



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:23 AM UTC

PDB ID : 5SCF / pdb_00005scf
Title : Structure of liver pyruvate kinase in complex with anthraquinone derivative 99
Authors : Lulla, A.; Foller, A.; Nain-Perez, A.; Grotli, M.; Brear, P.; Hyvonen, M.
Deposited on : 2021-12-01
Resolution : 2.19 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

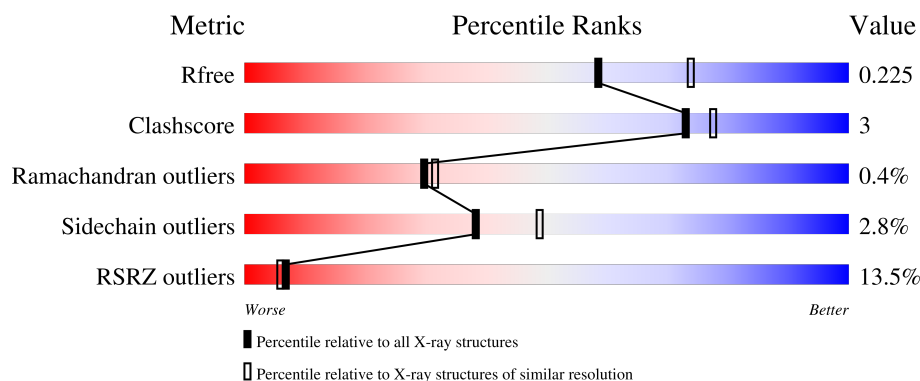
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	23% 84% 9% 6%
1	B	447	20% 85% 11% ..
1	C	447	9% 85% 9% 5%
1	D	447	5% 86% 8% 5%
1	E	447	24% 85% 8% 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 27934 atoms, of which 44 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	13	0
			3238	2033	581	604	20			
1	B	434	Total	C	N	O	S	3	8	0
			3340	2099	602	619	20			
1	C	425	Total	C	N	O	S	0	7	0
			3264	2053	585	607	19			
1	D	425	Total	C	N	O	S	0	8	0
			3261	2048	590	604	19			
1	E	420	Total	C	N	O	S	0	13	0
			3261	2051	585	605	20			
1	F	432	Total	C	N	O	S	0	8	0
			3327	2094	597	616	20			
1	G	422	Total	C	N	O	S	0	8	0
			3246	2042	582	603	19			
1	H	425	Total	C	N	O	S	0	9	0
			3277	2057	597	604	19			

There are 48 discrepancies between the modelled and reference sequences:

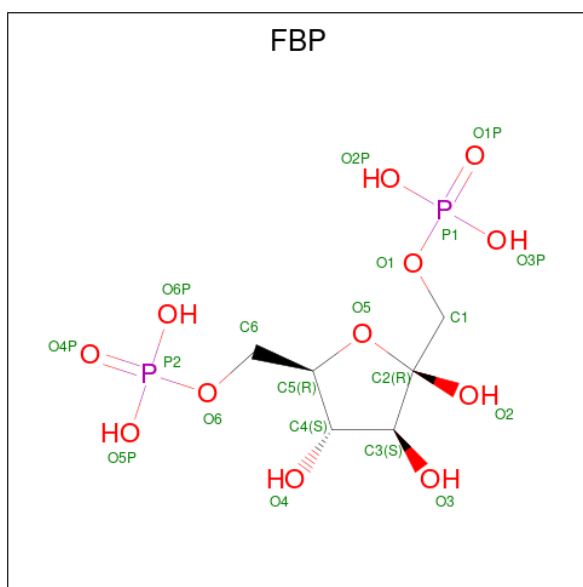
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q16716
A	0	SER	-	expression tag	UNP Q16716
A	12	ASP	SER	conflict	UNP Q16716
A	130	GLY	-	linker	UNP Q16716
A	131	SER	-	linker	UNP Q16716
A	230	GLY	-	linker	UNP Q16716
B	-1	GLY	-	expression tag	UNP Q16716
B	0	SER	-	expression tag	UNP Q16716
B	12	ASP	SER	conflict	UNP Q16716
B	130	GLY	-	linker	UNP Q16716
B	229	SER	-	linker	UNP Q16716
B	230	GLY	-	linker	UNP Q16716
C	-1	GLY	-	expression tag	UNP Q16716

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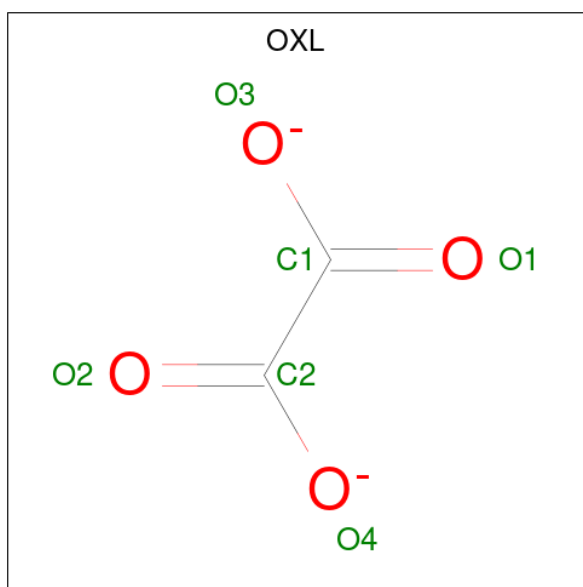
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP Q16716
C	12	ASP	SER	conflict	UNP Q16716
C	130	GLY	-	linker	UNP Q16716
C	131	SER	-	linker	UNP Q16716
C	132	GLY	-	linker	UNP Q16716
D	-1	GLY	-	expression tag	UNP Q16716
D	0	SER	-	expression tag	UNP Q16716
D	12	ASP	SER	conflict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

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



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

- Molecule 3 is OXALATE ION (CCD ID: OXL) (formula: C_2O_4).



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

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

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

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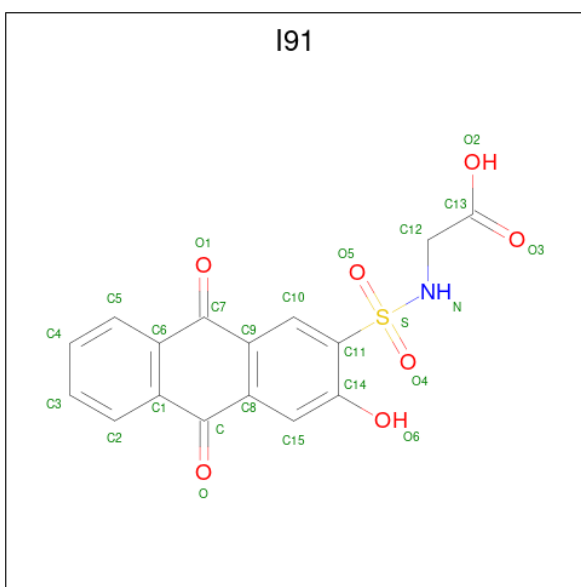
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total 1	Mg 1	0	0
4	F	1	Total 1	Mg 1	0	0
4	G	1	Total 1	Mg 1	0	0
4	H	1	Total 1	Mg 1	0	0

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

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

- Molecule 6 is N-(3-hydroxy-9,10-dioxo-9,10-dihydroanthracene-2-sulfonyl)glycine (CCD ID: I91) (formula: C₁₆H₁₁NO₇S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total 36	C 16	H 11	N 1	O 7	S 1	11	0
6	C	1	Total 36	C 16	H 11	N 1	O 7	S 1	11	0
6	F	1	Total 36	C 16	H 11	N 1	O 7	S 1	11	0
6	G	1	Total 36	C 16	H 11	N 1	O 7	S 1	11	0

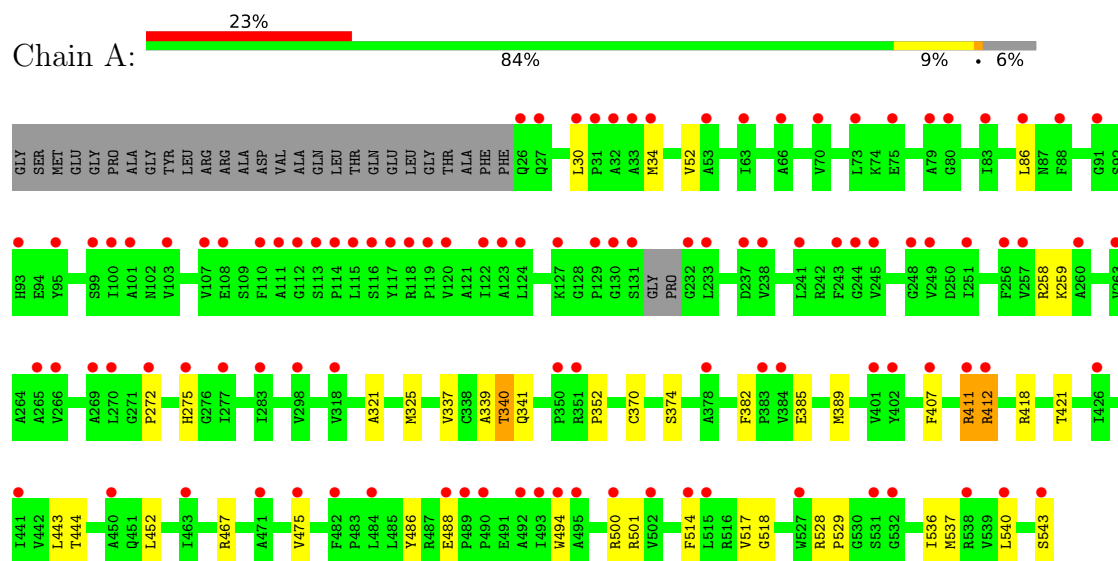
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	83	Total	O	0	0
			83	83		
7	B	122	Total	O	0	0
			122	122		
7	C	186	Total	O	0	0
			186	186		
7	D	240	Total	O	0	0
			240	240		
7	E	117	Total	O	0	0
			117	117		
7	F	161	Total	O	0	0
			161	161		
7	G	197	Total	O	0	0
			197	197		
7	H	246	Total	O	0	0
			246	246		

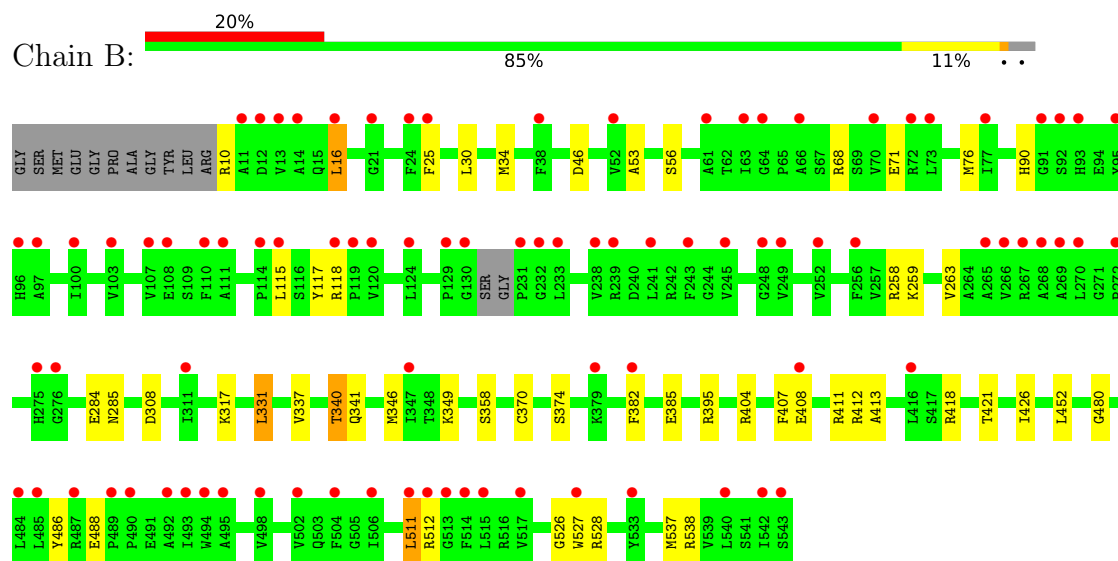
3 Residue-property plots [i](#)

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

• Molecule 1: Pyruvate kinase

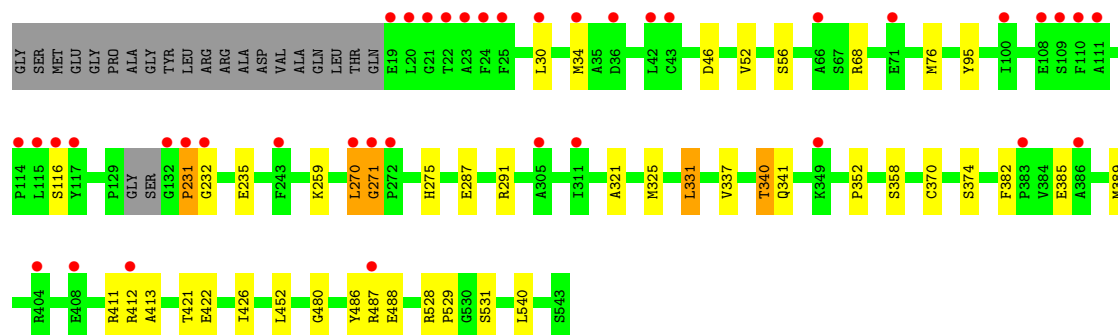


• Molecule 1: Pyruvate kinase



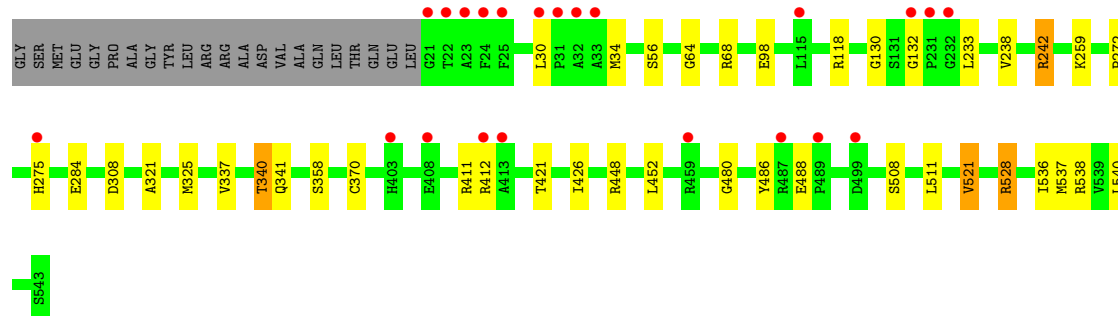
• Molecule 1: Pyruvate kinase

Chain C: 



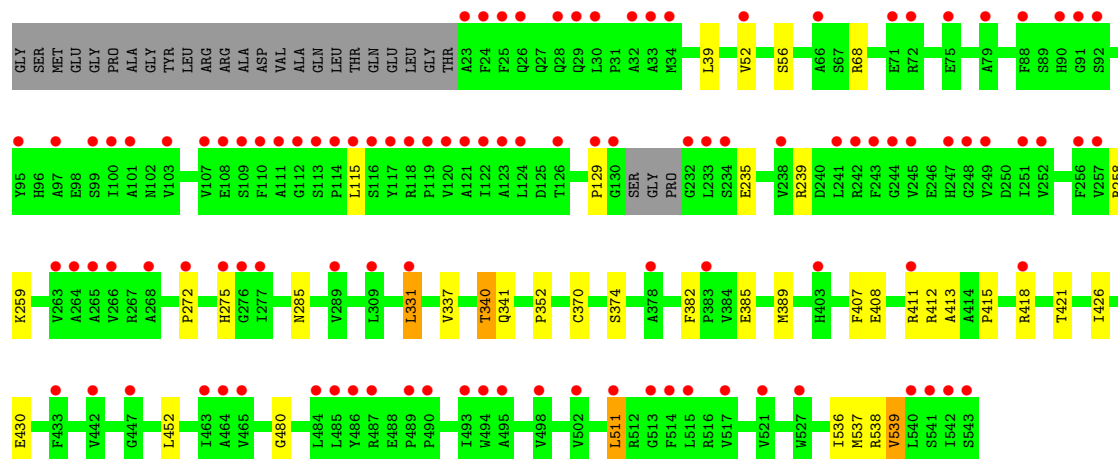
• Molecule 1: Pyruvate kinase

Chain D: 



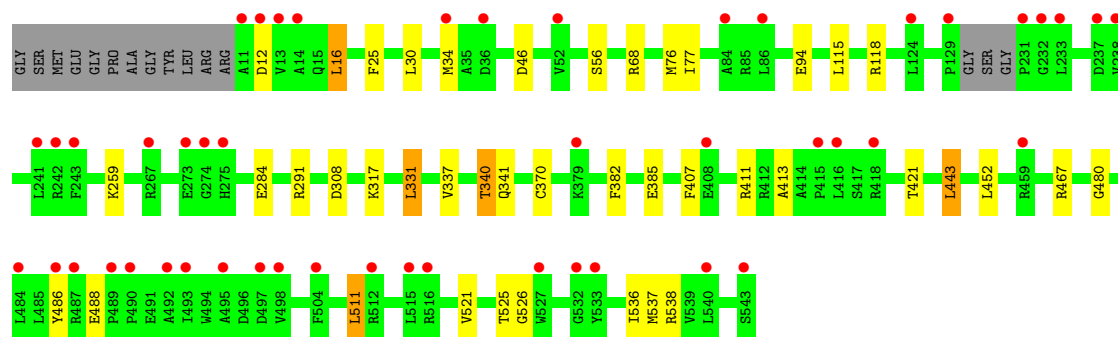
• Molecule 1: Pyruvate kinase

Chain E: 

