



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:34 PM UTC

PDB ID : 5SCI / pdb_00005sci
Title : Structure of liver pyruvate kinase in complex with anthraquinone derivative
105
Authors : Lulla, A.; Foller, A.; Nain-Perez, A.; Grotli, M.; Brear, P.; Hyvonen, M.
Deposited on : 2021-12-01
Resolution : 2.15 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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

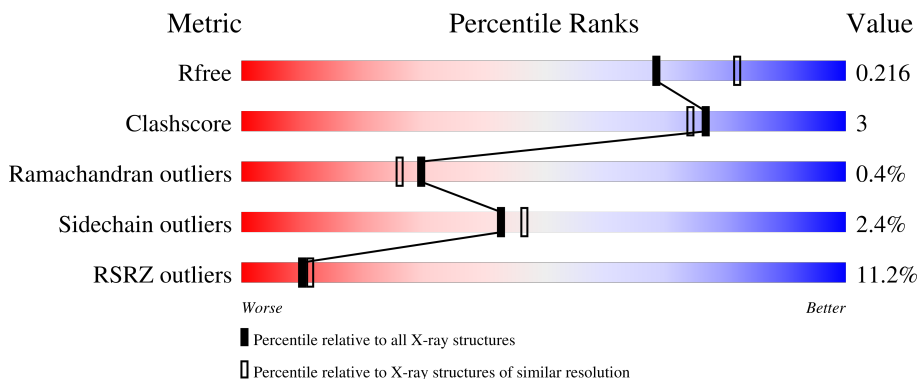
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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

Mol	Chain	Length	Quality of chain
1	A	447	 19% 85% 9% • 6%
1	B	447	 18% 89% 7% • •
1	C	447	 10% 85% 10% • 5%
1	D	447	 3% 87% 7% • 5%
1	E	447	 17% 86% 6% • 6%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXL	A	602	-	X	-	-
3	OXL	B	602	-	X	-	-
3	OXL	C	602	-	X	-	-
3	OXL	D	602	-	X	-	-
3	OXL	E	602	-	X	-	-
3	OXL	F	602	-	X	-	-
3	OXL	G	602	-	X	-	-
3	OXL	H	602	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28156 atoms, of which 104 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
			Total	C	N	O	S			
1	A	422	3236	2034	585	597	20	0	6	0
1	B	435	3325	2088	603	614	20	0	4	0
1	C	425	3247	2040	585	603	19	0	4	0
1	D	425	3252	2042	590	601	19	0	6	0
1	E	419	3210	2018	579	593	20	0	5	0
1	F	433	3325	2092	598	615	20	0	7	0
1	G	421	3231	2031	581	600	19	0	6	0
1	H	425	3251	2040	594	598	19	0	4	0

There are 48 discrepancies between the modelled and reference sequences:

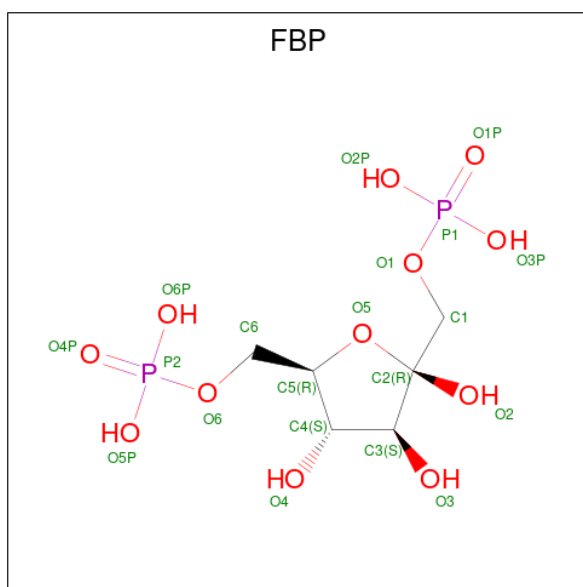
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q16716
A	0	SER	-	expression tag	UNP Q16716
A	12	ASP	SER	conflict	UNP Q16716
A	130	GLY	-	linker	UNP Q16716
A	131	SER	-	linker	UNP Q16716
A	132	GLY	-	linker	UNP Q16716
B	-1	GLY	-	expression tag	UNP Q16716
B	0	SER	-	expression tag	UNP Q16716
B	12	ASP	SER	conflict	UNP Q16716
B	130	GLY	-	linker	UNP Q16716
B	131	SER	-	linker	UNP Q16716
B	230	GLY	-	linker	UNP Q16716
C	-1	GLY	-	expression tag	UNP Q16716

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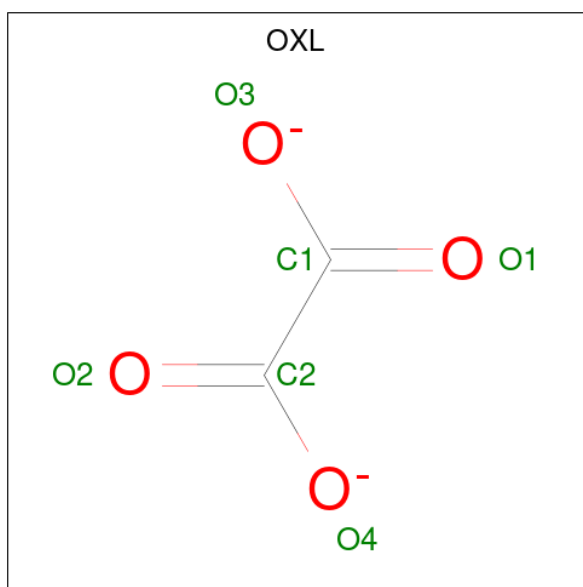
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP Q16716
C	12	ASP	SER	conflict	UNP Q16716
C	130	GLY	-	linker	UNP Q16716
C	131	SER	-	linker	UNP Q16716
C	132	GLY	-	linker	UNP Q16716
D	-1	GLY	-	expression tag	UNP Q16716
D	0	SER	-	expression tag	UNP Q16716
D	12	ASP	SER	conflict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

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



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

- Molecule 3 is OXALATE ION (CCD ID: OXL) (formula: C₂O₄).



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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

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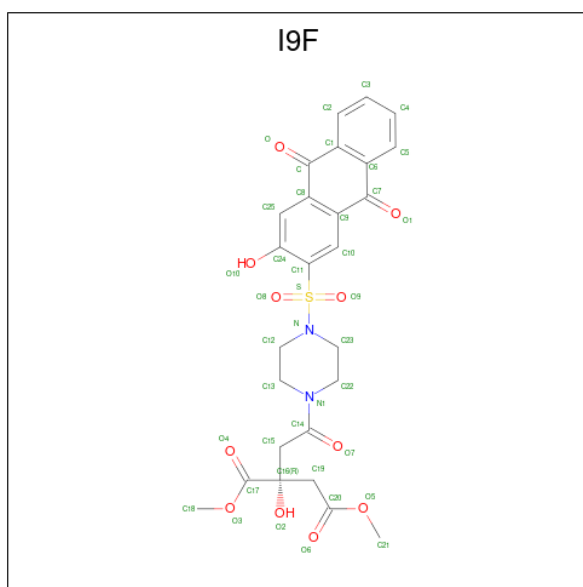
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0
4	G	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0

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

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

- Molecule 6 is dimethyl (2R)-2-hydroxy-2-{2-[4-(3-hydroxy-9,10-dioxo-9,10-dihydroan thracene-2-sulfonyl)piperazin-1-yl]-2-oxoethyl}butanedioate (CCD ID: I9F) (formula: C₂₆H₂₆N₂O₁₁S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			S
6	C	1	Total 66	C 26	H 26	N 2	O 11	S 1	26	0
6	E	1	Total 66	C 26	H 26	N 2	O 11	S 1	26	0
6	F	1	Total 66	C 26	H 26	N 2	O 11	S 1	26	0
6	G	1	Total 66	C 26	H 26	N 2	O 11	S 1	26	0

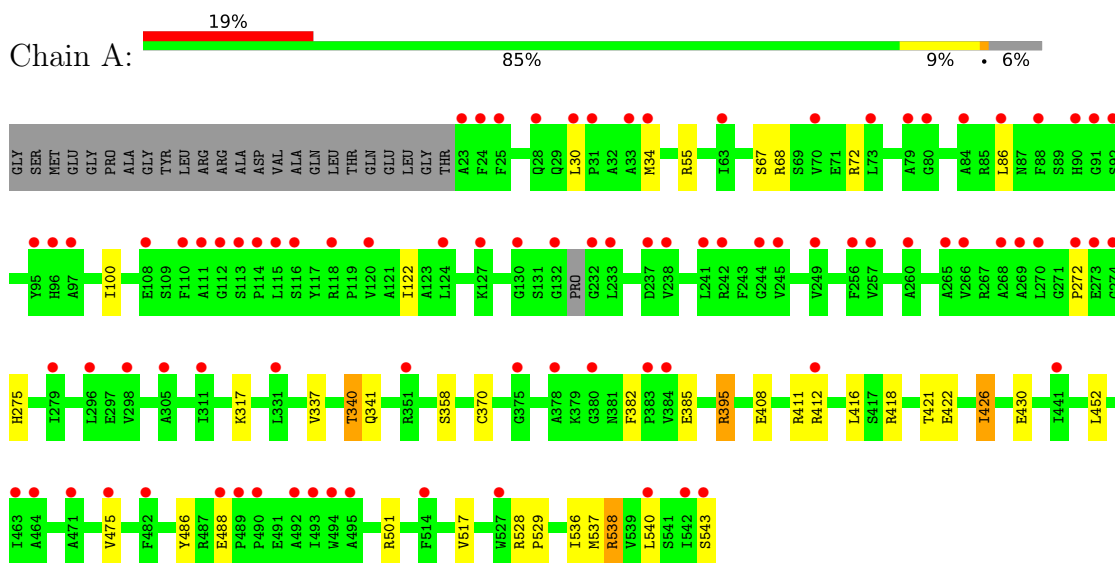
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	101	Total 101	O 101	0	0
7	B	133	Total 133	O 133	0	0
7	C	220	Total 220	O 220	0	0
7	D	246	Total 246	O 246	0	0
7	E	125	Total 125	O 125	0	0
7	F	196	Total 196	O 196	0	0
7	G	261	Total 261	O 261	0	0
7	H	309	Total 309	O 309	0	0

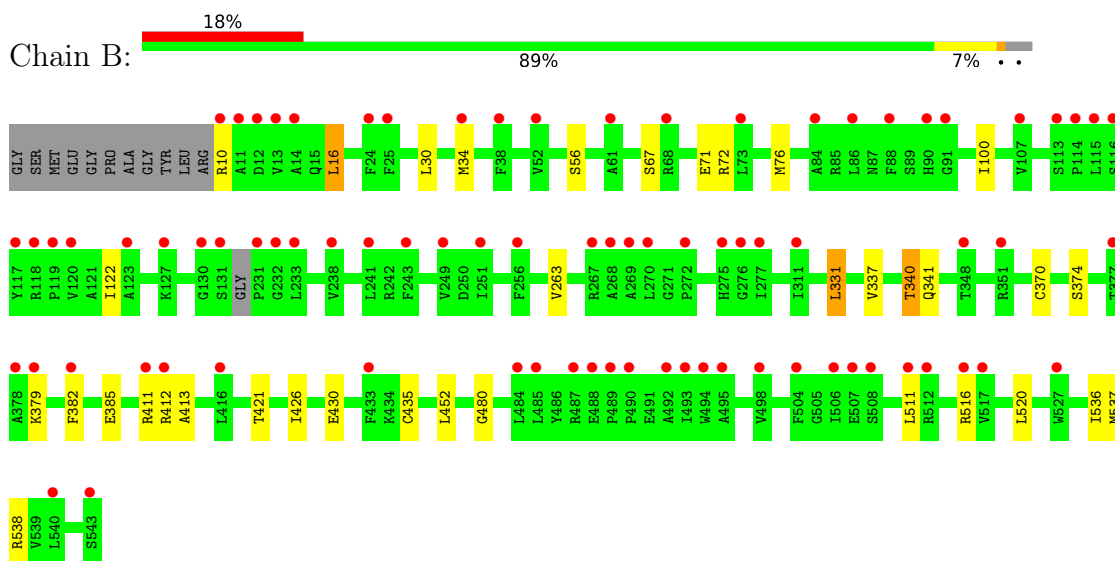
3 Residue-property plots

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


- Molecule 1: Pyruvate kinase

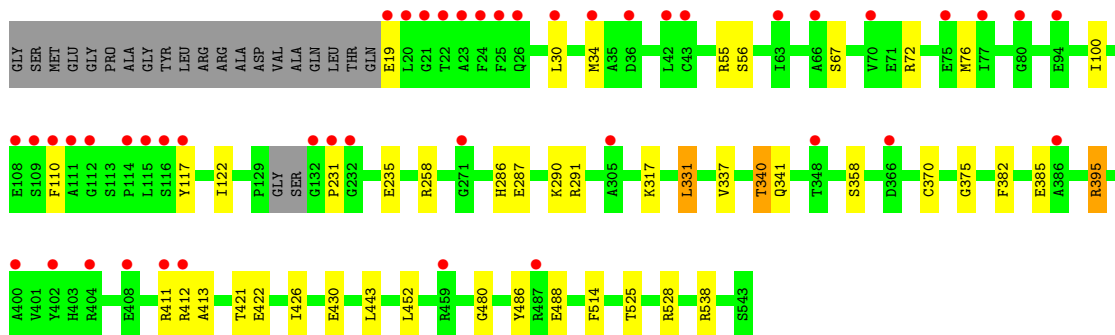


- Molecule 1: Pyruvate kinase




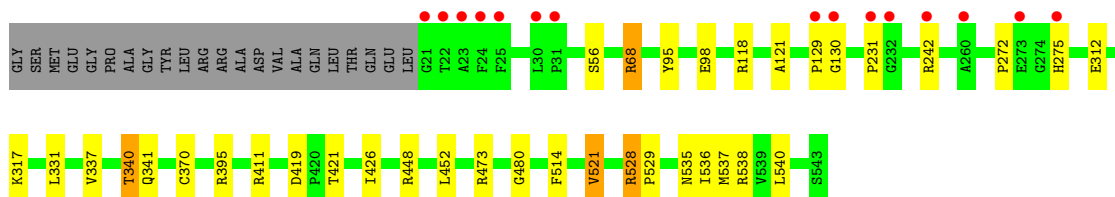
- Molecule 1: Pyruvate kinase

Chain C:  10% 85% 10% • 5%




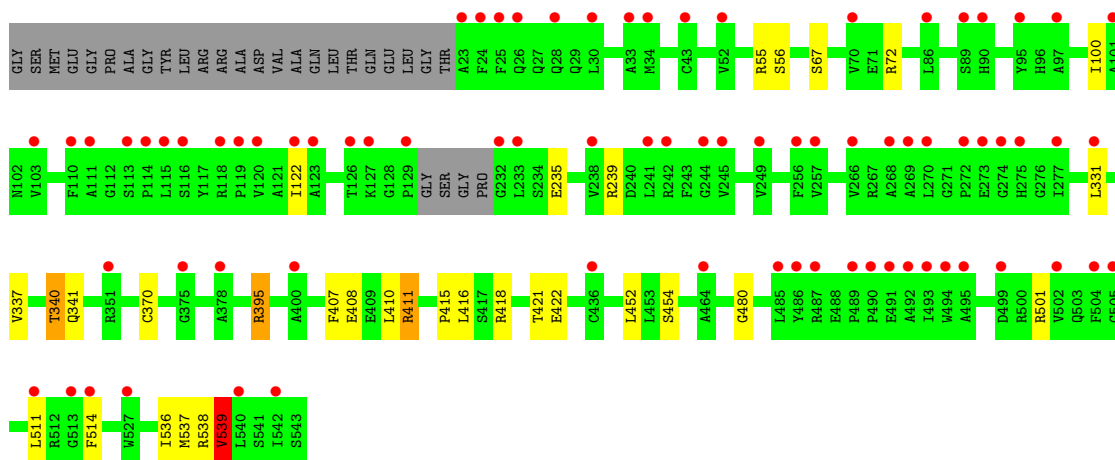
• Molecule 1: Pyruvate kinase

Chain D:  3% 87% 7% • 5%




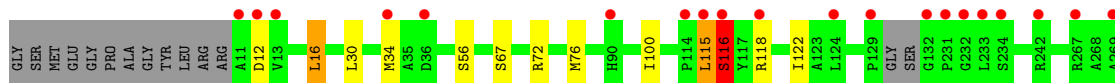
• Molecule 1: Pyruvate kinase

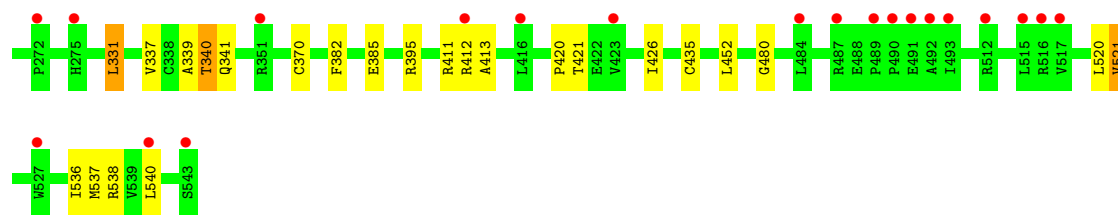
Chain E:  17% 86% 6% • 6%



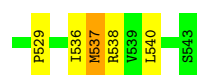
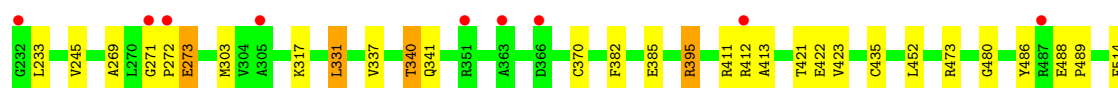
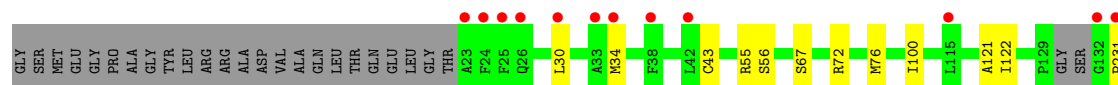
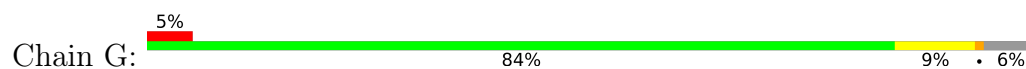
• Molecule 1: Pyruvate kinase

