



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:50 PM EDT

PDB ID : 5SCG / pdb_00005scg
Title : Structure of liver pyruvate kinase in complex with anthraquinone derivative 101
Authors : Lulla, A.; Foller, A.; Nain-Perez, A.; Grotli, M.; Brear, P.; Hyvonen, M.
Deposited on : 2021-12-01
Resolution : 1.94 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

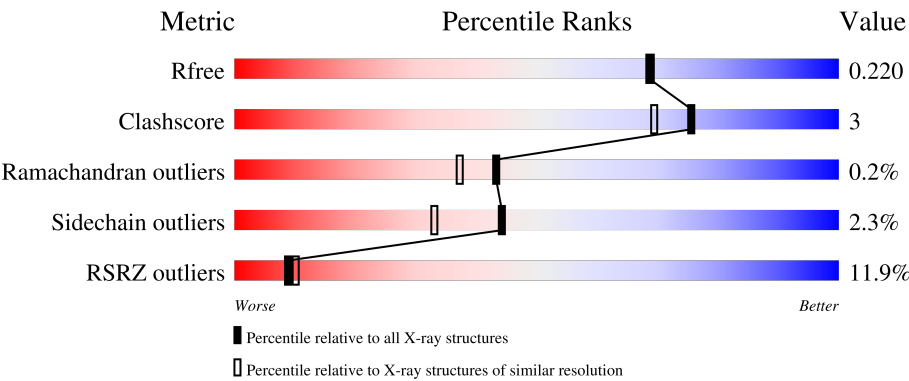
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	15% 84%9%6%
1	B	447	35% 88%9%
1	C	447	5% 86%9%5%
1	D	447	3% 87%7%5%
1	E	447	16% 86%7%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 29025 atoms, of which 102 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	436	Total	C	N	O	S	3	8	0
			3350	2104	604	622	20			
1	C	424	Total	C	N	O	S	0	7	0
			3260	2051	584	606	19			
1	D	425	Total	C	N	O	S	0	8	0
			3261	2048	590	604	19			
1	E	419	Total	C	N	O	S	0	13	0
			3257	2049	584	604	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	9	0
			3257	2048	586	604	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:

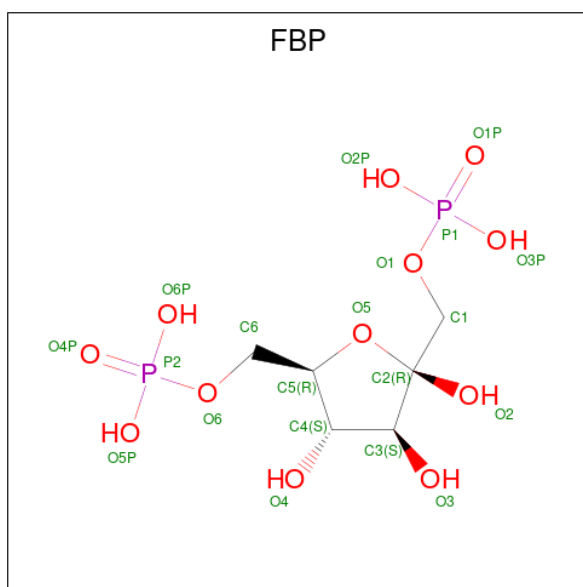
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q16716
A	0	SER	-	expression tag	UNP Q16716
A	12	ASP	SER	conflict	UNP Q16716
A	130	GLY	-	linker	UNP Q16716
A	131	SER	-	linker	UNP Q16716
A	230	GLY	-	linker	UNP Q16716
B	-1	GLY	-	expression tag	UNP Q16716
B	0	SER	-	expression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

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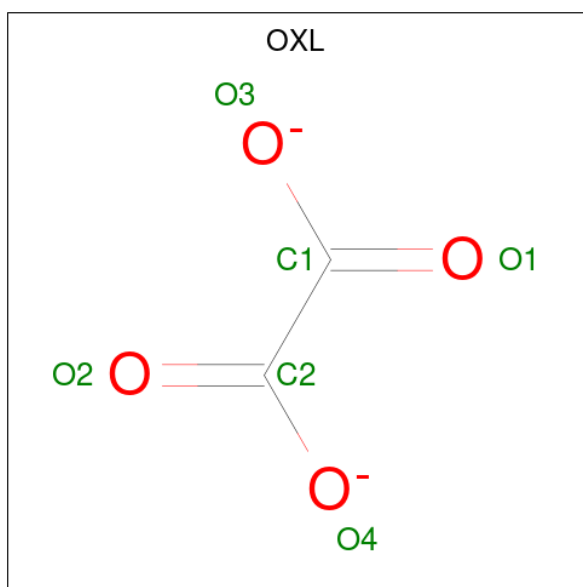
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP Q16716
C	12	ASP	SER	conflict	UNP Q16716
C	228	GLY	-	linker	UNP Q16716
C	229	SER	-	linker	UNP Q16716
C	230	GLY	-	linker	UNP Q16716
D	-1	GLY	-	expression tag	UNP Q16716
D	0	SER	-	expression tag	UNP Q16716
D	12	ASP	SER	conflict	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	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: $C_6H_{14}O_{12}P_2$).



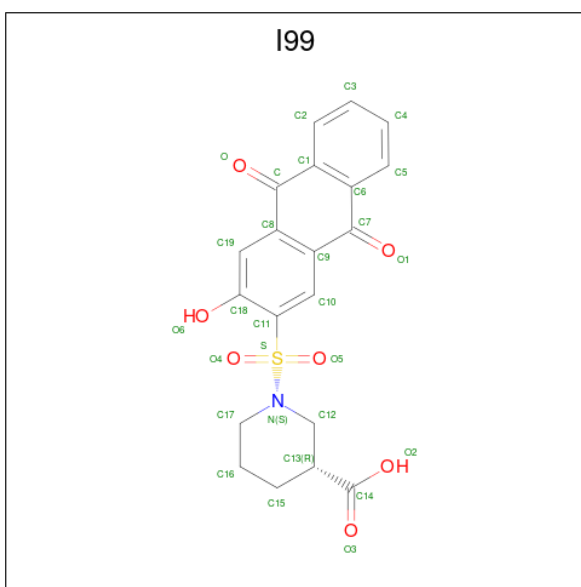
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		
2	E	1	Total	C	O	P	0	0
			20	6	12	2		
2	F	1	Total	C	O	P	0	0
			20	6	12	2		
2	G	1	Total	C	O	P	0	0
			20	6	12	2		
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 (3R)-1-(3-hydroxy-9,10-dioxo-9,10-dihydroanthracene-2-sulfonyl)piperidine-3-carboxylic acid (CCD ID: I99) (formula: C₂₀H₁₇NO₇S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 46	C 20	H 17	N 1	O 7	S 1	17	0
4	B	1	Total 46	C 20	H 17	N 1	O 7	S 1	17	0
4	C	1	Total 46	C 20	H 17	N 1	O 7	S 1	17	0
4	E	1	Total 46	C 20	H 17	N 1	O 7	S 1	17	0
4	F	1	Total 46	C 20	H 17	N 1	O 7	S 1	17	0
4	G	1	Total 46	C 20	H 17	N 1	O 7	S 1	17	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	206	Total 206	O 206	0	0
7	B	186	Total 186	O 186	0	0
7	C	319	Total 319	O 319	0	0
7	D	367	Total 367	O 367	0	0
7	E	208	Total 208	O 208	0	0
7	F	273	Total 273	O 273	0	0
7	G	347	Total 347	O 347	0	0

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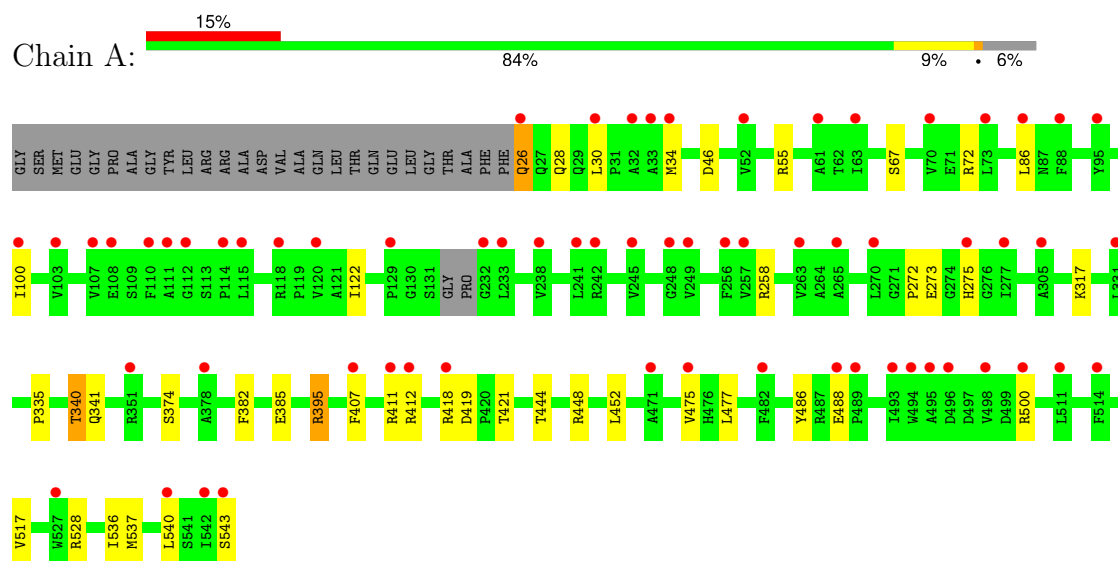
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	392	Total 392	O 392	0	0

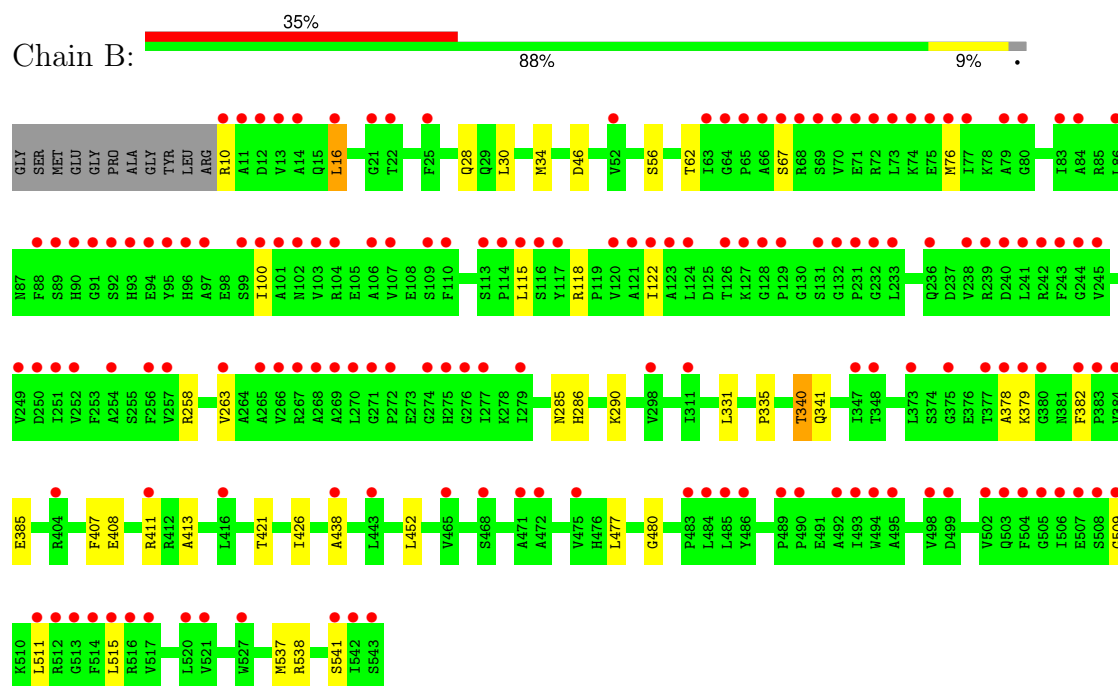
3 Residue-property plots [i](#)

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

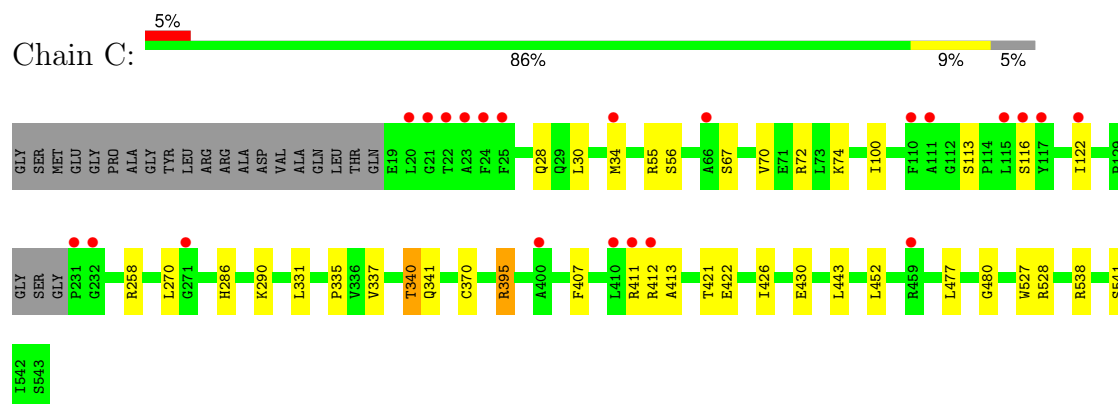
• Molecule 1: Pyruvate kinase



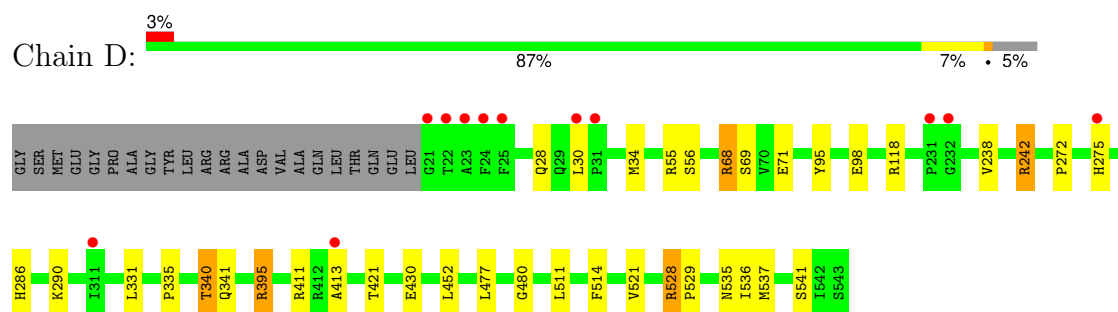
• Molecule 1: Pyruvate kinase



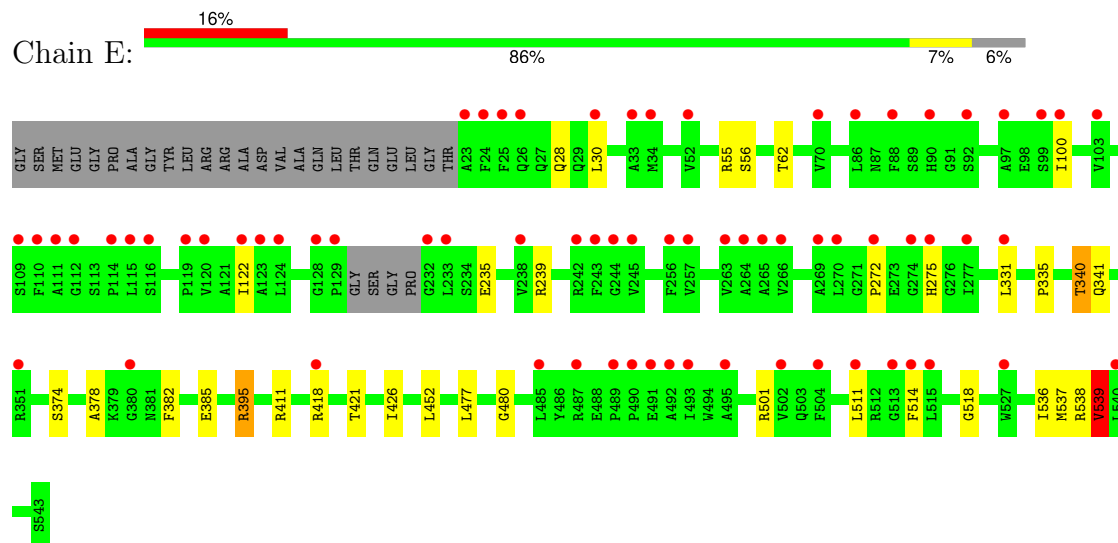
- Molecule 1: Pyruvate kinase



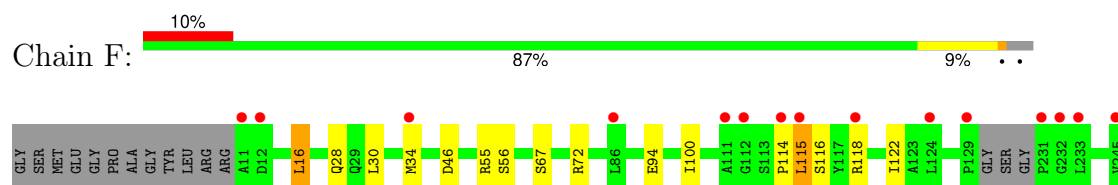
- Molecule 1: Pyruvate kinase

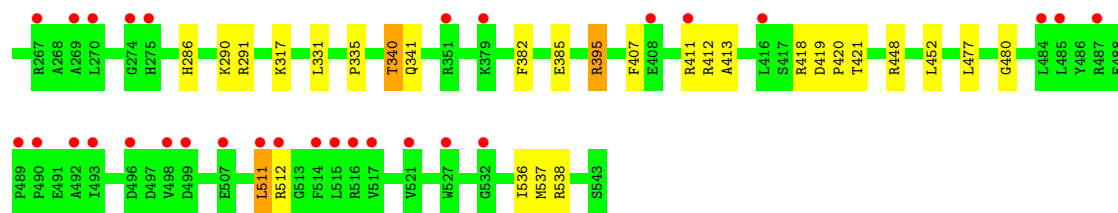


- Molecule 1: Pyruvate kinase

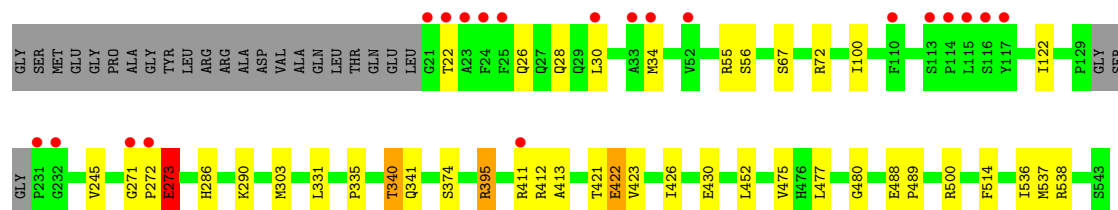
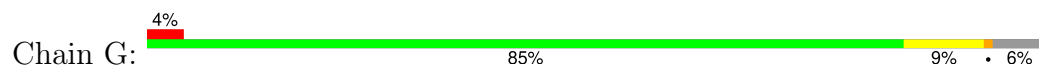


