



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:28 AM UTC

PDB ID : 5SCD / pdb_00005scd
Title : Structure of liver pyruvate kinase in complex with anthraquinone derivative
58
Authors : Lulla, A.; Foller, A.; Nain-Perez, A.; Grotli, M.; Brear, P.; Hyvonen, M.
Deposited on : 2021-12-01
Resolution : 2.04 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

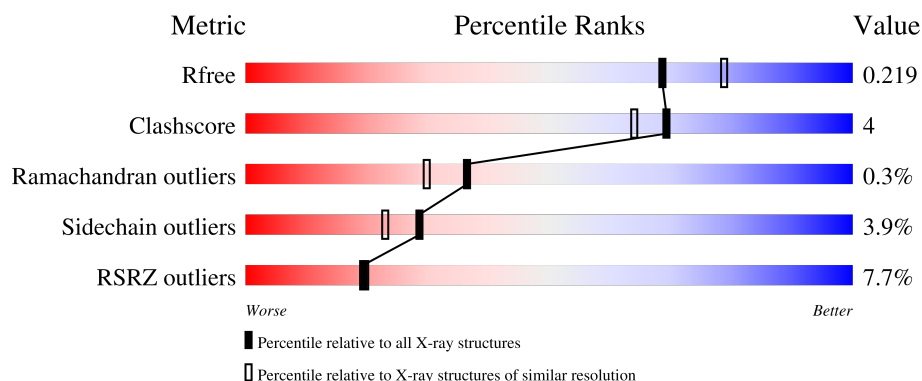
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	11% 82% 11% 6%
1	B	447	9% 88% 9% ..
1	C	447	5% 84% 10% 5%
1	D	447	4% 84% 9% 5%
1	E	447	16% 84% 10% 6%

Continued on next page...

Continued from previous page...

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 28080 atoms, of which 40 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	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:

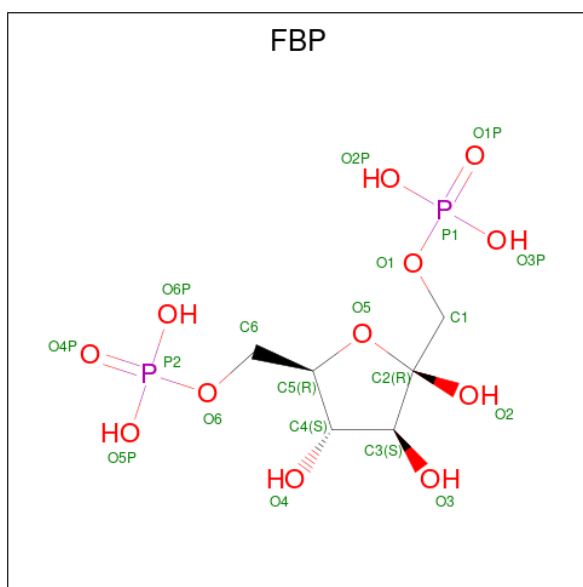
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q16716
A	0	SER	-	expression tag	UNP Q16716
A	12	ASP	SER	conflict	UNP Q16716
A	130	GLY	-	linker	UNP Q16716
A	131	SER	-	linker	UNP Q16716
A	230	GLY	-	linker	UNP Q16716
B	-1	GLY	-	expression tag	UNP Q16716
B	0	SER	-	expression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

Continued on next page...

Continued from previous page...