Chain F:  9% 89% 7% • •

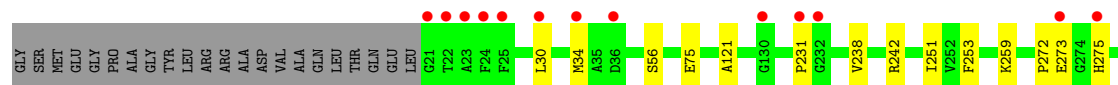
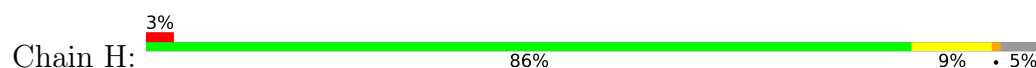




- Molecule 1: Pyruvate kinase



- Molecule 1: Pyruvate kinase



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	207.65Å 112.84Å 188.36Å 90.00° 91.67° 90.00°	Depositor
Resolution (Å)	188.28 – 2.15 188.28 – 2.15	Depositor EDS
% Data completeness (in resolution range)	78.0 (188.28-2.15) 78.0 (188.28-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.16Å)	Xtrriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, R_{free}	0.206 , 0.229 0.195 , 0.216	Depositor DCC
R_{free} test set	9067 reflections (3.87%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtrriage
Anisotropy	0.020	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	28156	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.88 % 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 2.9665e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: FBP, K, I9F, 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	0.66	0/3307	1.01	2/4469 (0.0%)
1	B	0.69	1/3391 (0.0%)	1.01	0/4583
1	C	0.73	0/3313	1.01	1/4479 (0.0%)
1	D	0.74	0/3326	1.03	1/4497 (0.0%)
1	E	0.64	0/3278	1.00	5/4430 (0.1%)
1	F	0.71	1/3400 (0.0%)	1.02	2/4597 (0.0%)
1	G	0.76	3/3303 (0.1%)	1.01	1/4465 (0.0%)
1	H	0.78	0/3316	1.03	3/4483 (0.1%)
All	All	0.72	5/26634 (0.0%)	1.01	15/36003 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	374	SER	CA-C	8.68	1.56	1.52
1	G	489	PRO	CA-C	5.78	1.55	1.51
1	F	116	SER	CA-C	5.54	1.60	1.52
1	G	303	MET	SD-CE	-5.22	1.66	1.79
1	G	537	MET	SD-CE	-5.11	1.66	1.79

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	422	GLU	CB-CG-CD	6.91	124.35	112.60
1	A	422	GLU	CB-CG-CD	6.82	124.19	112.60
1	C	514	PHE	CA-CB-CG	6.12	119.92	113.80
1	G	514	PHE	CA-CB-CG	5.86	119.66	113.80
1	E	539	VAL	N-CA-CB	5.83	118.03	111.21
1	H	514	PHE	CA-CB-CG	5.44	119.24	113.80
1	D	514	PHE	CA-CB-CG	5.34	119.14	113.80
1	H	339	ALA	CA-C-N	5.28	131.62	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	339	ALA	C-N-CA	5.28	131.62	121.54
1	F	339	ALA	CA-C-N	5.25	131.57	121.54
1	F	339	ALA	C-N-CA	5.25	131.57	121.54
1	E	514	PHE	CA-CB-CG	5.07	118.86	113.80
1	E	410	LEU	CA-C-N	5.01	127.24	120.38
1	E	410	LEU	C-N-CA	5.01	127.24	120.38
1	A	426	ILE	CB-CG1-CD1	5.00	124.30	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3236	0	3299	22	0
1	B	3325	0	3391	19	0
1	C	3247	0	3299	26	0
1	D	3252	0	3310	18	0
1	E	3210	0	3270	19	0
1	F	3325	0	3395	23	0
1	G	3231	0	3284	27	0
1	H	3251	0	3306	23	0
2	A	20	0	10	1	0
2	B	20	0	10	0	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
2	E	20	0	10	1	0
2	F	20	0	10	0	0
2	G	20	0	10	0	0
2	H	20	0	10	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	6	0	0	0	0
3	H	6	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	1	0	0	0	0
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	C	40	26	0	1	0
6	E	40	26	0	0	0
6	F	40	26	0	0	0
6	G	40	26	0	0	0
7	A	101	0	0	0	0
7	B	133	0	0	0	0
7	C	220	0	0	3	0
7	D	246	0	0	2	0
7	E	125	0	0	0	0
7	F	196	0	0	0	0
7	G	261	0	0	1	2
7	H	309	0	0	2	2
All	All	28052	104	26634	153	2

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 (153) 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:C:422[A]:GLU:HG3	1:C:452:LEU:HD13	1.62	0.80
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.65	0.78
1:C:411:ARG:HG3	1:C:426:ILE:HD11	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:538:ARG:HG2	1:H:536:ILE:HG12	1.66	0.78
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.65	0.78
1:A:408:GLU:OE2	1:B:411:ARG:NH2	2.21	0.74
1:A:418[A]:ARG:HG3	1:B:16:LEU:HD11	1.70	0.72
1:C:528:ARG:NH1	1:G:233:LEU:O	2.23	0.72
1:F:411:ARG:HG3	1:F:426:ILE:HD11	1.72	0.71
1:A:272:PRO:HA	1:A:275:HIS:NE2	2.05	0.71
1:E:408:GLU:OE2	1:F:411:ARG:NH2	2.23	0.71
1:B:411:ARG:HG3	1:B:426:ILE:HD11	1.74	0.68
1:G:537:MET:HE3	1:H:537:MET:HG2	1.80	0.63
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.81	0.63
1:F:56:SER:HB2	1:F:480:GLY:HA2	1.80	0.63
1:G:56:SER:HB2	1:G:480:GLY:HA2	1.80	0.62
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.82	0.62
1:G:536:ILE:HG12	1:H:538[A]:ARG:HG2	1.82	0.61
1:E:235:GLU:O	1:E:239:ARG:HD3	2.01	0.61
1:G:272:PRO:HD2	1:G:273:GLU:OE1	2.00	0.61
1:E:536:ILE:HG12	1:F:538:ARG:HG2	1.82	0.60
1:H:56:SER:HB2	1:H:480:GLY:HA2	1.83	0.60
1:E:56:SER:HB2	1:E:480:GLY:HA2	1.84	0.59
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.84	0.59
1:C:538:ARG:HG2	1:D:536:ILE:HG12	1.83	0.58
1:A:272:PRO:HA	1:A:275:HIS:CD2	2.39	0.58
1:E:538:ARG:HG2	1:F:536:ILE:HG12	1.86	0.58
1:H:272:PRO:HA	1:H:275[A]:HIS:CE1	2.39	0.57
1:D:411:ARG:HG3	1:D:426:ILE:HD11	1.86	0.57
1:E:539:VAL:HG22	1:F:420:PRO:HB3	1.88	0.56
1:D:272:PRO:HA	1:D:275[A]:HIS:CE1	2.40	0.56
1:A:538:ARG:HG3	1:B:536:ILE:HG12	1.88	0.56
1:C:375:GLY:HA2	6:C:605:I9F:O9	2.06	0.55
1:D:521:VAL:HG12	1:D:540:LEU:HB3	1.88	0.55
1:G:331:LEU:HD11	1:G:413:ALA:HB1	1.88	0.54
1:C:340:THR:HG22	1:C:341:GLN:HG3	1.90	0.54
1:E:331:LEU:HD22	1:G:43:CYS:SG	2.48	0.54
1:D:340:THR:HG22	1:D:341:GLN:HG3	1.90	0.53
1:B:340:THR:HG22	1:B:341:GLN:HG3	1.91	0.53
1:G:340:THR:HG22	1:G:341:GLN:HG3	1.91	0.53
1:A:340:THR:HG22	1:A:341:GLN:HG3	1.91	0.52
1:E:415:PRO:HB3	1:F:12:ASP:HA	1.91	0.52
1:B:382:PHE:HB3	1:B:385:GLU:HB2	1.91	0.52
1:D:535:ASN:OD1	1:D:536:ILE:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:407:PHE:O	1:E:411:ARG:HB2	2.10	0.52
1:E:340:THR:HG22	1:E:341:GLN:HG3	1.92	0.51
1:F:30:LEU:O	1:F:34:MET:HG2	2.10	0.51
1:F:67:SER:HA	1:F:72:ARG:HG2	1.93	0.51
1:A:67:SER:HA	1:A:72:ARG:HG2	1.92	0.51
1:A:517:VAL:HG22	1:A:543:SER:HB3	1.92	0.50
1:D:528:ARG:HD2	1:D:529:PRO:O	2.11	0.50
1:D:317:LYS:NZ	7:D:704:HOH:O	2.44	0.50
1:A:382:PHE:HB3	1:A:385:GLU:HB2	1.93	0.50
1:B:30:LEU:O	1:B:34:MET:HG2	2.12	0.50
1:A:30:LEU:O	1:A:34:MET:HG2	2.11	0.50
1:H:331:LEU:HD11	1:H:413:ALA:HB1	1.93	0.50
1:A:317:LYS:NZ	7:C:702:HOH:O	2.44	0.49
1:C:235:GLU:HG3	1:G:529:PRO:HG3	1.94	0.49
1:A:411:ARG:HG3	1:A:426:ILE:HD11	1.95	0.49
1:F:56:SER:HB2	1:F:480:GLY:CA	2.43	0.49
1:H:75:GLU:HG3	7:H:963:HOH:O	2.13	0.49
1:C:30:LEU:O	1:C:34:MET:HG2	2.13	0.49
1:C:538:ARG:HD3	7:C:778:HOH:O	2.12	0.49
1:B:421:THR:HG22	1:B:452:LEU:HD12	1.95	0.49
1:G:30:LEU:O	1:G:34:MET:HG2	2.13	0.48
1:H:30:LEU:O	1:H:34:MET:HG2	2.12	0.48
1:B:56:SER:HB2	1:B:480:GLY:CA	2.44	0.48
1:C:56:SER:HB2	1:C:480:GLY:CA	2.43	0.48
1:F:331:LEU:HD11	1:F:413:ALA:HB1	1.95	0.48
1:A:100:ILE:HG23	1:A:122:ILE:HD13	1.96	0.48
1:C:331:LEU:HD11	1:C:413:ALA:HB1	1.95	0.48
1:A:421:THR:HG22	1:A:452:LEU:HD12	1.96	0.48
1:C:110:PHE:O	1:C:117:TYR:HB2	2.14	0.48
1:F:421:THR:HG22	1:F:452:LEU:HD12	1.96	0.47
1:F:521:VAL:HG12	1:F:540[B]:LEU:HB3	1.96	0.47
1:H:340:THR:HG22	1:H:341:GLN:HG3	1.95	0.47
1:C:337:VAL:HG22	1:C:370:CYS:HB2	1.96	0.47
1:F:382:PHE:HB3	1:F:385:GLU:HB2	1.94	0.47
1:H:238:VAL:O	1:H:242:ARG:HG3	2.14	0.47
1:H:317:LYS:NZ	7:H:701:HOH:O	2.44	0.47
1:C:100:ILE:HG23	1:C:122:ILE:HD13	1.97	0.47
1:G:486:TYR:CZ	1:G:488:GLU:HB2	2.50	0.47
1:H:421:THR:HG22	1:H:452:LEU:HD12	1.97	0.47
1:F:100:ILE:HG23	1:F:122:ILE:HD13	1.97	0.47
1:B:337:VAL:HG22	1:B:370:CYS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:56:SER:HB2	1:G:480:GLY:CA	2.44	0.47
1:H:337:VAL:HG22	1:H:370:CYS:HB2	1.98	0.46
1:G:382:PHE:HB3	1:G:385:GLU:HB2	1.96	0.46
1:H:56:SER:HB2	1:H:480:GLY:CA	2.46	0.46
1:C:486:TYR:CZ	1:C:488:GLU:HB2	2.49	0.46
1:E:416:LEU:HB3	1:F:16:LEU:HD22	1.97	0.46
1:F:411:ARG:CG	1:F:426:ILE:HD11	2.44	0.46
1:G:317:LYS:NZ	7:G:704:HOH:O	2.44	0.46
1:E:337:VAL:HG22	1:E:370:CYS:HB2	1.97	0.46
1:H:523:VAL:HB	1:H:538[B]:ARG:HG2	1.98	0.46
1:F:337:VAL:HG22	1:F:370:CYS:HB2	1.97	0.46
1:B:100:ILE:HG23	1:B:122:ILE:HD13	1.97	0.45
1:G:421:THR:HG22	1:G:452:LEU:HD12	1.98	0.45
1:A:430:GLU:OE2	1:B:430:GLU:OE1	2.35	0.45
1:C:430[B]:GLU:OE2	1:D:411:ARG:HD2	2.17	0.45
1:A:486:TYR:CZ	1:A:488[B]:GLU:HB2	2.51	0.45
1:G:100:ILE:HG23	1:G:122:ILE:HD13	1.98	0.45
1:D:121:ALA:HA	1:D:473:ARG:HB3	1.98	0.45
1:G:337:VAL:HG22	1:G:370:CYS:HB2	1.99	0.45
1:C:67:SER:HA	1:C:72:ARG:HG2	1.98	0.45
1:F:340:THR:HG22	1:F:341:GLN:HG3	1.97	0.45
1:D:421:THR:HG22	1:D:452:LEU:HD12	1.98	0.45
1:G:67:SER:HA	1:G:72:ARG:HG2	1.98	0.45
1:C:287:GLU:HG2	1:C:291:ARG:HD2	1.98	0.45
1:D:419:ASP:OD2	1:D:448:ARG:NH2	2.50	0.45
1:E:421:THR:HG22	1:E:452:LEU:HD12	1.98	0.45
1:H:121:ALA:HA	1:H:473:ARG:HB3	1.99	0.44
1:A:337:VAL:HG22	1:A:370:CYS:HB2	1.98	0.44
1:B:411:ARG:CG	1:B:426:ILE:HD11	2.46	0.44
1:D:68:ARG:NH2	1:D:98:GLU:HB2	2.32	0.44
1:E:56:SER:HB2	1:E:480:GLY:CA	2.46	0.44
1:D:56:SER:HB2	1:D:480:GLY:CA	2.46	0.44
1:C:411:ARG:CG	1:C:426:ILE:HD11	2.43	0.44
1:F:115:LEU:O	1:F:116:SER:HB3	2.17	0.44
1:A:528:ARG:HD2	1:A:529:PRO:O	2.17	0.44
1:C:317:LYS:NZ	7:C:709:HOH:O	2.51	0.44
1:C:421:THR:HG22	1:C:452:LEU:HD12	1.99	0.44
1:G:423:VAL:HG21	1:H:435:CYS:HB3	1.99	0.44
1:B:435:CYS:HB2	1:B:520:LEU:HD12	2.00	0.43
1:E:67:SER:HA	1:E:72:ARG:HG2	2.00	0.43
1:G:269:ALA:C	1:G:271:GLY:H	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:537:MET:HE3	1:H:537:MET:CG	2.46	0.43
1:F:435:CYS:HB2	1:F:520:LEU:HD12	2.01	0.43
1:G:435:CYS:HB3	1:H:423:VAL:HG21	2.00	0.43
1:H:251:ILE:HG12	1:H:477:LEU:HD11	2.01	0.43
1:A:501:ARG:NH1	2:A:601:FBP:O2P	2.40	0.43
1:H:419:ASP:OD2	1:H:448:ARG:NH2	2.48	0.43
1:D:337:VAL:HG22	1:D:370:CYS:HB2	2.01	0.43
1:C:382:PHE:HB3	1:C:385:GLU:HB2	2.01	0.42
1:E:100:ILE:HG23	1:E:122:ILE:HD13	1.99	0.42
1:E:418:ARG:HG3	1:F:16:LEU:HD11	2.02	0.42
1:E:501:ARG:NH1	2:E:601:FBP:O1P	2.37	0.42
1:B:331:LEU:HD11	1:B:413:ALA:HB1	2.02	0.42
1:E:55:ARG:HB2	1:E:395:ARG:HG3	2.00	0.42
1:H:290:LYS:HA	1:H:290:LYS:HD2	1.85	0.42
1:H:253:PHE:HD1	1:H:280:ILE:HB	1.85	0.42
1:C:443:LEU:HD22	1:C:525:THR:HG22	2.02	0.41
1:G:245:VAL:CG1	1:G:273:GLU:HG2	2.50	0.41
1:D:312:GLU:HB3	7:D:851:HOH:O	2.20	0.41
1:A:55:ARG:HB2	1:A:395:ARG:HG3	2.01	0.41
1:C:286:HIS:CE1	1:C:290:LYS:HG3	2.56	0.41
1:B:67:SER:HA	1:B:72:ARG:HG2	2.03	0.41
1:A:416:LEU:HB3	1:B:16:LEU:HD22	2.02	0.41
1:G:55:ARG:HB2	1:G:395:ARG:HG3	2.02	0.40
1:F:521:VAL:HG12	1:F:540[A]:LEU:HB2	2.02	0.40
1:C:55:ARG:HB2	1:C:395:ARG:HG3	2.03	0.40
1:D:68:ARG:HD2	1:D:95:TYR:OH	2.21	0.40
1:G:121:ALA:HA	1:G:473:ARG:HB3	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:789:HOH:O	7:H:893:HOH:O[4_546]	1.99	0.21
7:G:785:HOH:O	7:H:893:HOH:O[4_546]	2.03	0.17