- Molecule 1: Pyruvate kinase

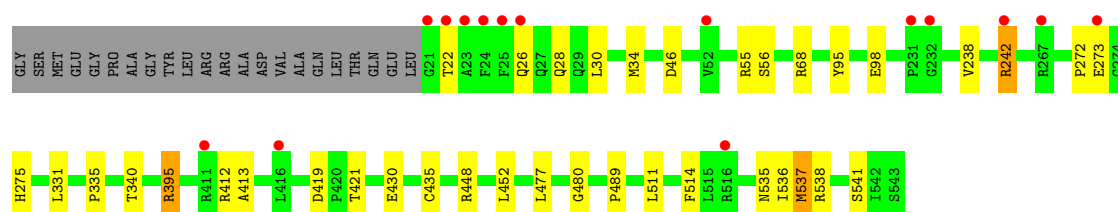
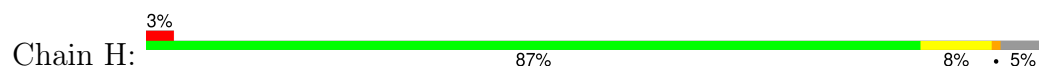




● Molecule 1: Pyruvate kinase



● Molecule 1: Pyruvate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	207.97Å 113.10Å 188.63Å 90.00° 91.73° 90.00°	Depositor
Resolution (Å)	188.54 – 1.94 188.54 – 1.94	Depositor EDS
% Data completeness (in resolution range)	77.3 (188.54-1.94) 77.3 (188.54-1.94)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.94Å)	Xtriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, R_{free}	0.200 , 0.229 0.192 , 0.220	Depositor DCC
R_{free} test set	12493 reflections (3.86%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	29025	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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 39.99 % 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 2.9250e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: I99, MG, FBP, OXL, 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	0.69	1/3328 (0.0%)	1.00	3/4497 (0.1%)
1	B	0.72	0/3429	1.00	1/4636 (0.0%)
1	C	0.77	0/3335	1.01	0/4508
1	D	0.80	0/3341	1.03	1/4517 (0.0%)
1	E	0.67	1/3350 (0.0%)	0.99	2/4527 (0.0%)
1	F	0.71	0/3405	1.00	1/4603 (0.0%)
1	G	0.79	2/3335 (0.1%)	1.00	2/4507 (0.0%)
1	H	0.79	1/3357 (0.0%)	1.00	2/4537 (0.0%)
All	All	0.74	5/26880 (0.0%)	1.00	12/36332 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	489	PRO	CA-C	5.51	1.55	1.52
1	G	303	MET	SD-CE	-5.50	1.65	1.79
1	A	374	SER	CA-C	5.46	1.55	1.52
1	G	489	PRO	CA-C	5.15	1.54	1.51
1	E	374	SER	CA-C	5.01	1.54	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	273	GLU	CB-CG-CD	7.06	124.60	112.60
1	E	539	VAL	N-CA-CB	5.77	117.96	111.21
1	G	514	PHE	CA-CB-CG	5.71	119.51	113.80
1	H	46	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	26	GLN	CA-C-N	5.50	130.74	120.95
1	A	26	GLN	C-N-CA	5.50	130.74	120.95
1	A	46	ASP	CA-CB-CG	5.36	117.96	112.60
1	D	514	PHE	CA-CB-CG	5.20	119.00	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	46	ASP	CA-CB-CG	5.16	117.76	112.60
1	H	514	PHE	CA-CB-CG	5.05	118.85	113.80
1	E	514	PHE	CA-CB-CG	5.04	118.83	113.80
1	B	46	ASP	CA-CB-CG	5.02	117.62	112.60

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	19	0
1	B	3350	0	3417	23	0
1	C	3260	0	3320	24	0
1	D	3261	0	3321	22	0
1	E	3257	0	3323	19	0
1	F	3327	0	3399	24	0
1	G	3257	0	3320	27	0
1	H	3277	0	3341	22	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
3	G	6	0	0	0	0
3	H	6	0	0	0	0
4	A	29	17	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	29	17	0	0	0
4	C	29	17	0	0	0
4	E	29	17	0	0	0
4	F	29	17	0	0	0
4	G	29	17	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	A	206	0	0	1	0
7	B	186	0	0	0	0
7	C	319	0	0	1	0
7	D	367	0	0	0	0
7	E	208	0	0	0	0
7	F	273	0	0	1	0
7	G	347	0	0	3	0
7	H	392	0	0	0	0
All	All	28923	102	26833	162	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 (162) 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	1.68	0.76
1:C:411:ARG:HG2	1:C:426:ILE:HD11	1.66	0.76
1:H:68:ARG:NH2	1:H:95:TYR:O	2.19	0.75
1:E:418[B]:ARG:HG3	1:F:16:LEU:HD11	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.71	0.72
1:G:538:ARG:HG2	1:H:536:ILE:HG12	1.70	0.71
1:A:418[B]:ARG:HG3	1:B:16:LEU:HD11	1.72	0.71
1:E:235:GLU:O	1:E:239:ARG:HD3	1.93	0.69
1:G:488:GLU:OE1	7:G:701:HOH:O	2.11	0.69
1:D:528:ARG:HD2	1:D:529:PRO:O	1.95	0.66
1:G:536:ILE:HG12	1:H:538[A]:ARG:HG2	1.77	0.66
1:A:272:PRO:HA	1:A:275:HIS:CE1	2.33	0.64
1:E:538:ARG:HG2	1:F:536:ILE:HG12	1.81	0.63
1:H:68:ARG:HH22	1:H:98:GLU:HB2	1.64	0.63
1:B:407:PHE:CE2	1:B:411:ARG:NH1	2.66	0.63
1:E:411:ARG:HG3	1:E:426:ILE:HD11	1.81	0.62
1:D:68:ARG:HH22	1:D:98:GLU:HB2	1.65	0.62
1:G:56:SER:HB2	1:G:480:GLY:HA2	1.84	0.60
1:F:115:LEU:HD22	1:F:511:LEU:HB3	1.84	0.59
1:A:407:PHE:CE2	1:A:411:ARG:NH1	2.69	0.59
1:D:272:PRO:HA	1:D:275[A]:HIS:CE1	2.38	0.58
1:C:538:ARG:HG2	1:D:536:ILE:HG12	1.83	0.58
1:E:272:PRO:HA	1:E:275[A]:HIS:CE1	2.39	0.58
1:G:411:ARG:HG3	1:G:426:ILE:HD11	1.83	0.58
1:H:272:PRO:HA	1:H:275[A]:HIS:CE1	2.39	0.58
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.85	0.57
1:F:407:PHE:CE2	1:F:411:ARG:NH1	2.72	0.57
1:E:536:ILE:HG12	1:F:538:ARG:HG2	1.86	0.56
1:H:56:SER:HB2	1:H:480:GLY:HA2	1.87	0.56
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.88	0.56
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.88	0.56
1:D:68:ARG:NH2	1:D:95:TYR:O	2.39	0.56
1:A:317:LYS:NZ	7:A:705:HOH:O	2.40	0.55
1:B:407:PHE:CD2	1:B:411:ARG:NH1	2.76	0.54
1:F:56:SER:HB2	1:F:480:GLY:HA2	1.89	0.54
1:G:245:VAL:CG1	1:G:273:GLU:HG2	2.38	0.54
1:D:71[B]:GLU:H	1:D:71[B]:GLU:CD	2.16	0.53
1:E:56:SER:HB2	1:E:480:GLY:HA2	1.90	0.53
1:G:430[A]:GLU:OE1	1:H:430[A]:GLU:OE1	2.27	0.52
1:B:438:ALA:HB3	1:B:515:LEU:HD23	1.91	0.52
1:H:535:ASN:OD1	1:H:536:ILE:HG13	2.10	0.52
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.93	0.51
1:G:430[B]:GLU:OE2	1:H:430[B]:GLU:OE1	2.29	0.51
1:G:500[A]:ARG:NH2	7:G:701:HOH:O	2.40	0.51
1:B:411:ARG:HG2	1:B:426:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:GLY:HA3	1:B:515:LEU:HD12	1.92	0.51
1:E:539:VAL:HG22	1:F:420:PRO:HB3	1.93	0.50
1:C:411:ARG:HH12	1:D:411:ARG:HH21	1.59	0.50
1:G:537:MET:HE3	1:H:537:MET:HG2	1.94	0.50
1:B:62:THR:HG22	1:B:378:ALA:HB2	1.94	0.49
1:F:114:PRO:O	1:F:512:ARG:NH2	2.40	0.49
1:F:116:SER:O	1:F:118:ARG:HD2	2.11	0.49
1:A:100:ILE:HG23	1:A:122:ILE:HD13	1.94	0.49
1:F:100:ILE:HG23	1:F:122:ILE:HD13	1.94	0.49
1:B:258:ARG:HD3	1:B:285:ASN:HD21	1.77	0.49
1:C:430[B]:GLU:OE2	1:D:430[B]:GLU:OE1	2.30	0.49
1:C:100:ILE:HG23	1:C:122:ILE:HD13	1.93	0.49
1:G:100:ILE:HG23	1:G:122:ILE:HD13	1.94	0.49
1:E:100:ILE:HG23	1:E:122:ILE:HD13	1.95	0.49
1:B:30:LEU:O	1:B:34:MET:HG2	2.13	0.48
1:B:408:GLU:HG3	1:B:411:ARG:NH2	2.28	0.48
1:F:30:LEU:O	1:F:34:MET:HG2	2.13	0.48
1:B:115:LEU:HD11	1:B:511:LEU:HB2	1.95	0.48
1:B:331:LEU:HD11	1:B:413:ALA:HB1	1.96	0.48
1:E:501:ARG:NH1	2:E:601:FBP:O1P	2.40	0.48
1:C:30:LEU:O	1:C:34:MET:HG2	2.14	0.48
1:G:30:LEU:O	1:G:34:MET:HG2	2.14	0.47
1:A:30:LEU:O	1:A:34:MET:HG2	2.14	0.47
1:C:67:SER:HA	1:C:72:ARG:HG2	1.96	0.47
1:B:340:THR:HG22	1:B:341:GLN:HG3	1.97	0.47
1:F:28:GLN:HG3	1:F:30:LEU:HG	1.96	0.47
1:H:28:GLN:HG3	1:H:30:LEU:HG	1.96	0.47
1:E:335:PRO:HB3	1:E:477:LEU:O	2.14	0.47
1:A:486:TYR:CZ	1:A:488[B]:GLU:HB2	2.50	0.47
1:B:100:ILE:HG23	1:B:122:ILE:HD13	1.96	0.47
1:G:56:SER:HB2	1:G:480:GLY:CA	2.44	0.47
1:H:30:LEU:O	1:H:34:MET:HG2	2.15	0.47
1:H:68:ARG:NH2	1:H:98:GLU:HB2	2.27	0.47
1:C:55:ARG:HB2	1:C:395:ARG:HG3	1.97	0.47
1:A:340:THR:HG22	1:A:341:GLN:HG3	1.97	0.46
1:F:67:SER:HA	1:F:72:ARG:HG2	1.98	0.46
1:H:56:SER:HB2	1:H:480:GLY:CA	2.45	0.46
1:E:28:GLN:HG3	1:E:30:LEU:HG	1.98	0.46
1:G:67:SER:HA	1:G:72:ARG:HG2	1.97	0.46
1:G:340:THR:HG22	1:G:341:GLN:HG3	1.98	0.46
1:H:335:PRO:HB3	1:H:477:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:THR:HG22	1:C:452:LEU:HD12	1.97	0.46
1:F:56:SER:HB2	1:F:480:GLY:CA	2.45	0.46
1:C:28:GLN:HG3	1:C:30:LEU:HG	1.98	0.46
1:D:28:GLN:HG3	1:D:30:LEU:HG	1.97	0.46
1:A:67:SER:HA	1:A:72:ARG:HG2	1.96	0.46
1:B:335:PRO:HB3	1:B:477:LEU:O	2.16	0.46
1:B:28:GLN:HG3	1:B:30:LEU:HG	1.97	0.46
1:A:28:GLN:HG3	1:A:30:LEU:HG	1.98	0.45
1:A:335:PRO:HB3	1:A:477:LEU:O	2.16	0.45
1:A:517:VAL:HG13	1:A:543:SER:HB3	1.98	0.45
1:G:272:PRO:HD2	1:G:273:GLU:OE1	2.16	0.45
1:D:335:PRO:HB3	1:D:477:LEU:O	2.16	0.45
1:B:56:SER:HB2	1:B:480:GLY:CA	2.46	0.45
1:F:335:PRO:HB3	1:F:477:LEU:O	2.17	0.45
1:D:56:SER:HB2	1:D:480:GLY:CA	2.46	0.45
1:G:374[B]:SER:OG	4:G:603:I99:O4	2.32	0.45
1:H:331:LEU:HD11	1:H:413:ALA:HB1	1.97	0.45
1:F:331:LEU:HD11	1:F:413:ALA:HB1	1.99	0.44
1:G:28:GLN:HG3	1:G:30:LEU:HG	1.98	0.44
1:A:55:ARG:HB2	1:A:395:ARG:HG3	1.98	0.44
1:C:331:LEU:HD11	1:C:413:ALA:HB1	1.98	0.44
1:G:55:ARG:HB2	1:G:395:ARG:HG3	2.00	0.44
1:H:55:ARG:HB2	1:H:395:ARG:HG3	1.99	0.44
1:E:340:THR:HG22	1:E:341:GLN:HG3	2.00	0.44
1:C:286:HIS:CE1	1:C:290:LYS:HG3	2.53	0.44
1:E:55:ARG:HB2	1:E:395:ARG:HG3	1.99	0.44
1:G:421:THR:HG22	1:G:452:LEU:HD12	1.99	0.44
1:H:419:ASP:OD2	1:H:448:ARG:NH2	2.48	0.44
1:A:517:VAL:HG22	1:A:543:SER:CB	2.48	0.44
1:F:421:THR:HG22	1:F:452:LEU:HD12	2.00	0.44
1:H:22:THR:O	1:H:26:GLN:HG2	2.18	0.44
1:C:340:THR:HG22	1:C:341:GLN:HG3	2.00	0.43
1:D:340:THR:HG22	1:D:341:GLN:HG3	2.00	0.43
1:G:331:LEU:HD11	1:G:413:ALA:HB1	2.00	0.43
1:G:335:PRO:HB3	1:G:477:LEU:O	2.19	0.43
1:F:317:LYS:NZ	7:F:709:HOH:O	2.49	0.43
1:D:55:ARG:HB2	1:D:395:ARG:HG3	2.00	0.43
1:C:335:PRO:HB3	1:C:477:LEU:O	2.18	0.43
1:C:538:ARG:HD3	7:C:810:HOH:O	2.18	0.43
1:B:382:PHE:HB3	1:B:385:GLU:HB2	2.01	0.42
1:E:62:THR:HG22	1:E:378:ALA:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:PHE:HB3	1:A:385:GLU:HB2	2.01	0.42
1:G:271:GLY:HA2	7:G:773:HOH:O	2.19	0.42
1:D:331:LEU:HD11	1:D:413:ALA:HB1	2.01	0.42
1:G:22:THR:O	1:G:26:GLN:HG2	2.19	0.42
1:B:421:THR:HG22	1:B:452:LEU:HD12	2.01	0.42
1:C:430[A]:GLU:OE1	1:D:430[A]:GLU:OE1	2.38	0.42
1:G:286:HIS:CE1	1:G:290:LYS:HG3	2.55	0.42
1:C:56:SER:HB2	1:C:480:GLY:CA	2.50	0.42
1:C:407:PHE:CZ	1:C:411:ARG:HD2	2.55	0.42
1:E:518:GLY:O	1:F:418:ARG:NH2	2.53	0.42
1:F:419:ASP:OD2	1:F:448:ARG:NH2	2.52	0.42
1:A:419:ASP:OD2	1:A:448:ARG:NH2	2.50	0.42
1:A:421:THR:HG22	1:A:452:LEU:HD12	2.02	0.42
1:F:382:PHE:HB3	1:F:385:GLU:HB2	2.01	0.41
1:H:421:THR:HG22	1:H:452:LEU:HD12	2.02	0.41
1:F:286:HIS:CE1	1:F:290:LYS:HG3	2.55	0.41
1:C:527:TRP:CE2	1:C:528:ARG:HG2	2.56	0.41
1:C:70:VAL:HG12	1:C:74:LYS:HE3	2.03	0.41
1:E:56:SER:HB2	1:E:480:GLY:CA	2.49	0.41
1:D:68:ARG:NH2	1:D:98:GLU:HB2	2.33	0.41
1:A:444:THR:OG1	2:A:601:FBP:O6P	2.38	0.41
1:D:421:THR:HG22	1:D:452:LEU:HD12	2.03	0.41
1:F:55:ARG:HB2	1:F:395:ARG:HG3	2.02	0.41
1:F:340:THR:HG22	1:F:341:GLN:HG3	2.02	0.41
1:H:238:VAL:O	1:H:242[B]:ARG:HG3	2.20	0.41
1:E:421:THR:HG22	1:E:452:LEU:HD12	2.02	0.40
1:B:67:SER:HB2	1:B:76[B]:MET:SD	2.61	0.40
1:C:337:VAL:HG22	1:C:370:CYS:HB2	2.03	0.40
1:C:411:ARG:NH1	1:D:411:ARG:NH2	2.70	0.40
1:D:238:VAL:O	1:D:242[B]:ARG:HG3	2.21	0.40
1:E:382:PHE:HB3	1:E:385:GLU:HB2	2.03	0.40
1:G:423:VAL:HG21	1:H:435:CYS:HB3	2.02	0.40
1:B:286:HIS:CE1	1:B:290:LYS:HG3	2.57	0.40
1:D:286:HIS:CE1	1:D:290:LYS:HG3	2.57	0.40
1:D:535:ASN:OD1	1:D:536:ILE:HG13	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%)	422 (99%)	4 (1%)	1 (0%)	43	37
1	B	442/447 (99%)	434 (98%)	7 (2%)	1 (0%)	43	37
1	C	427/447 (96%)	420 (98%)	6 (1%)	1 (0%)	43	37
1	D	431/447 (96%)	427 (99%)	3 (1%)	1 (0%)	43	37
1	E	428/447 (96%)	424 (99%)	3 (1%)	1 (0%)	43	37
1	F	436/447 (98%)	432 (99%)	3 (1%)	1 (0%)	43	37
1	G	427/447 (96%)	419 (98%)	7 (2%)	1 (0%)	43	37
1	H	432/447 (97%)	426 (99%)	5 (1%)	1 (0%)	43	37
All	All	3450/3576 (96%)	3404 (99%)	38 (1%)	8 (0%)	43	37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	THR
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