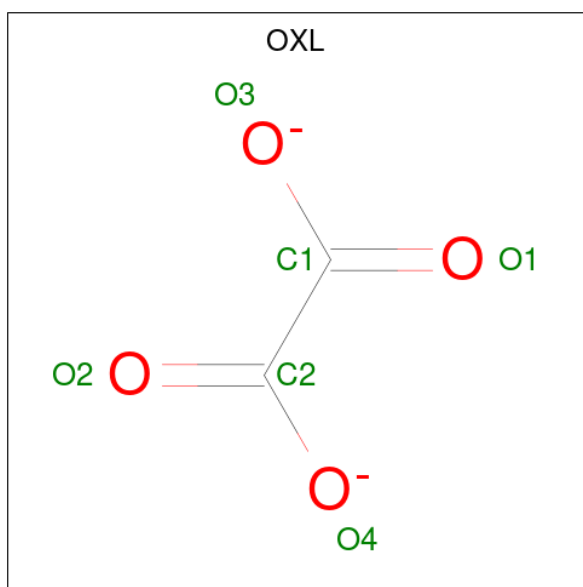
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP Q16716
C	12	ASP	SER	conflict	UNP Q16716
C	130	GLY	-	linker	UNP Q16716
C	131	SER	-	linker	UNP Q16716
C	132	GLY	-	linker	UNP Q16716
D	-1	GLY	-	expression tag	UNP Q16716
D	0	SER	-	expression tag	UNP Q16716
D	12	ASP	SER	conflict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

Continued on next page...

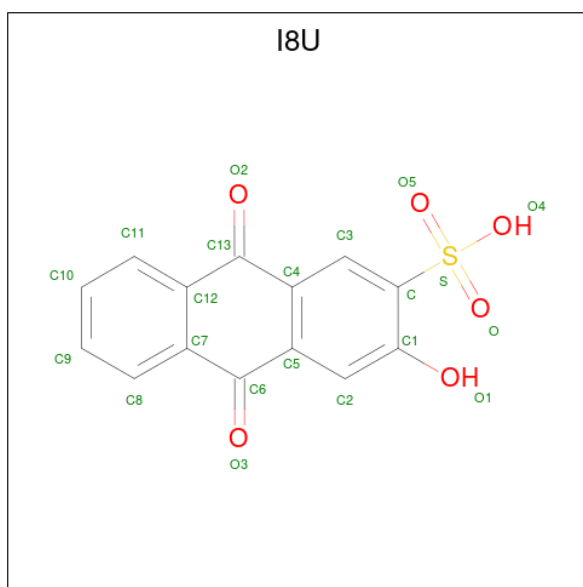
Continued from previous page...

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 3-hydroxy-9,10-dioxo-9,10-dihydroanthracene-2-sulfonic acid (CCD ID: I8U) (formula: C₁₄H₈O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	H	O	S	8	0
			29	14	8	6	1		
6	C	1	Total	C	H	O	S	8	0
			29	14	8	6	1		
6	E	1	Total	C	H	O	S	8	0
			29	14	8	6	1		
6	F	1	Total	C	H	O	S	8	0
			29	14	8	6	1		
6	G	1	Total	C	H	O	S	8	0
			29	14	8	6	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	116	Total	O	0	0
			116	116		
7	B	137	Total	O	0	0
			137	137		
7	C	213	Total	O	0	0
			213	213		
7	D	234	Total	O	0	0
			234	234		
7	E	104	Total	O	0	0
			104	104		
7	F	164	Total	O	0	0
			164	164		
7	G	249	Total	O	0	0
			249	249		

Continued on next page...