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	424/447 (95%)	420 (99%)	3 (1%)	1 (0%)	43	44
1	B	435/447 (97%)	430 (99%)	4 (1%)	1 (0%)	43	44
1	C	425/447 (95%)	419 (99%)	4 (1%)	2 (0%)	24	20
1	D	429/447 (96%)	421 (98%)	4 (1%)	4 (1%)	14	9
1	E	420/447 (94%)	416 (99%)	3 (1%)	1 (0%)	43	44
1	F	436/447 (98%)	428 (98%)	6 (1%)	2 (0%)	24	20
1	G	423/447 (95%)	416 (98%)	5 (1%)	2 (0%)	24	20
1	H	427/447 (96%)	422 (99%)	3 (1%)	2 (0%)	24	20
All	All	3419/3576 (96%)	3372 (99%)	32 (1%)	15 (0%)	30	26

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	116	SER
1	C	231	PRO
1	D	130	GLY
1	D	231	PRO
1	G	231	PRO
1	B	340	THR
1	C	340	THR
1	D	340	THR
1	E	340	THR
1	F	340	THR
1	G	340	THR
1	H	340	THR
1	A	340	THR
1	H	231	PRO
1	D	129	PRO

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	340/352 (97%)	330 (97%)	10 (3%)	37	39
1	B	349/352 (99%)	336 (96%)	13 (4%)	30	30
1	C	341/352 (97%)	333 (98%)	8 (2%)	44	49
1	D	342/352 (97%)	332 (97%)	10 (3%)	37	39
1	E	338/352 (96%)	330 (98%)	8 (2%)	43	47
1	F	350/352 (99%)	339 (97%)	11 (3%)	35	37
1	G	340/352 (97%)	332 (98%)	8 (2%)	43	47
1	H	340/352 (97%)	333 (98%)	7 (2%)	47	52
All	All	2740/2816 (97%)	2665 (97%)	75 (3%)	43	41

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ARG
1	A	86	LEU
1	A	358	SER
1	A	395	ARG
1	A	412	ARG
1	A	475	VAL
1	A	537[A]	MET
1	A	537[B]	MET
1	A	538	ARG
1	A	540	LEU
1	B	10	ARG
1	B	16	LEU
1	B	71	GLU
1	B	76[A]	MET
1	B	76[B]	MET
1	B	263	VAL
1	B	331	LEU
1	B	379	LYS
1	B	412	ARG

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Mol	Chain	Res	Type
1	B	511	LEU
1	B	516	ARG
1	B	537[A]	MET
1	B	537[B]	MET
1	C	19	GLU
1	C	76[A]	MET
1	C	76[B]	MET
1	C	258	ARG
1	C	331	LEU
1	C	358	SER
1	C	395	ARG
1	C	412	ARG
1	D	68	ARG
1	D	118	ARG
1	D	242[A]	ARG
1	D	242[B]	ARG
1	D	331	LEU
1	D	395	ARG
1	D	521	VAL
1	D	528	ARG
1	D	537	MET
1	D	538	ARG
1	E	395	ARG
1	E	411	ARG
1	E	454[A]	SER
1	E	454[B]	SER
1	E	511	LEU
1	E	537[A]	MET
1	E	537[B]	MET
1	E	539	VAL
1	F	16	LEU
1	F	76[A]	MET
1	F	76[B]	MET
1	F	115	LEU
1	F	118	ARG
1	F	331	LEU
1	F	395	ARG
1	F	412	ARG
1	F	521	VAL
1	F	537[A]	MET
1	F	537[B]	MET
1	G	76[A]	MET

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Mol	Chain	Res	Type
1	G	76[B]	MET
1	G	273	GLU
1	G	331	LEU
1	G	395	ARG
1	G	411	ARG
1	G	412	ARG
1	G	540	LEU
1	H	259	LYS
1	H	273	GLU
1	H	331	LEU
1	H	395	ARG
1	H	412	ARG
1	H	537	MET
1	H	541	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	405	GLN
1	B	405	GLN
1	C	27	GLN
1	C	275	HIS
1	C	405	GLN
1	D	405	GLN
1	D	535	ASN
1	E	27	GLN
1	E	405	GLN
1	F	405	GLN
1	G	27	GLN
1	G	405	GLN
1	H	27	GLN
1	H	405	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 16 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FBP	F	601	-	18,20,20	0.34	0	21,32,32	0.62	0
3	OXL	H	602	4	5,5,5	1.82	2 (40%)	6,6,6	1.93	2 (33%)
2	FBP	E	601	-	18,20,20	0.50	0	21,32,32	0.65	1 (4%)
2	FBP	G	601	-	18,20,20	0.49	0	21,32,32	0.63	0
2	FBP	B	601	-	18,20,20	0.71	0	21,32,32	0.81	1 (4%)
6	I9F	E	605	-	43,43,43	0.21	0	61,65,65	0.43	0
3	OXL	F	602	4	5,5,5	2.81	4 (80%)	6,6,6	2.45	3 (50%)
6	I9F	G	605	-	43,43,43	0.27	0	61,65,65	0.58	1 (1%)
2	FBP	C	601	-	18,20,20	0.76	1 (5%)	21,32,32	0.62	0
2	FBP	A	601	-	18,20,20	0.44	0	21,32,32	0.67	0
6	I9F	C	605	-	43,43,43	0.29	0	61,65,65	0.44	0
3	OXL	B	602	4	5,5,5	2.28	2 (40%)	6,6,6	0.77	0
3	OXL	C	602	4	5,5,5	2.00	2 (40%)	6,6,6	1.00	1 (16%)
2	FBP	H	601	-	18,20,20	0.77	0	21,32,32	0.81	1 (4%)
3	OXL	A	602	4	5,5,5	1.89	2 (40%)	6,6,6	2.35	3 (50%)
3	OXL	E	602	4	5,5,5	2.43	2 (40%)	6,6,6	1.50	2 (33%)
6	I9F	F	605	-	43,43,43	0.31	0	61,65,65	0.41	0
3	OXL	D	602	4	5,5,5	2.32	2 (40%)	6,6,6	2.14	3 (50%)
3	OXL	G	602	4	5,5,5	2.15	2 (40%)	6,6,6	2.26	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FBP	D	601	-	18,20,20	0.52	0	21,32,32	0.80	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
3	OXL	H	602	4	-	4/4/4/4	-
2	FBP	E	601	-	-	2/13/32/32	0/1/1/1
2	FBP	G	601	-	-	2/13/32/32	0/1/1/1
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
6	I9F	E	605	-	-	5/36/62/62	0/4/4/4
3	OXL	F	602	4	-	4/4/4/4	-
6	I9F	G	605	-	-	13/36/62/62	0/4/4/4
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
6	I9F	C	605	-	-	13/36/62/62	0/4/4/4
3	OXL	B	602	4	-	4/4/4/4	-
3	OXL	C	602	4	-	4/4/4/4	-
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1
3	OXL	A	602	4	-	4/4/4/4	-
3	OXL	E	602	4	-	4/4/4/4	-
6	I9F	F	605	-	-	15/36/62/62	0/4/4/4
3	OXL	D	602	4	-	4/4/4/4	-
3	OXL	G	602	4	-	4/4/4/4	-
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	OXL	O1-C1	4.74	1.34	1.22
3	B	602	OXL	O2-C2	3.97	1.32	1.22
3	D	602	OXL	O2-C2	3.80	1.31	1.22
3	F	602	OXL	O3-C1	-3.58	1.20	1.30
3	C	602	OXL	O1-C1	3.49	1.31	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	OXL	O2-C2	3.47	1.31	1.22
3	G	602	OXL	O3-C1	-3.42	1.21	1.30
3	B	602	OXL	O4-C2	-3.18	1.21	1.30
3	F	602	OXL	O1-C1	3.15	1.30	1.22
3	D	602	OXL	O4-C2	-3.15	1.22	1.30
3	G	602	OXL	O1-C1	3.10	1.30	1.22
3	F	602	OXL	O2-C2	3.03	1.30	1.22
3	H	602	OXL	O2-C2	2.73	1.29	1.22
3	H	602	OXL	O4-C2	-2.71	1.23	1.30
3	C	602	OXL	O3-C1	-2.71	1.23	1.30
3	F	602	OXL	O4-C2	-2.47	1.23	1.30
3	E	602	OXL	O3-C1	-2.42	1.24	1.30
3	A	602	OXL	O4-C2	-2.34	1.24	1.30
2	C	601	FBP	P1-O3P	-2.26	1.46	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	602	OXL	O4-C2-C1	4.40	121.37	112.83
3	A	602	OXL	O4-C2-C1	4.30	121.18	112.83
3	H	602	OXL	O4-C2-C1	4.03	120.65	112.83
3	G	602	OXL	O3-C1-C2	3.87	120.34	112.83
3	D	602	OXL	O3-C1-C2	3.58	119.77	112.83
3	G	602	OXL	O4-C2-C1	3.14	118.92	112.83
3	F	602	OXL	O3-C1-C2	3.07	118.78	112.83
3	A	602	OXL	O2-C2-C1	-2.75	114.90	120.63
3	D	602	OXL	O4-C2-C1	2.73	118.12	112.83
3	A	602	OXL	O3-C1-C2	2.54	117.76	112.83
3	E	602	OXL	O4-C2-C1	2.51	117.70	112.83
3	F	602	OXL	O2-C2-C1	-2.48	115.47	120.63
2	D	601	FBP	O5P-P2-O6	2.37	112.86	106.67
3	D	602	OXL	O1-C1-C2	-2.36	115.71	120.63
3	E	602	OXL	O3-C1-C2	2.35	117.39	112.83
2	B	601	FBP	O3P-P1-O2P	2.29	116.39	107.80
3	H	602	OXL	O2-C2-C1	-2.21	116.02	120.63
6	G	605	I9F	C16-C15-C14	2.16	120.23	114.66
3	C	602	OXL	O3-C1-C2	2.12	116.94	112.83
2	H	601	FBP	O5P-P2-O6	2.11	112.17	106.67
2	E	601	FBP	O3P-P1-O2P	2.08	115.61	107.80

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	605	I9F	C24-C11-S-O9
6	C	605	I9F	C24-C11-S-O8
6	C	605	I9F	C15-C16-C17-O4
6	C	605	I9F	O2-C16-C17-O4
6	C	605	I9F	C15-C16-C17-O3
6	C	605	I9F	O2-C16-C17-O3
6	C	605	I9F	C19-C16-C17-O3
6	C	605	I9F	C16-C17-O3-C18
6	C	605	I9F	C19-C20-O5-C21
6	C	605	I9F	O6-C20-O5-C21
6	E	605	I9F	C19-C16-C17-O4
6	E	605	I9F	C15-C16-C17-O3
6	E	605	I9F	C19-C16-C17-O3
6	F	605	I9F	C16-C17-O3-C18
6	F	605	I9F	C19-C20-O5-C21
6	F	605	I9F	O6-C20-O5-C21
6	G	605	I9F	C24-C11-S-O9
6	G	605	I9F	C24-C11-S-O8
6	F	605	I9F	O4-C17-O3-C18
6	F	605	I9F	C12-N-S-C11
6	C	605	I9F	O4-C17-O3-C18
6	G	605	I9F	O7-C14-N1-C22
6	F	605	I9F	C12-N-S-O8
6	G	605	I9F	C23-N-S-C11
6	F	605	I9F	C23-N-S-O8
6	F	605	I9F	C23-N-S-O9
2	A	601	FBP	C4-C5-C6-O6
2	B	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6
2	E	601	FBP	C4-C5-C6-O6
2	F	601	FBP	C4-C5-C6-O6
2	H	601	FBP	C4-C5-C6-O6
6	F	605	I9F	C24-C11-S-O9
6	G	605	I9F	C15-C14-N1-C22
6	F	605	I9F	C15-C16-C19-C20
6	F	605	I9F	C23-N-S-C11
2	D	601	FBP	C4-C5-C6-O6
2	G	601	FBP	C4-C5-C6-O6
6	G	605	I9F	C23-N-S-O9
6	F	605	I9F	C17-C16-C19-C20
6	G	605	I9F	C17-C16-C19-C20
6	G	605	I9F	O2-C16-C19-C20
2	A	601	FBP	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	E	601	FBP	O5-C5-C6-O6
2	H	601	FBP	O5-C5-C6-O6
2	B	601	FBP	O5-C5-C6-O6
2	C	601	FBP	O5-C5-C6-O6
2	F	601	FBP	O5-C5-C6-O6
6	E	605	I9F	C24-C11-S-O8
6	G	605	I9F	C12-N-S-O9
2	D	601	FBP	O5-C5-C6-O6
3	D	602	OXL	O3-C1-C2-O4
3	H	602	OXL	O3-C1-C2-O4
6	F	605	I9F	O2-C16-C19-C20
6	G	605	I9F	C15-C16-C19-C20
6	C	605	I9F	C19-C16-C17-O4
6	E	605	I9F	C15-C16-C17-O4
6	G	605	I9F	C19-C16-C17-O4
3	A	602	OXL	O3-C1-C2-O4
3	C	602	OXL	O3-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O4
3	F	602	OXL	O3-C1-C2-O4
3	G	602	OXL	O3-C1-C2-O4
3	B	602	OXL	O3-C1-C2-O4
6	G	605	I9F	C19-C16-C17-O3
3	A	602	OXL	O1-C1-C2-O2
3	C	602	OXL	O1-C1-C2-O2
3	F	602	OXL	O1-C1-C2-O2
3	B	602	OXL	O1-C1-C2-O2
3	E	602	OXL	O1-C1-C2-O2
3	G	602	OXL	O1-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O2
6	C	605	I9F	O2-C16-C19-C20
6	G	605	I9F	C12-N-S-C11
2	G	601	FBP	O5-C5-C6-O6
3	D	602	OXL	O1-C1-C2-O4
3	H	602	OXL	O3-C1-C2-O2
6	F	605	I9F	C12-N-S-O9
6	F	605	I9F	C24-C11-S-O8
3	A	602	OXL	O1-C1-C2-O4
3	C	602	OXL	O1-C1-C2-O4
3	C	602	OXL	O3-C1-C2-O2
3	F	602	OXL	O1-C1-C2-O4
3	A	602	OXL	O3-C1-C2-O2