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	18
1	B	353/352 (100%)	345 (98%)	8 (2%)	44	33
1	C	344/352 (98%)	334 (97%)	10 (3%)	37	24
1	D	344/352 (98%)	332 (96%)	12 (4%)	32	18
1	E	346/352 (98%)	340 (98%)	6 (2%)	53	44
1	F	351/352 (100%)	342 (97%)	9 (3%)	40	28
1	G	344/352 (98%)	338 (98%)	6 (2%)	53	44
1	H	345/352 (98%)	337 (98%)	8 (2%)	44	33
All	All	2772/2816 (98%)	2701 (97%)	71 (3%)	44	28

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	86	LEU
1	A	258	ARG
1	A	273	GLU
1	A	395	ARG
1	A	412	ARG
1	A	475	VAL
1	A	500	ARG
1	A	528	ARG
1	A	537[A]	MET
1	A	537[B]	MET
1	A	540	LEU
1	B	10	ARG
1	B	16	LEU
1	B	118	ARG
1	B	263	VAL
1	B	379	LYS
1	B	537[A]	MET
1	B	537[B]	MET
1	B	541	SER
1	C	113	SER
1	C	116[A]	SER
1	C	116[B]	SER
1	C	258	ARG
1	C	270[A]	LEU
1	C	270[B]	LEU
1	C	395	ARG

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Mol	Chain	Res	Type
1	C	412	ARG
1	C	443	LEU
1	C	541	SER
1	D	34	MET
1	D	68	ARG
1	D	69	SER
1	D	118	ARG
1	D	242[A]	ARG
1	D	242[B]	ARG
1	D	395	ARG
1	D	511	LEU
1	D	521	VAL
1	D	528	ARG
1	D	537	MET
1	D	541	SER
1	E	331	LEU
1	E	395	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	94	GLU
1	F	115	LEU
1	F	291	ARG
1	F	395	ARG
1	F	412	ARG
1	F	511	LEU
1	F	537[A]	MET
1	F	537[B]	MET
1	G	273	GLU
1	G	395	ARG
1	G	412	ARG
1	G	422[A]	GLU
1	G	422[B]	GLU
1	G	475	VAL
1	H	242[A]	ARG
1	H	242[B]	ARG
1	H	273	GLU
1	H	395	ARG
1	H	412	ARG
1	H	511	LEU

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Mol	Chain	Res	Type
1	H	537	MET
1	H	541	SER

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	405	GLN
1	B	27	GLN
1	B	405	GLN
1	C	275	HIS
1	C	405	GLN
1	D	27	GLN
1	D	405	GLN
1	D	535	ASN
1	E	27	GLN
1	E	405	GLN
1	F	405	GLN
1	G	405	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 38 ligands modelled in this entry, 16 are monoatomic - leaving 22 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
4	I99	B	603	-	32,32,32	0.18	0	48,49,49	0.39	0
3	OXL	B	602	5	5,5,5	2.32	2 (40%)	6,6,6	1.34	1 (16%)
2	FBP	F	601	-	18,20,20	0.48	0	21,32,32	0.70	0
3	OXL	E	602	5	5,5,5	2.36	2 (40%)	6,6,6	1.43	2 (33%)
2	FBP	D	601	-	18,20,20	0.59	0	21,32,32	1.03	1 (4%)
3	OXL	D	602	5	5,5,5	2.09	2 (40%)	6,6,6	2.10	2 (33%)
3	OXL	C	602	5	5,5,5	1.81	2 (40%)	6,6,6	1.43	1 (16%)
2	FBP	B	601	-	18,20,20	0.74	0	21,32,32	0.93	2 (9%)
2	FBP	H	601	-	18,20,20	0.94	0	21,32,32	0.87	1 (4%)
3	OXL	H	602	5	5,5,5	1.79	2 (40%)	6,6,6	1.87	2 (33%)
4	I99	E	603	-	32,32,32	0.19	0	48,49,49	0.40	0
3	OXL	G	602	5	5,5,5	2.12	3 (60%)	6,6,6	2.68	3 (50%)
2	FBP	E	601	-	18,20,20	0.50	0	21,32,32	0.73	1 (4%)
2	FBP	C	601	-	18,20,20	0.68	0	21,32,32	0.79	0
2	FBP	G	601	-	18,20,20	0.67	1 (5%)	21,32,32	0.78	0
2	FBP	A	601	-	18,20,20	0.41	0	21,32,32	0.83	0
4	I99	C	603	-	32,32,32	0.29	0	48,49,49	0.50	0
4	I99	G	603	-	32,32,32	0.23	0	48,49,49	0.81	2 (4%)
4	I99	F	603	-	32,32,32	0.22	0	48,49,49	0.46	0
4	I99	A	603	-	32,32,32	0.19	0	48,49,49	0.40	0
3	OXL	A	602	5	5,5,5	1.93	2 (40%)	6,6,6	2.21	3 (50%)
3	OXL	F	602	5	5,5,5	2.88	4 (80%)	6,6,6	2.42	3 (50%)

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
4	I99	B	603	-	-	2/16/42/42	0/4/4/4
3	OXL	B	602	5	-	4/4/4/4	-
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
3	OXL	E	602	5	-	4/4/4/4	-
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OXL	D	602	5	-	4/4/4/4	-
3	OXL	C	602	5	-	4/4/4/4	-
2	FBP	B	601	-	-	3/13/32/32	0/1/1/1
2	FBP	H	601	-	-	3/13/32/32	0/1/1/1
3	OXL	H	602	5	-	4/4/4/4	-
4	I99	E	603	-	-	2/16/42/42	0/4/4/4
3	OXL	G	602	5	-	4/4/4/4	-
2	FBP	E	601	-	-	2/13/32/32	0/1/1/1
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
2	FBP	G	601	-	-	2/13/32/32	0/1/1/1
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
4	I99	C	603	-	-	10/16/42/42	1/4/4/4
4	I99	G	603	-	-	7/16/42/42	1/4/4/4
4	I99	F	603	-	-	3/16/42/42	0/4/4/4
4	I99	A	603	-	-	2/16/42/42	0/4/4/4
3	OXL	A	602	5	-	4/4/4/4	-
3	OXL	F	602	5	-	4/4/4/4	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	OXL	O1-C1	4.37	1.33	1.22
3	B	602	OXL	O2-C2	4.01	1.32	1.22
3	A	602	OXL	O2-C2	3.51	1.31	1.22
3	D	602	OXL	O2-C2	3.51	1.31	1.22
3	F	602	OXL	O2-C2	3.30	1.30	1.22
3	F	602	OXL	O1-C1	3.28	1.30	1.22
3	F	602	OXL	O3-C1	-3.25	1.21	1.30
3	B	602	OXL	O4-C2	-3.23	1.21	1.30
3	H	602	OXL	O4-C2	-3.04	1.22	1.30
3	G	602	OXL	O3-C1	-3.01	1.22	1.30
3	G	602	OXL	O1-C1	2.96	1.29	1.22
3	C	602	OXL	O1-C1	2.95	1.29	1.22
3	D	602	OXL	O4-C2	-2.92	1.22	1.30
3	C	602	OXL	O3-C1	-2.68	1.23	1.30
3	E	602	OXL	O3-C1	-2.68	1.23	1.30
3	H	602	OXL	O2-C2	2.47	1.28	1.22
3	A	602	OXL	O4-C2	-2.45	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	602	OXL	O4-C2	-2.41	1.24	1.30
2	G	601	FBP	P2-O6P	-2.02	1.47	1.54
3	G	602	OXL	C2-C1	-2.01	1.51	1.54

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	602	OXL	O3-C1-C2	4.67	121.89	112.83
3	F	602	OXL	O4-C2-C1	4.17	120.92	112.83
3	A	602	OXL	O4-C2-C1	4.04	120.66	112.83
3	H	602	OXL	O4-C2-C1	3.98	120.55	112.83
2	D	601	FBP	O5P-P2-O6	3.56	115.94	106.67
3	D	602	OXL	O4-C2-C1	3.34	119.30	112.83
3	F	602	OXL	O3-C1-C2	3.28	119.20	112.83
4	G	603	I99	C12-N-S	3.18	122.91	117.17
3	D	602	OXL	O3-C1-C2	3.11	118.86	112.83
3	C	602	OXL	O3-C1-C2	3.06	118.77	112.83
3	G	602	OXL	O1-C1-C2	-3.02	114.33	120.63
3	G	602	OXL	O4-C2-C1	2.99	118.63	112.83
3	B	602	OXL	O3-C1-C2	2.57	117.82	112.83
2	B	601	FBP	O3P-P1-O2P	2.56	117.39	107.80
3	A	602	OXL	O3-C1-C2	2.55	117.78	112.83
3	E	602	OXL	O4-C2-C1	2.43	117.55	112.83
3	A	602	OXL	O2-C2-C1	-2.42	115.58	120.63
2	E	601	FBP	O3P-P1-O2P	2.42	116.86	107.80
4	G	603	I99	C17-N-C12	2.39	115.34	112.66
3	F	602	OXL	O2-C2-C1	-2.34	115.76	120.63
2	H	601	FBP	O5P-P2-O6	2.34	112.76	106.67
3	E	602	OXL	O3-C1-C2	2.27	117.22	112.83
2	B	601	FBP	O5P-P2-O6	2.06	112.04	106.67
3	H	602	OXL	O2-C2-C1	-2.04	116.38	120.63

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	I99	C18-C11-S-O5
4	A	603	I99	C18-C11-S-O4
4	B	603	I99	C18-C11-S-O5
4	B	603	I99	C18-C11-S-O4
4	C	603	I99	C18-C11-S-O5
4	C	603	I99	C18-C11-S-O4

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Mol	Chain	Res	Type	Atoms
4	C	603	I99	C12-C13-C14-O2
4	E	603	I99	C18-C11-S-O5
4	E	603	I99	C18-C11-S-O4
4	F	603	I99	C18-C11-S-O5
4	F	603	I99	C18-C11-S-O4
4	G	603	I99	C12-N-S-C11
4	G	603	I99	C18-C11-S-O5
4	G	603	I99	C18-C11-S-O4
4	C	603	I99	C17-N-S-O5
4	C	603	I99	C17-N-S-O4
4	C	603	I99	C17-N-S-C11
4	G	603	I99	C17-N-S-O4
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	F	601	FBP	C4-C5-C6-O6
4	G	603	I99	C12-N-S-O4
4	G	603	I99	C17-N-S-C11
2	D	601	FBP	C4-C5-C6-O6
2	E	601	FBP	C4-C5-C6-O6
2	G	601	FBP	C4-C5-C6-O6
2	H	601	FBP	C4-C5-C6-O6
4	G	603	I99	C12-N-S-O5
4	C	603	I99	C12-N-S-O5
4	C	603	I99	C12-N-S-O4
2	A	601	FBP	O5-C5-C6-O6
2	B	601	FBP	O5-C5-C6-O6
2	D	601	FBP	O5-C5-C6-O6
2	E	601	FBP	O5-C5-C6-O6
2	F	601	FBP	O5-C5-C6-O6
4	C	603	I99	C12-N-S-C11
2	C	601	FBP	O5-C5-C6-O6
2	G	601	FBP	O5-C5-C6-O6
2	H	601	FBP	O5-C5-C6-O6
4	C	603	I99	C12-C13-C14-O3
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	A	602	OXL	O3-C1-C2-O4
3	D	602	OXL	O3-C1-C2-O4
3	A	602	OXL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	F	602	OXL	O1-C1-C2-O2
3	G	602	OXL	O1-C1-C2-O2
3	B	602	OXL	O3-C1-C2-O4
3	H	602	OXL	O3-C1-C2-O4
3	C	602	OXL	O1-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O2
3	B	602	OXL	O1-C1-C2-O2
3	E	602	OXL	O1-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O2
2	H	601	FBP	C6-O6-P2-O4P
3	H	602	OXL	O3-C1-C2-O2
3	A	602	OXL	O1-C1-C2-O4
3	A	602	OXL	O3-C1-C2-O2
3	C	602	OXL	O1-C1-C2-O4
3	C	602	OXL	O3-C1-C2-O2
3	D	602	OXL	O3-C1-C2-O2
3	E	602	OXL	O1-C1-C2-O4
3	F	602	OXL	O1-C1-C2-O4
3	F	602	OXL	O3-C1-C2-O2
3	G	602	OXL	O1-C1-C2-O4
3	G	602	OXL	O3-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O4
3	B	602	OXL	O3-C1-C2-O2
2	B	601	FBP	C1-O1-P1-O1P
4	F	603	I99	C12-C13-C14-O2
3	B	602	OXL	O1-C1-C2-O4

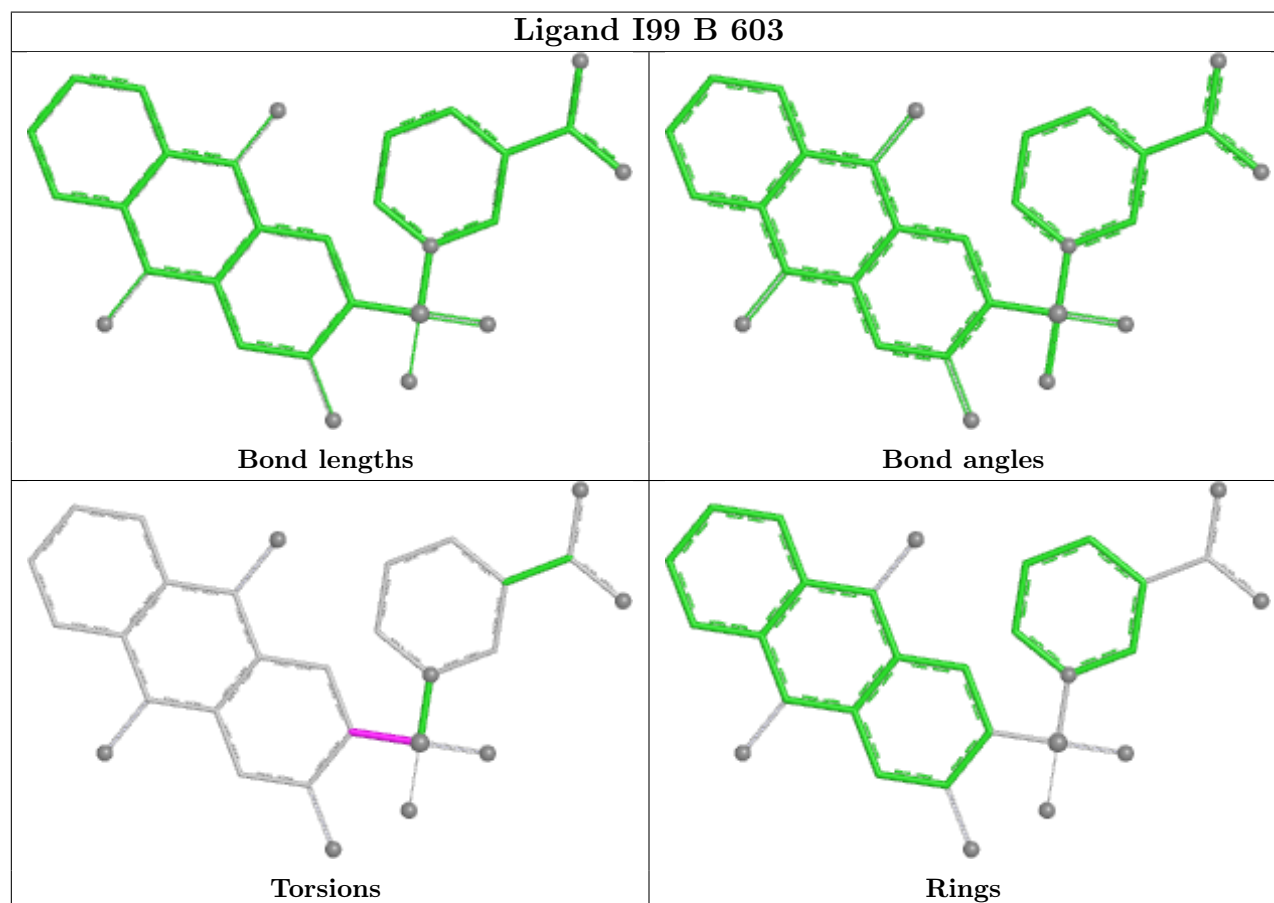
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	603	I99	C12-C13-C15-C16-C17-N
4	C	603	I99	C12-C13-C15-C16-C17-N