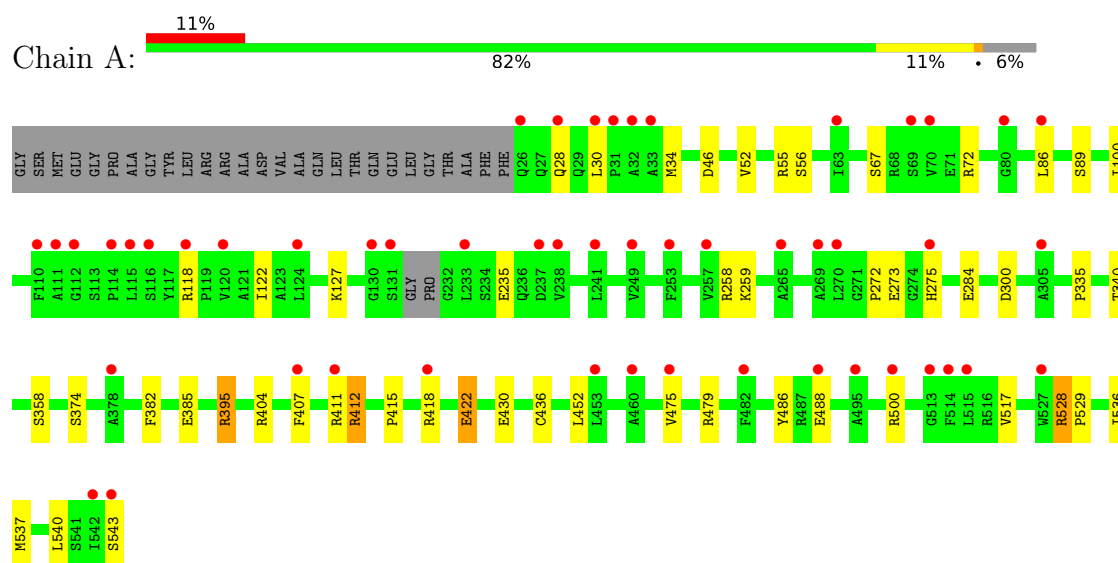
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	270	Total 270	O 270	0	0

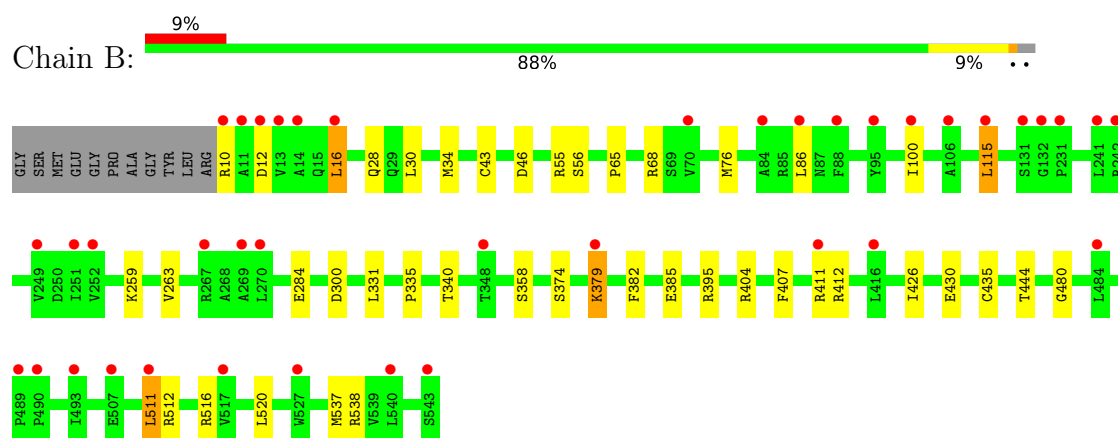
3 Residue-property plots [i](#)

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.

