77,78	0
6	HVI	B	601	28/28	0.94	0.16	31,46,52,58	0
2	FBP	G	601	20/20	0.96	0.13	38,47,58,61	0
2	FBP	C	601	20/20	0.96	0.17	37,42,56,57	0
2	FBP	E	601	20/20	0.96	0.13	41,48,56,61	0
6	HVI	H	601	28/28	0.96	0.14	31,38,45,48	0
2	FBP	D	602	20/20	0.97	0.12	40,49,55,62	0
6	HVI	D	601	28/28	0.97	0.14	33,45,55,59	0
6	HVI	F	601	28/28	0.97	0.15	31,38,46,50	0
3	MN	B	603	1/1	0.97	0.15	87,87,87,87	0
5	PYR	A	604	6/6	0.98	0.15	50,59,65,65	0
2	FBP	F	602	20/20	0.98	0.12	31,41,47,48	0
5	PYR	C	604	6/6	0.98	0.12	52,60,68,72	0
3	MN	C	602	1/1	0.98	0.15	67,67,67,67	0
2	FBP	A	601	20/20	0.98	0.10	39,46,56,61	0
2	FBP	H	602	20/20	0.98	0.11	35,41,51,51	0
3	MN	A	602	1/1	0.99	0.05	61,61,61,61	0
2	FBP	B	602	20/20	0.99	0.13	32,39,44,47	0