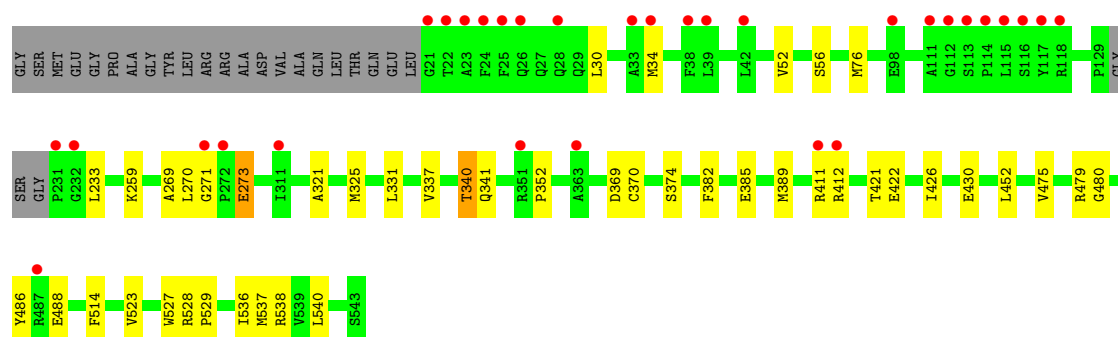
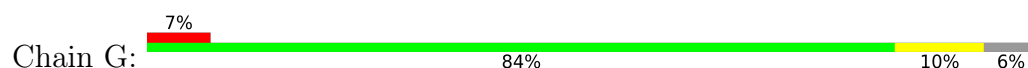


• Molecule 1: Pyruvate kinase

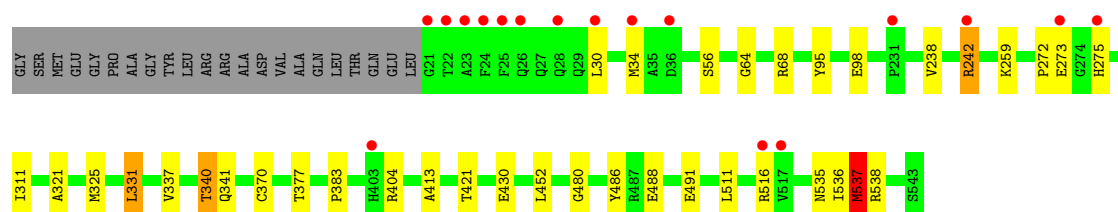
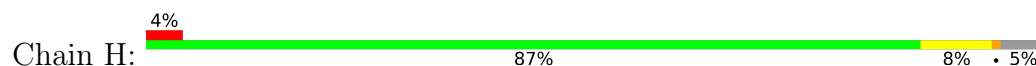
Chain F: 



• Molecule 1: Pyruvate kinase



• Molecule 1: Pyruvate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	207.19Å 112.92Å 188.59Å 90.00° 92.15° 90.00°	Depositor
Resolution (Å)	188.46 – 2.19 188.46 – 2.19	Depositor EDS
% Data completeness (in resolution range)	64.8 (188.46-2.19) 64.7 (188.46-2.19)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.18Å)	Xtriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, R_{free}	0.206 , 0.238 0.197 , 0.225	Depositor DCC
R_{free} test set	7172 reflections (3.19%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27934	wwPDB-VP
Average B, all atoms (Å ²)	57.0	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 50.34 % 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 6.5611e-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: OXL, FBP, I91, MG, K

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.70	1/3328 (0.0%)	1.03	3/4497 (0.1%)
1	B	0.74	2/3418 (0.1%)	1.05	1/4619 (0.0%)
1	C	0.78	1/3339 (0.0%)	1.06	5/4514 (0.1%)
1	D	0.80	0/3341	1.08	1/4517 (0.0%)
1	E	0.69	1/3354 (0.0%)	1.03	1/4532 (0.0%)
1	F	0.75	0/3405	1.07	1/4603 (0.0%)
1	G	0.81	0/3324	1.06	4/4493 (0.1%)
1	H	0.83	1/3357 (0.0%)	1.09	1/4537 (0.0%)
All	All	0.76	6/26866 (0.0%)	1.06	17/36312 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	374	SER	CA-C	6.01	1.55	1.52
1	E	374	SER	CA-C	5.95	1.55	1.52
1	H	537	MET	SD-CE	-5.79	1.65	1.79
1	C	374	SER	CA-C	5.67	1.55	1.52
1	B	374[A]	SER	CA-C	5.13	1.55	1.52
1	B	374[B]	SER	CA-C	5.13	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	273	GLU	CB-CG-CD	5.90	122.63	112.60
1	F	46	ASP	CA-CB-CG	5.84	118.44	112.60
1	G	270	LEU	CA-C-N	5.77	130.93	121.87
1	G	270	LEU	C-N-CA	5.77	130.93	121.87
1	B	46	ASP	CA-CB-CG	5.53	118.13	112.60
1	D	528	ARG	CB-CG-CD	-5.47	98.71	111.30
1	G	514	PHE	CA-CB-CG	5.46	119.26	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	311	ILE	CB-CA-C	5.28	115.71	111.06
1	C	46	ASP	CA-CB-CG	5.26	117.86	112.60
1	E	539	VAL	N-CA-CB	5.22	117.32	111.21
1	C	270[A]	LEU	CA-C-N	5.08	129.84	121.87
1	C	270[A]	LEU	C-N-CA	5.08	129.84	121.87
1	C	270[B]	LEU	CA-C-N	5.08	129.84	121.87
1	C	270[B]	LEU	C-N-CA	5.08	129.84	121.87
1	A	514	PHE	CA-CB-CG	5.07	118.87	113.80
1	A	339	ALA	CA-C-N	5.06	131.21	121.54
1	A	339	ALA	C-N-CA	5.06	131.21	121.54

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	3238	0	3312	23	0
1	B	3340	0	3409	30	0
1	C	3264	0	3322	23	0
1	D	3261	0	3321	24	0
1	E	3261	0	3326	21	0
1	F	3327	0	3399	25	0
1	G	3246	0	3308	25	0
1	H	3277	0	3341	21	0
2	A	20	0	10	2	0
2	B	20	0	10	1	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
2	E	20	0	10	0	0
2	F	20	0	10	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	6	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0
3	G	6	0	0	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	B	25	11	0	1	0
6	C	25	11	0	0	0
6	F	25	11	0	0	0
6	G	25	11	0	1	0
7	A	83	0	0	0	0
7	B	122	0	0	0	0
7	C	186	0	0	0	0
7	D	240	0	0	3	0
7	E	117	0	0	0	0
7	F	161	0	0	2	0
7	G	197	0	0	0	0
7	H	246	0	0	1	0
All	All	27890	44	26818	169	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (169) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.55	0.87
1:C:528:ARG:NH1	1:G:233:LEU:O	2.08	0.86
1:C:422[A]:GLU:HG3	1:C:452:LEU:HD13	1.56	0.86
1:A:272:PRO:HA	1:A:275:HIS:NE2	2.01	0.76
1:G:537:MET:HE3	1:H:537:MET:HG2	1.68	0.75
1:B:115:LEU:HD11	1:B:511:LEU:HB3	1.70	0.73
1:G:536:ILE:HG12	1:H:538[A]:ARG:HG2	1.72	0.71
1:B:258:ARG:HD3	1:B:285:ASN:HD21	1.55	0.71
1:G:56:SER:HB2	1:G:480:GLY:HA2	1.74	0.69
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.76	0.68
1:H:56:SER:HB2	1:H:480:GLY:HA2	1.77	0.67
1:E:536:ILE:HG12	1:F:538:ARG:HG2	1.75	0.66
1:F:56:SER:HB2	1:F:480:GLY:HA2	1.76	0.66
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.76	0.66
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.78	0.66
1:E:538:ARG:HG2	1:F:536:ILE:HG12	1.79	0.65
1:G:538:ARG:HG2	1:H:536:ILE:HG12	1.77	0.64
1:E:418[B]:ARG:HG3	1:F:16:LEU:HD11	1.79	0.64
1:D:68:ARG:HH22	1:D:98:GLU:HB2	1.60	0.64
1:E:56:SER:HB2	1:E:480:GLY:HA2	1.79	0.64
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.80	0.63
1:E:415:PRO:HB3	1:F:12:ASP:HA	1.80	0.62
1:A:411:ARG:NH2	1:B:411:ARG:NH2	2.48	0.61
1:H:68:ARG:NH2	1:H:95:TYR:O	2.34	0.60
1:D:68:ARG:NH2	1:D:98:GLU:HB2	2.18	0.59
1:D:340:THR:HG22	1:D:341:GLN:HG3	1.85	0.57
1:C:411:ARG:NH2	1:D:411:ARG:HE	2.02	0.57
1:A:407:PHE:CE2	1:A:411:ARG:NH1	2.72	0.57
1:G:340:THR:HG22	1:G:341:GLN:HG3	1.87	0.57
1:C:340:THR:HG22	1:C:341:GLN:HG3	1.87	0.57
1:F:407:PHE:CE2	1:F:411:ARG:NH1	2.72	0.56
1:A:340:THR:HG22	1:A:341:GLN:HG3	1.88	0.56
1:A:494:TRP:NE1	1:A:529:PRO:HB3	2.20	0.56
1:C:528:ARG:NH2	1:C:529:PRO:O	2.39	0.55
1:G:411:ARG:HG3	1:G:426:ILE:HD11	1.88	0.55
1:E:411:ARG:HG3	1:E:426:ILE:HD11	1.88	0.55
1:H:68:ARG:HH22	1:H:98:GLU:HB2	1.72	0.54
1:D:64:GLY:O	1:D:68:ARG:HG3	2.07	0.54
1:F:407:PHE:CD2	1:F:411:ARG:NH1	2.76	0.54
1:A:467:ARG:NH2	1:A:486:TYR:HE2	2.05	0.54
1:D:130:GLY:C	1:D:132:GLY:H	2.16	0.54
1:E:235:GLU:O	1:E:239:ARG:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:ARG:HH22	1:D:411:ARG:HE	1.57	0.53
1:H:340:THR:HG22	1:H:341:GLN:HG3	1.90	0.53
1:B:340:THR:HG22	1:B:341:GLN:HG3	1.91	0.53
1:G:56:SER:HB2	1:G:480:GLY:CA	2.39	0.52
1:C:56:SER:HB2	1:C:480:GLY:CA	2.39	0.52
1:C:411:ARG:HG3	1:C:426:ILE:HD11	1.91	0.52
1:E:340:THR:HG22	1:E:341:GLN:HG3	1.90	0.52
1:H:56:SER:HB2	1:H:480:GLY:CA	2.40	0.52
1:A:501:ARG:HH12	2:A:601:FBP:P1	2.33	0.52
1:A:421:THR:HG22	1:A:452:LEU:HD12	1.92	0.51
1:E:115:LEU:HB3	1:E:511:LEU:HD12	1.92	0.51
1:B:421:THR:HG22	1:B:452:LEU:HD12	1.94	0.50
1:B:56:SER:HB2	1:B:480:GLY:CA	2.42	0.50
1:G:374[B]:SER:OG	6:G:603:I91:O5	2.29	0.50
1:F:421:THR:HG22	1:F:452:LEU:HD12	1.94	0.50
1:E:421:THR:HG22	1:E:452:LEU:HD12	1.93	0.50
1:B:71:GLU:H	1:B:71:GLU:CD	2.20	0.50
1:F:77:ILE:HG22	1:F:118:ARG:HD3	1.94	0.49
1:B:30:LEU:O	1:B:34:MET:HG2	2.12	0.49
1:B:382:PHE:HB3	1:B:385:GLU:HB2	1.94	0.49
1:F:337:VAL:HG22	1:F:370:CYS:HB2	1.93	0.49
1:B:411:ARG:HG2	1:B:426:ILE:HD11	1.95	0.49
1:F:56:SER:HB2	1:F:480:GLY:CA	2.41	0.49
1:H:421:THR:HG22	1:H:452:LEU:HD12	1.95	0.49
1:F:443:LEU:HD22	1:F:525:THR:HG22	1.94	0.48
1:A:486:TYR:CZ	1:A:488[B]:GLU:HB2	2.49	0.48
1:H:331:LEU:HD11	1:H:413:ALA:HB1	1.96	0.48
1:C:382:PHE:HB3	1:C:385:GLU:HB2	1.95	0.48
1:F:340:THR:HG22	1:F:341:GLN:HG3	1.94	0.48
1:G:421:THR:HG22	1:G:452:LEU:HD12	1.94	0.48
1:F:30:LEU:O	1:F:34:MET:HG2	2.14	0.48
1:B:16:LEU:HD23	1:B:25:PHE:HZ	1.79	0.48
1:A:444:THR:OG1	2:A:601:FBP:O6P	2.29	0.48
1:B:527:TRP:CE2	1:B:528:ARG:HG2	2.49	0.48
1:C:337:VAL:HG22	1:C:370:CYS:HB2	1.96	0.48
1:C:421:THR:HG22	1:C:452:LEU:HD12	1.95	0.48
1:D:56:SER:HB2	1:D:480:GLY:CA	2.43	0.48
1:E:56:SER:HB2	1:E:480:GLY:CA	2.43	0.48
1:E:272:PRO:HA	1:E:275[A]:HIS:CE1	2.49	0.47
1:A:494:TRP:HE1	1:A:529:PRO:HB3	1.78	0.47
1:E:39:LEU:HG	1:G:331:LEU:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:272:PRO:HA	1:H:275[A]:HIS:CE1	2.49	0.47
1:A:382:PHE:HB3	1:A:385:GLU:HB2	1.95	0.47
1:E:382:PHE:HB3	1:E:385:GLU:HB2	1.96	0.47
1:C:486:TYR:CZ	1:C:488:GLU:HB2	2.49	0.47
1:H:30:LEU:O	1:H:34:MET:HG2	2.14	0.47
1:E:430:GLU:OE1	1:F:411:ARG:HD2	2.15	0.47
1:C:287:GLU:HG2	1:C:291:ARG:HD2	1.97	0.47
1:E:331:LEU:HD11	1:E:413:ALA:HB1	1.96	0.46
1:B:526:GLY:HA3	2:B:601:FBP:O3	2.16	0.46
1:D:421:THR:HG22	1:D:452:LEU:HD12	1.98	0.46
1:B:337:VAL:HG22	1:B:370:CYS:HB2	1.97	0.46
1:A:337:VAL:HG22	1:A:370:CYS:HB2	1.97	0.46
1:C:68:ARG:NE	1:C:95:TYR:CZ	2.83	0.46
1:F:317:LYS:NZ	7:F:705:HOH:O	2.46	0.46
1:G:486:TYR:CZ	1:G:488:GLU:HB2	2.51	0.46
1:C:30:LEU:O	1:C:34:MET:HG2	2.15	0.46
1:H:491:GLU:HB3	7:H:764:HOH:O	2.16	0.45
1:G:30:LEU:O	1:G:34:MET:HG2	2.16	0.45
1:F:526:GLY:HA3	2:F:601:FBP:O3	2.16	0.45
1:F:382:PHE:HB3	1:F:385:GLU:HB2	1.99	0.45
1:D:411:ARG:HG2	1:D:426:ILE:HD11	1.98	0.45
1:E:337:VAL:HG22	1:E:370:CYS:HB2	1.98	0.45
1:B:317:LYS:NZ	7:D:701:HOH:O	2.50	0.45
1:B:331:LEU:HD11	1:B:413:ALA:HB1	1.99	0.45
1:D:272:PRO:HA	1:D:275[A]:HIS:CE1	2.51	0.44
1:E:408[B]:GLU:OE2	1:F:411:ARG:NH2	2.50	0.44
1:G:352:PRO:HG3	1:G:389:MET:HG2	1.98	0.44
1:H:337:VAL:HG22	1:H:370:CYS:HB2	2.00	0.44
1:F:115:LEU:HD21	1:F:511:LEU:HB3	1.99	0.44
1:H:238:VAL:O	1:H:242[B]:ARG:HG3	2.17	0.44
1:G:430[A]:GLU:OE1	1:H:430[A]:GLU:OE1	2.36	0.44
1:D:130:GLY:C	1:D:132:GLY:N	2.76	0.44
1:A:517:VAL:HG22	1:A:543:SER:HB3	2.00	0.43
1:G:382:PHE:HB3	1:G:385:GLU:HB2	1.99	0.43
1:A:321:ALA:O	1:A:325:MET:HG3	2.18	0.43
1:D:337:VAL:HG22	1:D:370:CYS:HB2	2.01	0.43
1:C:411:ARG:HH12	1:D:411:ARG:NH2	2.15	0.43
1:G:337:VAL:HG22	1:G:370:CYS:HB2	2.01	0.43
1:G:269:ALA:C	1:G:271:GLY:H	2.26	0.43
1:H:64:GLY:O	1:H:68:ARG:HG3	2.18	0.43
1:H:486:TYR:CZ	1:H:488:GLU:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:GLY:O	1:C:275:HIS:CE1	2.71	0.43
1:C:321:ALA:O	1:C:325:MET:HG3	2.17	0.43
1:F:331:LEU:HD11	1:F:413:ALA:HB1	2.00	0.43
1:C:352:PRO:HG3	1:C:389:MET:HG2	2.01	0.43
1:C:331:LEU:HD11	1:C:413:ALA:HB1	2.00	0.43
1:F:16:LEU:HD23	1:F:25:PHE:HZ	1.84	0.43
1:A:30:LEU:O	1:A:34:MET:HG2	2.18	0.42
1:D:30:LEU:O	1:D:34:MET:HG3	2.19	0.42
1:E:352:PRO:HG3	1:E:389:MET:HG2	2.01	0.42
1:B:90:HIS:HB2	6:B:603:I91:C7	2.50	0.42
1:B:117:TYR:C	1:B:118:ARG:HG3	2.44	0.42
1:G:527:TRP:CD2	1:G:528:ARG:HG2	2.54	0.42
1:A:518:GLY:O	1:B:418:ARG:NH2	2.52	0.42
1:G:321:ALA:O	1:G:325:MET:HG3	2.19	0.42
1:C:231:PRO:HB2	1:C:232:GLY:H	1.71	0.42
1:E:258:ARG:HD3	1:E:285:ASN:HD21	1.84	0.42
1:A:352:PRO:HG3	1:A:389:MET:HG2	2.01	0.42
1:D:521:VAL:HG12	1:D:540:LEU:HB3	2.01	0.42
1:G:412:ARG:CZ	1:H:404:ARG:HD3	2.49	0.42
1:B:407:PHE:CD2	1:B:411:ARG:NH1	2.88	0.42
1:F:467:ARG:HD2	7:F:719:HOH:O	2.19	0.42
1:A:528:ARG:HD2	1:A:529:PRO:O	2.20	0.41
1:B:408:GLU:HG2	1:B:411:ARG:NH2	2.35	0.41
1:F:486:TYR:CZ	1:F:488:GLU:HB2	2.55	0.41
1:D:284:GLU:HB3	1:D:308:ASP:HB2	2.03	0.41
1:E:407:PHE:O	1:E:411:ARG:HB2	2.20	0.41
1:A:411:ARG:HH21	1:B:411:ARG:NH2	2.17	0.41
1:D:238:VAL:O	1:D:242[B]:ARG:HG3	2.20	0.41
1:D:448:ARG:HD3	7:D:739:HOH:O	2.19	0.41
1:A:418[B]:ARG:HG3	1:B:16:LEU:HD11	2.03	0.41
1:B:346:MET:HA	1:B:349:LYS:O	2.21	0.41
1:H:377:THR:HA	1:H:383:PRO:HB3	2.03	0.41
1:F:284:GLU:HB3	1:F:308:ASP:HB2	2.03	0.41
1:G:369:ASP:HA	1:G:479:ARG:HB2	2.03	0.40
1:A:412:ARG:NH1	1:B:404:ARG:HH11	2.19	0.40
1:G:523:VAL:HG21	1:G:540[A]:LEU:HD12	2.03	0.40
1:H:321:ALA:O	1:H:325:MET:HG3	2.21	0.40
1:B:53:ALA:O	1:B:395:ARG:NH2	2.51	0.40
1:B:486:TYR:CZ	1:B:488:GLU:HB2	2.55	0.40
1:D:233:LEU:HD12	1:D:233:LEU:HA	1.93	0.40
1:D:486:TYR:CZ	1:D:488:GLU:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:536:ILE:HD11	7:D:933:HOH:O	2.22	0.40
1:B:284:GLU:HB3	1:B:308:ASP:HB2	2.03	0.40
1:C:235:GLU:HG3	1:G:529:PRO:HG3	2.03	0.40
1:D:321:ALA:O	1:D:325:MET:HG3	2.22	0.40