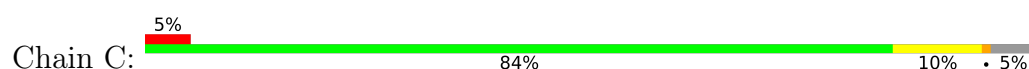
• Molecule 1: Pyruvate kinase

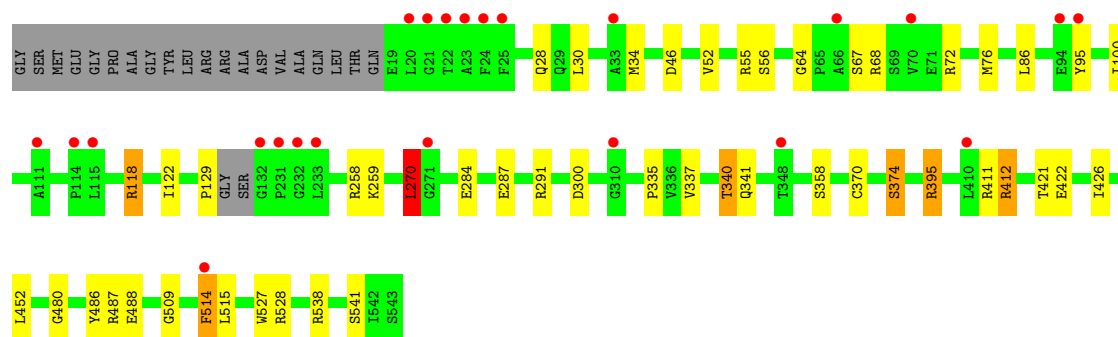


• Molecule 1: Pyruvate kinase

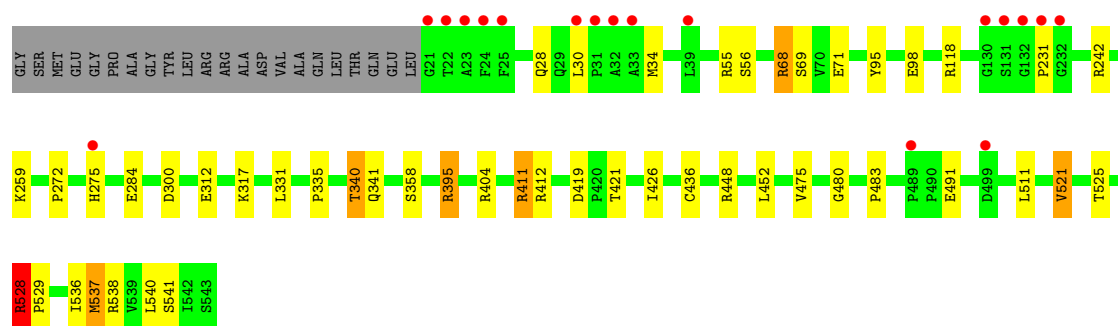
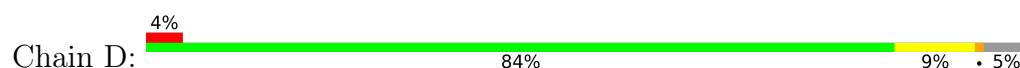


• Molecule 1: Pyruvate kinase

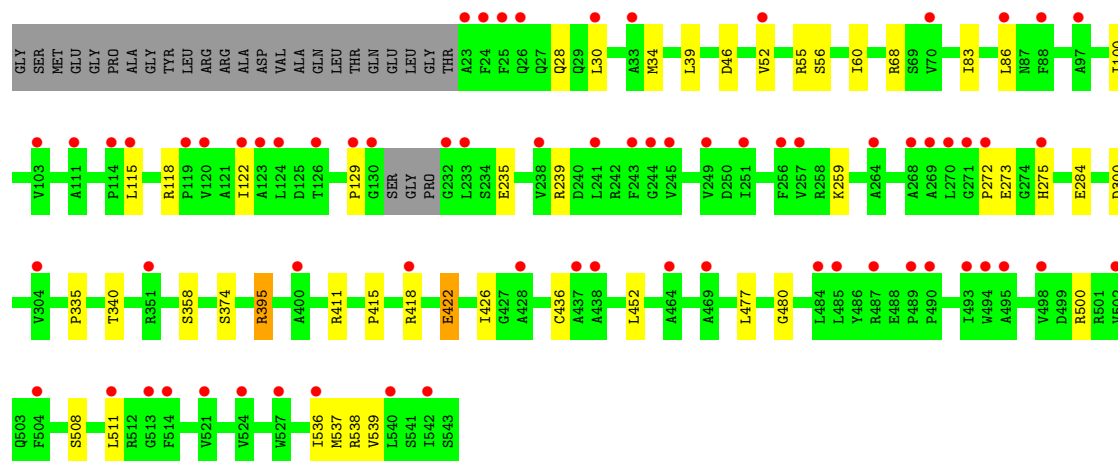
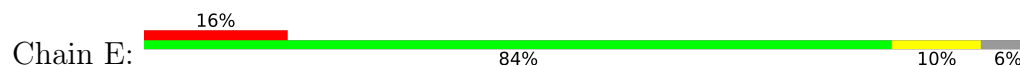