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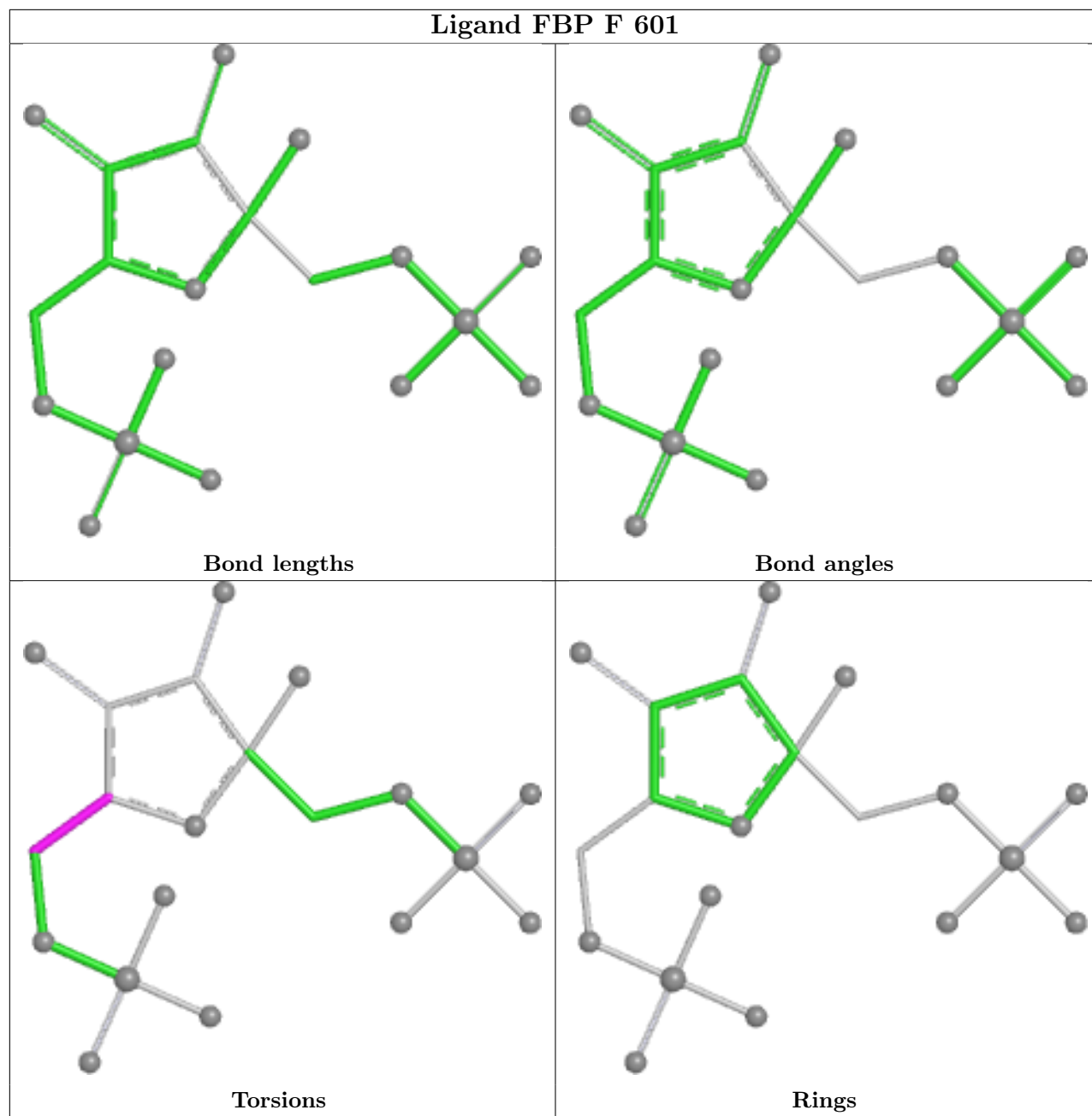
Mol	Chain	Res	Type	Atoms
3	B	602	OXL	O3-C1-C2-O2
3	E	602	OXL	O1-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O2
3	F	602	OXL	O3-C1-C2-O2
3	G	602	OXL	O3-C1-C2-O2
3	B	602	OXL	O1-C1-C2-O4
3	G	602	OXL	O1-C1-C2-O4
3	D	602	OXL	O3-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O4

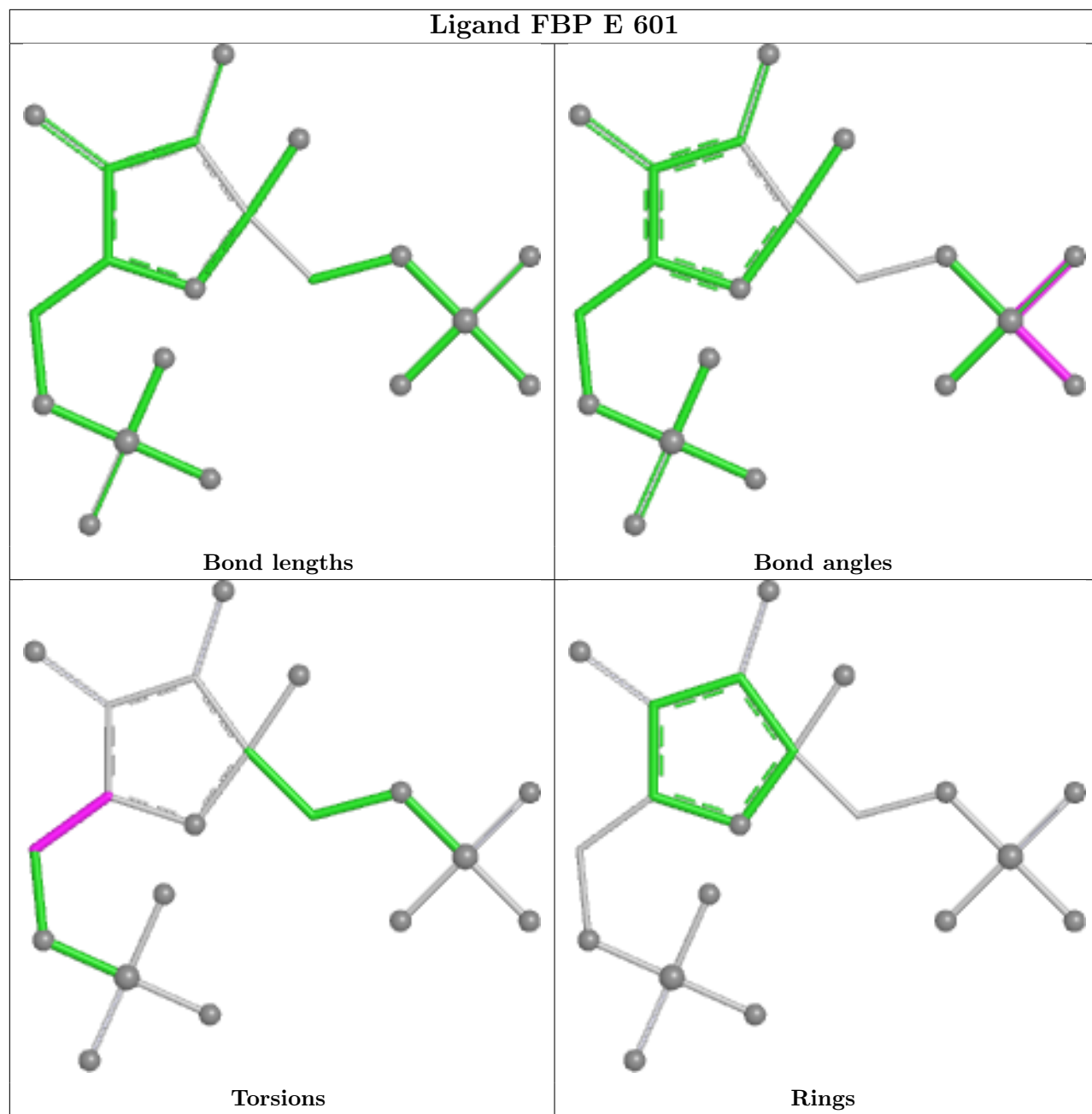
There are no ring outliers.

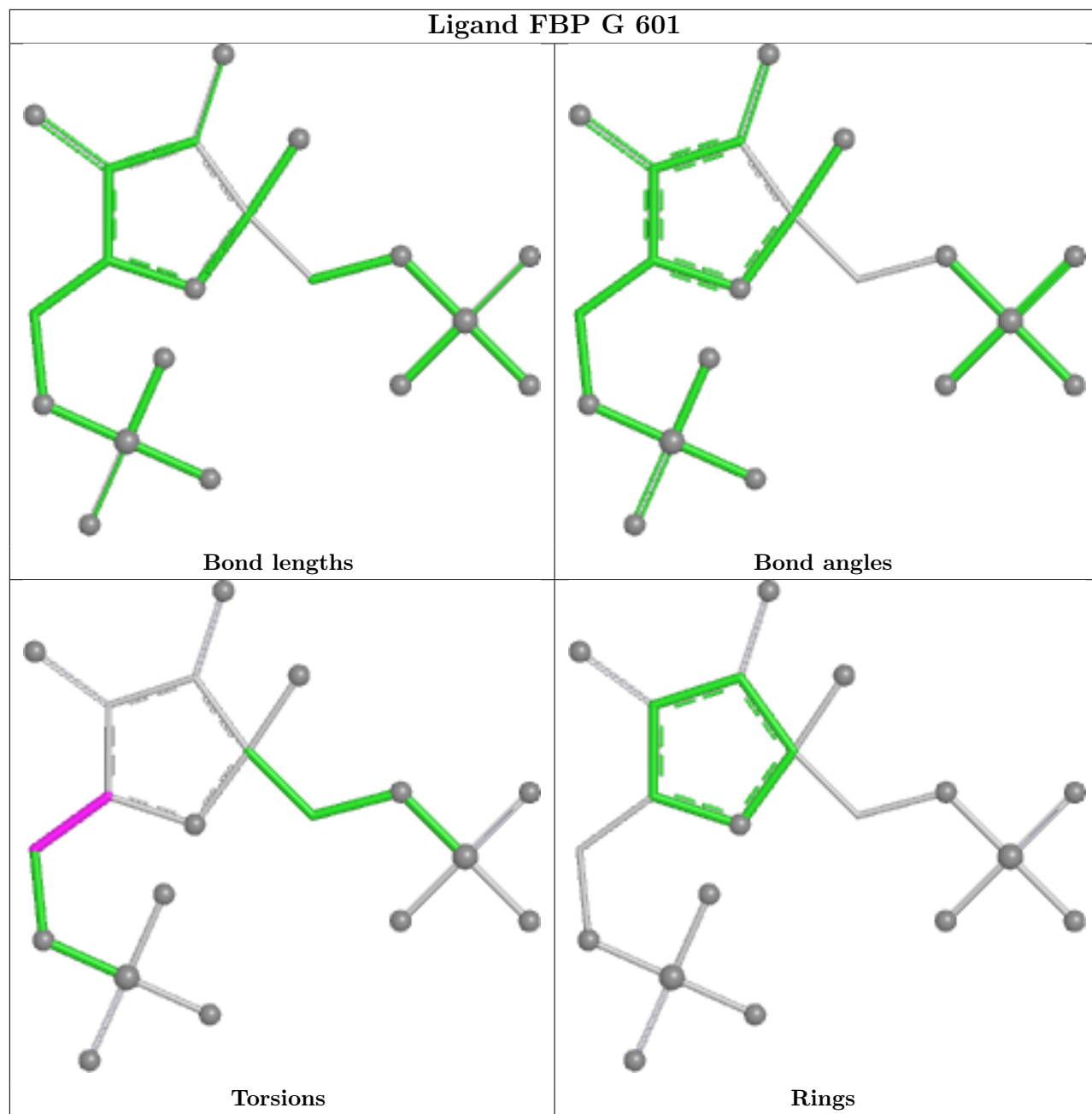
3 monomers are involved in 3 short contacts:

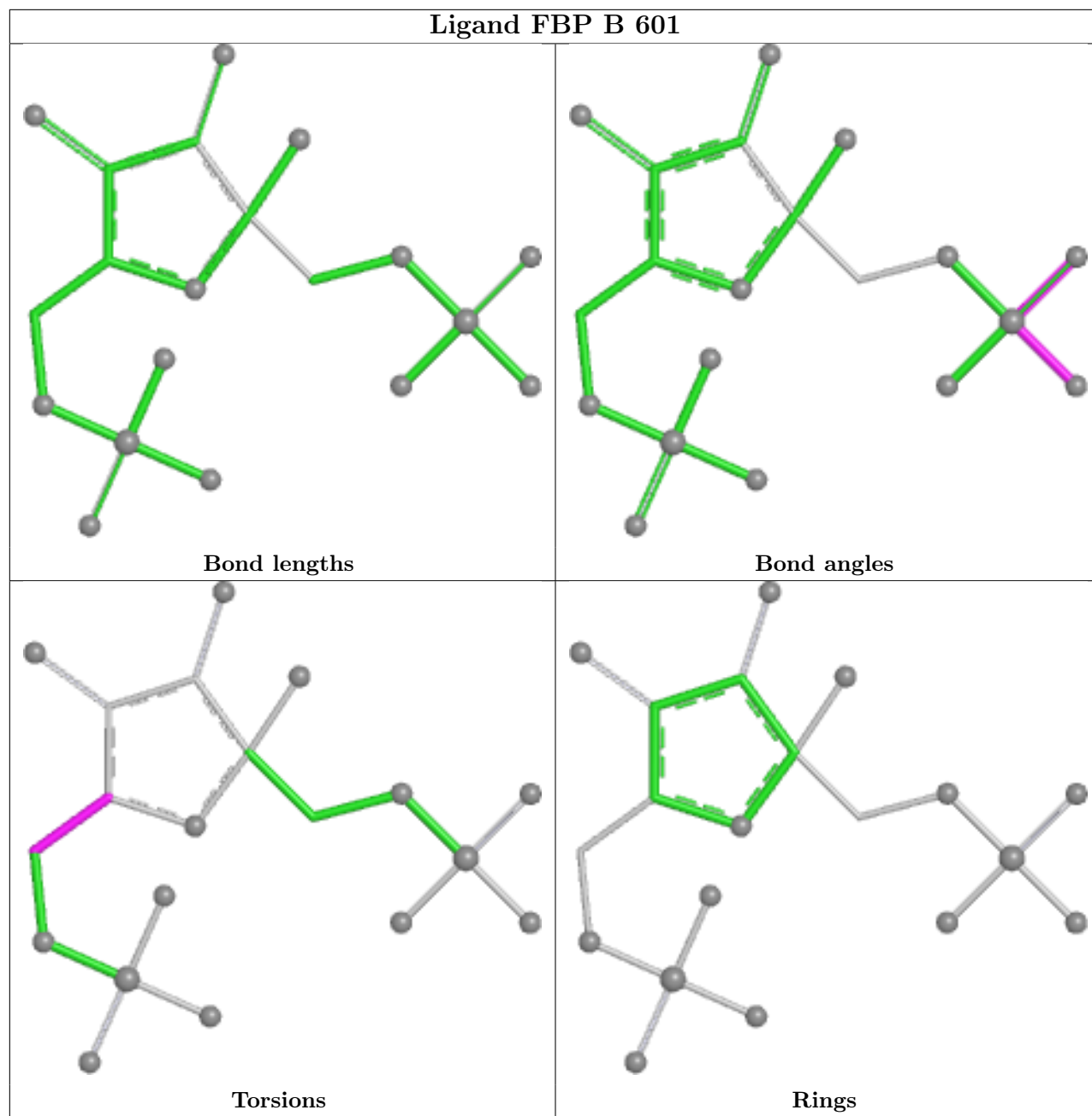
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	601	FBP	1	0
2	A	601	FBP	1	0
6	C	605	I9F	1	0

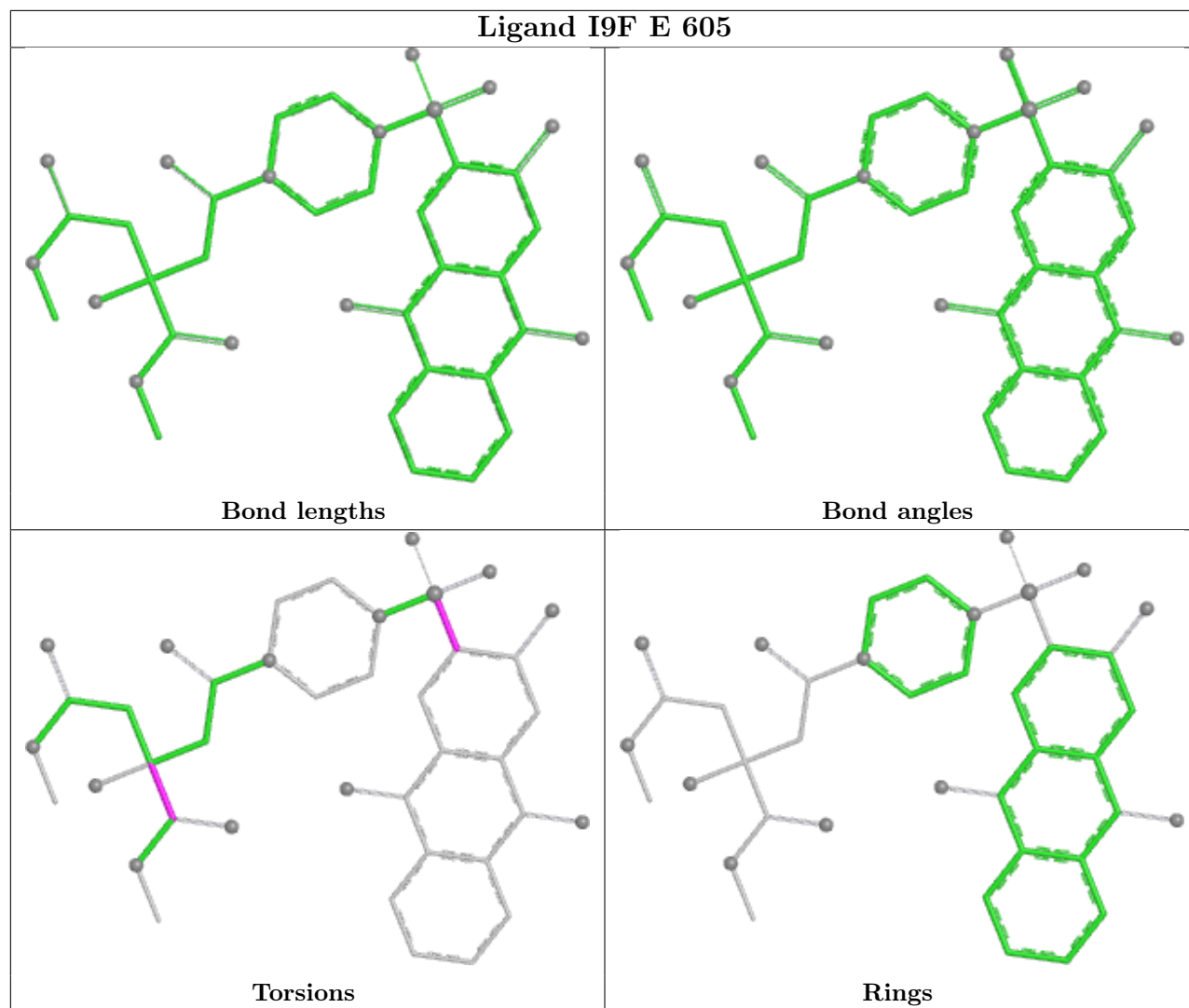
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