There are no symmetry-related clashes.

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	427/447 (96%)	421 (99%)	5 (1%)	1 (0%)	43	49
1	B	438/447 (98%)	432 (99%)	5 (1%)	1 (0%)	43	49
1	C	428/447 (96%)	420 (98%)	5 (1%)	3 (1%)	18	17
1	D	431/447 (96%)	424 (98%)	6 (1%)	1 (0%)	43	49
1	E	429/447 (96%)	424 (99%)	3 (1%)	2 (0%)	24	25
1	F	436/447 (98%)	431 (99%)	4 (1%)	1 (0%)	43	49
1	G	426/447 (95%)	420 (99%)	5 (1%)	1 (0%)	43	49
1	H	432/447 (97%)	425 (98%)	5 (1%)	2 (0%)	24	25
All	All	3447/3576 (96%)	3397 (98%)	38 (1%)	12 (0%)	30	39

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	231	PRO
1	A	340	THR
1	B	340	THR
1	D	340	THR
1	E	340	THR
1	F	340	THR

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Mol	Chain	Res	Type
1	H	340	THR
1	H	535	ASN
1	C	340	THR
1	G	340	THR
1	C	271	GLY
1	E	129	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/352 (98%)	333 (96%)	12 (4%)	32	40
1	B	352/352 (100%)	338 (96%)	14 (4%)	28	35
1	C	344/352 (98%)	330 (96%)	14 (4%)	27	33
1	D	344/352 (98%)	332 (96%)	12 (4%)	32	40
1	E	346/352 (98%)	337 (97%)	9 (3%)	40	51
1	F	351/352 (100%)	338 (96%)	13 (4%)	30	38
1	G	343/352 (97%)	337 (98%)	6 (2%)	53	66
1	H	345/352 (98%)	337 (98%)	8 (2%)	44	56
All	All	2770/2816 (98%)	2682 (97%)	88 (3%)	38	43

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	86	LEU
1	A	258	ARG
1	A	259	LYS
1	A	411	ARG
1	A	412	ARG
1	A	443	LEU
1	A	475	VAL
1	A	500	ARG

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Mol	Chain	Res	Type
1	A	537[A]	MET
1	A	537[B]	MET
1	A	540	LEU
1	B	10	ARG
1	B	16	LEU
1	B	68	ARG
1	B	76[A]	MET
1	B	76[B]	MET
1	B	259	LYS
1	B	263	VAL
1	B	331	LEU
1	B	358	SER
1	B	412	ARG
1	B	511	LEU
1	B	512	ARG
1	B	537[A]	MET
1	B	537[B]	MET
1	C	52	VAL
1	C	76[A]	MET
1	C	76[B]	MET
1	C	116[A]	SER
1	C	116[B]	SER
1	C	259	LYS
1	C	270[A]	LEU
1	C	270[B]	LEU
1	C	331	LEU
1	C	358	SER
1	C	412	ARG
1	C	487	ARG
1	C	531	SER
1	C	540	LEU
1	D	118	ARG
1	D	242[A]	ARG
1	D	242[B]	ARG
1	D	259	LYS
1	D	358	SER
1	D	412	ARG
1	D	508	SER
1	D	511	LEU
1	D	521	VAL
1	D	528	ARG
1	D	537	MET

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Mol	Chain	Res	Type
1	D	538	ARG
1	E	52	VAL
1	E	68	ARG
1	E	259	LYS
1	E	331	LEU
1	E	412	ARG
1	E	511	LEU
1	E	537[A]	MET
1	E	537[B]	MET
1	E	539	VAL
1	F	16	LEU
1	F	68	ARG
1	F	76[A]	MET
1	F	76[B]	MET
1	F	94	GLU
1	F	259	LYS
1	F	291	ARG
1	F	331	LEU
1	F	443	LEU
1	F	511	LEU
1	F	521	VAL
1	F	537[A]	MET
1	F	537[B]	MET
1	G	52	VAL
1	G	76[A]	MET
1	G	76[B]	MET
1	G	259	LYS
1	G	273	GLU
1	G	475	VAL
1	H	242[A]	ARG
1	H	242[B]	ARG
1	H	259	LYS
1	H	273	GLU
1	H	331	LEU
1	H	511	LEU
1	H	516	ARG
1	H	537	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	GLN

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Mol	Chain	Res	Type
1	A	405	GLN
1	B	405	GLN
1	C	26	GLN
1	C	275	HIS
1	C	405	GLN
1	D	405	GLN
1	E	405	GLN
1	F	405	GLN
1	G	275	HIS
1	G	405	GLN
1	H	390	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	0.50	0	21,32,32	0.60	0
2	FBP	G	601	-	18,20,20	0.57	1 (5%)	21,32,32	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OXL	D	602	4	5,5,5	2.11	2 (40%)	6,6,6	2.37	3 (50%)
3	OXL	H	602	4	5,5,5	1.74	2 (40%)	6,6,6	2.16	2 (33%)
6	I91	C	603	-	27,27,27	0.22	0	40,41,41	0.28	0
6	I91	B	603	-	27,27,27	0.23	0	40,41,41	1.70	1 (2%)
2	FBP	H	601	-	18,20,20	0.69	0	21,32,32	0.83	1 (4%)
3	OXL	B	602	4	5,5,5	2.17	1 (20%)	6,6,6	1.60	1 (16%)
3	OXL	C	602	4	5,5,5	1.95	2 (40%)	6,6,6	1.56	1 (16%)
6	I91	G	603	-	27,27,27	0.22	0	40,41,41	0.45	0
2	FBP	E	601	-	18,20,20	0.54	0	21,32,32	0.83	1 (4%)
2	FBP	D	601	-	18,20,20	0.78	1 (5%)	21,32,32	1.24	2 (9%)
2	FBP	A	601	-	18,20,20	0.79	1 (5%)	21,32,32	0.81	0
2	FBP	B	601	-	18,20,20	0.68	0	21,32,32	0.86	1 (4%)
3	OXL	A	602	4	5,5,5	2.00	2 (40%)	6,6,6	2.46	3 (50%)
2	FBP	C	601	-	18,20,20	0.76	1 (5%)	21,32,32	0.81	0
3	OXL	G	602	4	5,5,5	2.32	2 (40%)	6,6,6	2.39	3 (50%)
3	OXL	F	602	4	5,5,5	2.78	4 (80%)	6,6,6	2.46	3 (50%)
3	OXL	E	602	4	5,5,5	2.29	2 (40%)	6,6,6	1.34	2 (33%)
6	I91	F	603	-	27,27,27	0.19	0	40,41,41	0.27	0

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	-	-	8/13/32/32	0/1/1/1
2	FBP	G	601	-	-	2/13/32/32	0/1/1/1
3	OXL	D	602	4	-	4/4/4/4	-
3	OXL	H	602	4	-	4/4/4/4	-
6	I91	C	603	-	-	2/12/28/28	0/3/3/3
6	I91	B	603	-	-	3/12/28/28	0/3/3/3
2	FBP	H	601	-	-	3/13/32/32	0/1/1/1
3	OXL	B	602	4	-	4/4/4/4	-
3	OXL	C	602	4	-	4/4/4/4	-
6	I91	G	603	-	-	4/12/28/28	0/3/3/3
2	FBP	E	601	-	-	3/13/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
2	FBP	A	601	-	-	7/13/32/32	0/1/1/1
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
3	OXL	A	602	4	-	4/4/4/4	-
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
3	OXL	G	602	4	-	4/4/4/4	-
3	OXL	F	602	4	-	4/4/4/4	-
3	OXL	E	602	4	-	4/4/4/4	-
6	I91	F	603	-	-	8/12/28/28	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	OXL	O2-C2	4.34	1.33	1.22
3	F	602	OXL	O3-C1	-3.85	1.20	1.30
3	E	602	OXL	O1-C1	3.81	1.32	1.22
3	A	602	OXL	O2-C2	3.57	1.31	1.22
3	G	602	OXL	O3-C1	-3.54	1.20	1.30
3	C	602	OXL	O1-C1	3.32	1.30	1.22
3	D	602	OXL	O2-C2	3.22	1.30	1.22
3	G	602	OXL	O1-C1	3.21	1.30	1.22
3	F	602	OXL	O2-C2	3.13	1.30	1.22
3	D	602	OXL	O4-C2	-3.10	1.22	1.30
3	E	602	OXL	O3-C1	-2.99	1.22	1.30
3	H	602	OXL	O4-C2	-2.88	1.22	1.30
3	C	602	OXL	O3-C1	-2.72	1.23	1.30
3	F	602	OXL	O1-C1	2.72	1.29	1.22
3	F	602	OXL	O4-C2	-2.56	1.23	1.30
3	A	602	OXL	O4-C2	-2.49	1.23	1.30
2	C	601	FBP	P1-O3P	-2.45	1.45	1.54
3	H	602	OXL	O2-C2	2.34	1.28	1.22
2	A	601	FBP	P2-O6P	-2.34	1.46	1.54
2	D	601	FBP	P1-O1	-2.31	1.53	1.60
2	G	601	FBP	P2-O6P	-2.00	1.47	1.54

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	603	I91	C12-N-S	10.57	142.00	119.80
3	H	602	OXL	O4-C2-C1	4.54	121.63	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	FBP	O5P-P2-O6	4.45	118.28	106.67
3	A	602	OXL	O4-C2-C1	4.37	121.31	112.83
3	F	602	OXL	O4-C2-C1	4.19	120.96	112.83
3	D	602	OXL	O4-C2-C1	3.70	120.01	112.83
3	G	602	OXL	O4-C2-C1	3.64	119.89	112.83
3	D	602	OXL	O3-C1-C2	3.58	119.77	112.83
3	G	602	OXL	O3-C1-C2	3.40	119.43	112.83
3	F	602	OXL	O3-C1-C2	3.38	119.39	112.83
3	C	602	OXL	O3-C1-C2	3.08	118.80	112.83
3	A	602	OXL	O3-C1-C2	3.05	118.74	112.83
3	B	602	OXL	O4-C2-C1	2.91	118.47	112.83
2	H	601	FBP	O5P-P2-O6	2.55	113.32	106.67
3	A	602	OXL	O2-C2-C1	-2.54	115.35	120.63
3	G	602	OXL	O2-C2-C1	-2.48	115.47	120.63
2	D	601	FBP	O6-P2-O4P	-2.44	99.84	106.44
3	H	602	OXL	O2-C2-C1	-2.40	115.63	120.63
2	B	601	FBP	O3P-P1-O2P	2.39	116.76	107.80
3	F	602	OXL	O2-C2-C1	-2.38	115.68	120.63
3	E	602	OXL	O3-C1-C2	2.32	117.33	112.83
2	E	601	FBP	O3P-P1-O2P	2.27	116.30	107.80
3	E	602	OXL	O4-C2-C1	2.17	117.03	112.83
3	D	602	OXL	O1-C1-C2	-2.04	116.39	120.63

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FBP	C1-O1-P1-O1P
2	A	601	FBP	C1-O1-P1-O2P
2	A	601	FBP	C1-O1-P1-O3P
2	A	601	FBP	O1-C1-C2-O2
2	A	601	FBP	O1-C1-C2-O5
2	A	601	FBP	O5-C5-C6-O6
2	F	601	FBP	C1-O1-P1-O2P
2	F	601	FBP	C1-O1-P1-O3P
2	F	601	FBP	O1-C1-C2-O2
2	F	601	FBP	O1-C1-C2-C3
2	F	601	FBP	O1-C1-C2-O5
6	G	603	I91	N-C12-C13-O3
6	C	603	I91	C12-N-S-C11
6	G	603	I91	C12-N-S-O5
2	A	601	FBP	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	B	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6
2	D	601	FBP	C4-C5-C6-O6
2	E	601	FBP	C4-C5-C6-O6
2	F	601	FBP	C4-C5-C6-O6
2	G	601	FBP	C4-C5-C6-O6
2	H	601	FBP	C4-C5-C6-O6
6	G	603	I91	N-C12-C13-O2
6	G	603	I91	C12-N-S-C11
6	F	603	I91	C12-N-S-O5
2	B	601	FBP	O5-C5-C6-O6
2	E	601	FBP	O5-C5-C6-O6
2	F	601	FBP	O5-C5-C6-O6
6	F	603	I91	C12-N-S-O4
6	F	603	I91	C12-N-S-C11
2	D	601	FBP	O5-C5-C6-O6
2	C	601	FBP	O5-C5-C6-O6
2	H	601	FBP	O5-C5-C6-O6
2	F	601	FBP	C1-O1-P1-O1P
2	G	601	FBP	O5-C5-C6-O6
3	H	602	OXL	O3-C1-C2-O4
6	C	603	I91	C12-N-S-O5
3	E	602	OXL	O3-C1-C2-O4
3	B	602	OXL	O3-C1-C2-O4
3	C	602	OXL	O3-C1-C2-O4
3	F	602	OXL	O3-C1-C2-O4
3	G	602	OXL	O3-C1-C2-O4
3	F	602	OXL	O1-C1-C2-O2
3	A	602	OXL	O3-C1-C2-O4
3	D	602	OXL	O3-C1-C2-O4
3	A	602	OXL	O1-C1-C2-O2
3	B	602	OXL	O1-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O2
3	C	602	OXL	O1-C1-C2-O2
3	E	602	OXL	O1-C1-C2-O2
3	G	602	OXL	O1-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O2
2	E	601	FBP	C1-O1-P1-O1P
2	H	601	FBP	C1-O1-P1-O1P
6	F	603	I91	C10-C11-S-O5
6	B	603	I91	C13-C12-N-S
3	H	602	OXL	O3-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	F	603	I91	C14-C11-S-O4
6	B	603	I91	N-C12-C13-O3
6	F	603	I91	N-C12-C13-O3
3	F	602	OXL	O3-C1-C2-O2
3	B	602	OXL	O3-C1-C2-O2
3	D	602	OXL	O3-C1-C2-O2
3	C	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	O1-C1-C2-O4
3	A	602	OXL	O1-C1-C2-O4
3	A	602	OXL	O3-C1-C2-O2
3	B	602	OXL	O1-C1-C2-O4
3	C	602	OXL	O1-C1-C2-O4
3	D	602	OXL	O1-C1-C2-O4
3	G	602	OXL	O1-C1-C2-O4
3	G	602	OXL	O3-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O4
6	B	603	I91	N-C12-C13-O2
6	F	603	I91	N-C12-C13-O2
6	F	603	I91	C10-C11-S-N