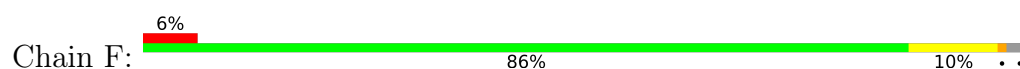
• Molecule 1: Pyruvate kinase



• Molecule 1: Pyruvate kinase

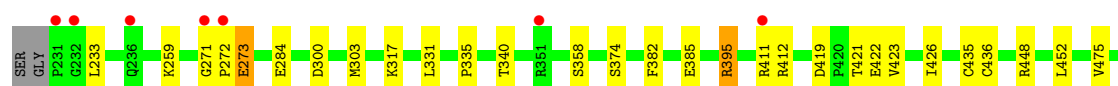
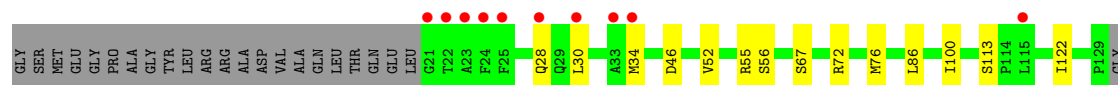
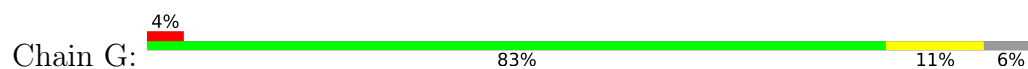


• Molecule 1: Pyruvate kinase

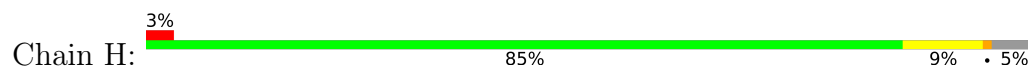




● Molecule 1: Pyruvate kinase



● 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	207.72Å 113.01Å 188.82Å 90.00° 91.63° 90.00°	Depositor
Resolution (Å)	103.82 – 2.04 103.82 – 2.04	Depositor EDS
% Data completeness (in resolution range)	62.5 (103.82-2.04) 62.5 (103.82-2.04)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.03Å)	Xtriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, R_{free}	0.202 , 0.226 0.194 , 0.219	Depositor DCC
R_{free} test set	8722 reflections (3.15%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.4	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	28080	wwPDB-VP
Average B, all atoms (Å ²)	53.0	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 50.52 % 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 6.3949e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OXL, K, FBP, I8U, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.72	1/3328 (0.0%)	1.05	1/4497 (0.0%)
1	B	0.74	2/3429 (0.1%)	1.05	1/4636 (0.0%)
1	C	0.79	1/3339 (0.0%)	1.07	7/4514 (0.2%)
1	D	0.78	1/3341 (0.0%)	1.05	3/4517 (0.1%)
1	E	0.68	1/3354 (0.0%)	1.02	1/4532 (0.0%)
1	F	0.72	0/3405	1.05	5/4603 (0.1%)
1	G	0.79	1/3324 (0.0%)	1.05	2/4493 (0.0%)
1	H	0.78	1/3357 (0.0%)	1.04	5/4537 (0.1%)
All	All	0.75	8/26877 (0.0%)	1.05	25/36329 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	374	SER	CA-C	8.02	1.56	1.52
1	B	374[A]	SER	CA-C	7.86	1.56	1.52
1	B	374[B]	SER	CA-C	7.86	1.56	1.52
1	C	374	SER	CA-C	7.36	1.56	1.52
1	E	374	SER	CA-C	6.89	1.55	1.52
1	G	303	MET	SD-CE	-5.53	1.65	1.79
1	D	537	MET	CA-C	5.52	1.59	1.52
1	H	303	MET	SD-CE	-5.35	1.66	1.79