3	MN	E	602	1/1	0.99	0.13	93,93,93,93	0

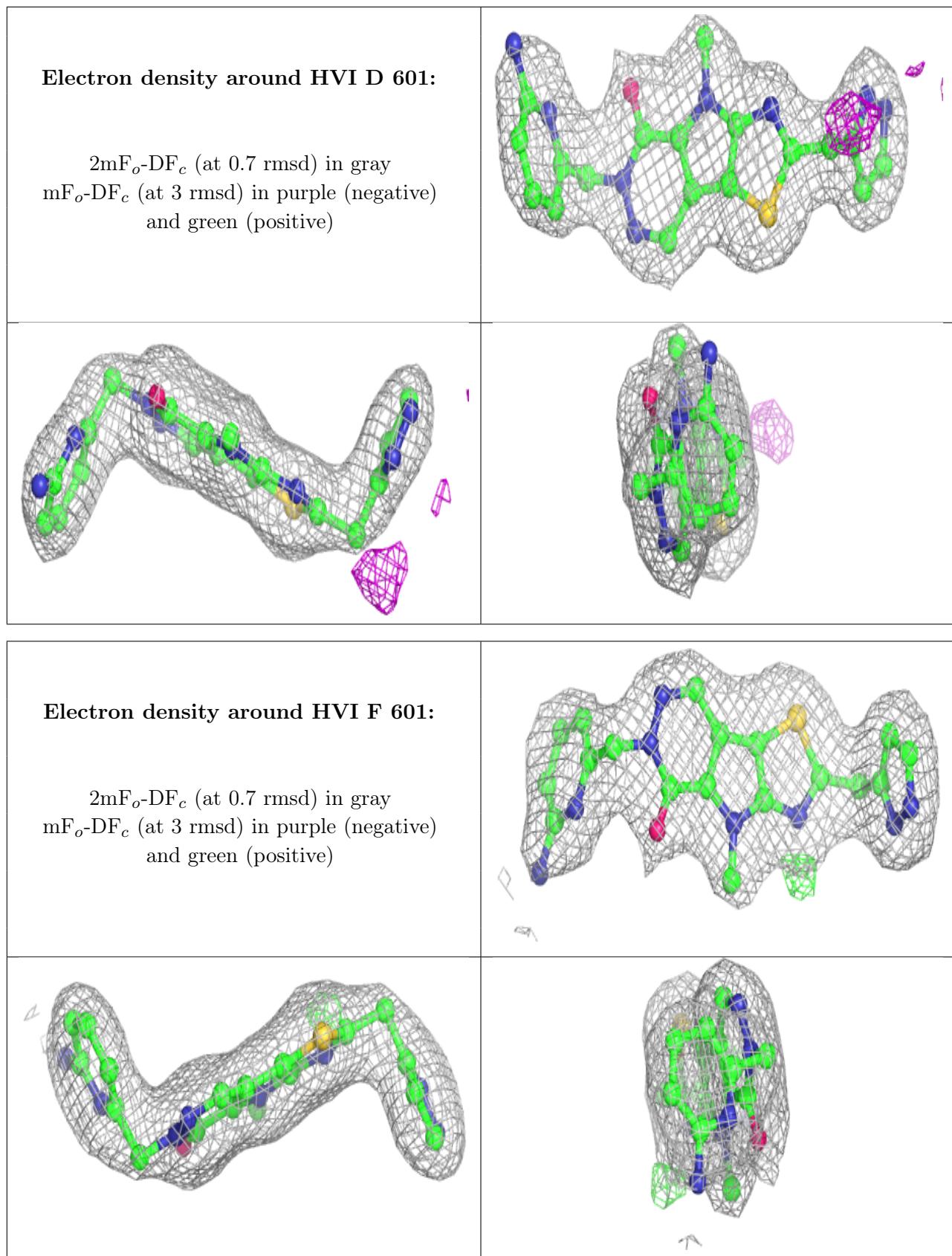
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

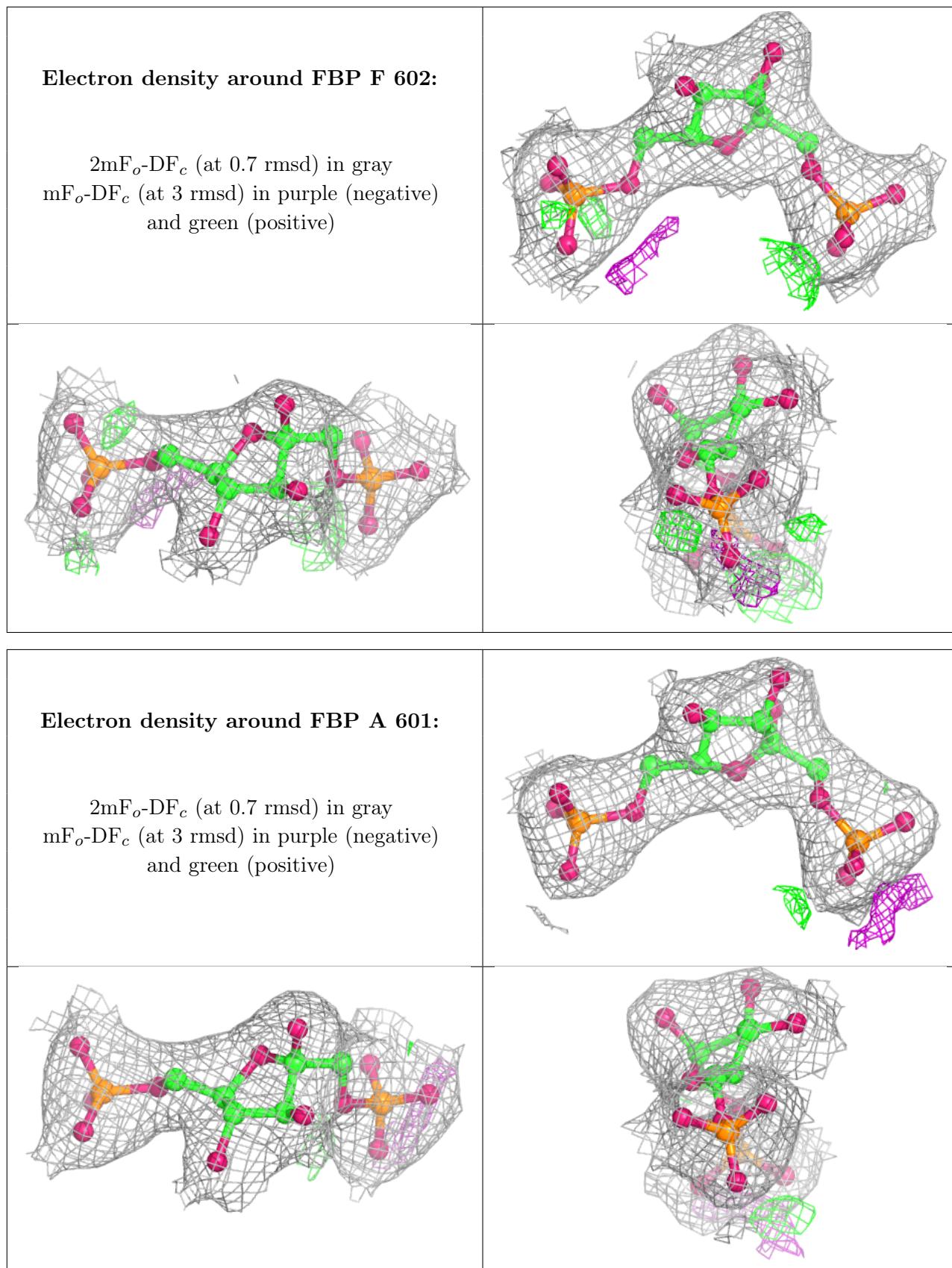
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

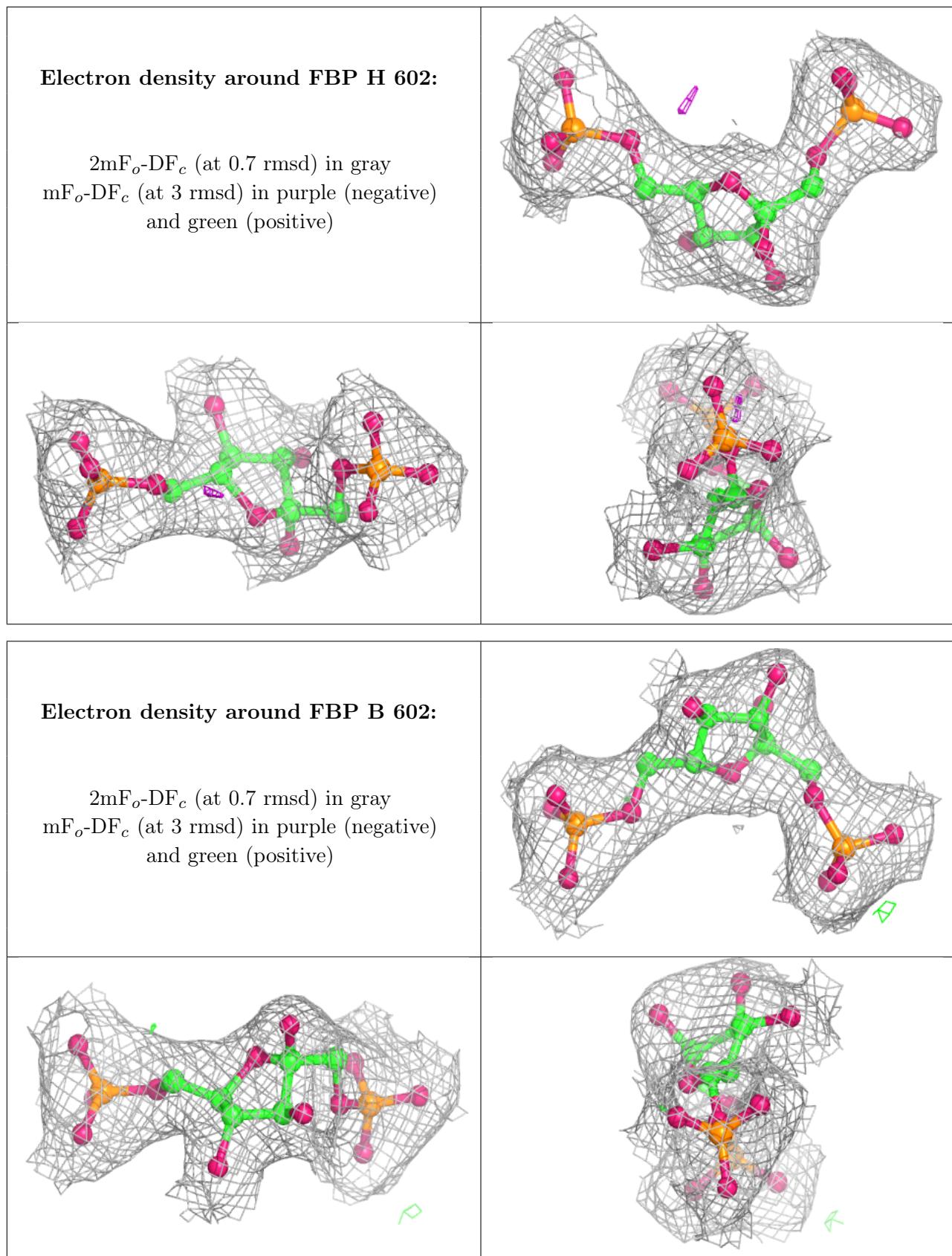












6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.