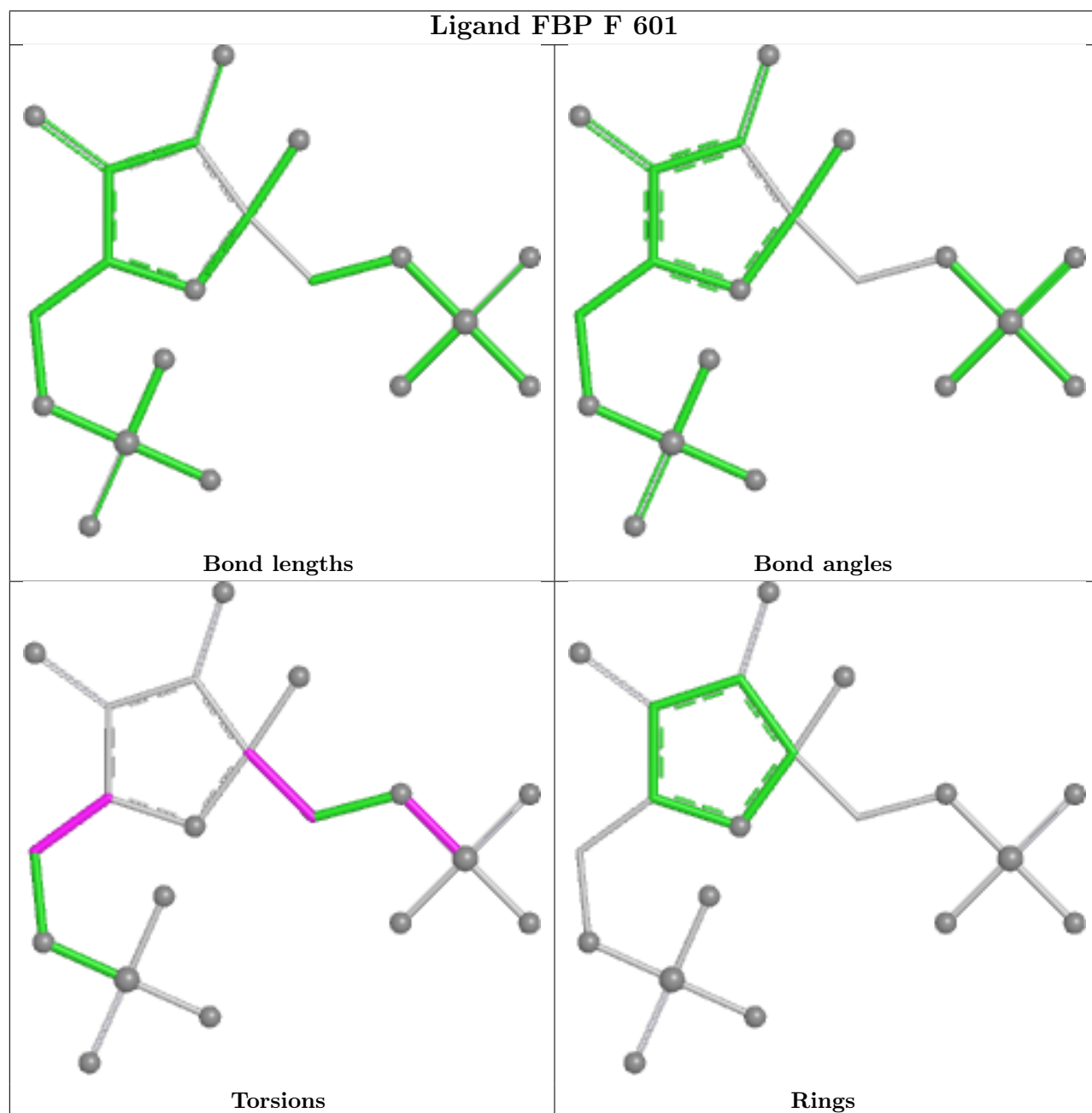
There are no ring outliers.

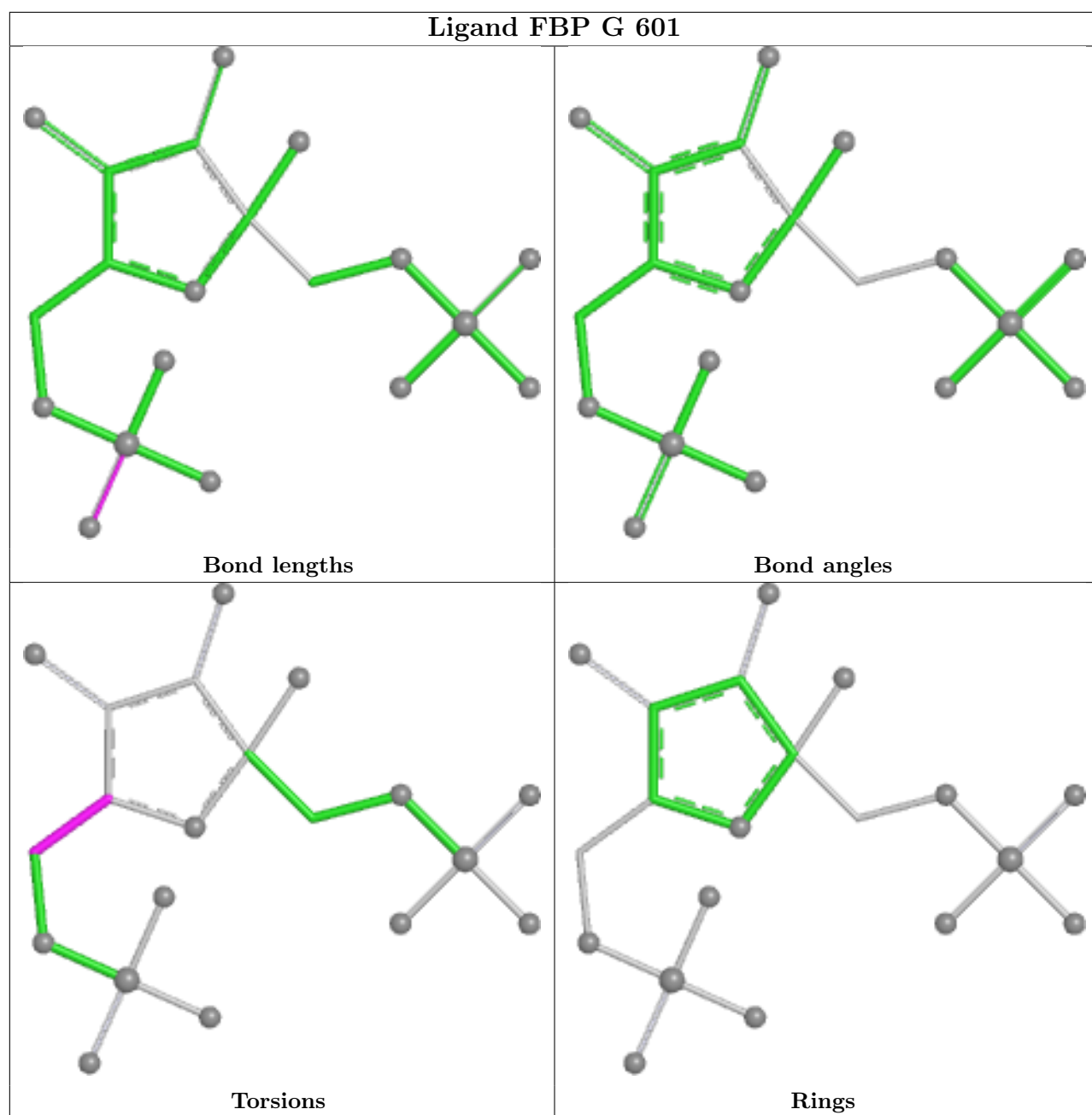
5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	601	FBP	1	0
6	B	603	I91	1	0
6	G	603	I91	1	0
2	A	601	FBP	2	0
2	B	601	FBP	1	0

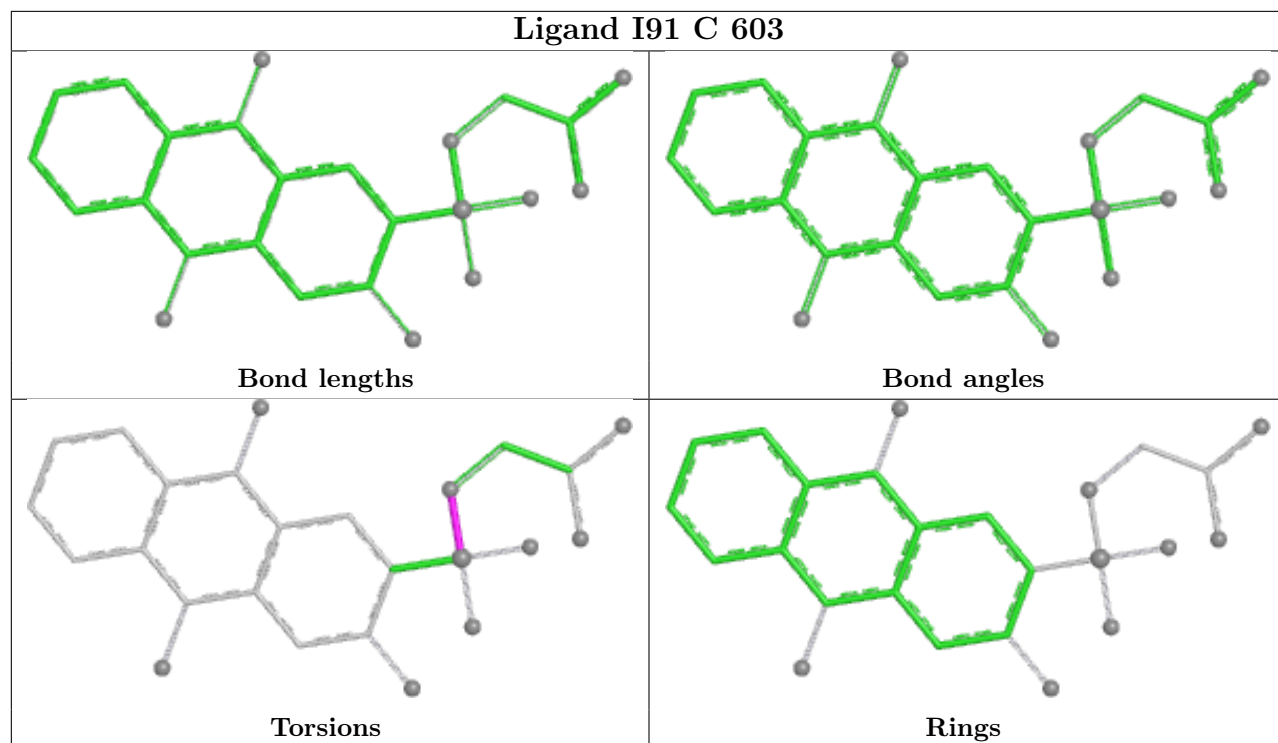
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