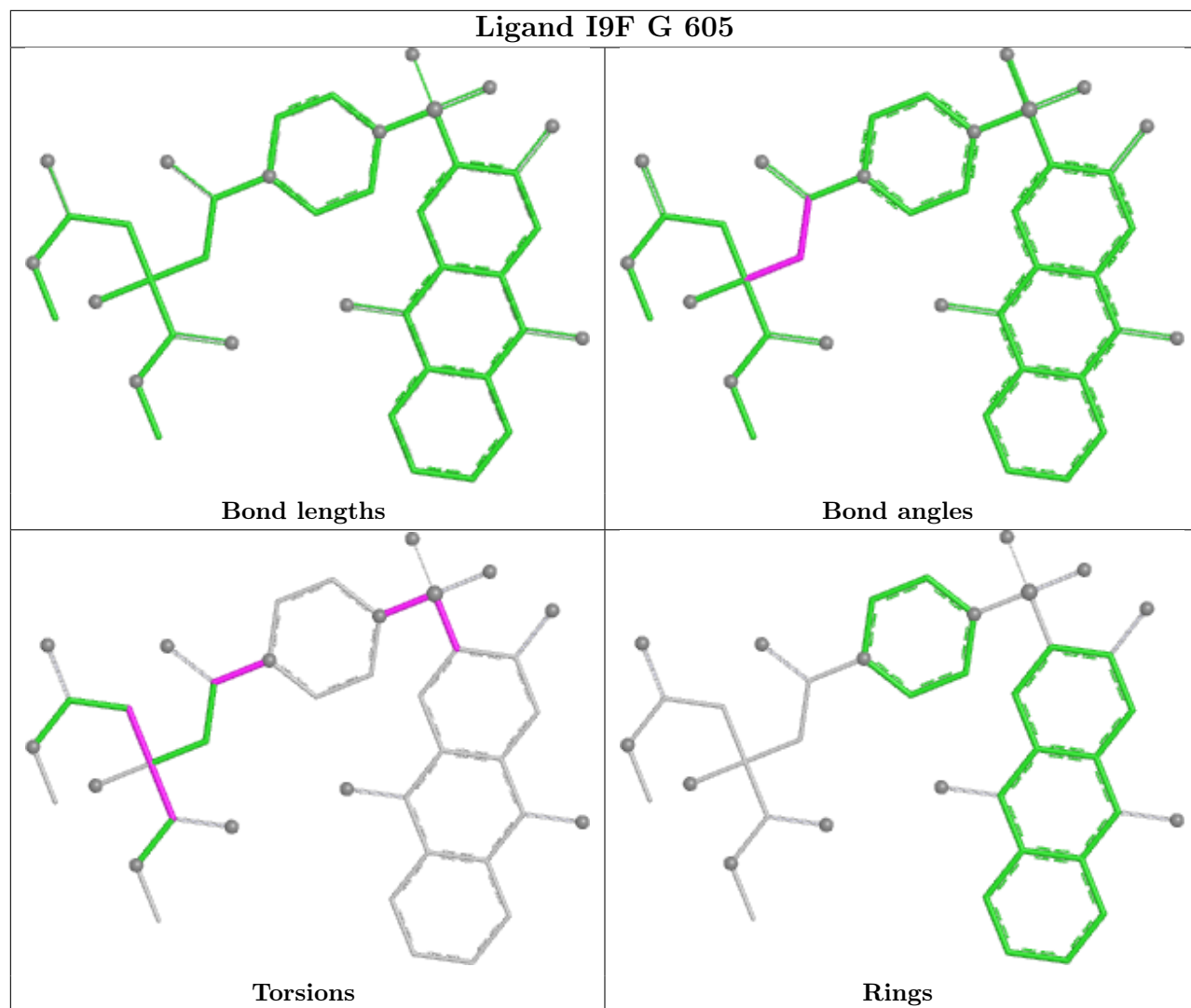


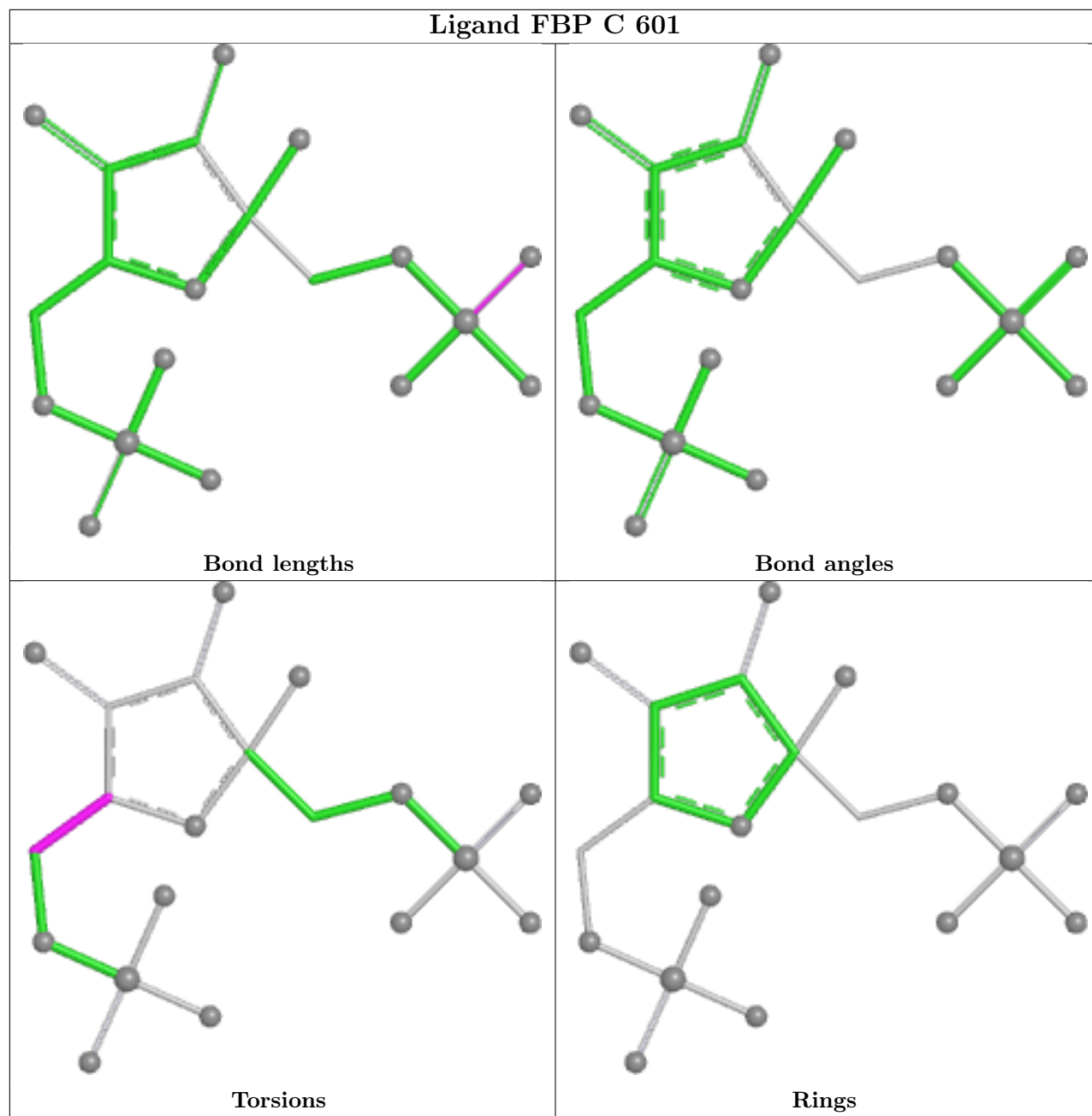


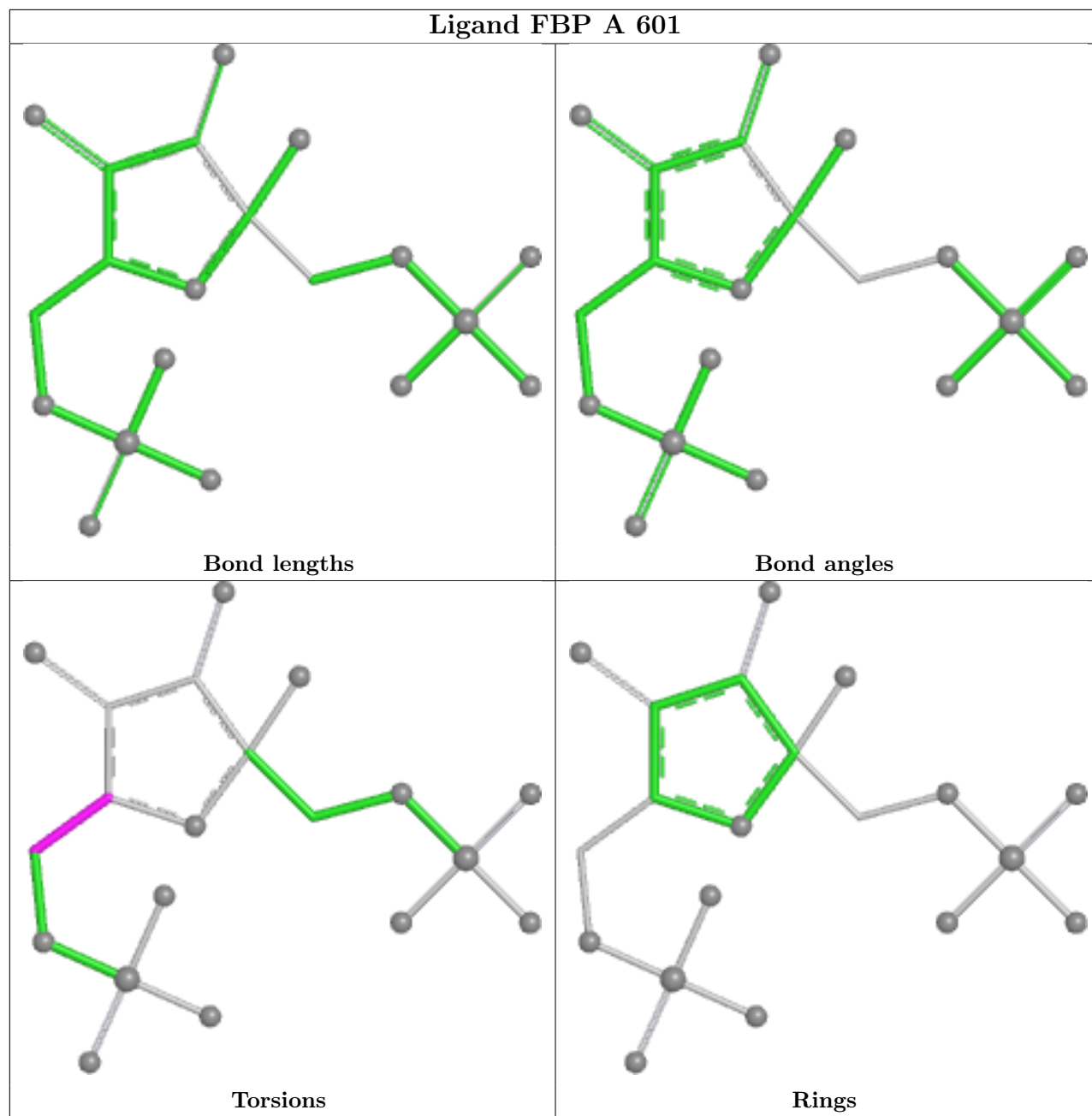


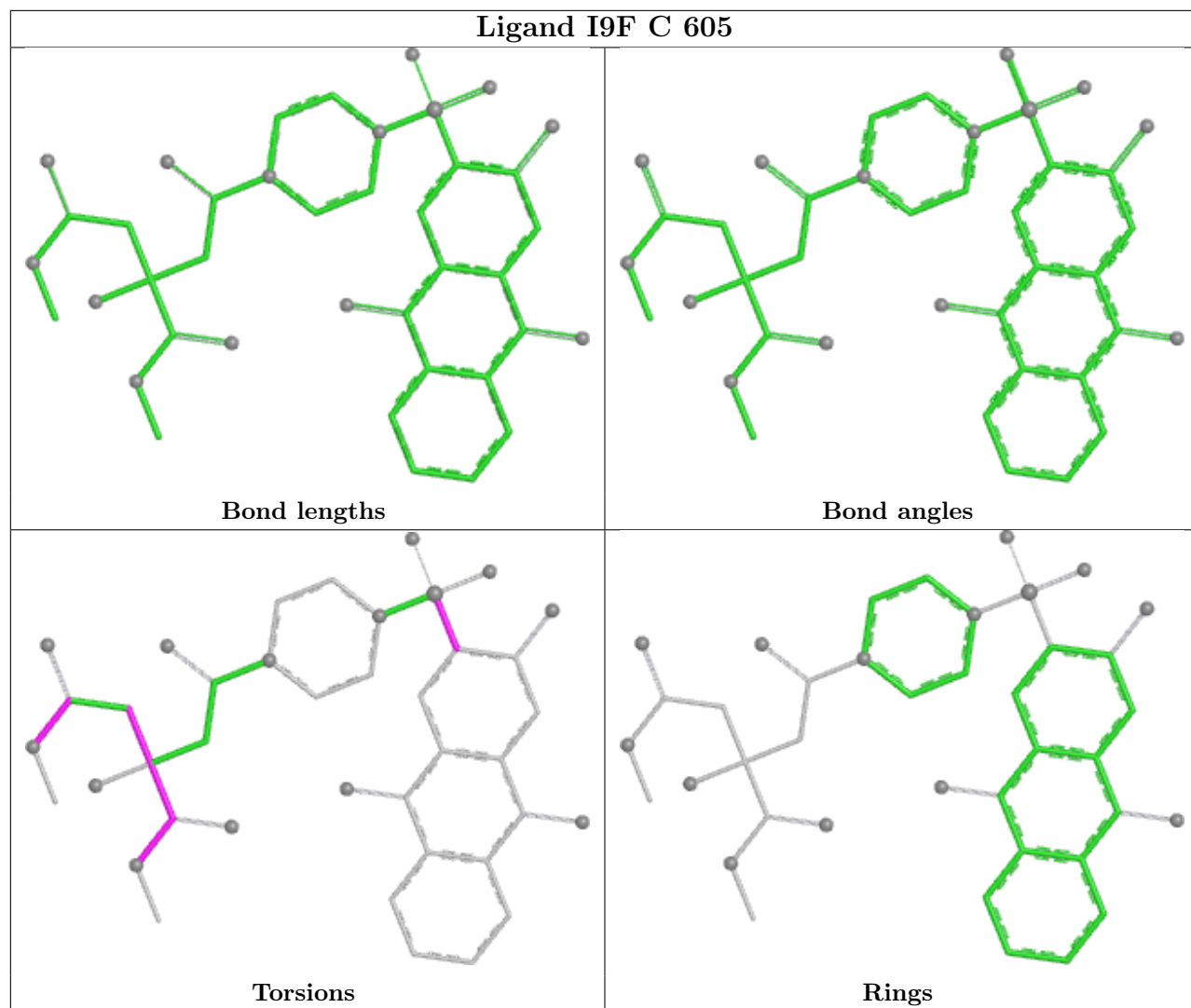


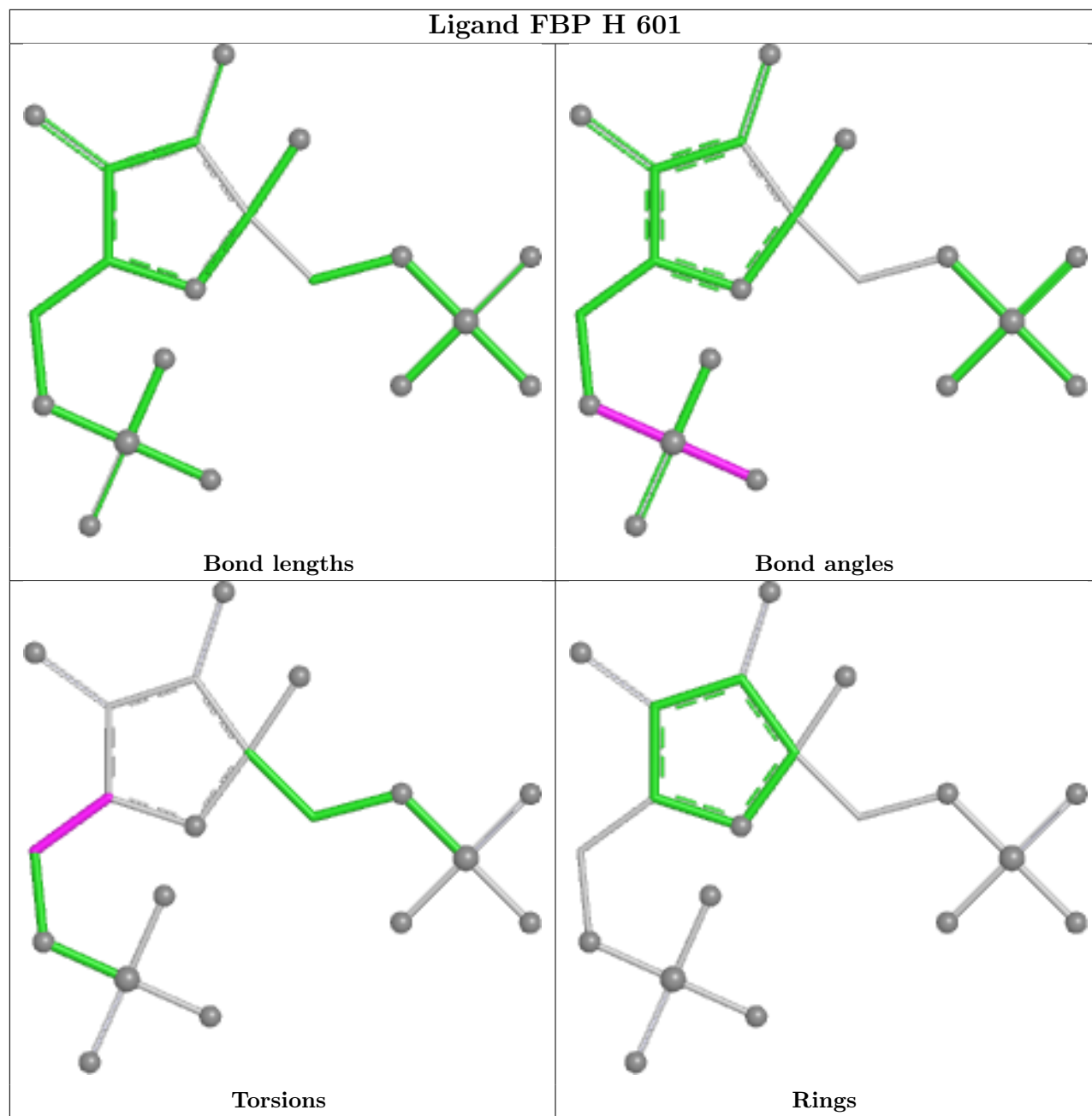


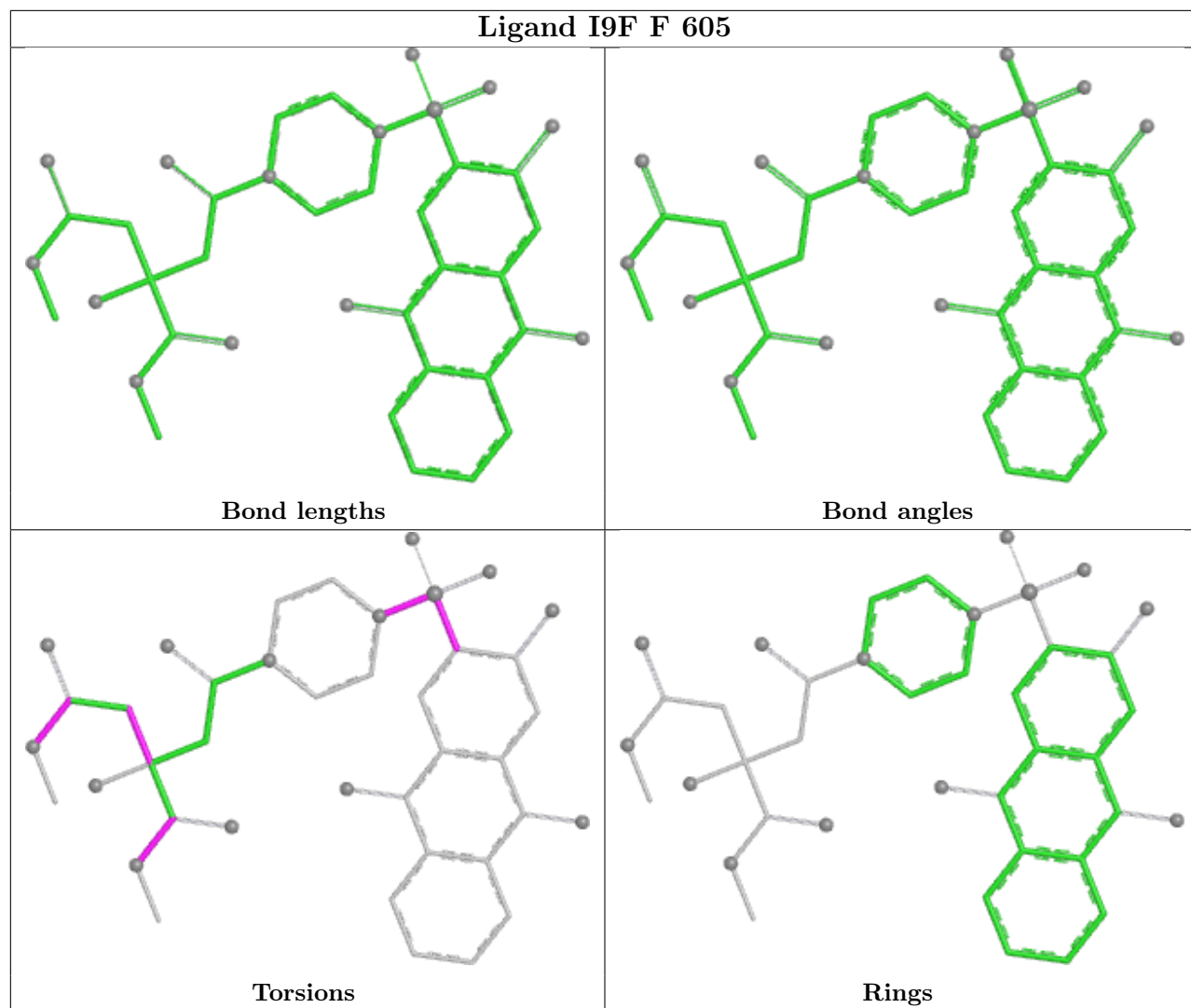


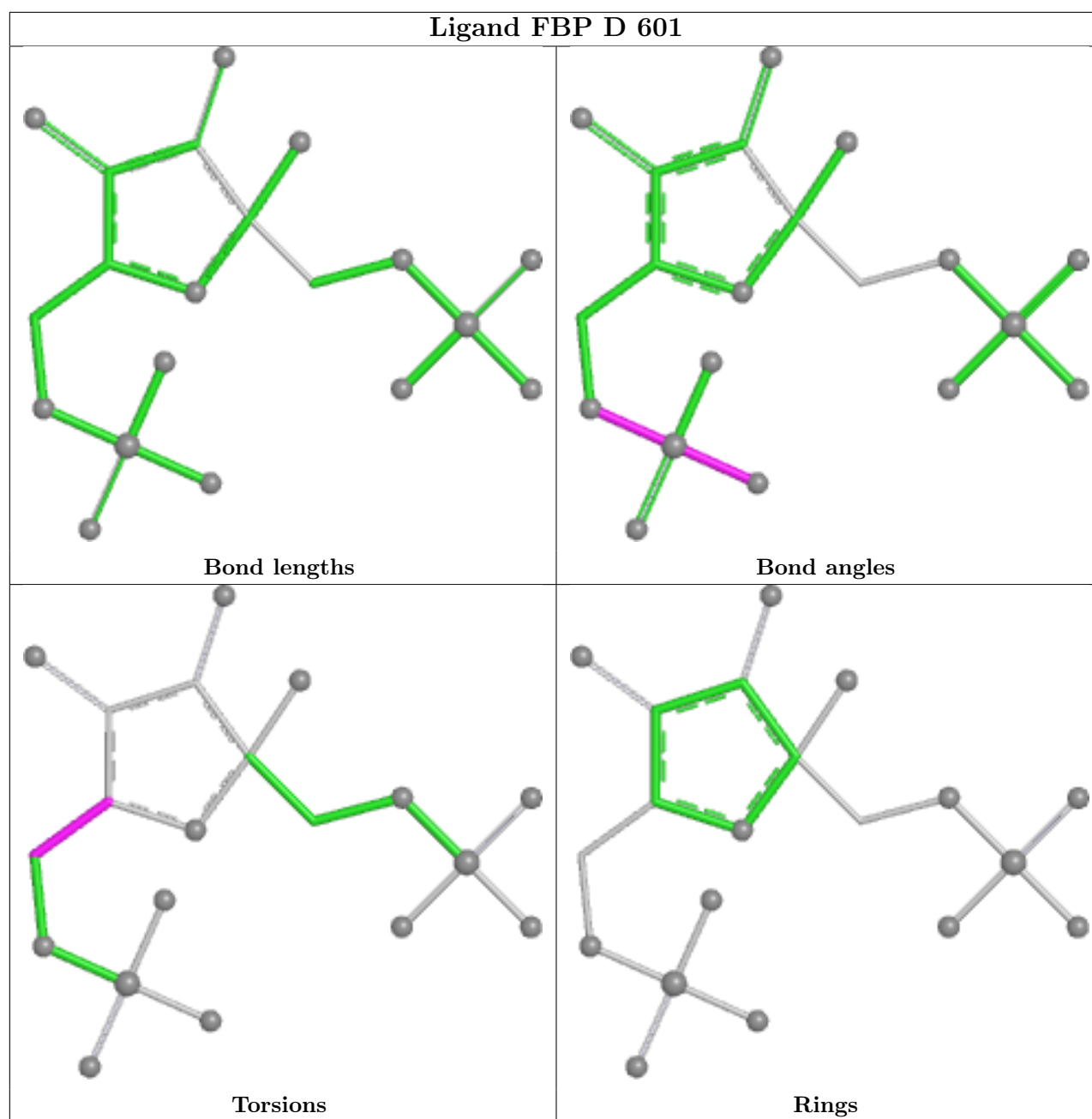












5.7 Other polymers [i](#)

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	422/447 (94%)	1.29	87 (20%) 2 3	34, 66, 94, 116	6 (1%)
1	B	435/447 (97%)	1.19	81 (18%) 3 4	34, 59, 89, 105	4 (0%)
1	C	425/447 (95%)	0.64	45 (10%) 11 12	27, 49, 77, 133	4 (0%)
1	D	425/447 (95%)	0.19	15 (3%) 47 51	21, 41, 70, 121	6 (1%)
1	E	419/447 (93%)	1.18	78 (18%) 3 4	33, 62, 94, 112	5 (1%)
1	F	433/447 (96%)	0.67	40 (9%) 14 16	29, 50, 79, 98	7 (1%)
1	G	421/447 (94%)	0.27	21 (4%) 34 38	25, 43, 67, 101	7 (1%)
1	H	425/447 (95%)	0.03	15 (3%) 47 51	20, 37, 65, 112	4 (0%)
All	All	3405/3576 (95%)	0.68	382 (11%) 10 11	20, 52, 86, 133	43 (1%)

All (382) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	115	LEU	11.0
1	C	20	LEU	8.6
1	D	25	PHE	7.2
1	B	114	PRO	6.9
1	B	231	PRO	6.6
1	F	115	LEU	6.4
1	H	21	GLY	6.4
1	B	511	LEU	6.1
1	A	25	PHE	6.0
1	E	25	PHE	5.9
1	F	114	PRO	5.8
1	C	23	ALA	5.8
1	G	23	ALA	5.8
1	A	132	GLY	5.8
1	A	232	GLY	5.6
1	F	231	PRO	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	116	SER	5.4
1	D	24	PHE	5.4
1	F	116	SER	5.3
1	G	271	GLY	5.3
1	D	23	ALA	5.2
1	D	21	GLY	5.1
1	E	23	ALA	5.1
1	F	232	GLY	5.1
1	G	25	PHE	5.0
1	A	241	LEU	4.9
1	A	482	PHE	4.9
1	B	232	GLY	4.8
1	G	24	PHE	4.8
1	H	25	PHE	4.8
1	E	115	LEU	4.7
1	E	129	PRO	4.7
1	C	115	LEU	4.7
1	B	527	TRP	4.6
1	A	238	VAL	4.6
1	B	490	PRO	4.6
1	H	24	PHE	4.6
1	C	22	THR	4.6
1	A	24	PHE	4.6
1	C	232	GLY	4.5
1	F	512	ARG	4.4
1	G	132	GLY	4.4
1	A	23	ALA	4.4
1	D	22	THR	4.3
1	H	23	ALA	4.3
1	E	24	PHE	4.3
1	F	267[A]	ARG	4.3
1	C	34	MET	4.3
1	A	543	SER	4.3
1	B	13	VAL	4.2
1	C	132	GLY	4.2
1	C	271	GLY	4.1
1	F	484	LEU	4.1
1	E	114	PRO	4.1
1	B	267[A]	ARG	4.1
1	B	512	ARG	4.0
1	E	232	GLY	4.0
1	F	132	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	111	ALA	3.9
1	C	114	PRO	3.9
1	B	379	LYS	3.9
1	B	489	PRO	3.9
1	C	25	PHE	3.9
1	C	231	PRO	3.9
1	E	489	PRO	3.9
1	B	117	TYR	3.9
1	E	495	ALA	3.9
1	A	34	MET	3.9
1	E	275	HIS	3.8
1	C	21	GLY	3.8
1	E	244	GLY	3.8
1	A	488[A]	GLU	3.8
1	E	233	LEU	3.8
1	F	489	PRO	3.8
1	E	120	VAL	3.8
1	B	118	ARG	3.7
1	E	493	ILE	3.7
1	F	527	TRP	3.6
1	B	11	ALA	3.6
1	D	231	PRO	3.6
1	A	527	TRP	3.6
1	F	487	ARG	3.6
1	C	19	GLU	3.5
1	A	114	PRO	3.5
1	C	66	ALA	3.5
1	G	34	MET	3.5
1	E	490	PRO	3.5
1	A	30	LEU	3.5
1	B	484	LEU	3.5
1	F	516	ARG	3.5
1	H	22	THR	3.5
1	D	275[A]	HIS	3.5
1	A	475	VAL	3.4
1	A	63	ILE	3.4
1	E	272	PRO	3.4
1	F	11	ALA	3.4
1	E	502	VAL	3.3
1	A	115	LEU	3.3
1	E	540	LEU	3.3
1	E	249	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	495	ALA	3.3
1	E	257	VAL	3.2
1	A	378	ALA	3.2
1	F	233	LEU	3.2
1	E	492	ALA	3.1
1	C	117	TYR	3.1
1	A	33	ALA	3.1
1	F	13	VAL	3.1
1	F	492	ALA	3.1
1	F	493	ILE	3.1
1	C	24	PHE	3.1
1	A	249	VAL	3.1
1	E	103	VAL	3.1
1	A	112	GLY	3.1
1	C	408	GLU	3.1
1	B	416	LEU	3.1
1	B	485	LEU	3.1
1	C	305	ALA	3.0
1	B	517	VAL	3.0
1	G	42	LEU	3.0
1	D	232	GLY	3.0
1	G	232	GLY	3.0
1	A	124	LEU	3.0
1	A	266	VAL	3.0
1	B	12	ASP	3.0
1	A	110	PHE	3.0
1	G	38	PHE	3.0
1	F	269	ALA	2.9
1	C	70	VAL	2.9
1	E	110	PHE	2.9
1	E	514	PHE	2.9
1	F	34	MET	2.9
1	A	88	PHE	2.9
1	E	238	VAL	2.9
1	F	12	ASP	2.9
1	B	251	ILE	2.9
1	G	231	PRO	2.9
1	C	110	PHE	2.9
1	B	378	ALA	2.9
1	B	91	GLY	2.9
1	B	487	ARG	2.8
1	D	30	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	30	LEU	2.8
1	H	411	ARG	2.8
1	H	231	PRO	2.8
1	E	400	ALA	2.8
1	B	52	VAL	2.8
1	B	348	THR	2.8
1	F	118	ARG	2.8
1	D	130	GLY	2.8
1	E	331	LEU	2.8
1	B	272	PRO	2.8
1	H	516	ARG	2.8
1	H	275[A]	HIS	2.8
1	B	61	ALA	2.8
1	A	540	LEU	2.8
1	A	493	ILE	2.8
1	B	90	HIS	2.7
1	E	375	GLY	2.7
1	E	101	ALA	2.7
1	E	269	ALA	2.7
1	E	464	ALA	2.7