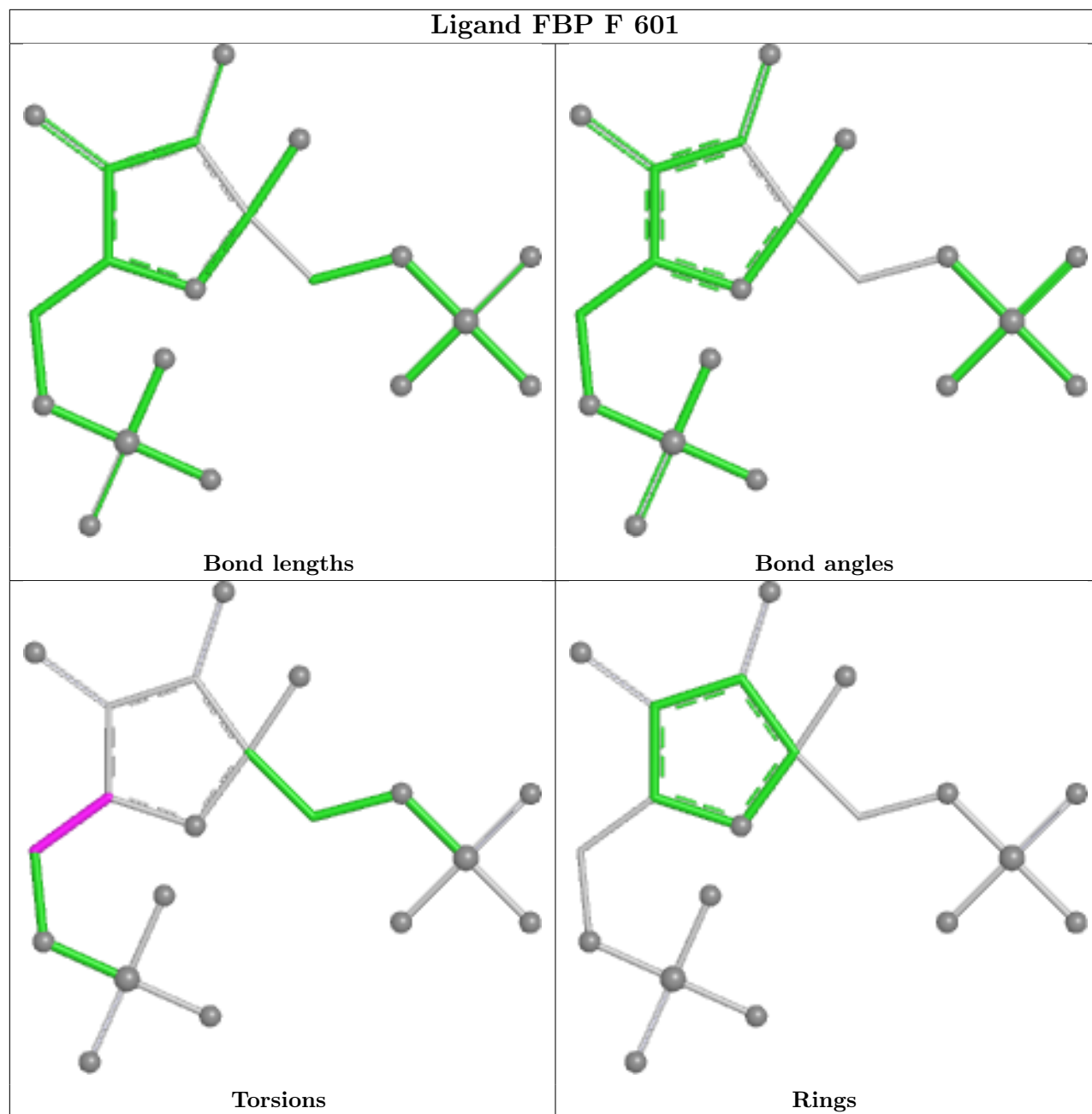
3 monomers are involved in 3 short contacts:

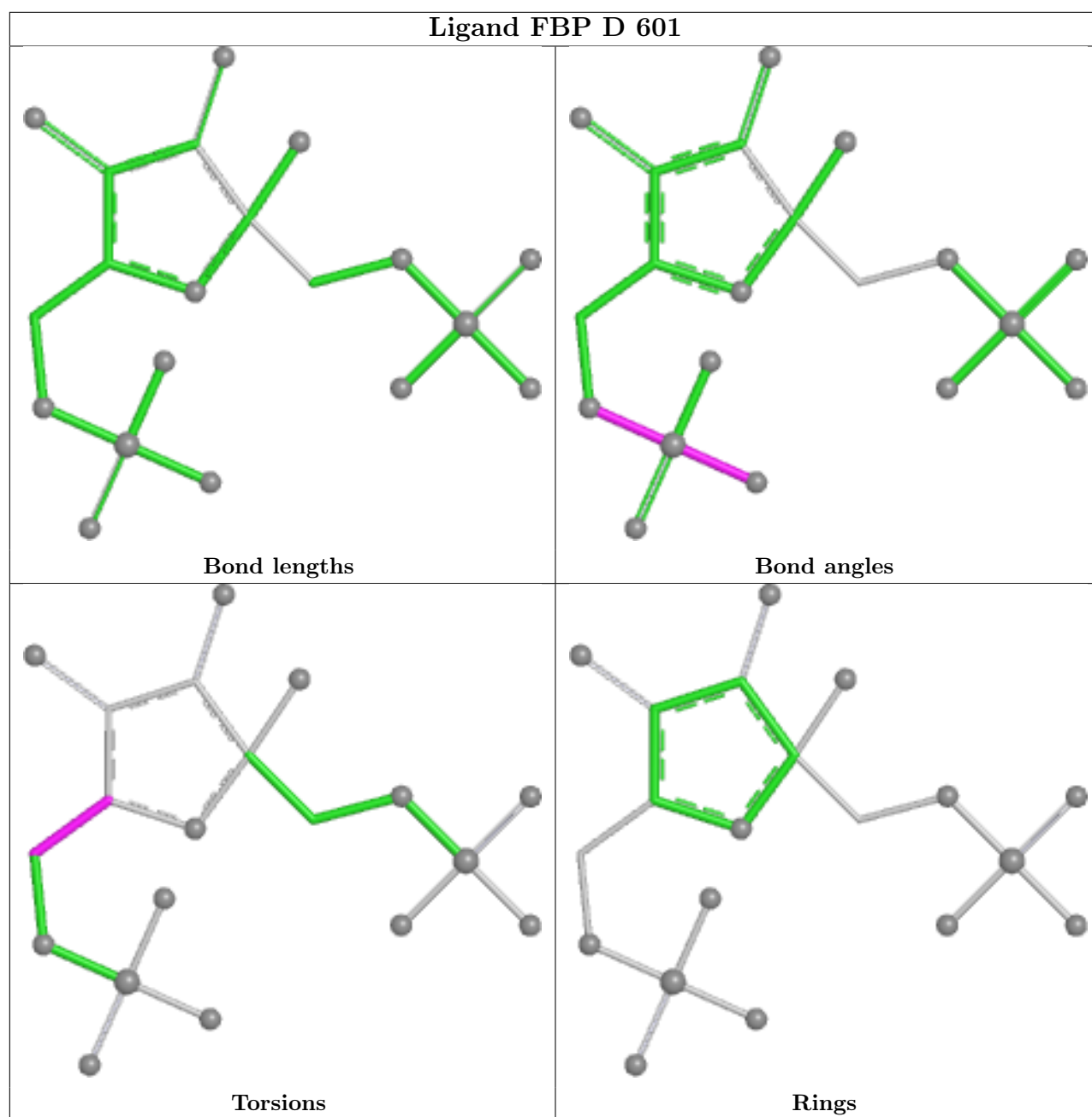
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	601	FBP	1	0
2	A	601	FBP	1	0
4	G	603	I99	1	0

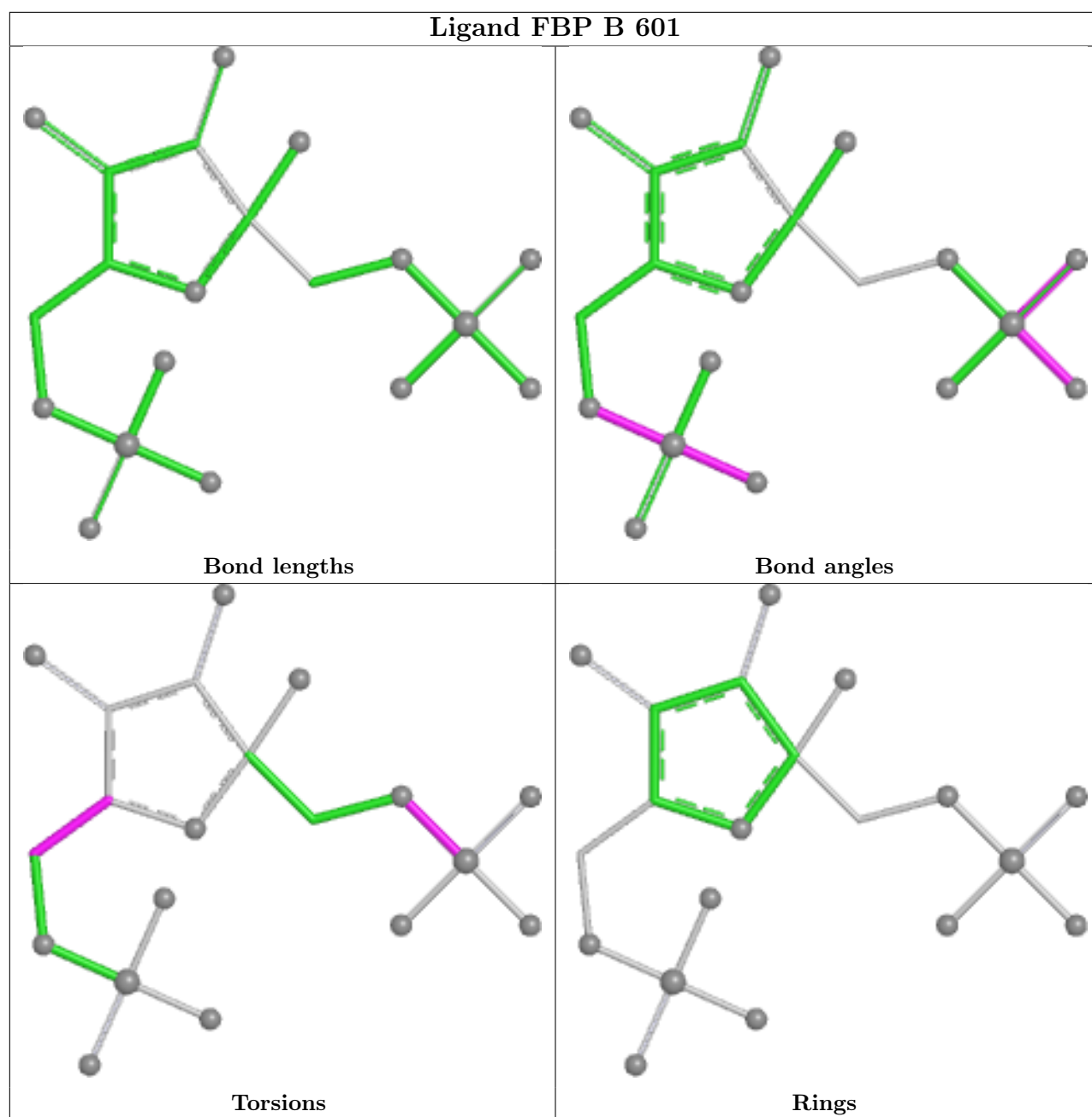
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