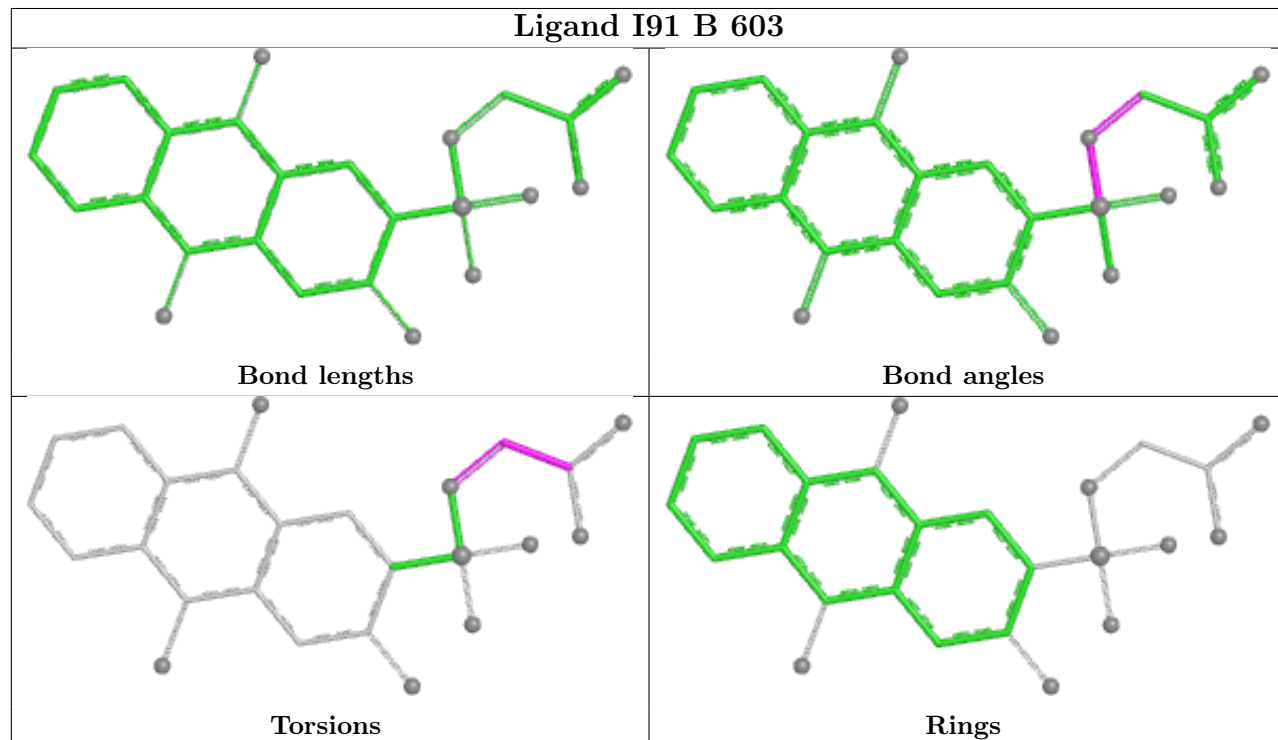


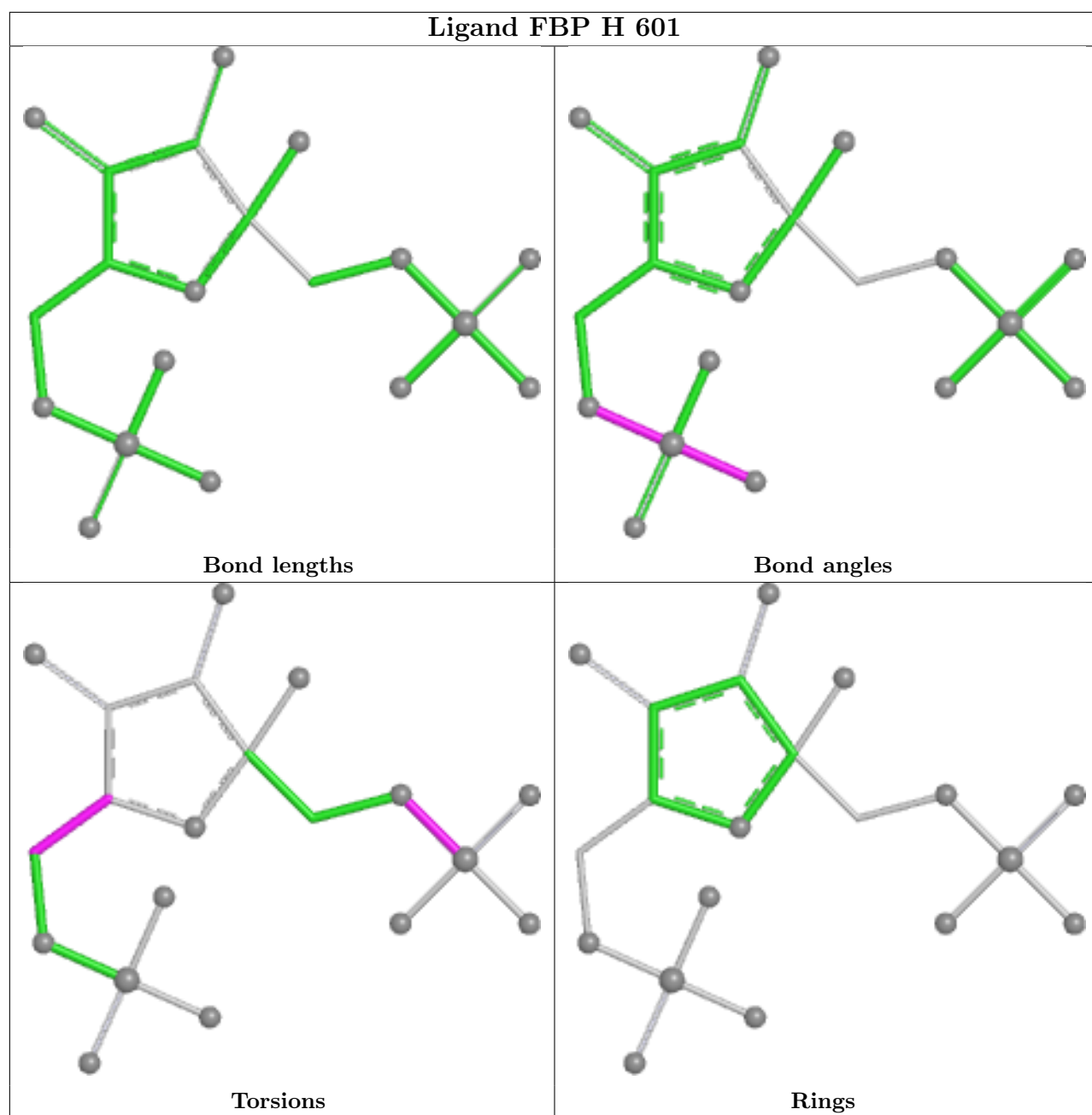


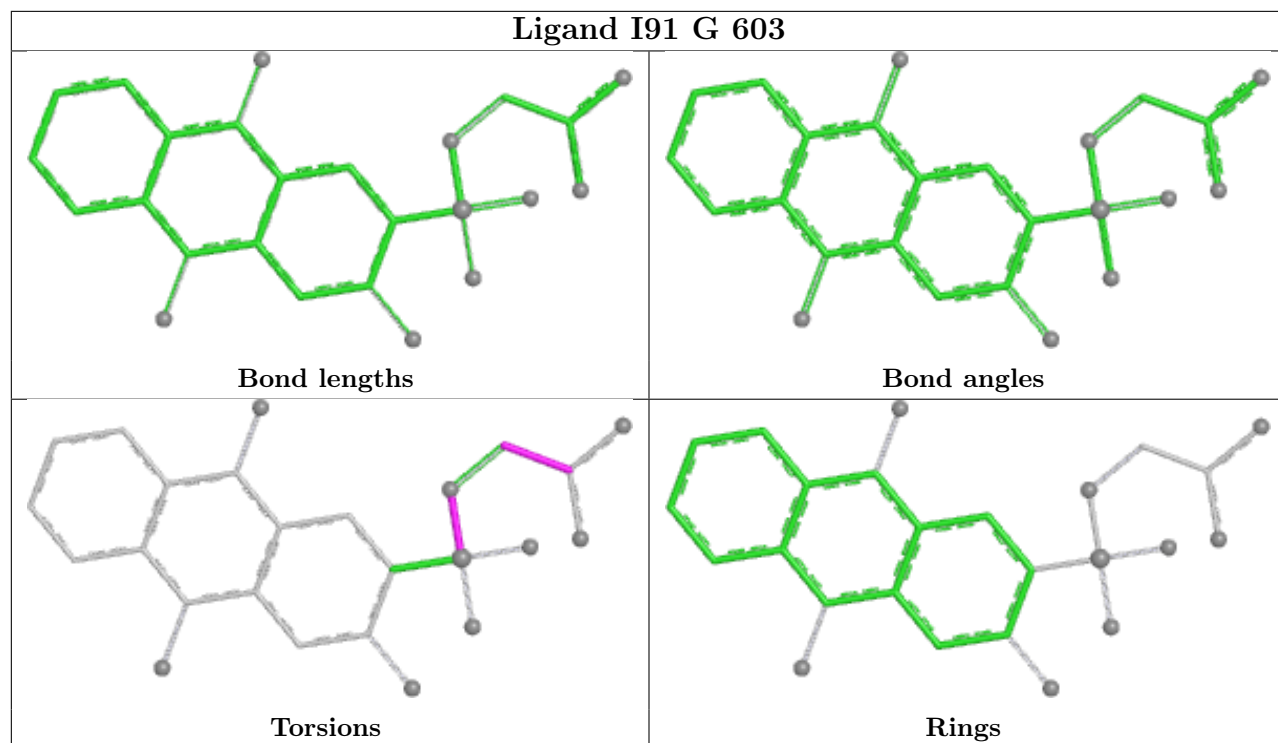
Ligand I91 C 603



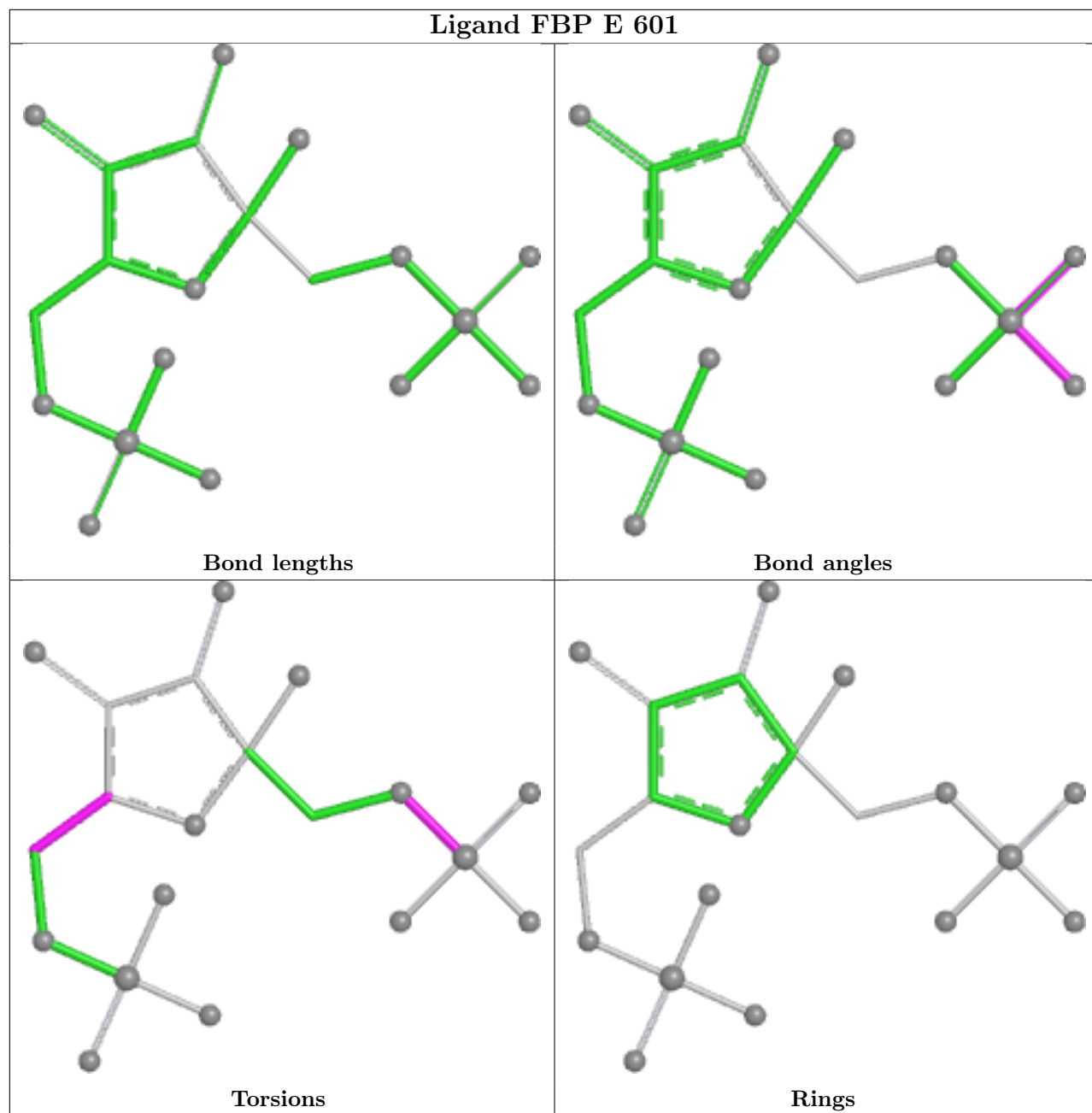
Ligand I91 B 603

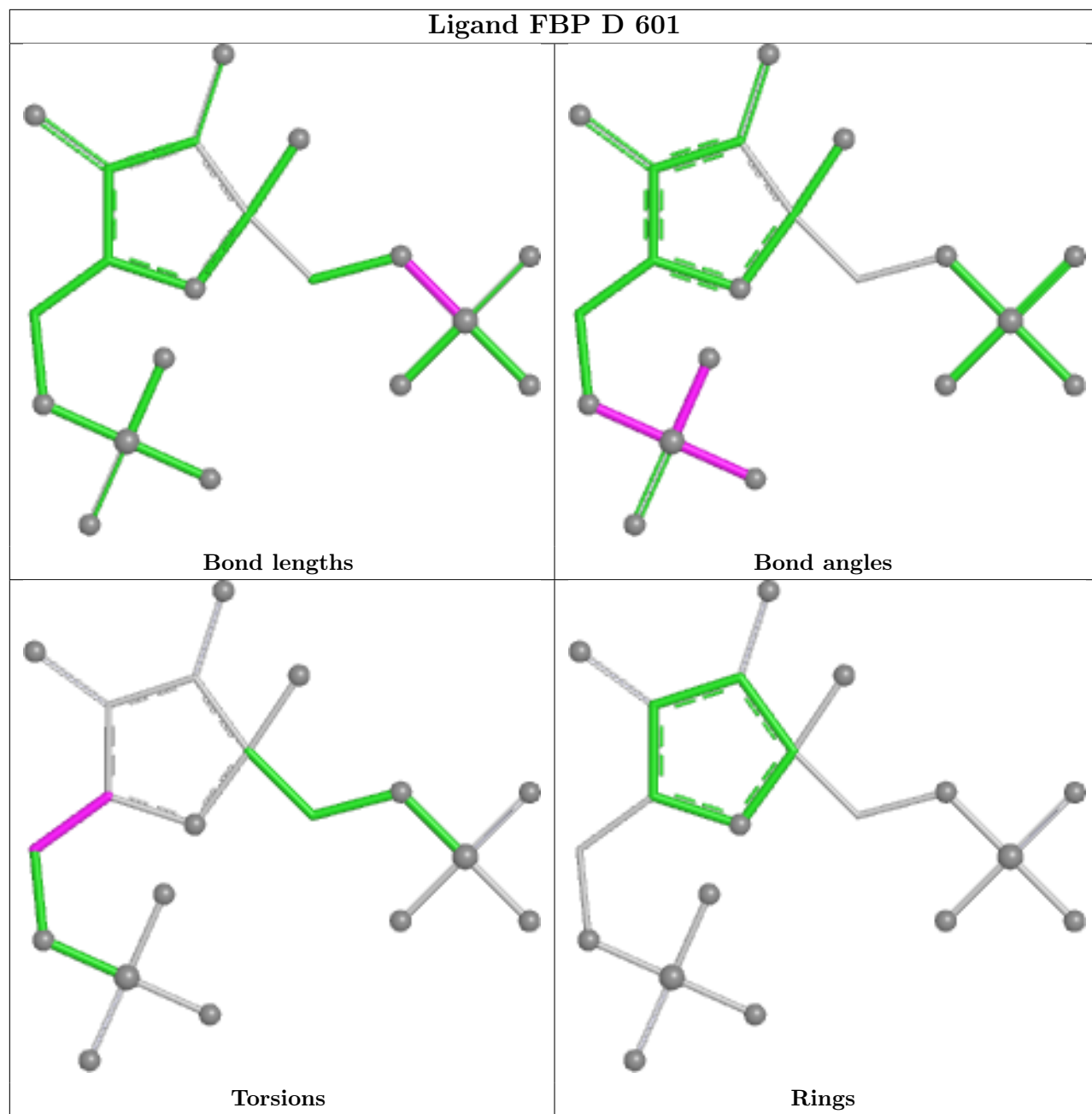


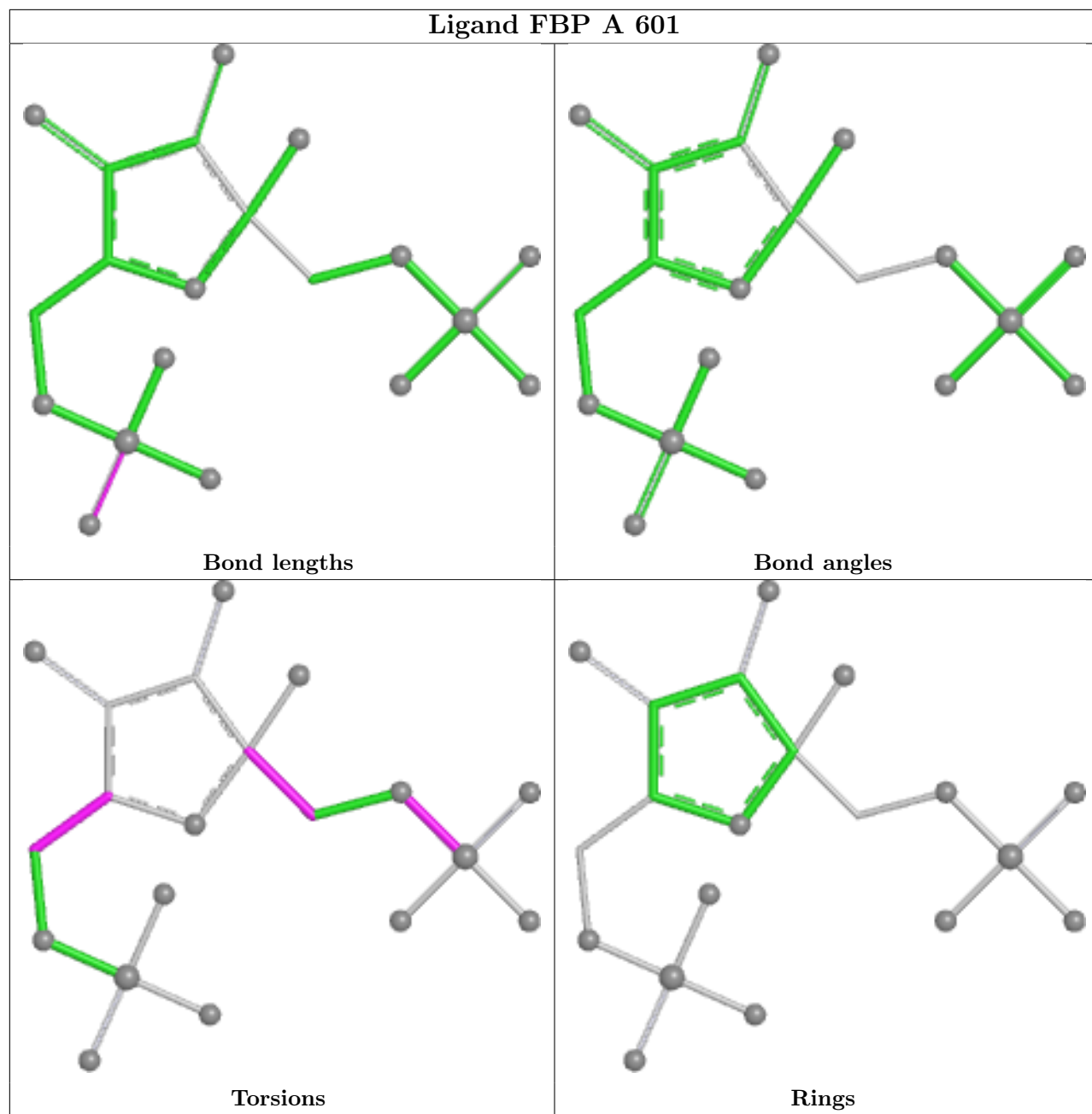




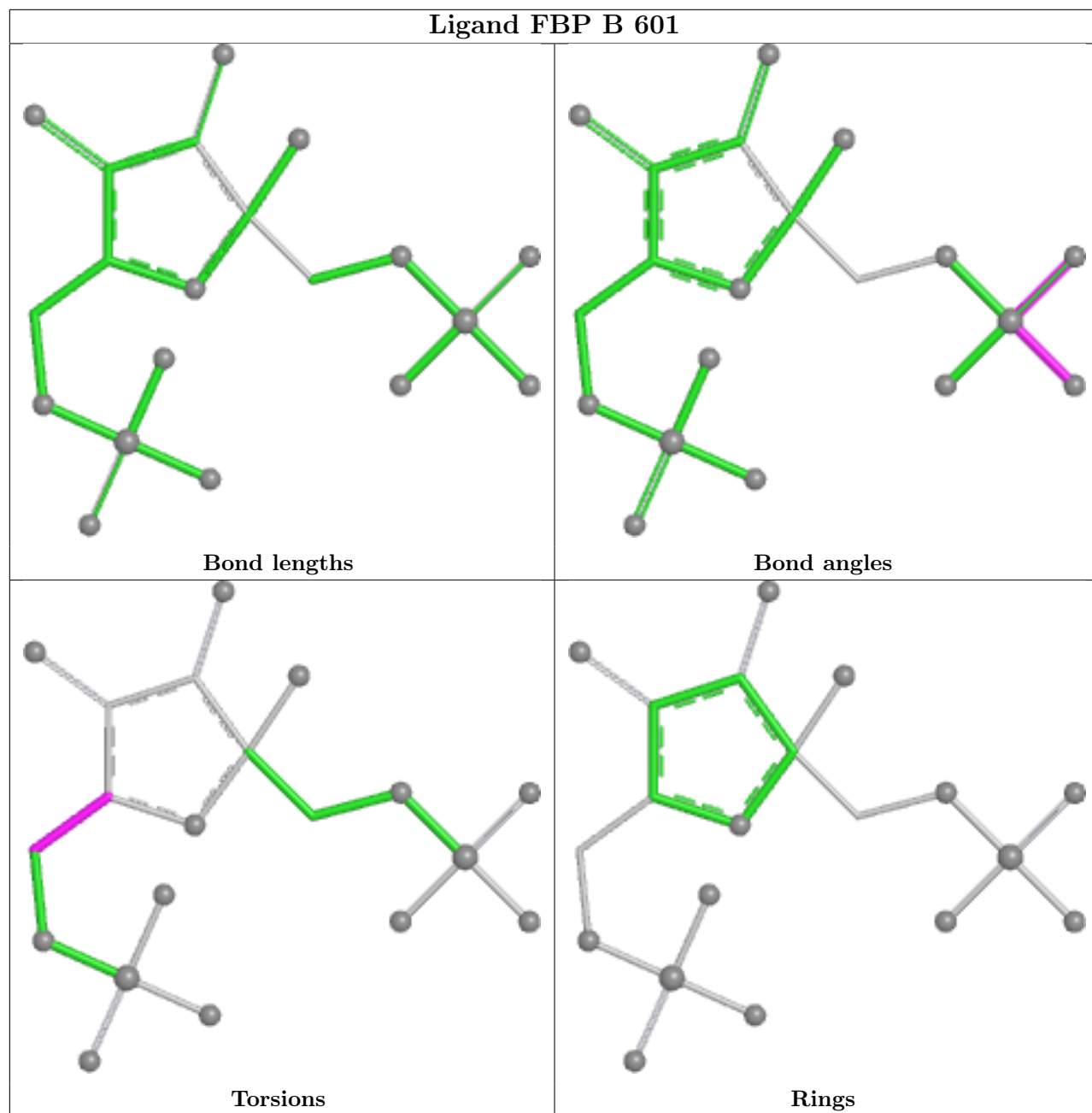
Ligand FBP E 601

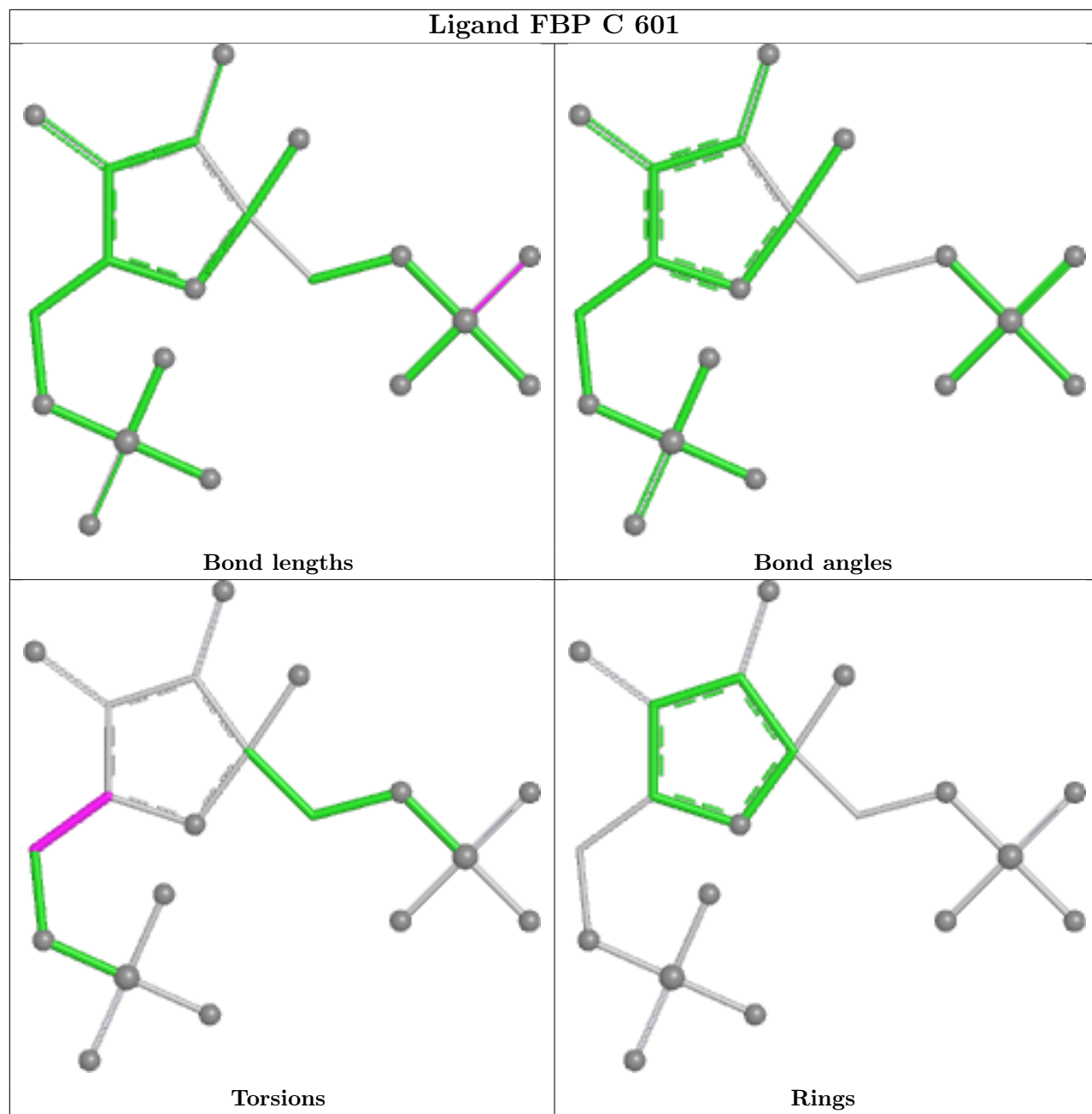


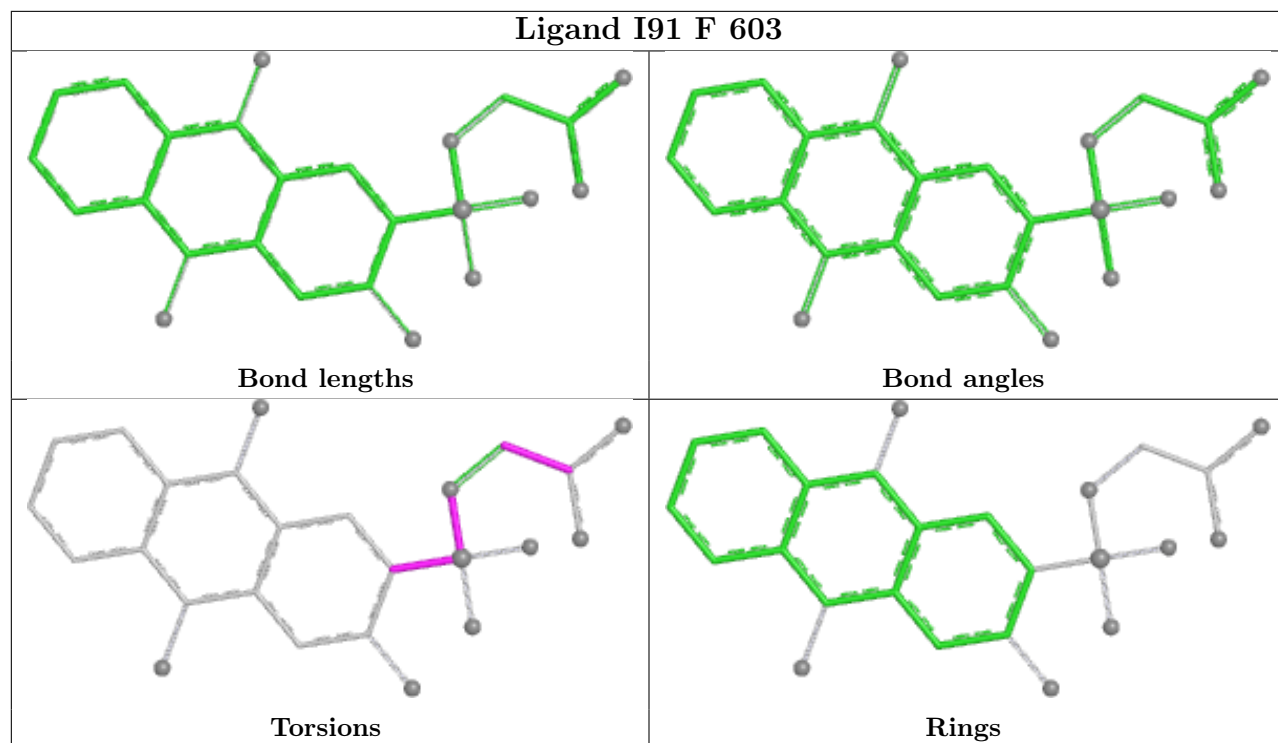




Ligand FBP B 601







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	418/447 (93%)	1.53	105 (25%) 1 1	37, 71, 105, 119	13 (3%)
1	B	434/447 (97%)	1.14	89 (20%) 2 2	30, 59, 90, 104	8 (1%)
1	C	425/447 (95%)	0.64	39 (9%) 14 13	27, 49, 80, 130	7 (1%)
1	D	425/447 (95%)	0.24	22 (5%) 33 32	21, 40, 69, 126	8 (1%)
1	E	420/447 (93%)	1.43	108 (25%) 1 1	30, 65, 102, 115	13 (3%)
1	F	432/447 (96%)	0.78	48 (11%) 10 9	31, 54, 82, 102	8 (1%)
1	G	422/447 (94%)	0.42	31 (7%) 21 20	22, 44, 78, 125	9 (2%)
1	H	425/447 (95%)	0.11	17 (4%) 42 41	18, 38, 69, 122	9 (2%)
All	All	3401/3576 (95%)	0.78	459 (13%) 7 6	18, 53, 92, 130	75 (2%)