1	B	270	LEU	2.7
1	B	10	ARG	2.7
1	F	490	PRO	2.7
1	E	126	THR	2.7
1	E	270	LEU	2.7
1	A	70	VAL	2.7
1	A	245	VAL	2.7
1	C	75	GLU	2.7
1	A	116	SER	2.7
1	B	543	SER	2.7
1	E	116	SER	2.7
1	B	268	ALA	2.7
1	C	411	ARG	2.7
1	G	33	ALA	2.6
1	G	30	LEU	2.6
1	C	36	ASP	2.6
1	F	36	ASP	2.6
1	E	505	GLY	2.6
1	E	241	LEU	2.6
1	F	129	PRO	2.6
1	A	311	ILE	2.6
1	B	107	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	265	ALA	2.6
1	E	123	ALA	2.6
1	A	272	PRO	2.6
1	A	490	PRO	2.6
1	E	511	LEU	2.6
1	B	113	SER	2.6
1	C	116	SER	2.6
1	C	487	ARG	2.6
1	E	351	ARG	2.6
1	A	28	GLN	2.6
1	B	249	VAL	2.6
1	G	26	GLN	2.6
1	E	34	MET	2.6
1	E	33	ALA	2.6
1	B	88	PHE	2.5
1	E	491	GLU	2.5
1	B	120	VAL	2.5
1	B	506	ILE	2.5
1	E	122	ILE	2.5
1	A	412	ARG	2.5
1	F	351	ARG	2.5
1	B	269	ALA	2.5
1	A	244	GLY	2.5
1	B	130	GLY	2.5
1	B	275	HIS	2.5
1	C	402	TYR	2.5
1	A	118	ARG	2.5
1	F	242	ARG	2.5
1	A	273	GLU	2.5
1	B	492	ALA	2.5
1	D	31	PRO	2.5
1	E	119	PRO	2.5
1	E	378	ALA	2.5
1	C	42	LEU	2.5
1	H	34	MET	2.5
1	E	513	GLY	2.5
1	C	404	ARG	2.5
1	E	52	VAL	2.5
1	A	92	SER	2.5
1	A	79	ALA	2.5
1	B	119	PRO	2.5
1	B	495	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	400	ALA	2.5
1	E	111	ALA	2.5
1	F	540[A]	LEU	2.5
1	A	274	GLY	2.5
1	H	232	GLY	2.5
1	E	527	TRP	2.5
1	B	493	ILE	2.5
1	F	517	VAL	2.4
1	C	94	GLU	2.4
1	E	487	ARG	2.4
1	B	25	PHE	2.4
1	B	256	PHE	2.4
1	B	498	VAL	2.4
1	E	494	TRP	2.4
1	F	423	VAL	2.4
1	A	31	PRO	2.4
1	A	489	PRO	2.4
1	G	272	PRO	2.4
1	B	411	ARG	2.4
1	A	86	LEU	2.4
1	E	485	LEU	2.4
1	C	26	GLN	2.4
1	E	277	ILE	2.4
1	B	34	MET	2.4
1	B	131	SER	2.4
1	E	113	SER	2.4
1	F	275	HIS	2.4
1	B	233	LEU	2.4
1	B	540[A]	LEU	2.4
1	C	112	GLY	2.4
1	E	504	PHE	2.4
1	E	70	VAL	2.4
1	B	508	SER	2.4
1	E	89	SER	2.4
1	A	471	ALA	2.3
1	F	515	LEU	2.3
1	H	30	LEU	2.3
1	B	504	PHE	2.3
1	E	256	PHE	2.3
1	A	97	ALA	2.3
1	A	464	ALA	2.3
1	A	242	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	412	ARG	2.3
1	G	487	ARG	2.3
1	A	514	PHE	2.3
1	B	24	PHE	2.3
1	B	38	PHE	2.3
1	E	90	HIS	2.3
1	A	108	GLU	2.3
1	F	272	PRO	2.3
1	A	73	LEU	2.3
1	A	91	GLY	2.3
1	A	270	LEU	2.3
1	A	96	HIS	2.3
1	B	507	GLU	2.3
1	B	311	ILE	2.3
1	E	118	ARG	2.3
1	A	237	ASP	2.3
1	E	97	ALA	2.3
1	C	30	LEU	2.3
1	B	494	TRP	2.3
1	A	90	HIS	2.2
1	A	113	SER	2.2
1	C	109	SER	2.2
1	E	28	GLN	2.2
1	B	382	PHE	2.2
1	B	433	PHE	2.2
1	A	542	ILE	2.2
1	A	384	VAL	2.2
1	B	238	VAL	2.2
1	A	80	GLY	2.2
1	B	84	ALA	2.2
1	A	331[A]	LEU	2.2
1	B	488	GLU	2.2
1	H	273	GLU	2.2
1	C	412	ARG	2.2
1	A	441	ILE	2.2
1	A	257	VAL	2.2
1	H	130	GLY	2.2
1	A	492	ALA	2.2
1	F	124	LEU	2.2
1	A	494	TRP	2.2
1	A	127	LYS	2.2
1	A	256	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	383	PRO	2.2
1	D	129	PRO	2.2
1	E	542	ILE	2.2
1	A	120	VAL	2.2
1	A	260	ALA	2.2
1	F	90	HIS	2.2
1	B	73	LEU	2.2
1	F	416	LEU	2.2
1	A	351	ARG	2.2
1	D	242[A]	ARG	2.2
1	E	127	LYS	2.2
1	C	348	THR	2.2
1	G	366	ASP	2.2
1	A	279	ILE	2.1
1	B	243	PHE	2.1
1	A	298	VAL	2.1
1	B	14	ALA	2.1
1	C	386	ALA	2.1
1	B	351	ARG	2.1
1	C	43	CYS	2.1
1	E	86	LEU	2.1
1	E	436	CYS	2.1
1	E	273	GLU	2.1
1	A	130	GLY	2.1
1	E	242	ARG	2.1
1	G	351	ARG	2.1
1	B	123	ALA	2.1
1	E	268	ALA	2.1
1	B	241	LEU	2.1
1	F	543	SER	2.1
1	D	273	GLU	2.1
1	A	380	GLY	2.1
1	A	463	ILE	2.1
1	C	80	GLY	2.1
1	A	269	ALA	2.1
1	D	260	ALA	2.1
1	G	305	ALA	2.1
1	G	363	ALA	2.1
1	A	296	LEU	2.1
1	G	115	LEU	2.1
1	H	36	ASP	2.1
1	B	68	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	412	ARG	2.1
1	A	375	GLY	2.1
1	B	127	LYS	2.1
1	B	277	ILE	2.1
1	C	63	ILE	2.1
1	C	77	ILE	2.1
1	E	245	VAL	2.1
1	E	266	VAL	2.1
1	A	84	ALA	2.1
1	A	111	ALA	2.1
1	A	305	ALA	2.1
1	C	108	GLU	2.0
1	F	491	GLU	2.0
1	A	233	LEU	2.0
1	B	86	LEU	2.0
1	C	366	ASP	2.0
1	B	412	ARG	2.0
1	B	377	THR	2.0
1	E	274	GLY	2.0
1	E	486	TYR	2.0
1	F	234	SER	2.0
1	A	268	ALA	2.0
1	E	26	GLN	2.0
1	E	499	ASP	2.0
1	B	516	ARG	2.0
1	C	459	ARG	2.0
1	E	43	CYS	2.0
1	B	276	GLY	2.0
1	A	95	TYR	2.0
1	E	95	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