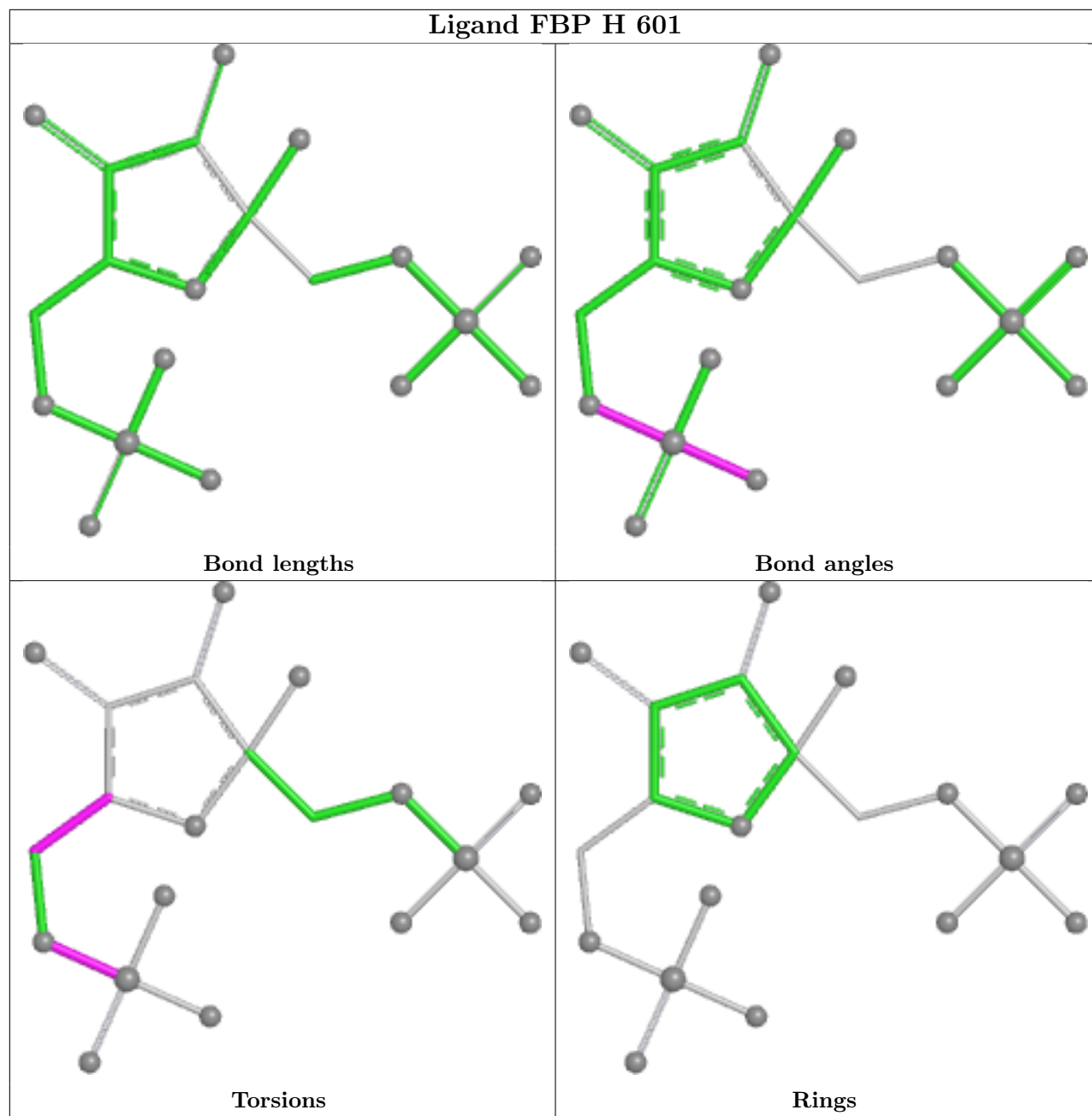


Ligand FBP F 601

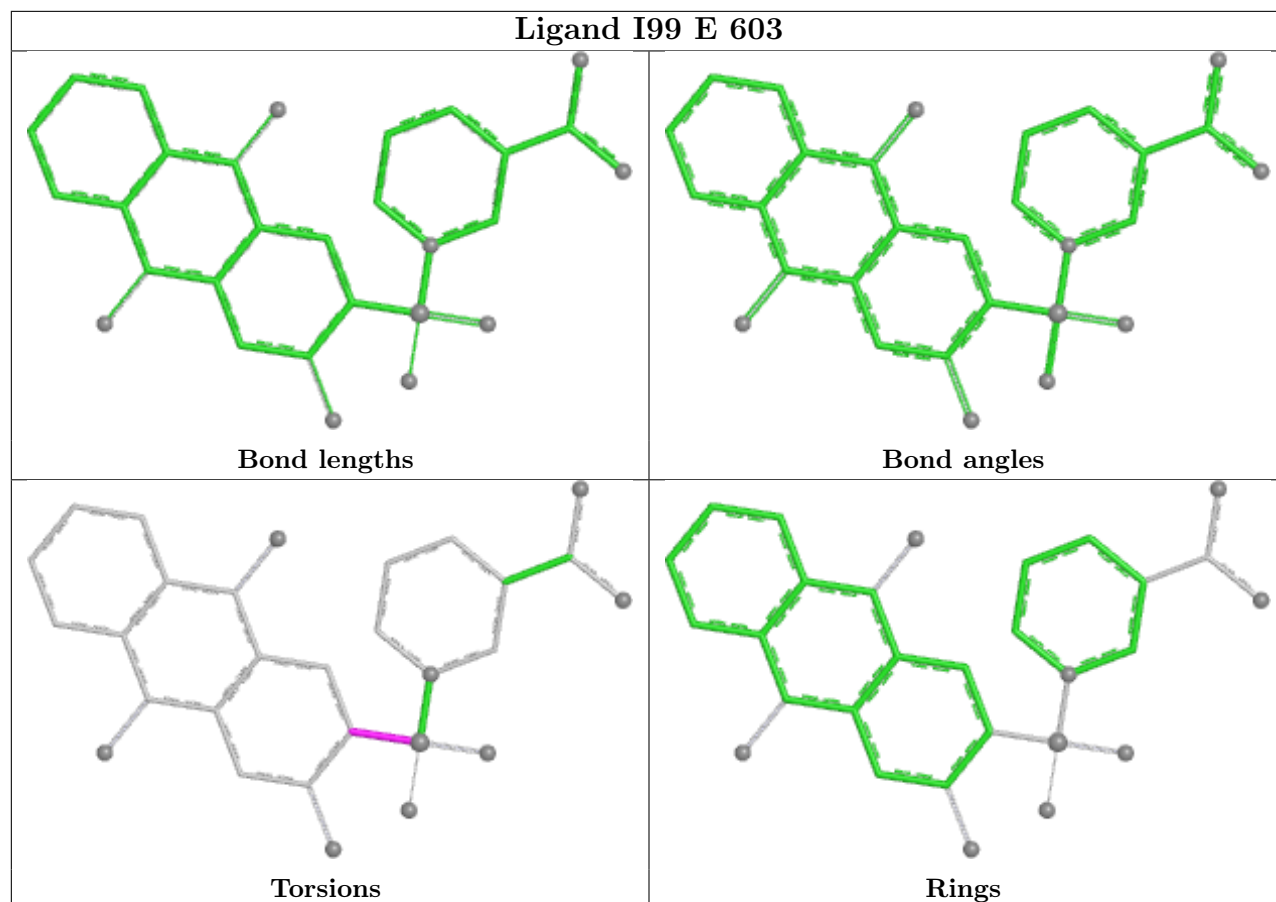




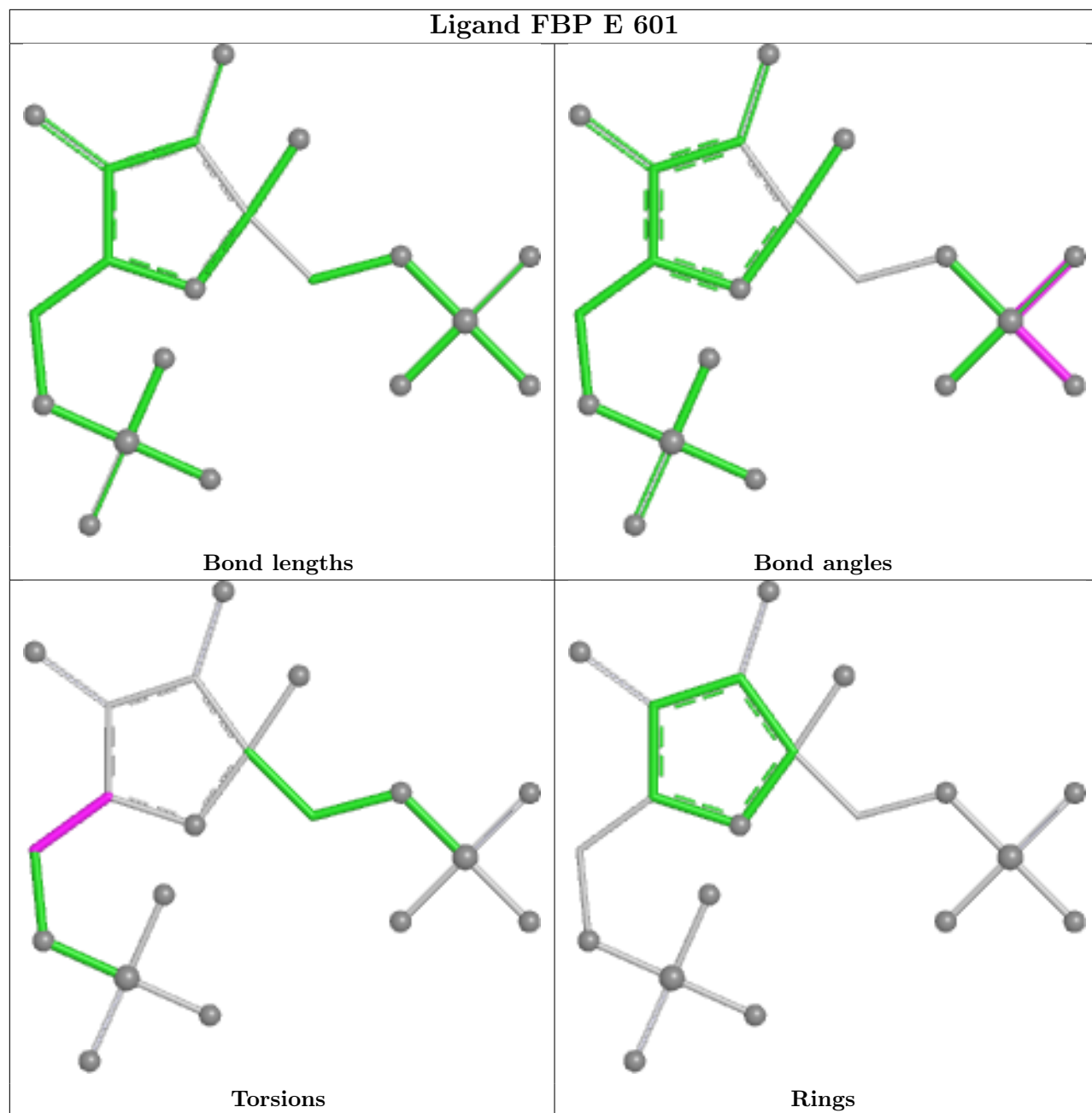


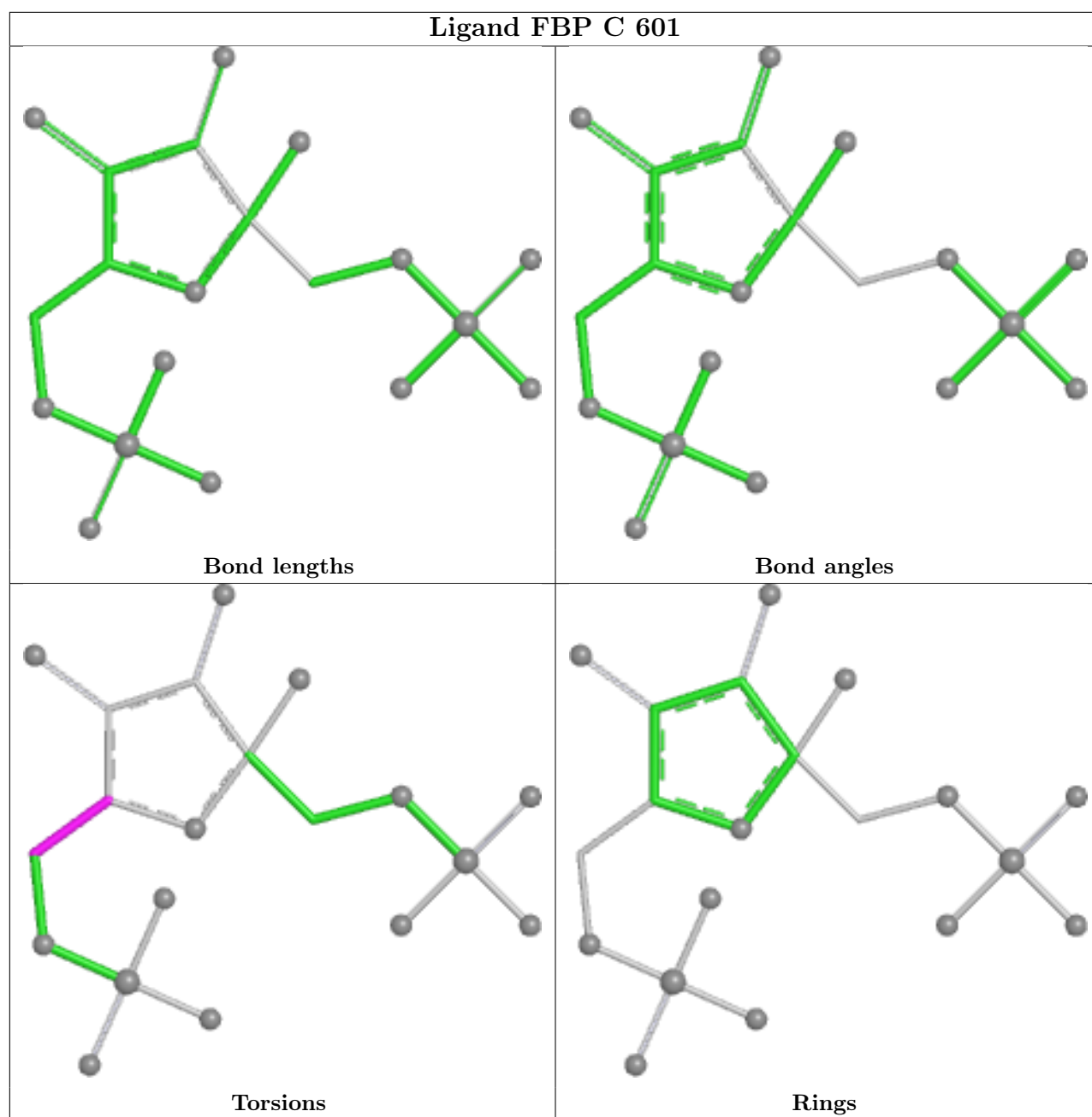


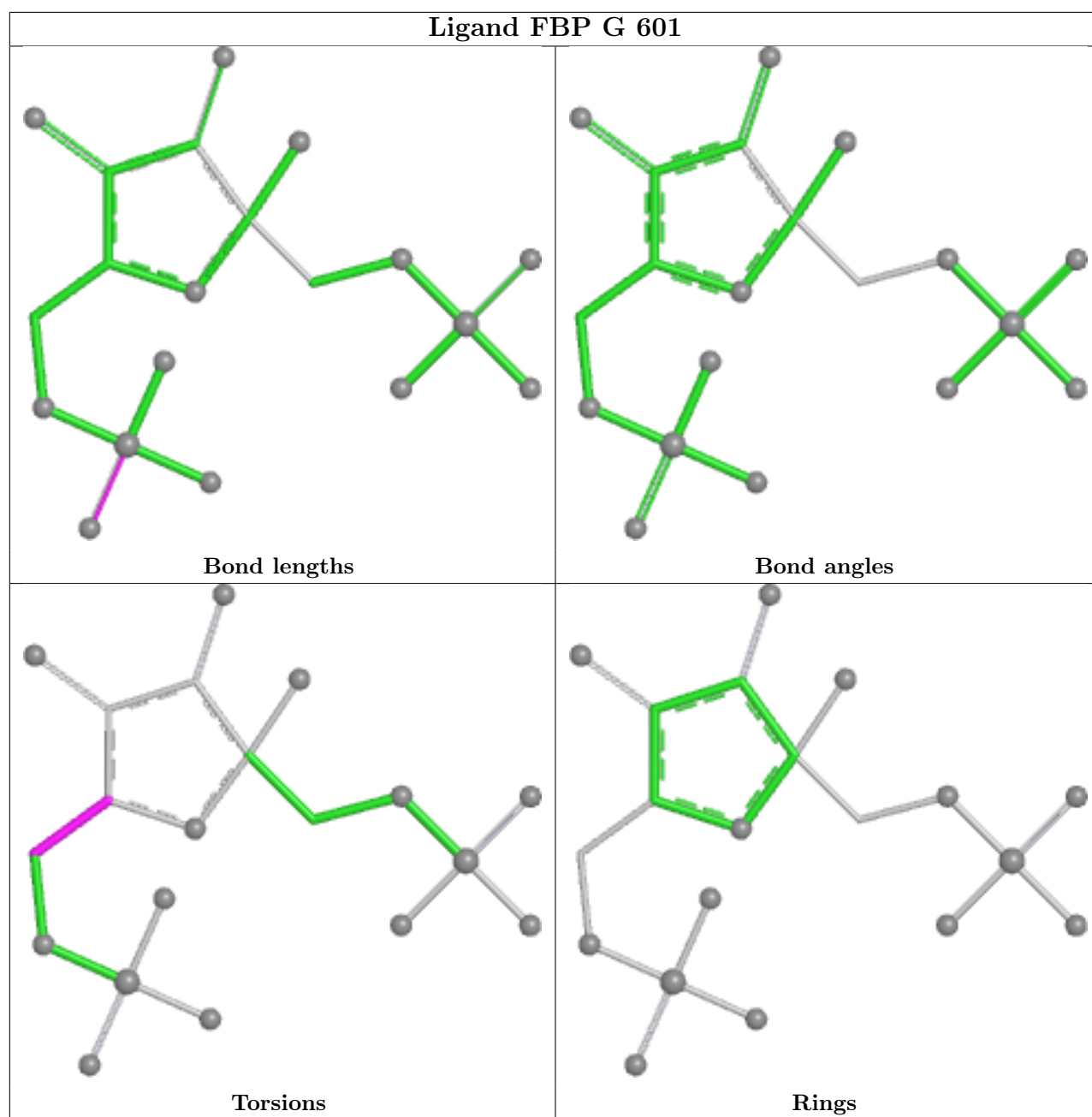
Ligand I99 E 603

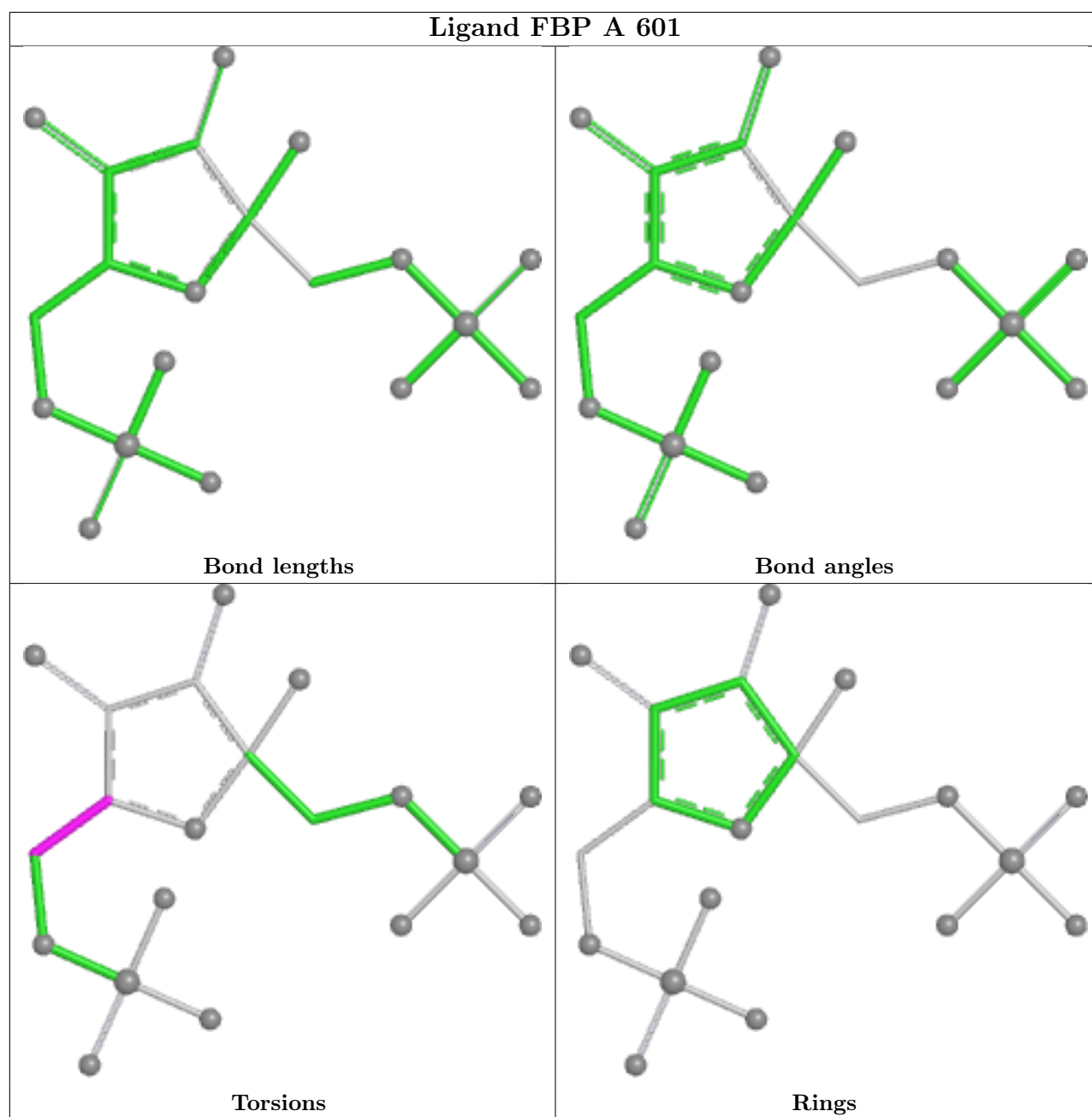


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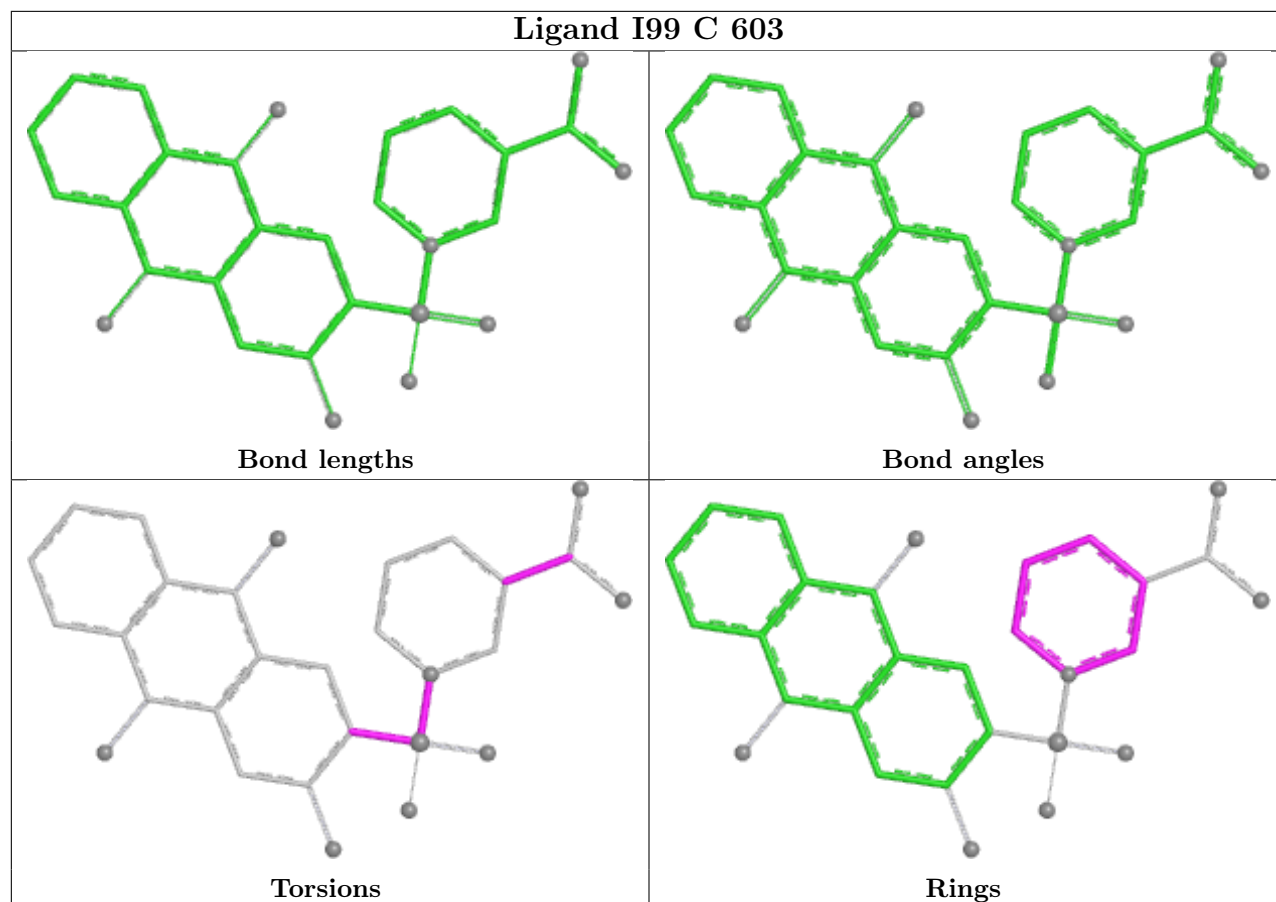