All (459) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	115	LEU	7.7
1	E	115	LEU	7.4
1	E	275[A]	HIS	6.5
1	D	25	PHE	6.4
1	C	20	LEU	6.3
1	E	114	PRO	6.2
1	E	25	PHE	6.1
1	D	24	PHE	6.0
1	F	231	PRO	6.0
1	E	23	ALA	5.9
1	G	24	PHE	5.9
1	B	231	PRO	5.9
1	A	30	LEU	5.8
1	C	132	GLY	5.8
1	D	231	PRO	5.8
1	H	21	GLY	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	115	LEU	5.7
1	G	25	PHE	5.5
1	G	116	SER	5.4
1	C	231	PRO	5.3
1	E	24	PHE	5.2
1	C	22	THR	5.2
1	G	231	PRO	5.2
1	A	232	GLY	5.2
1	A	241	LEU	5.2
1	G	23	ALA	5.1
1	A	490	PRO	5.1
1	C	25	PHE	5.1
1	H	25	PHE	5.1
1	G	21	GLY	5.1
1	B	517	VAL	4.9
1	D	21	GLY	4.9
1	B	11	ALA	4.8
1	H	24	PHE	4.8
1	D	23	ALA	4.7
1	G	271	GLY	4.7
1	A	482	PHE	4.7
1	G	114	PRO	4.7
1	H	22	THR	4.6
1	A	543	SER	4.6
1	E	33	ALA	4.5
1	C	21	GLY	4.5
1	E	123	ALA	4.4
1	B	527	TRP	4.4
1	E	130	GLY	4.3
1	F	11	ALA	4.3
1	B	95	TYR	4.3
1	A	114	PRO	4.3
1	A	26	GLN	4.3
1	E	116	SER	4.3
1	A	238	VAL	4.3
1	E	238	VAL	4.3
1	F	232	GLY	4.2
1	C	23	ALA	4.2
1	H	23	ALA	4.2
1	C	232	GLY	4.1
1	D	22	THR	4.1
1	A	116	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	512	ARG	4.1
1	B	490	PRO	4.1
1	B	267[A]	ARG	4.0
1	E	30	LEU	4.0
1	D	232	GLY	4.0
1	C	34	MET	4.0
1	A	500	ARG	4.0
1	E	495	ALA	3.9
1	G	22	THR	3.9
1	A	120	VAL	3.9
1	C	271	GLY	3.9
1	A	124	LEU	3.9
1	E	120	VAL	3.9
1	C	115	LEU	3.9
1	A	34	MET	3.9
1	F	267[A]	ARG	3.9
1	E	113	SER	3.8
1	E	490	PRO	3.8
1	A	249	VAL	3.8
1	F	233	LEU	3.8
1	A	112	GLY	3.8
1	A	493	ILE	3.8
1	G	33	ALA	3.8
1	F	489	PRO	3.8
1	F	492	ALA	3.7
1	E	489	PRO	3.7
1	B	543	SER	3.7
1	G	113	SER	3.7
1	E	103	VAL	3.7
1	E	502	VAL	3.7
1	G	487	ARG	3.6
1	E	119	PRO	3.6
1	F	484	LEU	3.6
1	A	80	GLY	3.5
1	E	244	GLY	3.5
1	A	130	GLY	3.5
1	B	504	PHE	3.5
1	A	495	ALA	3.4
1	E	257	VAL	3.4
1	A	463	ILE	3.4
1	B	511	LEU	3.4
1	D	275[A]	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	113	SER	3.4
1	A	378	ALA	3.4
1	B	14	ALA	3.4
1	A	95	TYR	3.3
1	B	130	GLY	3.3
1	E	233	LEU	3.3
1	F	516	ARG	3.3
1	D	499	ASP	3.3
1	A	33	ALA	3.3
1	B	100	ILE	3.3
1	C	24	PHE	3.3
1	E	110	PHE	3.3
1	A	527	TRP	3.3
1	E	122	ILE	3.3
1	E	277	ILE	3.3
1	F	12	ASP	3.3
1	A	266	VAL	3.2
1	B	61	ALA	3.2
1	A	233	LEU	3.2
1	E	232	GLY	3.2
1	B	13	VAL	3.2
1	A	488[A]	GLU	3.2
1	A	489	PRO	3.2
1	F	490	PRO	3.2
1	A	32	ALA	3.2
1	B	492	ALA	3.2
1	B	115	LEU	3.2
1	A	131	SER	3.2
1	D	132	GLY	3.2
1	B	233	LEU	3.1
1	B	243	PHE	3.1
1	B	489	PRO	3.1
1	B	66	ALA	3.1
1	E	464	ALA	3.1
1	A	79	ALA	3.1
1	A	63	ILE	3.1
1	E	493	ILE	3.1
1	F	487	ARG	3.1
1	F	408	GLU	3.1
1	A	111	ALA	3.1
1	A	122	ILE	3.1
1	A	248	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	415	PRO	3.0
1	C	408	GLU	3.0
1	A	260	ALA	3.0
1	A	502	VAL	3.0
1	B	498	VAL	3.0
1	E	540	LEU	3.0
1	B	77	ILE	3.0
1	B	272	PRO	3.0
1	C	19	GLU	3.0
1	F	275	HIS	3.0
1	B	495	ALA	3.0
1	C	66	ALA	3.0
1	E	28	GLN	3.0
1	B	540[A]	LEU	3.0
1	F	13	VAL	3.0
1	F	238	VAL	3.0
1	B	542	ILE	3.0
1	A	269	ALA	3.0
1	E	266	VAL	3.0
1	B	493	ILE	3.0
1	A	351	ARG	2.9
1	E	264	ALA	2.9
1	E	485	LEU	2.9
1	B	416	LEU	2.9
1	E	241	LEU	2.9
1	B	52	VAL	2.9
1	A	119	PRO	2.9
1	E	75	GLU	2.9
1	H	273	GLU	2.9
1	E	243	PHE	2.9
1	F	533	TYR	2.9
1	A	123	ALA	2.9
1	F	84	ALA	2.9
1	A	91	GLY	2.9
1	C	30	LEU	2.9
1	E	249	VAL	2.9
1	A	270	LEU	2.8
1	E	34	MET	2.8
1	F	498	VAL	2.8
1	A	100	ILE	2.8
1	A	243	PHE	2.8
1	B	110	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	243	PHE	2.8
1	E	112	GLY	2.8
1	E	517	VAL	2.8
1	A	237	ASP	2.8
1	A	514	PHE	2.8
1	E	95	TYR	2.8
1	A	265	ALA	2.8
1	F	14	ALA	2.8
1	E	494	TRP	2.8
1	A	127	LYS	2.8
1	B	72	ARG	2.8
1	E	99	SER	2.8
1	A	53	ALA	2.8
1	D	413	ALA	2.8
1	G	117	TYR	2.8
1	E	383	PRO	2.8
1	G	411	ARG	2.7
1	A	66	ALA	2.7
1	C	111	ALA	2.7
1	G	42	LEU	2.7
1	A	118	ARG	2.7
1	B	252	VAL	2.7
1	B	502	VAL	2.7
1	A	277	ILE	2.7
1	B	311	ILE	2.7
1	C	43	CYS	2.7
1	B	275	HIS	2.7
1	B	38	PHE	2.7
1	D	33	ALA	2.7
1	C	42	LEU	2.7
1	E	124	LEU	2.7
1	A	272	PRO	2.7
1	E	129	PRO	2.7
1	G	272	PRO	2.7
1	A	108	GLU	2.7
1	A	244	GLY	2.7
1	E	118	ARG	2.7
1	E	66	ALA	2.7
1	E	265	ALA	2.7
1	E	514	PHE	2.7
1	B	124	LEU	2.7
1	E	52	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	245	VAL	2.7
1	B	12	ASP	2.7
1	F	459	ARG	2.7
1	A	75[A]	GLU	2.6
1	A	256	PHE	2.6
1	E	256	PHE	2.6
1	B	16	LEU	2.6
1	A	383	PRO	2.6
1	B	379	LYS	2.6
1	C	311	ILE	2.6
1	A	538	ARG	2.6
1	D	412	ARG	2.6
1	B	408	GLU	2.6
1	A	275	HIS	2.6
1	A	110	PHE	2.6
1	B	73	LEU	2.6
1	C	110	PHE	2.6
1	F	515	LEU	2.6
1	E	442	VAL	2.6
1	E	542	ILE	2.6
1	G	26	GLN	2.6
1	G	232	GLY	2.6
1	A	492	ALA	2.6
1	D	32	ALA	2.6
1	A	31	PRO	2.6
1	A	86	LEU	2.6
1	D	115	LEU	2.6
1	E	272	PRO	2.6
1	G	28	GLN	2.6
1	E	111	ALA	2.6
1	E	378	ALA	2.6
1	G	111	ALA	2.6
1	B	514	PHE	2.5
1	E	26	GLN	2.5
1	G	98[A]	GLU	2.5
1	A	263	VAL	2.5
1	A	401	VAL	2.5
1	A	441	ILE	2.5
1	B	506	ILE	2.5
1	B	232	GLY	2.5
1	E	117	TYR	2.5
1	E	242	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	527	TRP	2.5
1	E	463	ILE	2.5
1	E	97	ALA	2.5
1	H	231	PRO	2.5
1	E	515	LEU	2.5
1	F	124	LEU	2.5
1	B	25	PHE	2.5
1	A	93	HIS	2.5
1	E	276	GLY	2.5
1	A	99	SER	2.5
1	A	484	LEU	2.5
1	B	485	LEU	2.5
1	B	515	LEU	2.5
1	E	511	LEU	2.5
1	C	404	ARG	2.5
1	G	412	ARG	2.5
1	E	91	GLY	2.5
1	E	248	GLY	2.5
1	B	245	VAL	2.4
1	A	350	PRO	2.4
1	C	305	ALA	2.4
1	B	241	LEU	2.4
1	B	484	LEU	2.4
1	C	487	ARG	2.4
1	H	275[A]	HIS	2.4
1	A	532	GLY	2.4
1	B	24	PHE	2.4
1	E	88	PHE	2.4
1	A	27	GLN	2.4
1	B	70	VAL	2.4
1	E	100	ILE	2.4
1	E	107	VAL	2.4
1	C	272	PRO	2.4
1	F	129	PRO	2.4
1	C	386	ALA	2.4
1	E	32	ALA	2.4
1	F	242	ARG	2.4
1	H	516	ARG	2.4
1	B	270	LEU	2.4
1	D	30	LEU	2.4
1	D	403	HIS	2.4
1	E	90	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	247	HIS	2.4
1	F	497	ASP	2.4
1	A	70	VAL	2.4
1	A	475	VAL	2.4
1	B	120	VAL	2.4
1	E	109	SER	2.4
1	G	34	MET	2.4
1	A	412	ARG	2.4
1	B	118	ARG	2.4
1	B	487	ARG	2.4
1	E	487	ARG	2.4
1	G	351	ARG	2.4
1	C	114	PRO	2.4
1	A	73	LEU	2.4
1	A	540	LEU	2.4
1	C	36	ASP	2.4
1	A	107	VAL	2.4
1	B	107	VAL	2.4
1	B	347	ILE	2.4
1	E	251	ILE	2.4
1	E	263	VAL	2.4
1	E	92	SER	2.4
1	F	379	LYS	2.4
1	B	93	HIS	2.4
1	A	117	TYR	2.3
1	A	450	ALA	2.3
1	B	111	ALA	2.3
1	E	121	ALA	2.3
1	E	484	LEU	2.3
1	F	36	ASP	2.3
1	F	237	ASP	2.3
1	F	504	PHE	2.3
1	E	289	VAL	2.3
1	E	498	VAL	2.3
1	A	129	PRO	2.3
1	D	31	PRO	2.3
1	E	126	THR	2.3
1	E	309	LEU	2.3
1	H	36	ASP	2.3
1	A	411	ARG	2.3
1	C	412	ARG	2.3
1	H	34	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	63	ILE	2.3
1	B	249	VAL	2.3
1	D	489	PRO	2.3
1	A	101	ALA	2.3
1	B	268	ALA	2.3
1	A	515	LEU	2.3
1	B	248	GLY	2.3
1	C	270[A]	LEU	2.3
1	A	407	PHE	2.3
1	C	108	GLU	2.3
1	E	234	SER	2.3
1	E	403	HIS	2.3
1	G	38	PHE	2.3
1	A	83	ILE	2.3
1	A	318	VAL	2.3
1	A	384	VAL	2.3
1	E	411	ARG	2.3
1	E	101	ALA	2.3
1	E	268	ALA	2.3
1	F	416	LEU	2.3
1	A	402	TYR	2.3
1	C	109	SER	2.2
1	E	541[A]	SER	2.2
1	E	543	SER	2.2
1	F	543	SER	2.2
1	B	382	PHE	2.2
1	E	465	VAL	2.2
1	B	512	ARG	2.2
1	B	21	GLY	2.2
1	E	29	GLN	2.2
1	H	28	GLN	2.2
1	B	256	PHE	2.2
1	A	298	VAL	2.2
1	C	349	LYS	2.2
1	F	493	ILE	2.2
1	B	91	GLY	2.2
1	B	269	ALA	2.2
1	E	108	GLU	2.2
1	G	363	ALA	2.2
1	A	531[A]	SER	2.2
1	B	92	SER	2.2
1	B	239	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	494	TRP	2.2
1	A	88	PHE	2.2
1	A	251	ILE	2.2
1	A	283	ILE	2.2
1	B	129	PRO	2.2
1	A	245	VAL	2.2
1	F	274	GLY	2.2
1	B	97	ALA	2.2
1	E	79	ALA	2.2
1	C	116[A]	SER	2.2
1	C	117	TYR	2.2
1	E	486	TYR	2.2
1	A	494	TRP	2.2
1	B	108	GLU	2.1
1	B	266	VAL	2.1
1	B	276	GLY	2.1
1	E	513	GLY	2.1
1	F	532	GLY	2.1
1	G	112	GLY	2.1
1	D	459	ARG	2.1
1	E	71	GLU	2.1
1	B	119	PRO	2.1
1	E	527	TRP	2.1
1	E	433	PHE	2.1
1	F	243	PHE	2.1
1	E	418[A]	ARG	2.1
1	A	471	ALA	2.1
1	F	241	LEU	2.1
1	C	383	PRO	2.1
1	B	513	GLY	2.1
1	G	118	ARG	2.1
1	H	242[A]	ARG	2.1
1	A	257	VAL	2.1
1	H	517	VAL	2.1
1	F	495	ALA	2.1
1	F	86	LEU	2.1
1	C	71	GLU	2.1
1	D	408	GLU	2.1
1	F	273	GLU	2.1
1	H	26	GLN	2.1
1	B	114	PRO	2.1
1	D	487	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	72	ARG	2.1
1	A	426	ILE	2.1
1	C	100	ILE	2.1
1	E	521	VAL	2.1
1	B	265	ALA	2.1
1	E	331	LEU	2.0
1	G	39	LEU	2.0
1	H	30	LEU	2.0
1	F	418	ARG	2.0
1	B	64	GLY	2.0
1	E	447	GLY	2.0
1	G	311	ILE	2.0
1	A	103	VAL	2.0
1	B	103	VAL	2.0
1	B	238	VAL	2.0
1	E	252	VAL	2.0
1	F	52	VAL	2.0
1	F	34	MET	2.0
1	F	540[A]	LEU	2.0
1	B	96	HIS	2.0
1	H	403	HIS	2.0
1	B	533	TYR	2.0
1	F	486	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.

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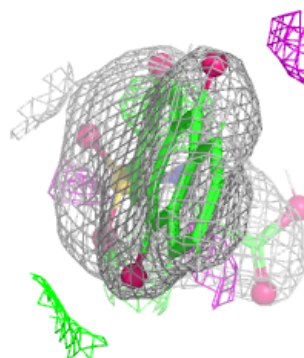
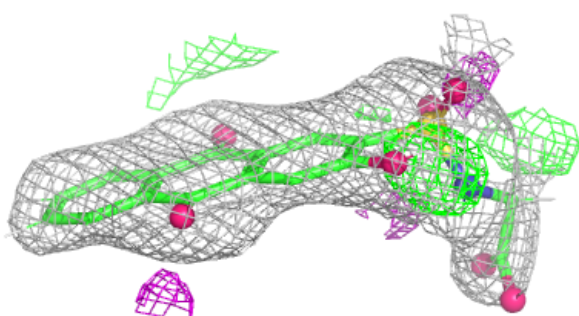
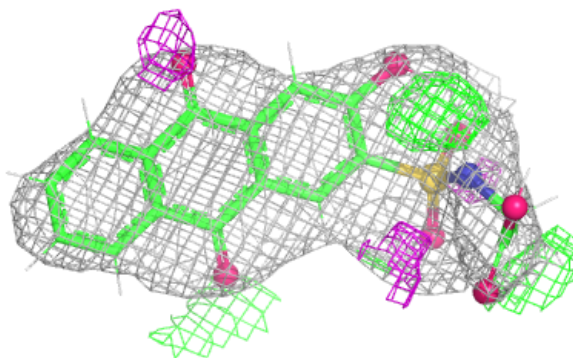
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	K	A	604	1/1	0.85	0.11	100,100,100,100	0
5	K	E	604	1/1	0.85	0.20	104,104,104,104	0
6	I91	G	603	25/25	0.87	0.16	78,80,84,84	11
6	I91	B	603	25/25	0.89	0.14	89,92,93,93	11
4	MG	B	604	1/1	0.90	0.09	58,58,58,58	0
4	MG	E	603	1/1	0.90	0.09	64,64,64,64	0
3	OXL	E	602	6/6	0.90	0.12	85,85,85,85	0
6	I91	C	603	25/25	0.91	0.13	81,82,86,86	11
2	FBP	E	601	20/20	0.92	0.10	63,65,68,68	0
5	K	C	605	1/1	0.92	0.10	72,72,72,72	0
6	I91	F	603	25/25	0.92	0.11	71,72,74,75	11
4	MG	A	603	1/1	0.92	0.08	80,80,80,80	0
3	OXL	A	602	6/6	0.93	0.08	71,71,72,72	0
5	K	B	605	1/1	0.93	0.10	95,95,95,95	0
3	OXL	B	602	6/6	0.93	0.07	52,53,54,55	0
2	FBP	A	601	20/20	0.93	0.10	64,69,71,72	0
4	MG	D	603	1/1	0.94	0.07	42,42,42,42	0
5	K	G	605	1/1	0.94	0.10	68,68,68,68	0
3	OXL	F	602	6/6	0.94	0.10	68,69,71,71	0
3	OXL	H	602	6/6	0.94	0.10	46,46,46,46	0
3	OXL	C	602	6/6	0.94	0.08	58,59,60,61	0
2	FBP	B	601	20/20	0.94	0.09	59,62,66,66	0
3	OXL	G	602	6/6	0.95	0.07	50,50,50,51	0
2	FBP	F	601	20/20	0.95	0.07	56,61,64,64	0
3	OXL	D	602	6/6	0.95	0.12	46,47,47,47	0
4	MG	F	604	1/1	0.96	0.06	53,53,53,53	0
5	K	F	605	1/1	0.97	0.05	77,77,77,77	0
5	K	H	604	1/1	0.97	0.12	59,59,59,59	0
2	FBP	H	601	20/20	0.98	0.05	28,30,32,33	0
5	K	D	604	1/1	0.98	0.11	57,57,57,57	0
2	FBP	D	601	20/20	0.98	0.04	31,33,35,35	0
4	MG	C	604	1/1	0.98	0.09	55,55,55,55	0
2	FBP	G	601	20/20	0.98	0.05	30,33,36,37	0
2	FBP	C	601	20/20	0.99	0.04	32,35,38,38	0
4	MG	G	604	1/1	0.99	0.04	37,37,37,37	0
4	MG	H	603	1/1	1.00	0.02	40,40,40,40	0

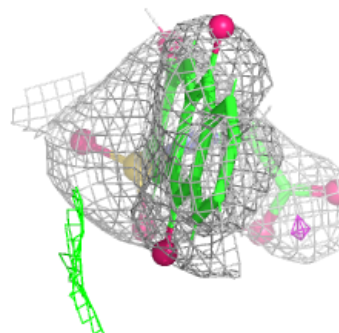
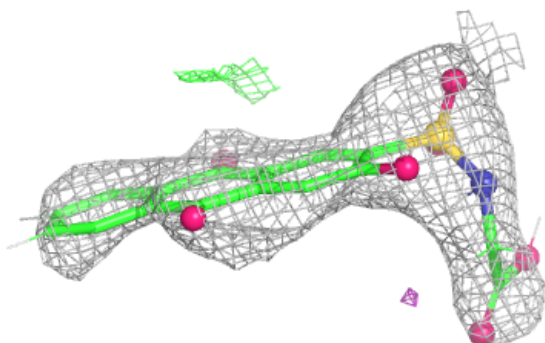
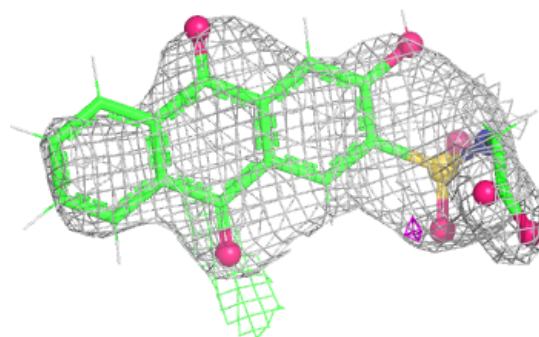
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around I91 G 603:

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

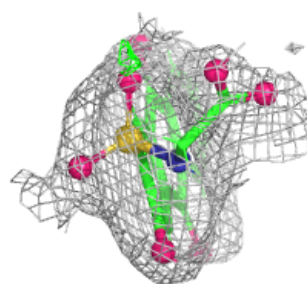
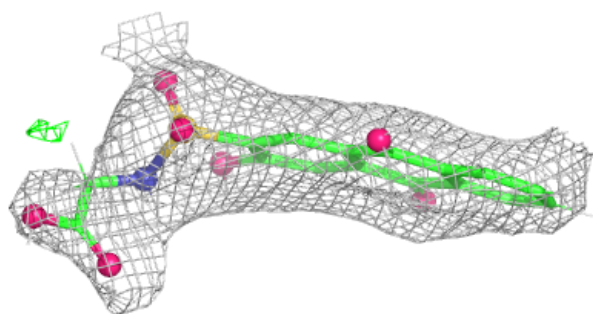
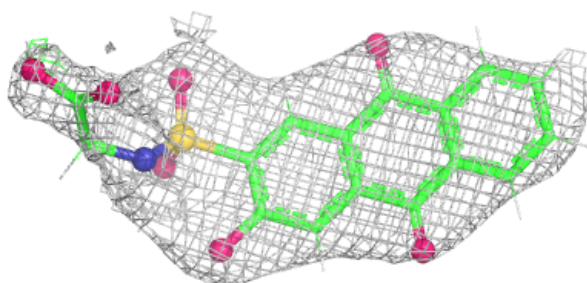
**Electron density around I91 B 603:**

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

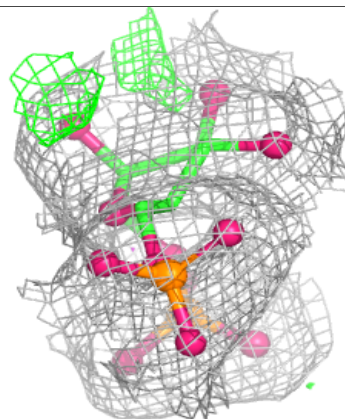
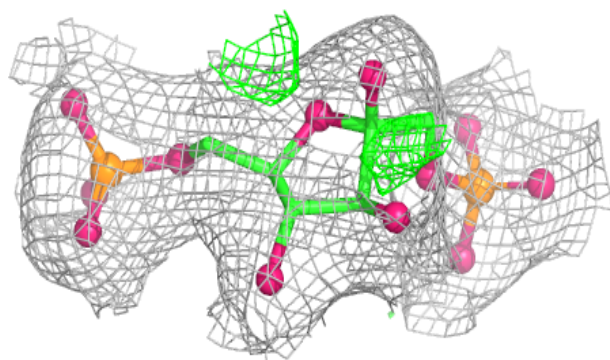
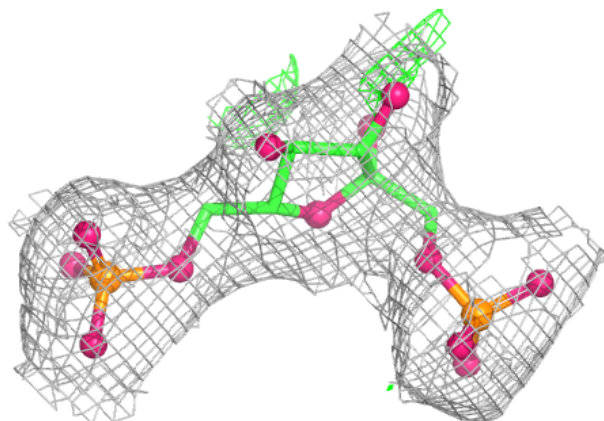