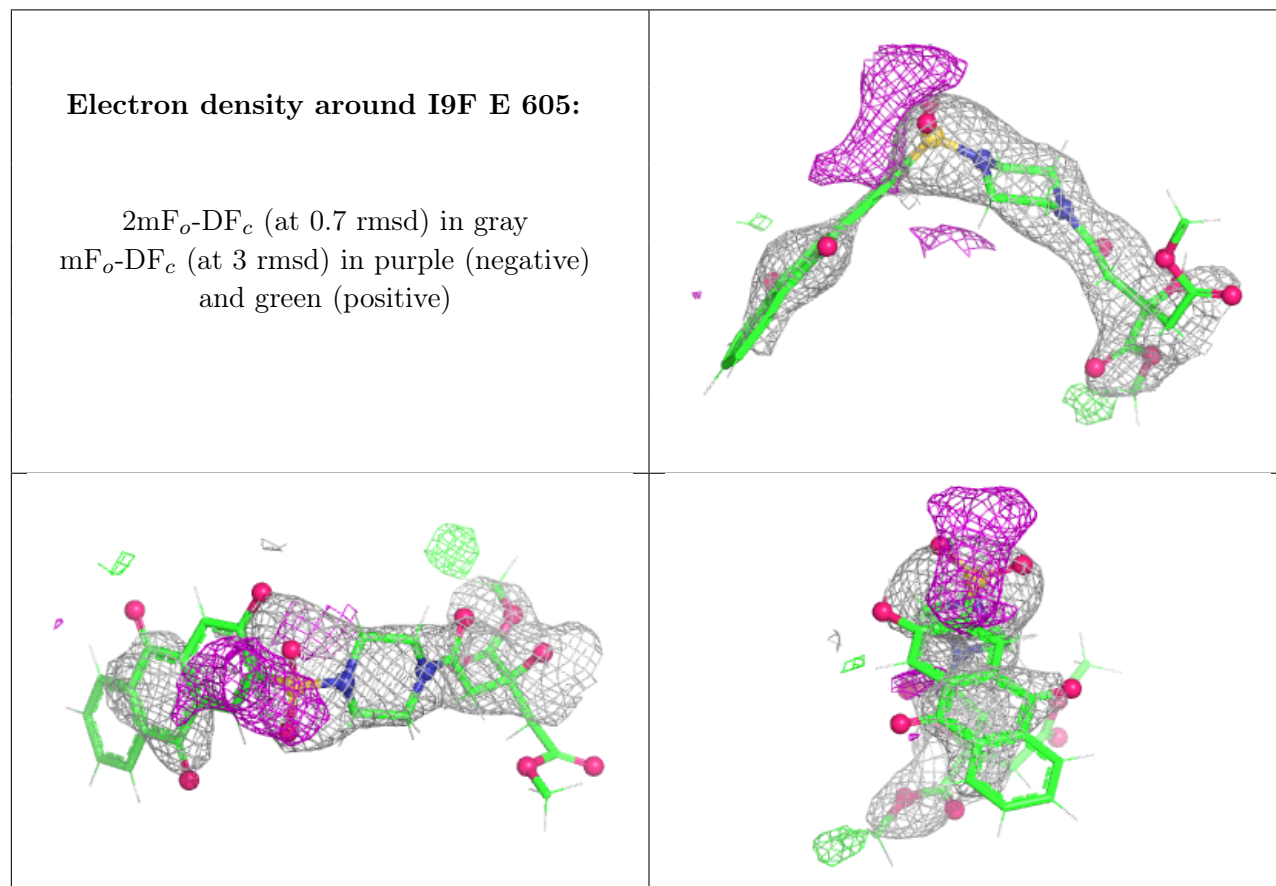
There are no oligosaccharides in this entry.

6.4 Ligands i

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

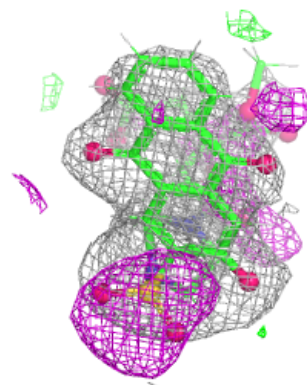
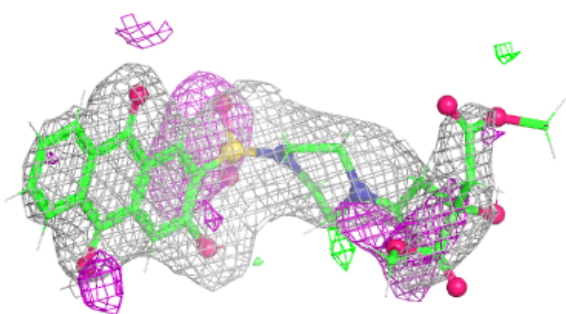
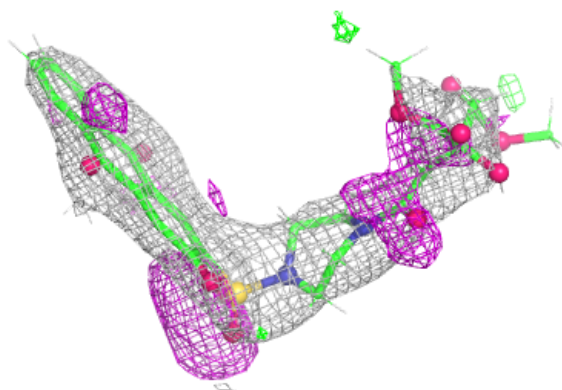
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	I9F	E	605	40/40	0.71	0.20	118,119,123,123	26
6	I9F	F	605	40/40	0.77	0.19	70,80,93,93	26
4	MG	H	603	1/1	0.78	0.19	53,53,53,53	0
6	I9F	G	605	40/40	0.80	0.18	77,80,91,91	26
6	I9F	C	605	40/40	0.81	0.17	83,87,96,96	26
4	MG	D	603	1/1	0.82	0.15	54,54,54,54	0
3	OXL	E	602	6/6	0.82	0.13	68,68,68,68	0
5	K	E	604	1/1	0.85	0.27	119,119,119,119	0
5	K	A	604	1/1	0.89	0.12	120,120,120,120	0
5	K	C	604	1/1	0.90	0.17	86,86,86,86	0
3	OXL	A	602	6/6	0.90	0.09	68,68,68,68	0
4	MG	C	603	1/1	0.91	0.11	55,55,55,55	0
5	K	G	604	1/1	0.91	0.16	74,74,74,74	0
3	OXL	D	602	6/6	0.92	0.09	48,48,49,50	0
4	MG	A	603	1/1	0.92	0.08	67,67,67,67	0
4	MG	E	603	1/1	0.92	0.09	62,62,62,62	0
4	MG	F	603	1/1	0.92	0.07	47,47,47,47	0
5	K	F	604	1/1	0.92	0.08	90,90,90,90	0
2	FBP	E	601	20/20	0.93	0.08	60,61,62,62	0
3	OXL	C	602	6/6	0.93	0.08	61,61,62,63	0
3	OXL	G	602	6/6	0.93	0.09	50,50,51,52	0
3	OXL	H	602	6/6	0.94	0.10	43,44,44,45	0
2	FBP	F	601	20/20	0.94	0.08	52,55,60,60	0
2	FBP	B	601	20/20	0.94	0.09	61,61,64,64	0
2	FBP	A	601	20/20	0.94	0.09	61,63,64,64	0
3	OXL	B	602	6/6	0.95	0.07	51,52,54,54	0
5	K	H	604	1/1	0.95	0.08	64,64,64,64	0
3	OXL	F	602	6/6	0.95	0.08	58,59,60,61	0
5	K	B	604	1/1	0.96	0.07	86,86,86,86	0
4	MG	B	603	1/1	0.96	0.07	65,65,65,65	0
2	FBP	H	601	20/20	0.98	0.05	28,30,32,33	0
2	FBP	C	601	20/20	0.98	0.05	34,36,38,39	0
2	FBP	D	601	20/20	0.98	0.05	33,35,37,37	0
5	K	D	604	1/1	0.98	0.12	57,57,57,57	0
4	MG	G	603	1/1	0.98	0.04	40,40,40,40	0
2	FBP	G	601	20/20	0.98	0.04	30,33,35,35	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.

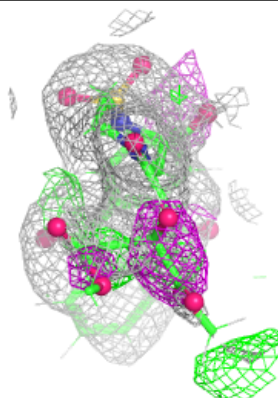
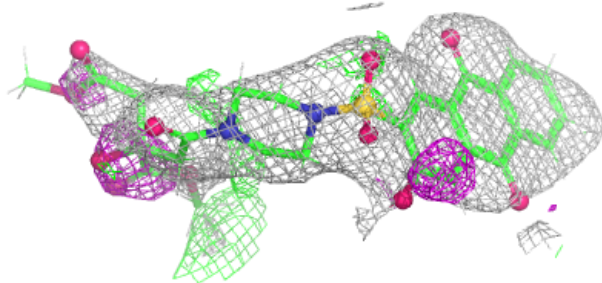
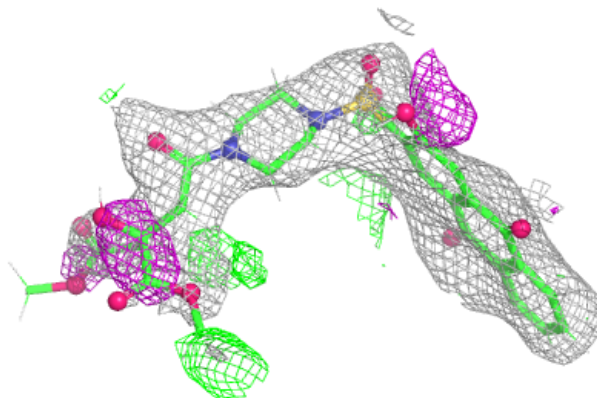


Electron density around I9F F 605:

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

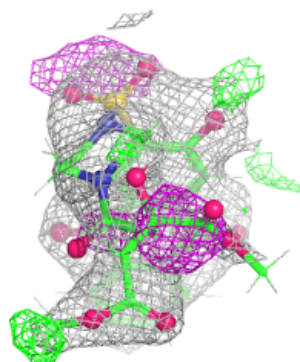
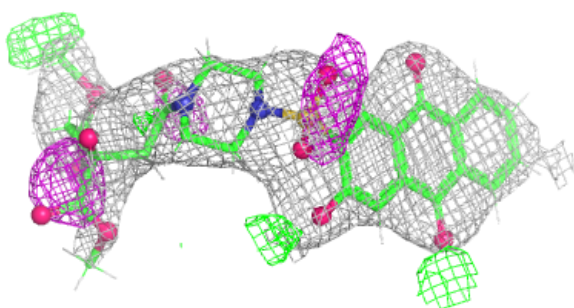
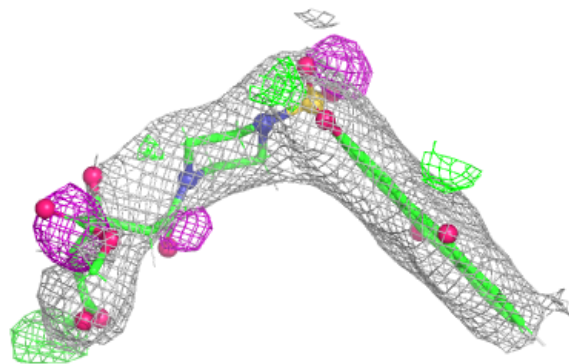
**Electron density around I9F G 605:**