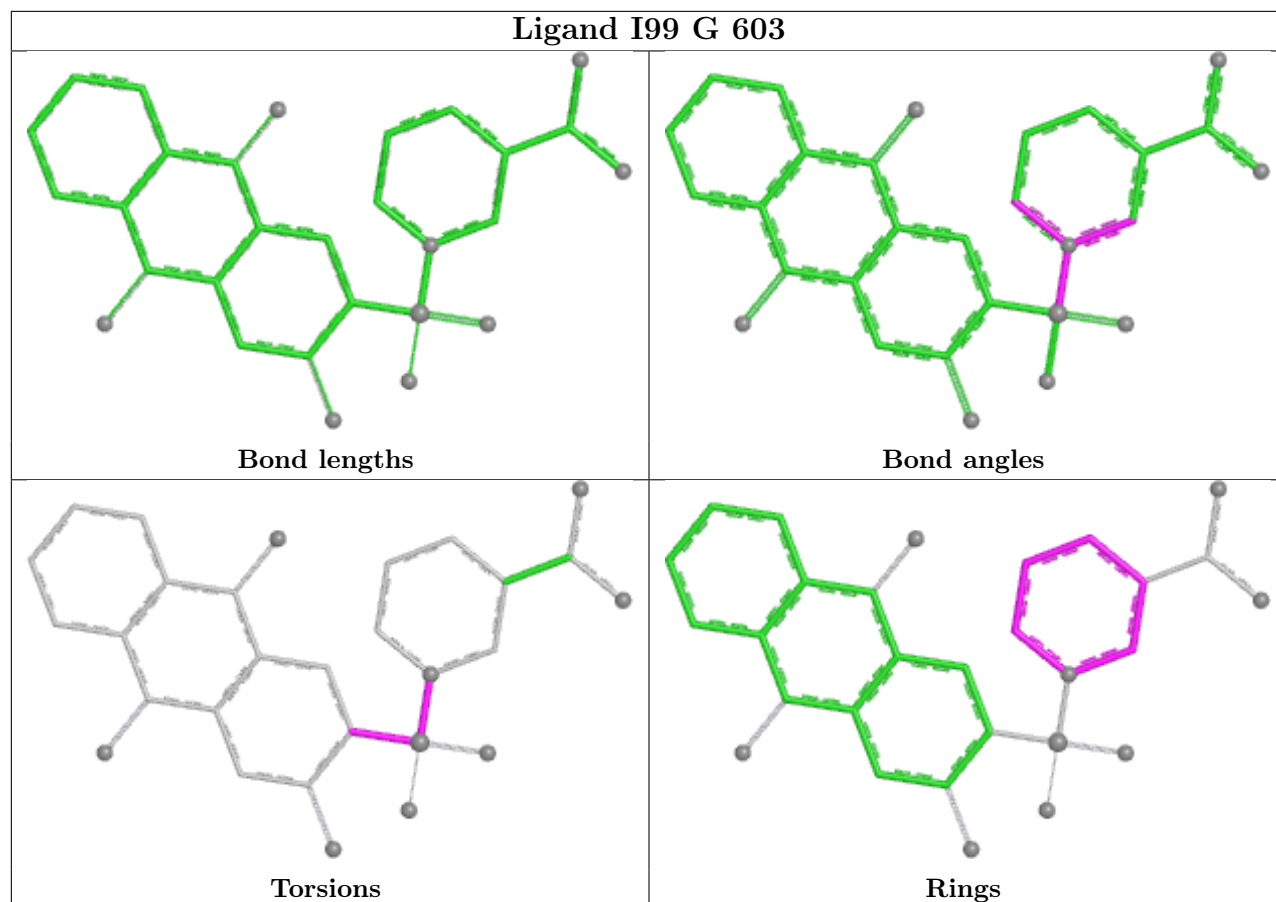


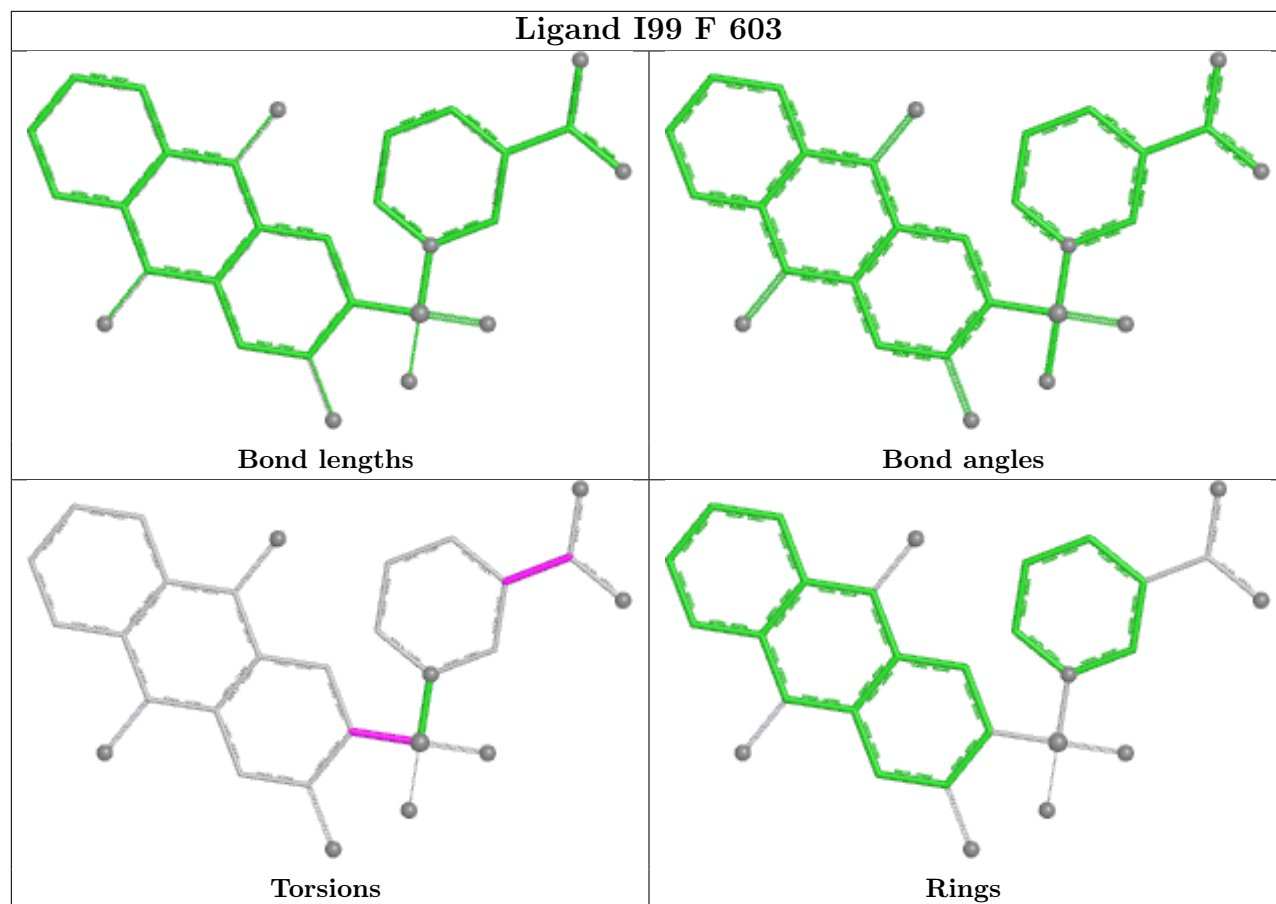


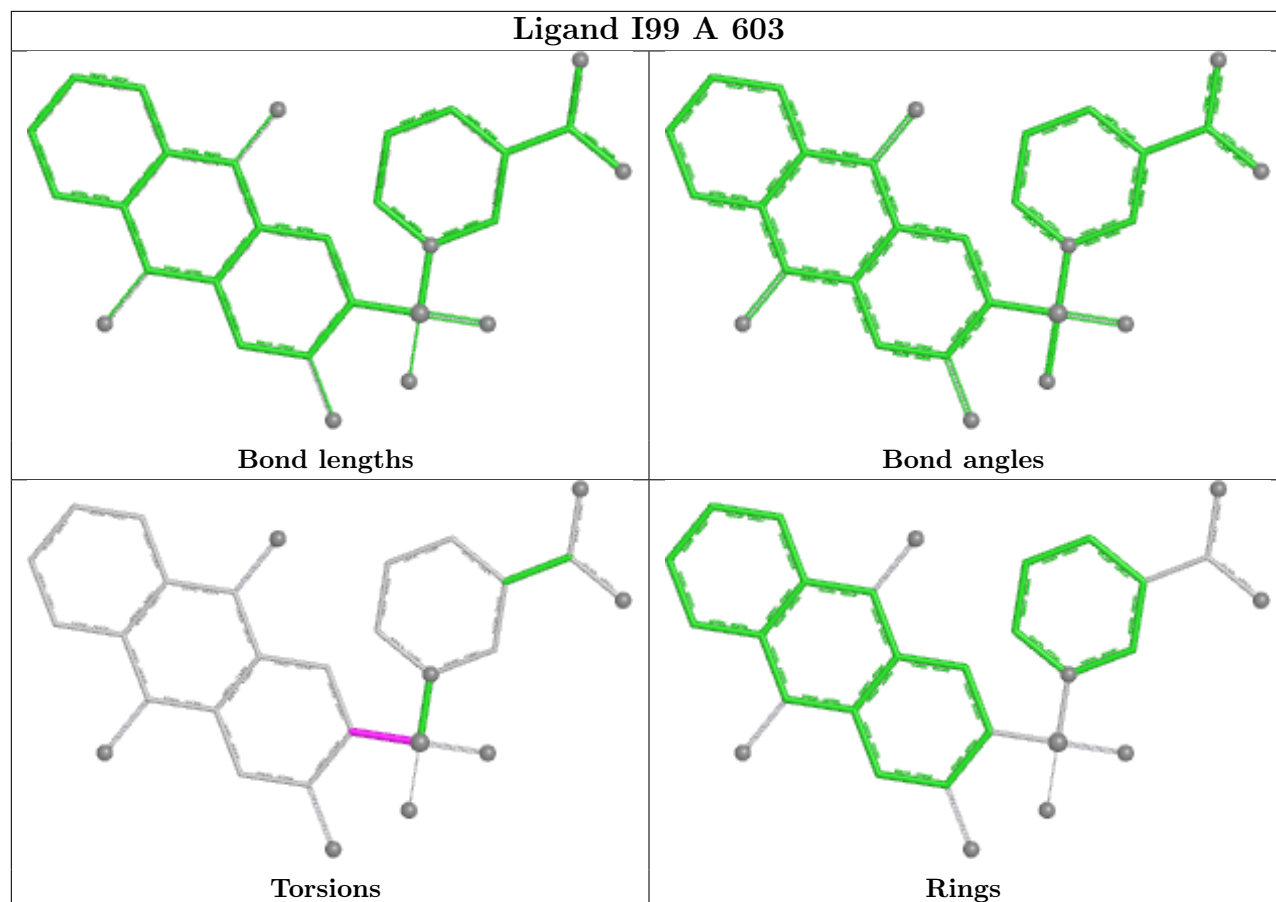
Ligand I99 C 603



Ligand I99 G 603







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	1.13	65 (15%) 5 5	29, 53, 78, 93	13 (3%)
1	B	436/447 (97%)	1.57	155 (35%) 1 0	27, 54, 89, 100	8 (1%)
1	C	424/447 (94%)	0.38	22 (5%) 33 37	23, 40, 62, 114	7 (1%)
1	D	425/447 (95%)	0.16	12 (2%) 55 62	18, 35, 59, 110	8 (1%)
1	E	419/447 (93%)	1.08	70 (16%) 4 4	28, 52, 81, 95	13 (3%)
1	F	432/447 (96%)	0.71	45 (10%) 11 13	25, 45, 70, 87	8 (1%)
1	G	422/447 (94%)	0.29	20 (4%) 36 41	16, 37, 59, 106	10 (2%)
1	H	425/447 (95%)	0.04	15 (3%) 47 53	18, 34, 57, 100	9 (2%)
All	All	3401/3576 (95%)	0.67	404 (11%) 9 10	16, 44, 77, 114	76 (2%)