Electron density around I91 C 603:

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

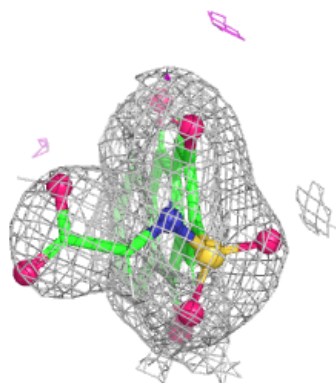
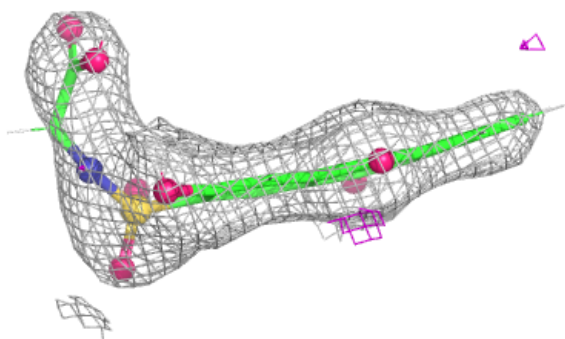
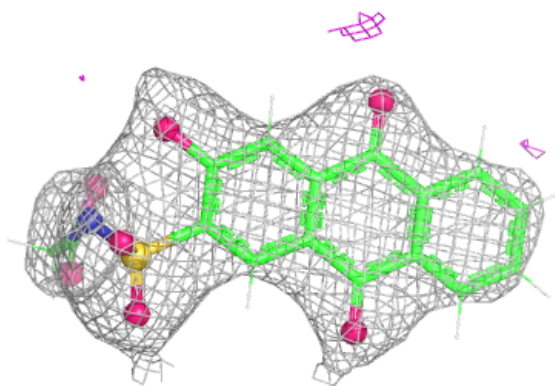
**Electron density around FBP E 601:**

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

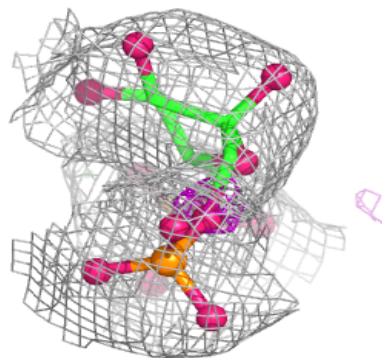
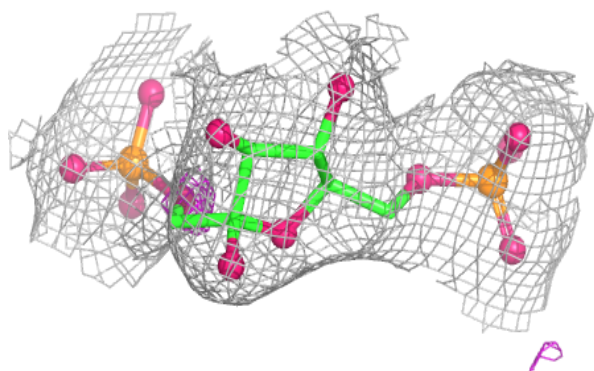
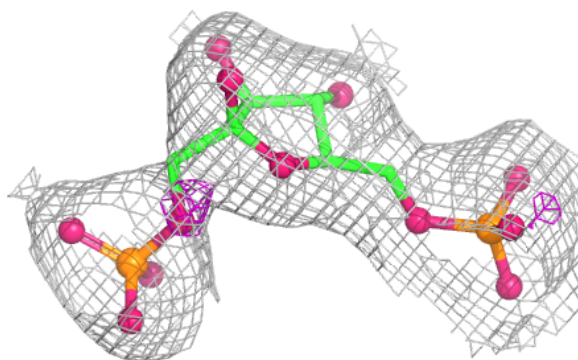


Electron density around I91 F 603:

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

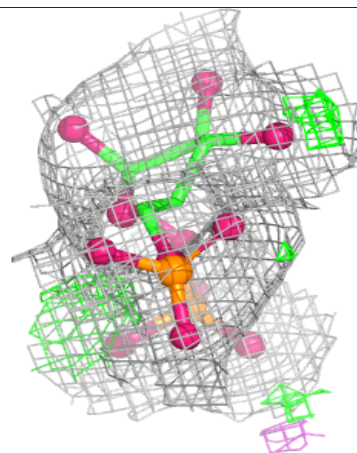
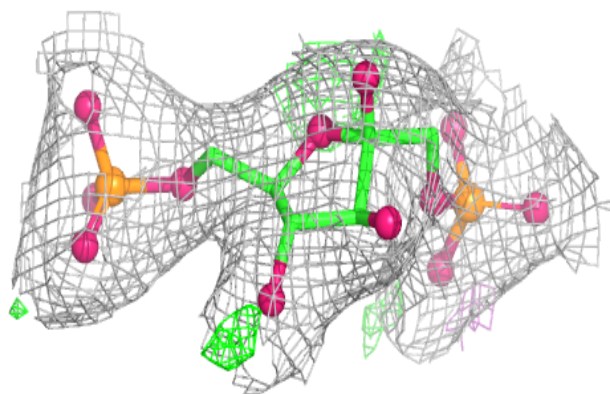
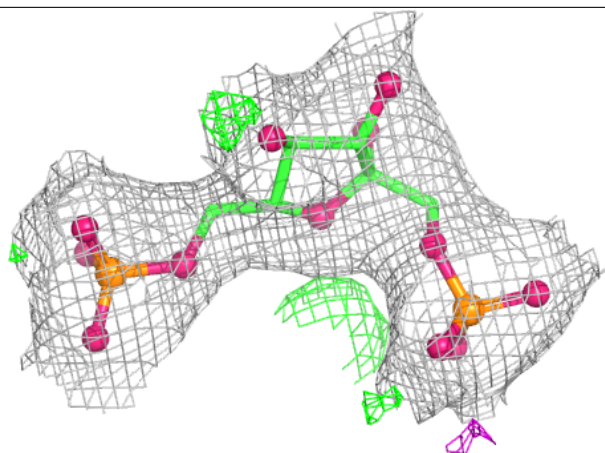
**Electron density around FBP A 601:**

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



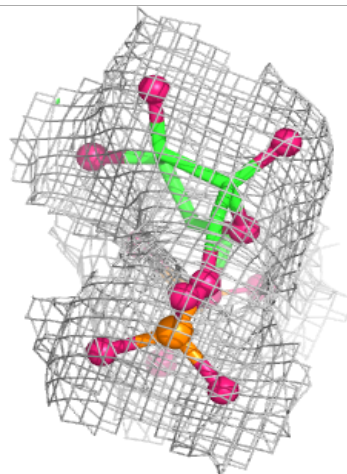
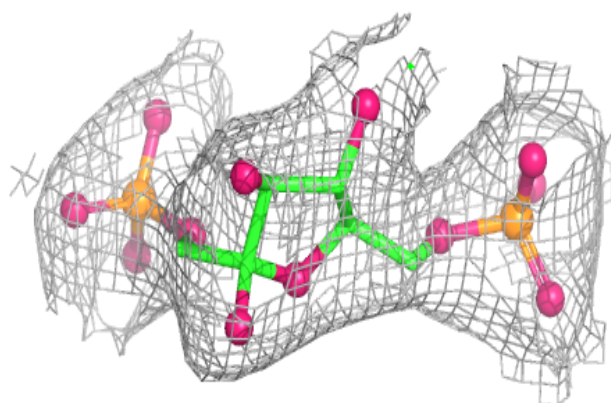
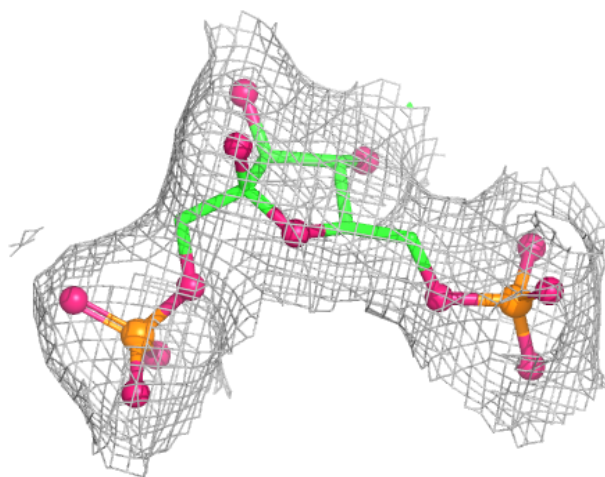
Electron density around FBP B 601:

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



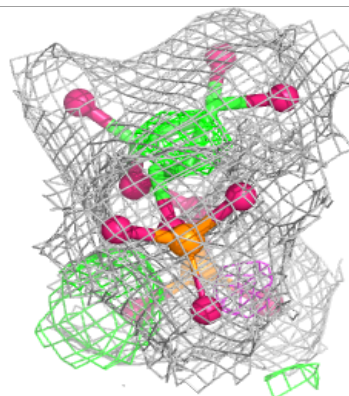
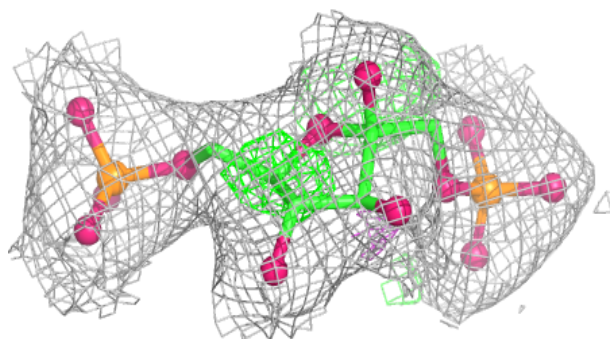
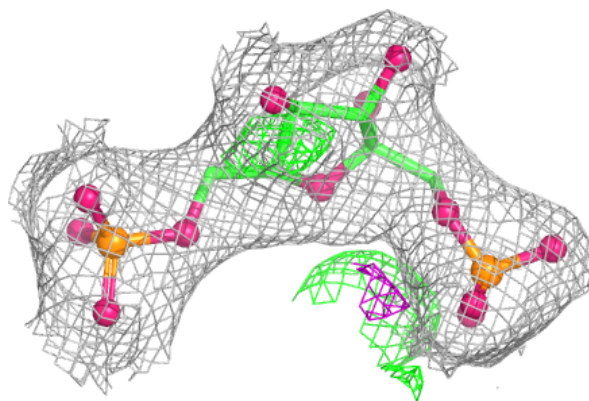
Electron density around FBP F 601:

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

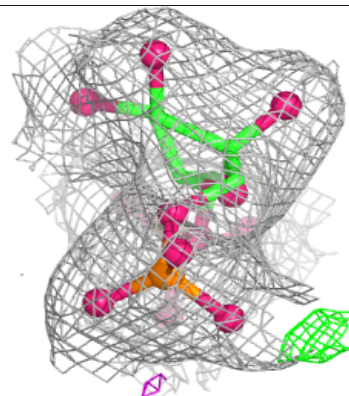
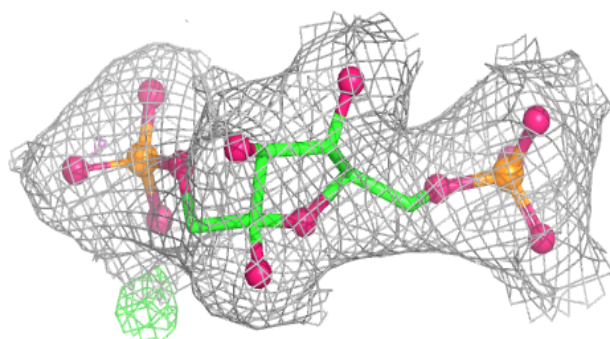
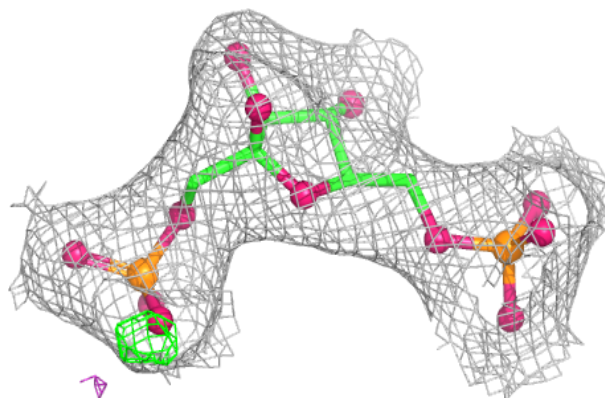


Electron density around FBP H 601:

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

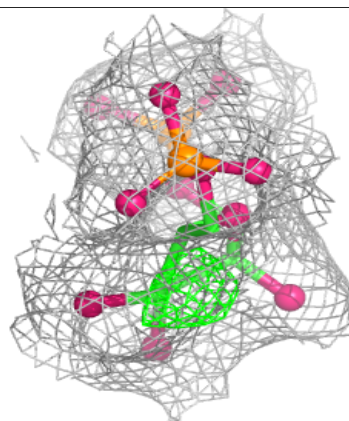
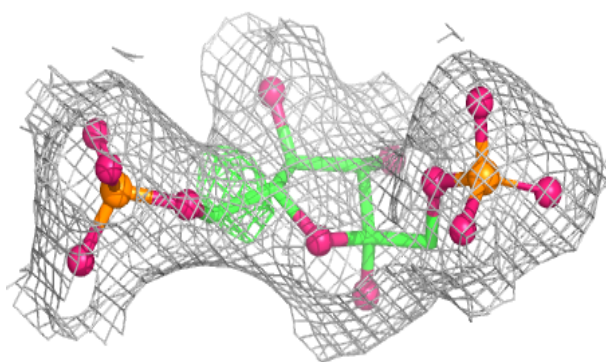
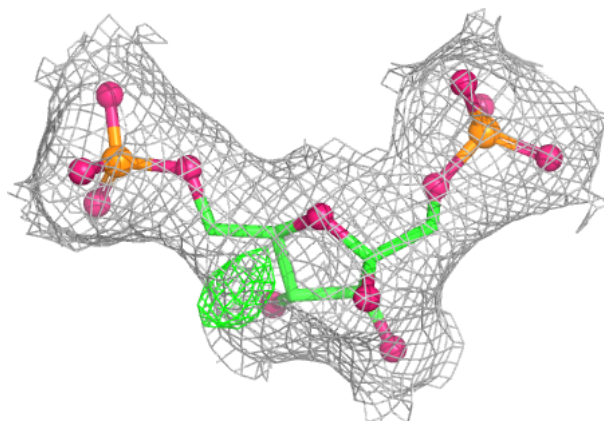
**Electron density around FBP D 601:**

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

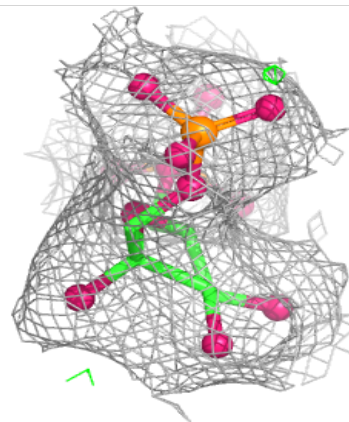
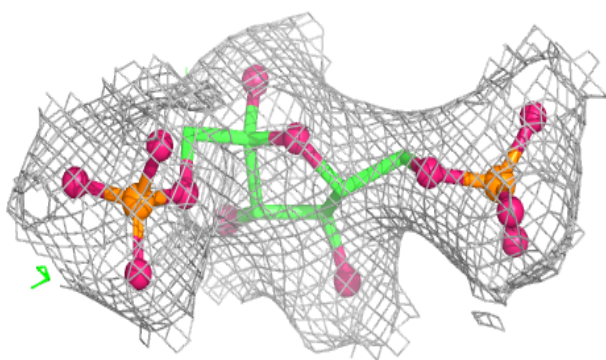
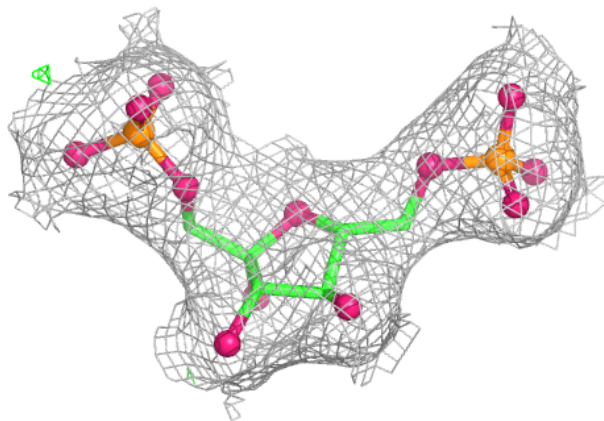


Electron density around FBP G 601:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.