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

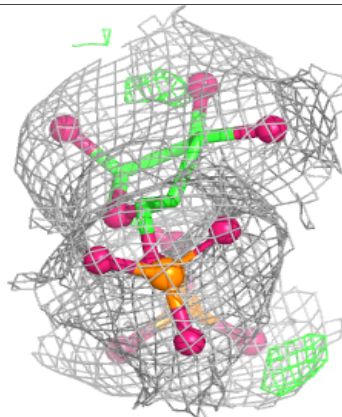
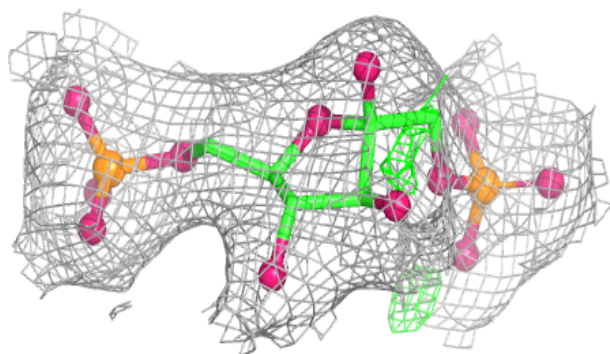
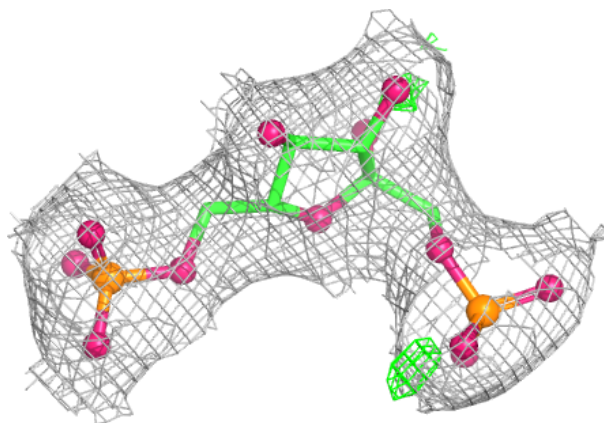


Electron density around I9F C 605:

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

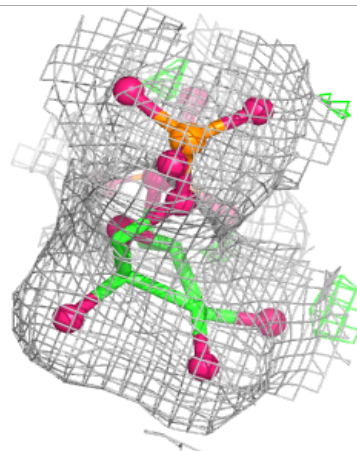
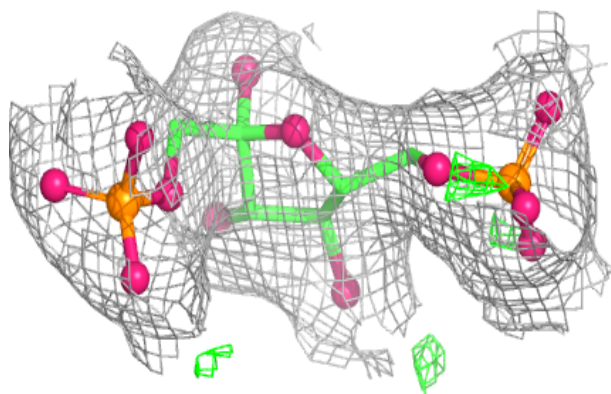
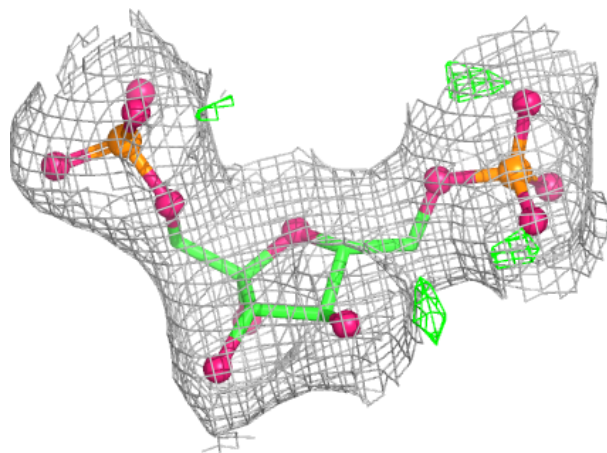
**Electron density around FBP E 601:**

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



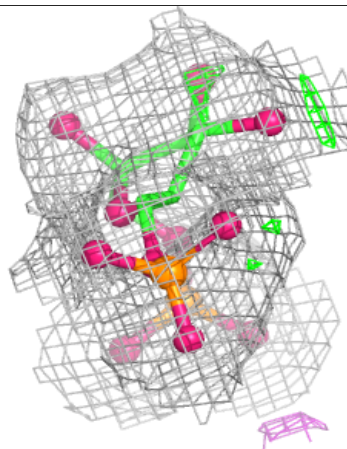
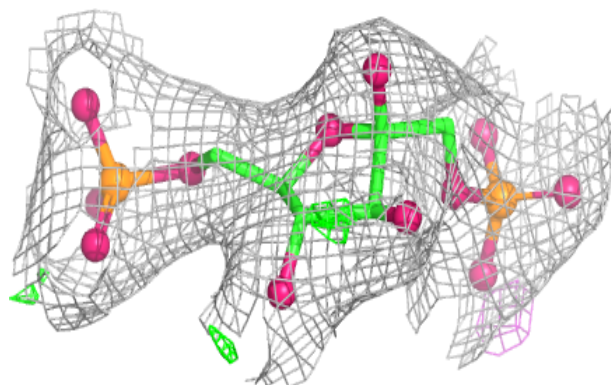
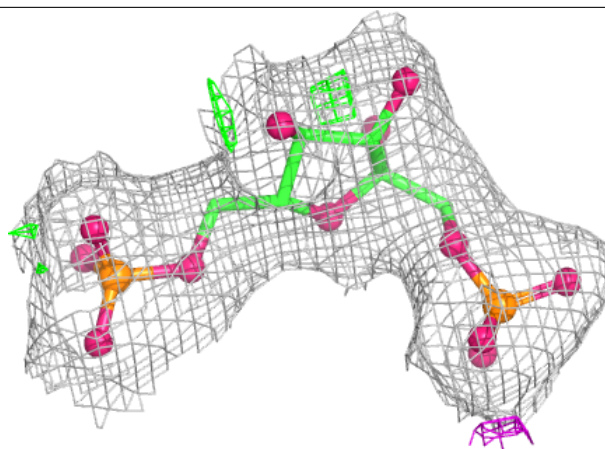
Electron density around FBP F 601:

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

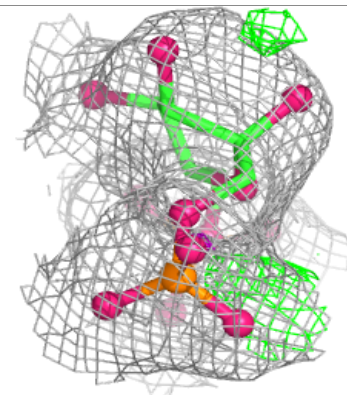
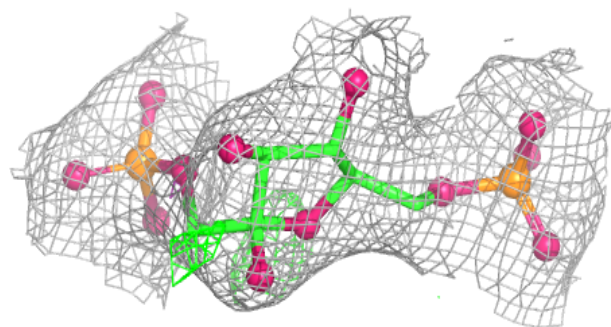
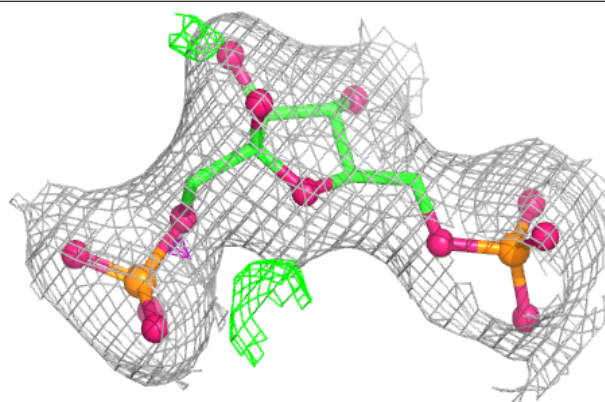


Electron density around FBP B 601:

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

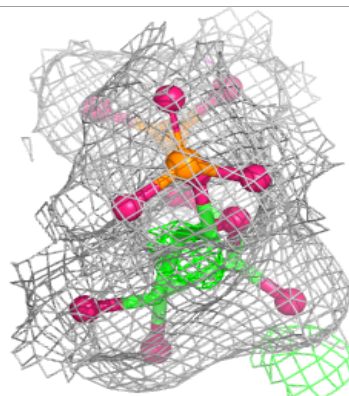
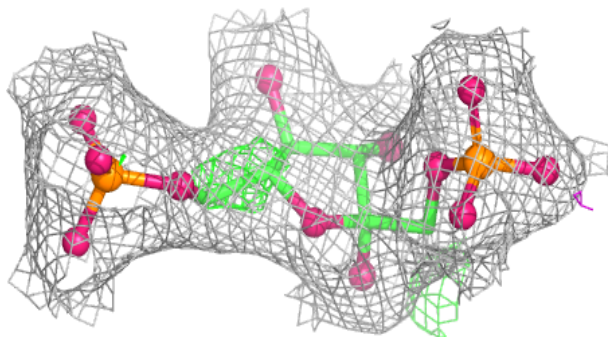
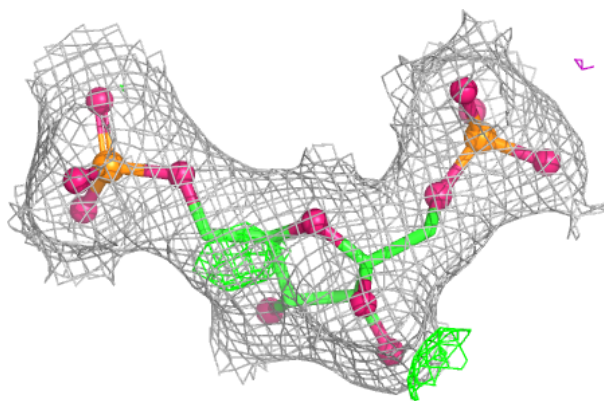
**Electron density around FBP A 601:**

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

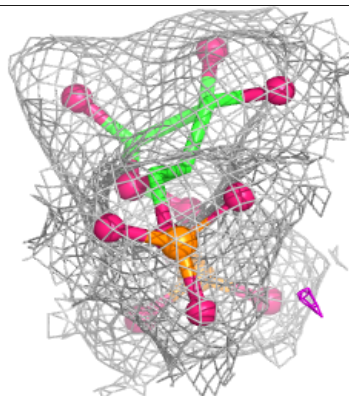
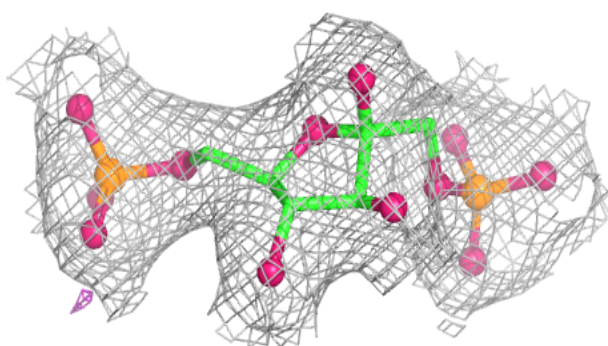
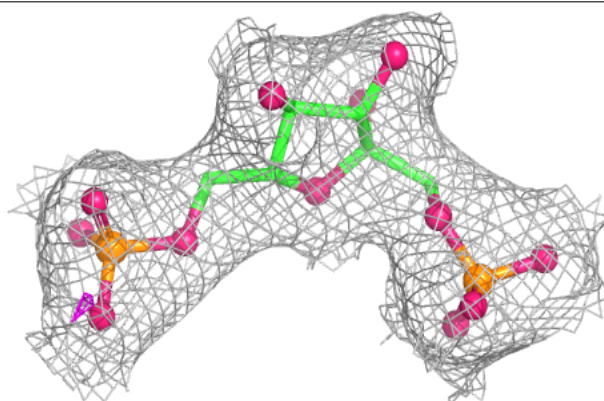


Electron density around FBP H 601:

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

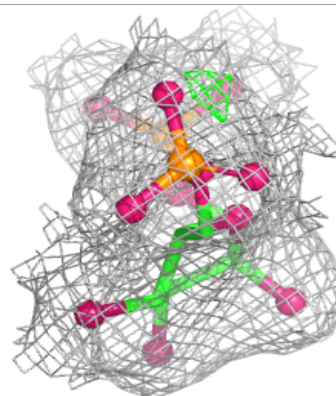
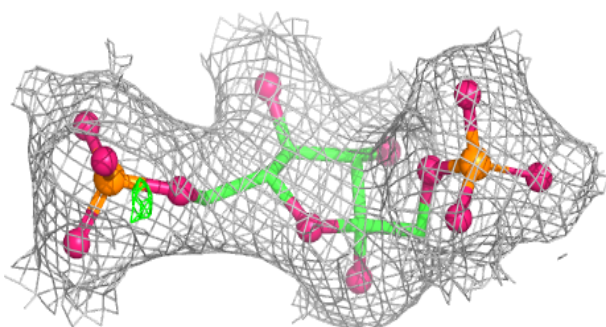
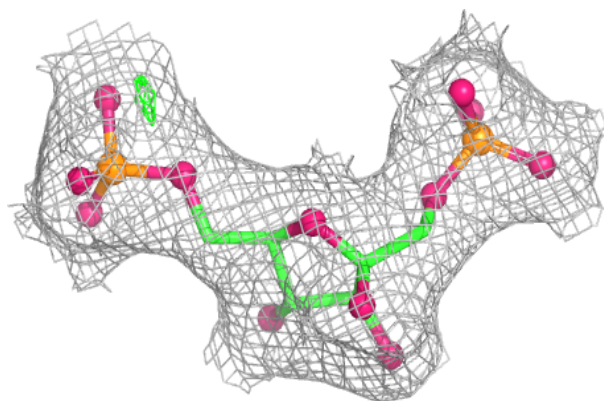
**Electron density around FBP C 601:**

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

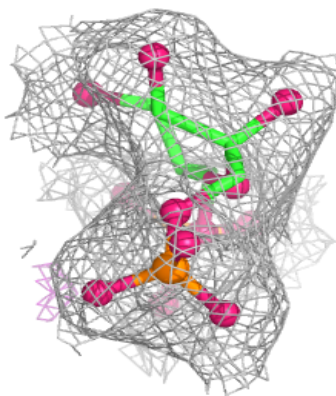
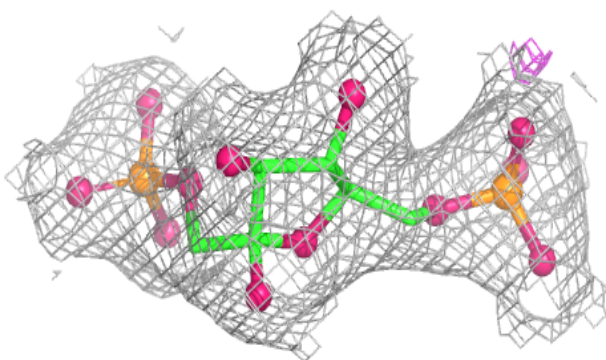
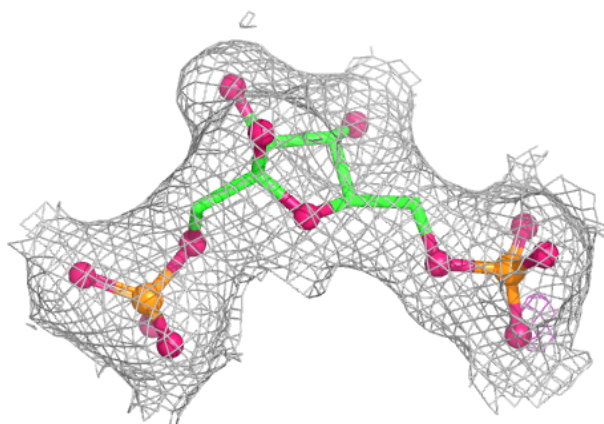


Electron density around FBP D 601:

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

**Electron density around FBP G 601:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.