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	514	PHE	CA-CB-CG	9.65	123.45	113.80
1	F	46	ASP	CA-CB-CG	6.23	118.83	112.60
1	G	514	PHE	CA-CB-CG	6.21	120.01	113.80
1	C	46	ASP	CA-CB-CG	5.62	118.22	112.60
1	C	515	LEU	N-CA-C	5.61	118.72	109.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	46	ASP	CA-CB-CG	5.46	118.06	112.60
1	C	270[A]	LEU	CA-C-N	5.45	130.43	121.87
1	C	270[A]	LEU	C-N-CA	5.45	130.43	121.87
1	C	270[B]	LEU	CA-C-N	5.45	130.43	121.87
1	C	270[B]	LEU	C-N-CA	5.45	130.43	121.87
1	F	497	ASP	CA-C-N	5.34	127.29	120.56
1	F	497	ASP	C-N-CA	5.34	127.29	120.56
1	E	46	ASP	CA-CB-CG	5.29	117.89	112.60
1	H	339	ALA	CA-C-N	5.24	131.54	121.54
1	H	339	ALA	C-N-CA	5.24	131.54	121.54
1	A	46	ASP	CA-CB-CG	5.20	117.80	112.60
1	D	528	ARG	CB-CG-CD	-5.19	99.37	111.30
1	H	46	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	46	ASP	CA-CB-CG	5.16	117.76	112.60
1	F	339	ALA	CA-C-N	5.12	131.32	121.54
1	F	339	ALA	C-N-CA	5.12	131.32	121.54
1	D	525	THR	CA-C-N	5.06	126.07	121.82
1	D	525	THR	C-N-CA	5.06	126.07	121.82
1	H	453	LEU	CA-C-N	5.00	126.98	120.28
1	H	453	LEU	C-N-CA	5.00	126.98	120.28

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	3350	0	3417	25	0
1	C	3264	0	3322	34	0
1	D	3261	0	3321	29	0
1	E	3261	0	3326	21	0
1	F	3327	0	3399	28	0
1	G	3246	0	3308	32	0
1	H	3277	0	3341	24	0
2	A	20	0	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	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	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	21	8	0	0	0
6	C	21	8	0	1	0
6	E	21	8	0	0	0
6	F	21	8	0	0	0
6	G	21	8	0	1	0
7	A	116	0	0	0	0
7	B	137	0	0	1	0
7	C	213	0	0	1	0
7	D	234	0	0	3	0
7	E	104	0	0	0	0
7	F	164	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	249	0	0	2	0
7	H	270	0	0	0	0
All	All	28040	40	26826	188	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 4.