All (404) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	LEU	6.7
1	G	271	GLY	6.2
1	D	25	PHE	6.1
1	E	25	PHE	6.0
1	E	275[A]	HIS	6.0
1	B	511	LEU	5.7
1	D	231	PRO	5.5
1	C	271	GLY	5.5
1	B	115	LEU	5.3
1	F	231	PRO	5.1
1	D	24	PHE	5.1
1	G	24	PHE	5.1
1	H	21	GLY	5.1
1	B	484	LEU	5.0
1	G	231	PRO	5.0
1	B	114	PRO	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	267[A]	ARG	4.8
1	G	25	PHE	4.8
1	B	249	VAL	4.8
1	H	25	PHE	4.5
1	B	485	LEU	4.5
1	E	24	PHE	4.4
1	A	500	ARG	4.4
1	E	232	GLY	4.3
1	D	22	THR	4.3
1	B	527	TRP	4.3
1	D	21	GLY	4.2
1	C	22	THR	4.2
1	B	270	LEU	4.2
1	F	267[A]	ARG	4.1
1	B	95	TYR	4.1
1	E	114	PRO	4.1
1	E	490	PRO	4.1
1	A	232	GLY	4.1
1	A	543	SER	4.1
1	B	517	VAL	4.1
1	C	23	ALA	4.0
1	B	70	VAL	4.0
1	C	25	PHE	4.0
1	B	241	LEU	4.0
1	B	64	GLY	3.9
1	G	21	GLY	3.9
1	E	115	LEU	3.9
1	D	23	ALA	3.9
1	B	106	ALA	3.9
1	B	67	SER	3.9
1	E	30	LEU	3.9
1	B	107	VAL	3.9
1	B	238	VAL	3.9
1	B	506	ILE	3.9
1	C	24	PHE	3.9
1	F	512	ARG	3.8
1	G	115	LEU	3.8
1	B	493	ILE	3.8
1	C	21	GLY	3.8
1	G	23	ALA	3.8
1	B	504	PHE	3.8
1	E	129	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	92	SER	3.7
1	B	100	ILE	3.7
1	A	238	VAL	3.7
1	F	516	ARG	3.7
1	B	103	VAL	3.6
1	B	88	PHE	3.6
1	G	116	SER	3.6
1	B	120	VAL	3.6
1	B	245	VAL	3.6
1	F	511	LEU	3.6
1	G	22	THR	3.6
1	B	110	PHE	3.6
1	A	241	LEU	3.6
1	F	233	LEU	3.6
1	B	505	GLY	3.5
1	E	493	ILE	3.5
1	B	498	VAL	3.5
1	A	495	ALA	3.5
1	B	73	LEU	3.5
1	B	378	ALA	3.5
1	B	508	SER	3.5
1	B	489	PRO	3.5
1	A	527	TRP	3.5
1	B	542	ILE	3.5
1	H	24	PHE	3.5
1	B	251	ILE	3.4
1	A	514	PHE	3.4
1	B	268	ALA	3.4
1	B	379	LYS	3.4
1	A	115	LEU	3.4
1	B	231	PRO	3.4
1	H	22	THR	3.4
1	B	66	ALA	3.4
1	E	492	ALA	3.4
1	B	90	HIS	3.4
1	B	77	ILE	3.4
1	B	86	LEU	3.4
1	B	515	LEU	3.4
1	B	252	VAL	3.3
1	A	33	ALA	3.3
1	A	249	VAL	3.3
1	B	97	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	23	ALA	3.3
1	B	124	LEU	3.3
1	E	233	LEU	3.3
1	F	484	LEU	3.3
1	A	114	PRO	3.3
1	B	513	GLY	3.3
1	B	495	ALA	3.2
1	E	269	ALA	3.2
1	F	11	ALA	3.2
1	B	13	VAL	3.2
1	B	91	GLY	3.2
1	F	493	ILE	3.2
1	D	30	LEU	3.2
1	A	542	ILE	3.2
1	B	348	THR	3.1
1	B	52	VAL	3.1
1	D	232	GLY	3.1
1	H	23	ALA	3.1
1	F	489	PRO	3.1
1	B	543	SER	3.1
1	E	109	SER	3.1
1	A	30	LEU	3.1
1	B	502	VAL	3.1
1	B	102	ASN	3.1
1	B	93	HIS	3.1
1	B	233	LEU	3.1
1	C	34	MET	3.1
1	F	270	LEU	3.0
1	B	76[A]	MET	3.0
1	B	382	PHE	3.0
1	A	233	LEU	3.0
1	B	72	ARG	3.0
1	B	256	PHE	3.0
1	B	272	PRO	3.0
1	A	73	LEU	3.0
1	B	269	ALA	3.0
1	A	86	LEU	2.9
1	F	115	LEU	2.9
1	C	232	GLY	2.9
1	E	122	ILE	2.9
1	A	26	GLN	2.9
1	E	270	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	99	SER	2.9
1	F	112	GLY	2.9
1	A	489	PRO	2.9
1	B	490	PRO	2.9
1	B	243	PHE	2.9
1	A	111	ALA	2.9
1	C	66	ALA	2.9
1	B	275	HIS	2.9
1	E	124	LEU	2.9
1	G	34	MET	2.9
1	A	120	VAL	2.9
1	B	232	GLY	2.9
1	H	232	GLY	2.9
1	B	123	ALA	2.9
1	A	270	LEU	2.9
1	B	384	VAL	2.8
1	B	514	PHE	2.8
1	B	131	SER	2.8
1	A	63	ILE	2.8
1	B	277	ILE	2.8
1	E	511	LEU	2.8
1	B	21	GLY	2.8
1	A	70	VAL	2.8
1	E	52	VAL	2.8
1	F	232	GLY	2.8
1	B	494	TRP	2.8
1	F	490	PRO	2.8
1	F	12	ASP	2.8
1	E	514	PHE	2.8
1	A	411	ARG	2.8
1	B	96	HIS	2.8
1	H	416	LEU	2.8
1	E	489	PRO	2.8
1	B	486	TYR	2.7
1	H	516	ARG	2.7
1	A	112	GLY	2.7
1	B	132	GLY	2.7
1	B	244	GLY	2.7
1	B	11	ALA	2.7
1	B	84	ALA	2.7
1	A	88	PHE	2.7
1	C	115	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	485	LEU	2.7
1	H	231	PRO	2.7
1	B	122	ILE	2.7
1	D	311	ILE	2.7
1	B	68	ARG	2.7
1	E	351	ARG	2.7
1	A	245	VAL	2.7
1	A	257	VAL	2.7
1	B	475	VAL	2.7
1	E	244	GLY	2.7
1	F	114	PRO	2.7
1	E	238	VAL	2.7
1	F	245	VAL	2.7
1	A	494	TRP	2.6
1	F	487	ARG	2.6
1	H	242[A]	ARG	2.6
1	F	514	PHE	2.6
1	B	65	PRO	2.6
1	A	32	ALA	2.6
1	B	472	ALA	2.6
1	G	114	PRO	2.6
1	B	274	GLY	2.6
1	A	107	VAL	2.6
1	C	111	ALA	2.6
1	B	520	LEU	2.6
1	A	34	MET	2.6
1	B	266	VAL	2.6
1	B	298	VAL	2.6
1	F	517	VAL	2.6
1	B	12	ASP	2.5
1	B	128	GLY	2.5
1	B	347	ILE	2.5
1	B	121	ALA	2.5
1	G	33	ALA	2.5
1	E	257	VAL	2.5
1	B	507	GLU	2.5
1	H	273	GLU	2.5
1	B	239	ARG	2.5
1	E	418[A]	ARG	2.5
1	F	351	ARG	2.5
1	B	471	ALA	2.5
1	F	498	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	52	VAL	2.5
1	G	272	PRO	2.5
1	B	380	GLY	2.5
1	C	410	LEU	2.5
1	A	118	ARG	2.5
1	B	63	ILE	2.5
1	B	74	LYS	2.5
1	B	250	ASP	2.5
1	B	276	GLY	2.4
1	C	412	ARG	2.4
1	F	411	ARG	2.4
1	A	275	HIS	2.4
1	B	25	PHE	2.4
1	E	256	PHE	2.4
1	A	378	ALA	2.4
1	E	123	ALA	2.4
1	A	263	VAL	2.4
1	C	411	ARG	2.4
1	E	487	ARG	2.4
1	H	411	ARG	2.4
1	B	271	GLY	2.4
1	E	128	GLY	2.4
1	A	108	GLU	2.4
1	D	275[A]	HIS	2.4
1	F	275	HIS	2.4
1	E	34	MET	2.4
1	E	116	SER	2.4
1	E	88	PHE	2.4
1	B	83	ILE	2.4
1	E	100	ILE	2.4
1	B	101	ALA	2.4
1	B	265	ALA	2.4
1	E	495	ALA	2.4
1	A	418[A]	ARG	2.4
1	B	411	ARG	2.4
1	E	263	VAL	2.4
1	B	503	GLN	2.4
1	B	80	GLY	2.4
1	C	116[A]	SER	2.4
1	E	86	LEU	2.4
1	C	117	TYR	2.4
1	B	240	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	242	ARG	2.4
1	D	413	ALA	2.4
1	A	488[A]	GLU	2.4
1	F	527	TRP	2.4
1	B	416	LEU	2.3
1	C	110	PHE	2.3
1	B	126	THR	2.3
1	B	279	ILE	2.3
1	B	311	ILE	2.3
1	F	532	GLY	2.3
1	A	475	VAL	2.3
1	E	99	SER	2.3
1	E	245	VAL	2.3
1	H	52	VAL	2.3
1	C	459	ARG	2.3
1	E	527	TRP	2.3
1	A	540	LEU	2.3
1	A	265	ALA	2.3
1	A	100	ILE	2.3
1	C	231	PRO	2.3
1	F	129	PRO	2.3
1	B	509	GLY	2.3
1	B	116	SER	2.3
1	E	92	SER	2.3
1	B	404	ARG	2.3
1	A	331[A]	LEU	2.3
1	F	34	MET	2.3
1	B	483	PRO	2.3
1	E	272	PRO	2.3
1	G	232	GLY	2.3
1	G	411	ARG	2.3
1	B	443	LEU	2.3
1	F	379	LYS	2.3
1	F	515	LEU	2.3
1	G	30	LEU	2.3
1	F	274	GLY	2.2
1	F	507	GLU	2.2
1	B	109	SER	2.2
1	C	122	ILE	2.2
1	A	52	VAL	2.2
1	E	120	VAL	2.2
1	B	22	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	416	LEU	2.2
1	E	380	GLY	2.2
1	A	305	ALA	2.2
1	E	97	ALA	2.2
1	A	110	PHE	2.2
1	E	243	PHE	2.2
1	A	412	ARG	2.2
1	E	502	VAL	2.2
1	F	521	VAL	2.2
1	B	94	GLU	2.2
1	F	408	GLU	2.2
1	B	373	LEU	2.2
1	B	113	SER	2.2
1	E	513	GLY	2.2
1	F	496	ASP	2.2
1	B	438	ALA	2.2
1	E	33	ALA	2.2
1	E	111	ALA	2.2
1	A	482	PHE	2.2
1	E	277	ILE	2.2
1	E	90	HIS	2.2
1	B	242	ARG	2.2
1	E	26	GLN	2.2
1	E	103	VAL	2.2
1	E	266	VAL	2.2
1	F	499	ASP	2.2
1	G	113	SER	2.2
1	F	86	LEU	2.2
1	D	31	PRO	2.2
1	A	61	ALA	2.2
1	E	264	ALA	2.2
1	E	491	GLU	2.1
1	A	277	ILE	2.1
1	A	496	ASP	2.1
1	A	498	VAL	2.1
1	B	465	VAL	2.1
1	E	112	GLY	2.1
1	E	274	GLY	2.1
1	E	331	LEU	2.1
1	E	540	LEU	2.1
1	F	124	LEU	2.1
1	B	75[A]	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	79	ALA	2.1
1	B	254	ALA	2.1
1	F	111	ALA	2.1
1	F	269	ALA	2.1
1	A	95	TYR	2.1
1	B	117	TYR	2.1
1	G	117	TYR	2.1
1	B	89	SER	2.1
1	A	351	ARG	2.1
1	B	257	VAL	2.1
1	B	16	LEU	2.1
1	C	400	ALA	2.1
1	G	110	PHE	2.1
1	A	493	ILE	2.1
1	A	242	ARG	2.1
1	B	104	ARG	2.1
1	B	512	ARG	2.1
1	H	267[A]	ARG	2.1
1	B	377	THR	2.1
1	A	103	VAL	2.1
1	A	129	PRO	2.1
1	B	383	PRO	2.1
1	E	515	LEU	2.1
1	A	471	ALA	2.1
1	B	14	ALA	2.1
1	B	492	ALA	2.1
1	E	265	ALA	2.1
1	F	492	ALA	2.1
1	B	499	ASP	2.1
1	A	407	PHE	2.0
1	B	71	GLU	2.0
1	E	110	PHE	2.0
1	E	504	PHE	2.0
1	B	69	SER	2.0
1	B	375	GLY	2.0
1	B	129	PRO	2.0
1	B	521	VAL	2.0
1	E	119	PRO	2.0
1	A	511	LEU	2.0
1	F	485	LEU	2.0
1	B	516	ARG	2.0
1	F	118	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	127	LYS	2.0
1	B	468	SER	2.0
1	B	541	SER	2.0
1	A	256	PHE	2.0
1	A	248	GLY	2.0
1	B	236	GLN	2.0
1	H	26	GLN	2.0
1	B	10	ARG	2.0
1	B	263	VAL	2.0
1	E	70	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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
4	I99	B	603	29/29	0.80	0.20	81,85,87,87	17
4	I99	A	603	29/29	0.86	0.15	83,85,87,87	17
3	OXL	E	602	6/6	0.87	0.12	62,63,63,63	0
6	K	E	605	1/1	0.88	0.21	93,93,93,93	0
4	I99	G	603	29/29	0.89	0.16	61,65,67,67	17
4	I99	E	603	29/29	0.89	0.13	89,89,90,90	17
6	K	B	605	1/1	0.91	0.12	80,80,80,80	0
4	I99	F	603	29/29	0.92	0.11	59,60,63,63	17
5	MG	B	604	1/1	0.93	0.09	65,65,65,65	0
3	OXL	A	602	6/6	0.94	0.08	57,57,58,58	0
6	K	A	605	1/1	0.94	0.11	86,86,86,86	0
2	FBP	B	601	20/20	0.94	0.08	49,51,54,55	0
4	I99	C	603	29/29	0.94	0.09	57,58,62,63	17

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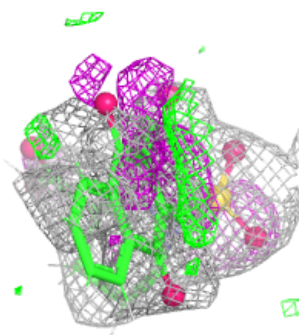
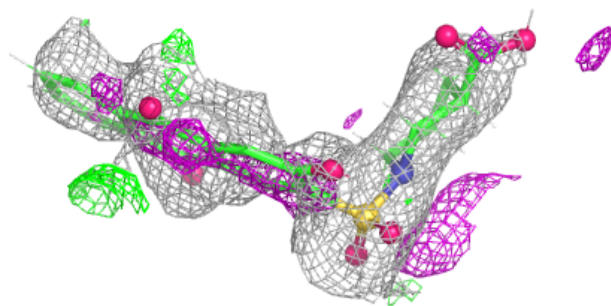
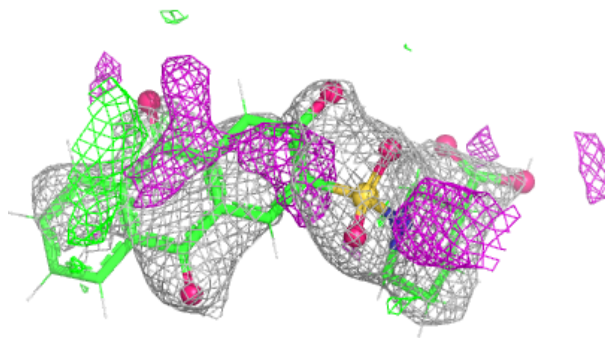
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	K	F	605	1/1	0.94	0.11	80,80,80,80	0
6	K	G	605	1/1	0.94	0.17	60,60,60,60	0
3	OXL	B	602	6/6	0.95	0.07	46,47,47,47	0
2	FBP	E	601	20/20	0.95	0.08	46,47,48,49	0
3	OXL	G	602	6/6	0.95	0.07	40,41,41,42	0
2	FBP	F	601	20/20	0.95	0.08	44,47,52,52	0
2	FBP	A	601	20/20	0.95	0.08	46,49,50,50	0
6	K	C	605	1/1	0.96	0.23	62,62,62,62	0
3	OXL	F	602	6/6	0.96	0.07	48,49,50,50	0
3	OXL	H	602	6/6	0.96	0.07	35,36,36,37	0
5	MG	A	604	1/1	0.96	0.06	62,62,62,62	0
3	OXL	C	602	6/6	0.97	0.06	44,45,45,45	0
3	OXL	D	602	6/6	0.97	0.06	38,39,39,40	0
2	FBP	D	601	20/20	0.98	0.04	27,29,30,32	0
6	K	D	604	1/1	0.98	0.13	51,51,51,51	0
5	MG	E	604	1/1	0.98	0.06	57,57,57,57	0
2	FBP	G	601	20/20	0.98	0.05	29,30,31,33	0
2	FBP	H	601	20/20	0.98	0.04	25,28,30,30	0
6	K	H	604	1/1	0.98	0.16	55,55,55,55	0
5	MG	G	604	1/1	0.99	0.06	38,38,38,38	0
5	MG	H	603	1/1	0.99	0.04	39,39,39,39	0
5	MG	C	604	1/1	0.99	0.04	46,46,46,46	0
5	MG	D	603	1/1	0.99	0.04	38,38,38,38	0
2	FBP	C	601	20/20	0.99	0.04	29,30,32,33	0
5	MG	F	604	1/1	1.00	0.02	42,42,42,42	0

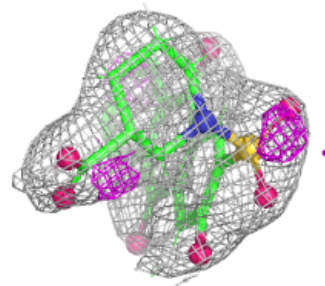
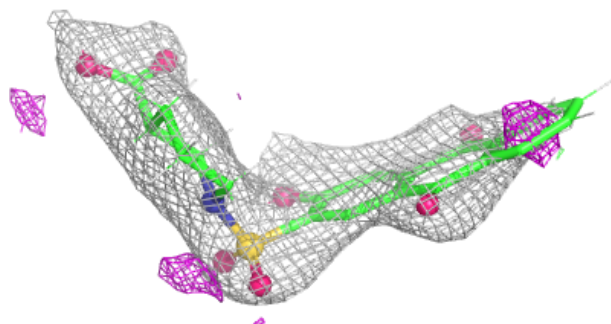
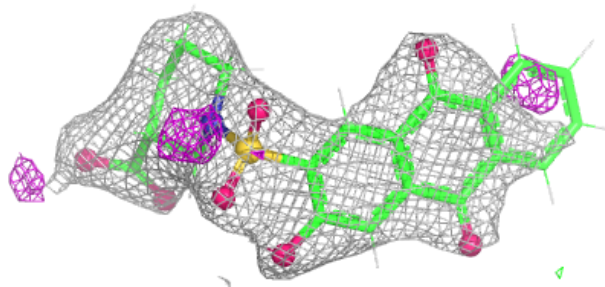
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around I99 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)

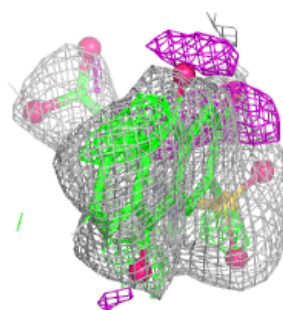
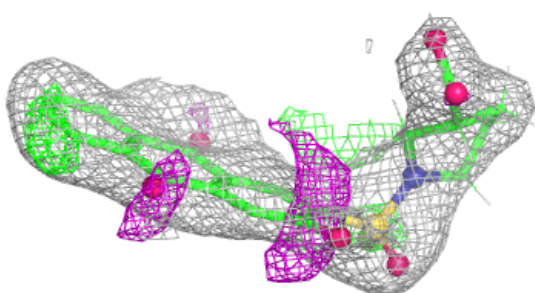
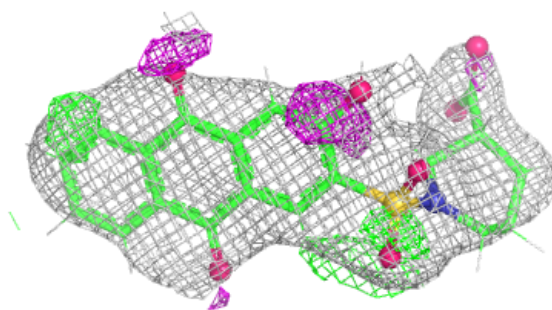
**Electron density around I99 A 603:**

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

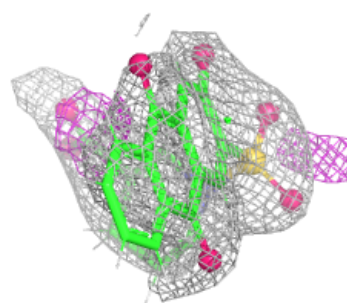
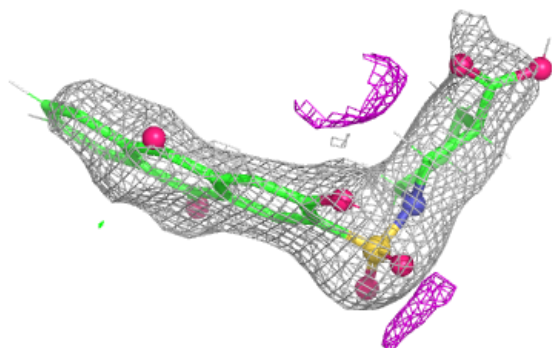
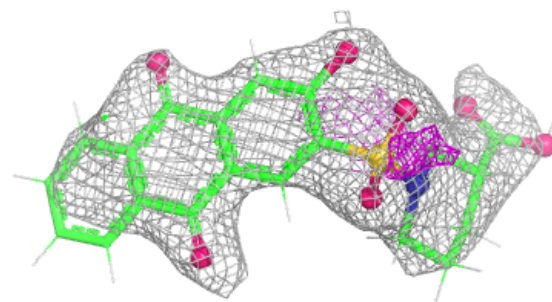


Electron density around I99 G 603:

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

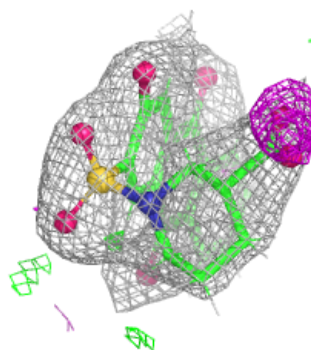
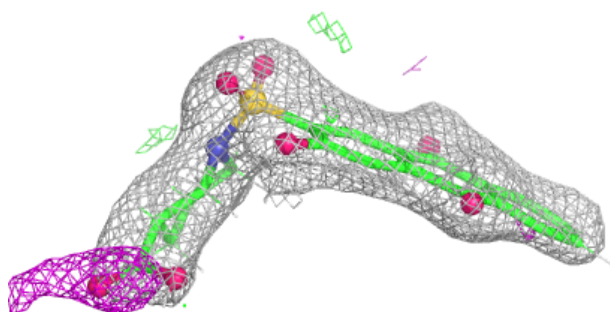
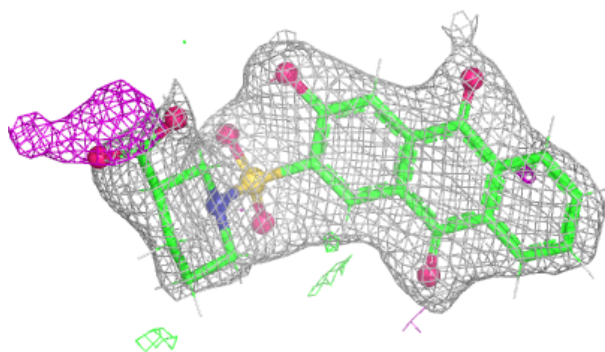
**Electron density around I99 E 603:**

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

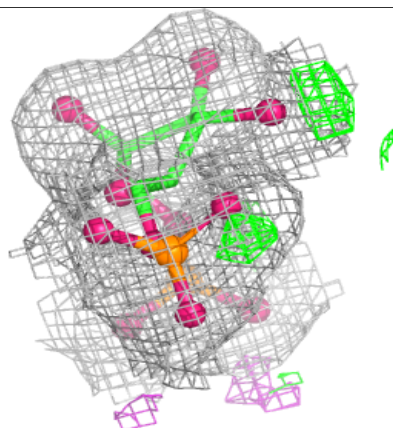
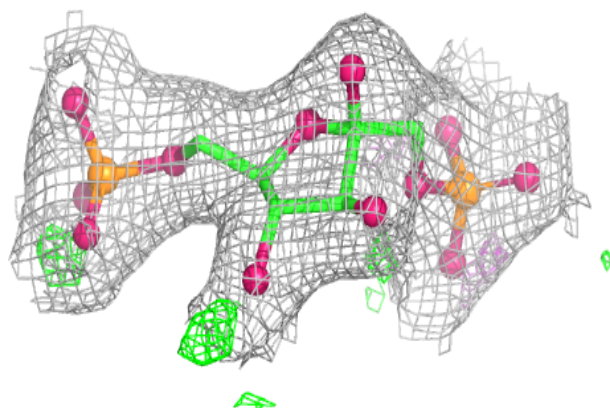
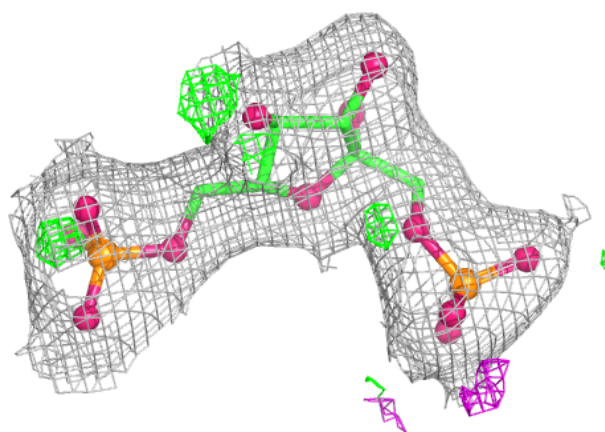


Electron density around I99 F 603:

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

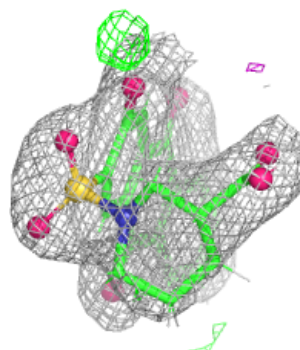
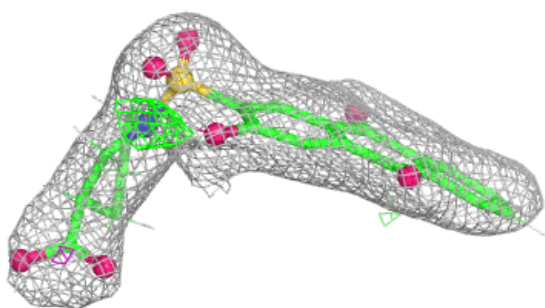
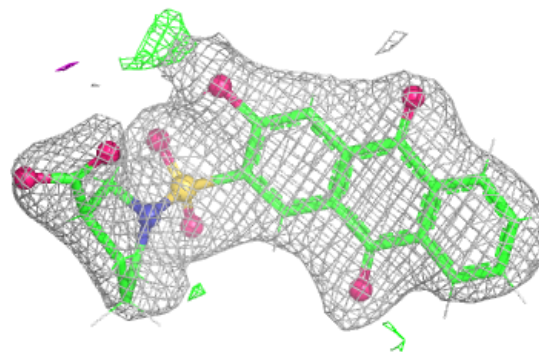
**Electron density around FBP B 601:**

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



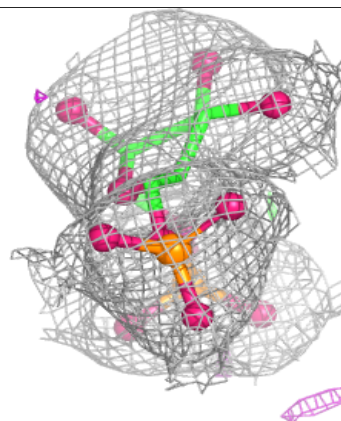
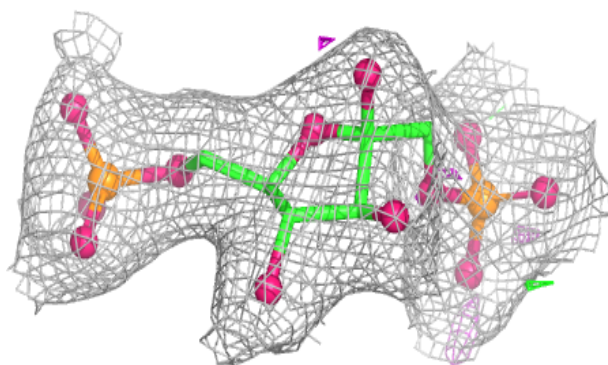
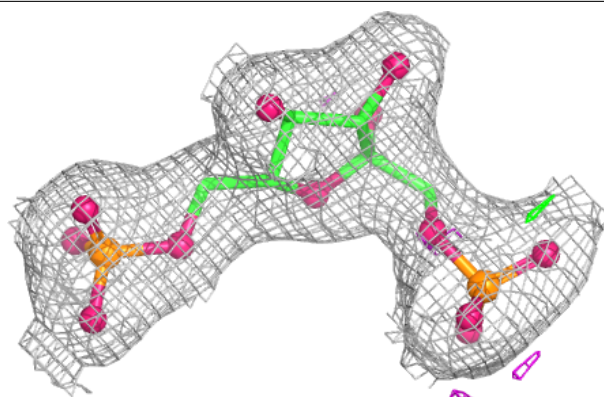
Electron density around I99 C 603:

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



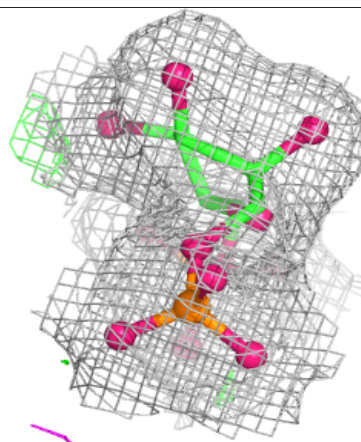
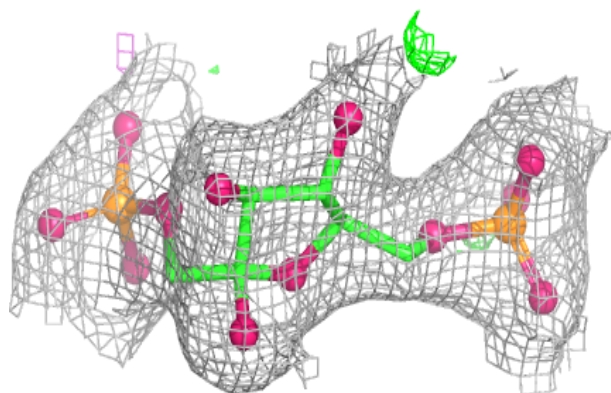
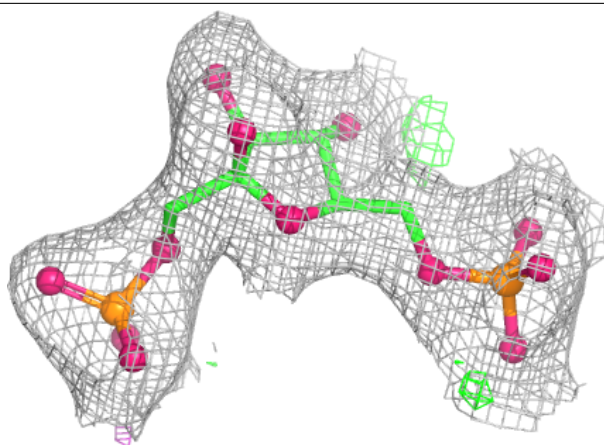
Electron density around FBP E 601:

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

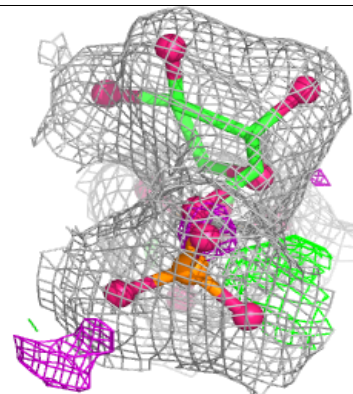
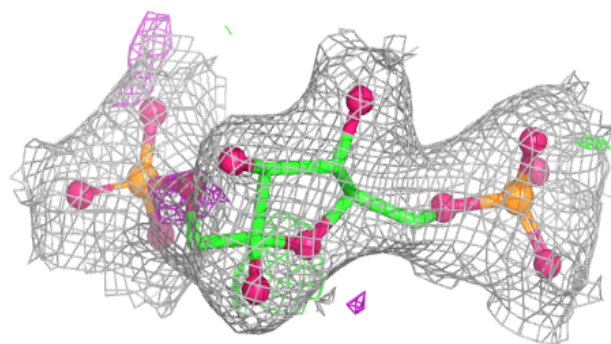
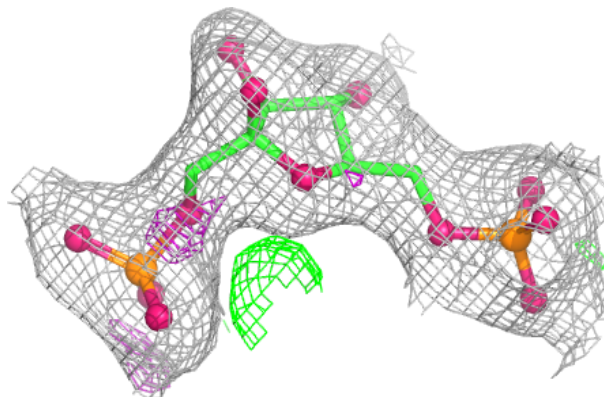


Electron density around FBP F 601:

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

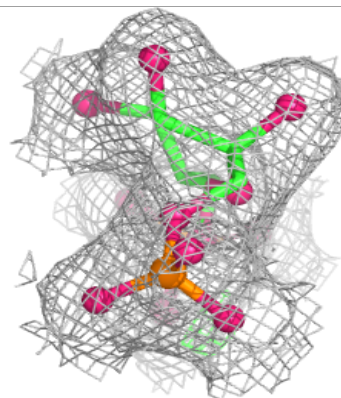
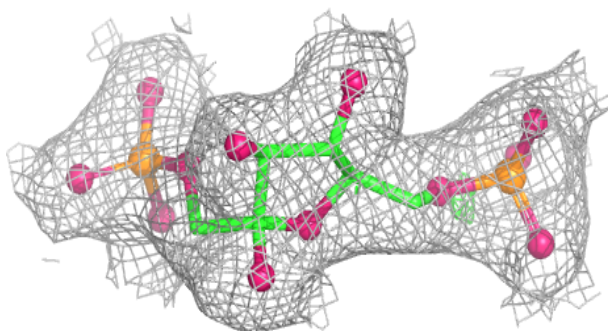
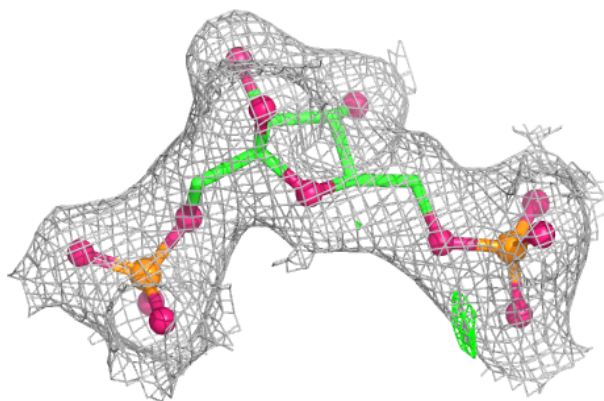
**Electron density around FBP A 601:**

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

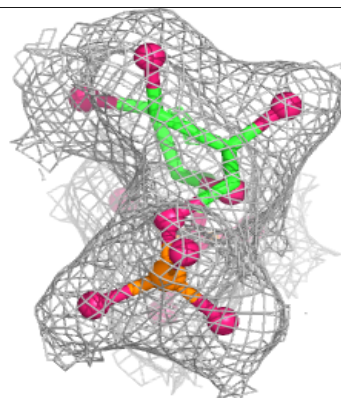
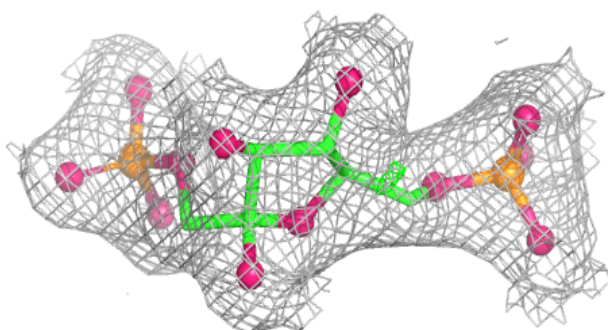
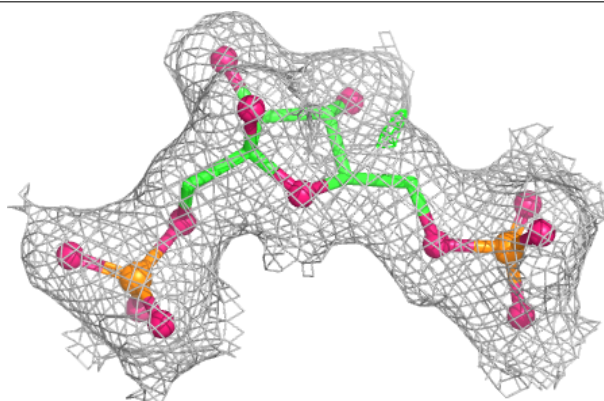


Electron density around FBP D 601:

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

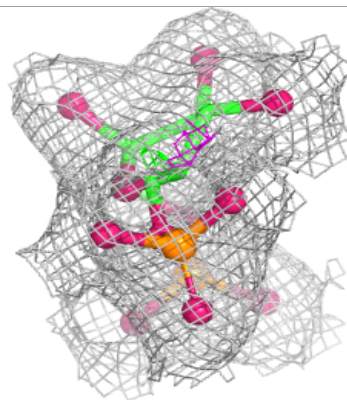
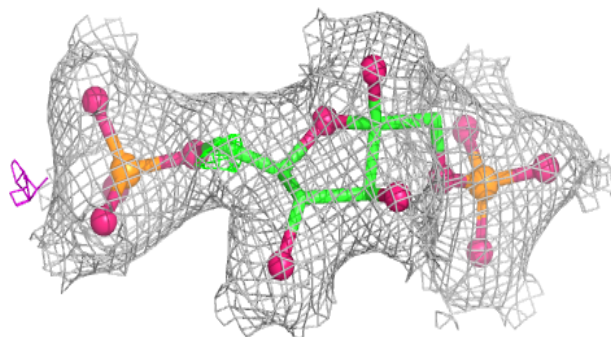
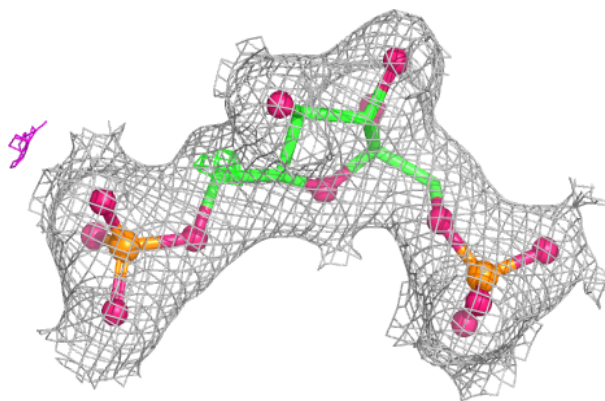
**Electron density around FBP G 601:**

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

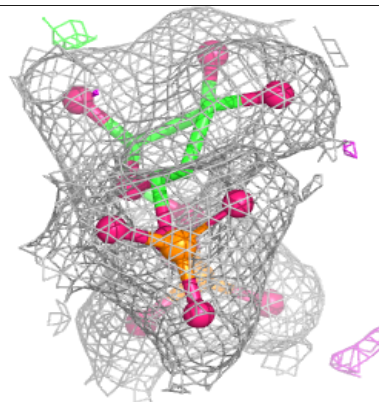
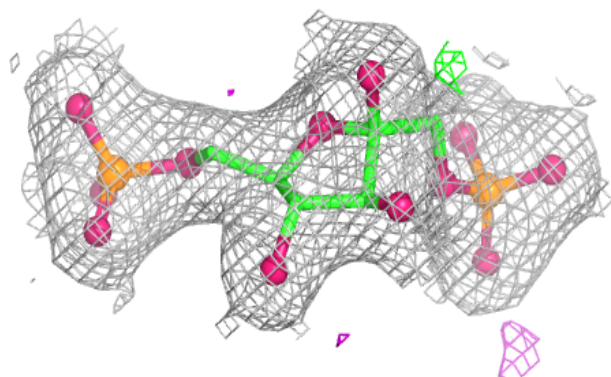
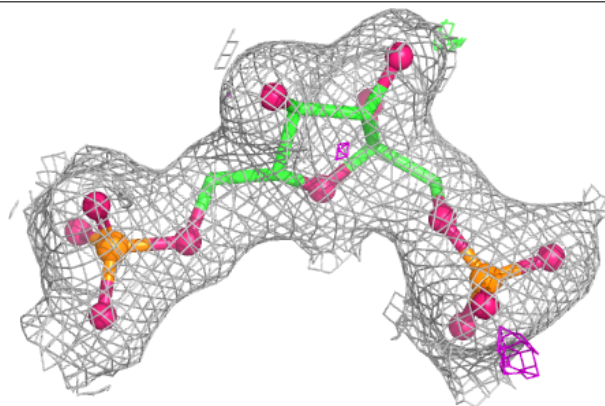


Electron density around FBP H 601:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.