All (188) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:415:PRO:HB3	1:F:12:ASP:HA	1.45	0.97
1:G:537:MET:HE3	1:H:537:MET:HG2	1.63	0.80
1:F:115:LEU:HD23	1:F:511:LEU:HB3	1.64	0.79
1:C:422[A]:GLU:HG3	1:C:452:LEU:HD13	1.67	0.77
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.69	0.75
1:E:415:PRO:HA	1:F:12:ASP:HB2	1.70	0.73
1:H:68:ARG:HH22	1:H:98:GLU:HB2	1.55	0.72
1:G:538:ARG:HG2	1:H:536:ILE:HG12	1.74	0.70
1:E:422:GLU:HG2	1:E:452:LEU:HD13	1.72	0.70
1:A:422:GLU:HG2	1:A:452:LEU:HD13	1.73	0.70
1:D:528:ARG:HD2	1:D:529:PRO:O	1.93	0.68
1:A:407:PHE:CE2	1:A:411:ARG:NH1	2.61	0.68
1:G:411:ARG:HG3	1:G:426:ILE:HD11	1.75	0.68
1:F:407:PHE:CE2	1:F:411:ARG:NH1	2.63	0.67
1:G:56:SER:HB2	1:G:480:GLY:HA2	1.76	0.66
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.76	0.66
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.78	0.66
1:H:68:ARG:NH2	1:H:95:TYR:O	2.28	0.66
1:E:235:GLU:O	1:E:239:ARG:HD3	1.96	0.66
1:E:418[B]:ARG:HG3	1:F:16:LEU:HD11	1.78	0.65
1:F:56:SER:HB2	1:F:480:GLY:HA2	1.79	0.64
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.80	0.63
1:D:68:ARG:NH2	1:D:95:TYR:O	2.31	0.63
1:A:418[B]:ARG:HG3	1:B:16:LEU:HD11	1.81	0.62
1:G:421:THR:HG22	1:G:452:LEU:HD12	1.81	0.62
1:D:68:ARG:HH22	1:D:98:GLU:HB2	1.64	0.61
1:H:56:SER:HB2	1:H:480:GLY:HA2	1.83	0.61
1:A:272:PRO:HA	1:A:275:HIS:NE2	2.16	0.60
1:E:415:PRO:CB	1:F:12:ASP:HA	2.25	0.59
1:E:56:SER:HB2	1:E:480:GLY:HA2	1.83	0.59
1:A:528:ARG:HD2	1:A:529:PRO:O	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:411:ARG:HG3	1:E:426:ILE:HD11	1.84	0.59
1:G:536:ILE:HG12	1:H:538[A]:ARG:HG2	1.85	0.58
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.85	0.58
1:C:538:ARG:HG2	1:D:536:ILE:HG12	1.86	0.56
1:E:538:ARG:HG2	1:F:536:ILE:HG12	1.87	0.56
1:H:68:ARG:NH2	1:H:98:GLU:HB2	2.21	0.55
1:G:537:MET:HE3	1:H:537:MET:CG	2.35	0.54
1:B:407:PHE:CE2	1:B:411:ARG:NH1	2.75	0.54
1:G:486:TYR:CZ	1:G:488:GLU:HB2	2.43	0.54
1:G:272:PRO:HD2	1:G:273:GLU:OE1	2.08	0.54
1:H:331:LEU:HD11	1:H:413:ALA:HB1	1.90	0.54
1:D:491:GLU:HB3	7:D:851:HOH:O	2.09	0.53
1:C:412:ARG:NH1	1:D:404:ARG:HH11	2.06	0.53
1:C:411:ARG:HH12	1:D:411:ARG:HH21	1.56	0.53
1:C:64:GLY:O	1:C:68:ARG:HG3	2.09	0.52
1:F:67:SER:HA	1:F:72:ARG:HG2	1.92	0.52
1:B:115:LEU:HD11	1:B:511:LEU:HB2	1.91	0.52
1:B:382:PHE:HB3	1:B:385:GLU:HB2	1.92	0.52
1:D:411:ARG:HG2	1:D:426:ILE:HD11	1.91	0.51
1:C:287:GLU:HG2	1:C:291:ARG:HD2	1.92	0.51
1:C:68:ARG:NE	1:C:95:TYR:CZ	2.79	0.51
1:D:272:PRO:HA	1:D:275[A]:HIS:CE1	2.46	0.51
1:G:374[B]:SER:OG	6:G:603:I8U:O	2.30	0.50
1:G:317:LYS:NZ	7:G:704:HOH:O	2.44	0.50
1:C:56:SER:HB2	1:C:480:GLY:CA	2.41	0.50
1:C:129:PRO:HG3	1:C:258:ARG:HH21	1.77	0.50
1:F:56:SER:HB2	1:F:480:GLY:CA	2.42	0.50
1:B:407:PHE:CD2	1:B:411:ARG:NH1	2.80	0.49
1:G:56:SER:HB2	1:G:480:GLY:CA	2.41	0.49
1:B:65:PRO:HG2	1:B:379:LYS:HZ2	1.76	0.49
1:E:536:ILE:HG12	1:F:538:ARG:HG2	1.93	0.49
1:F:233:LEU:HD12	7:F:737:HOH:O	2.12	0.49
1:B:411:ARG:HG2	1:B:426:ILE:HD11	1.94	0.49
1:F:287:GLU:OE2	1:F:291:ARG:NH1	2.46	0.49
1:F:30:LEU:O	1:F:34:MET:HG2	2.12	0.48
1:H:272:PRO:HA	1:H:275[A]:HIS:CE1	2.48	0.48
1:A:30:LEU:O	1:A:34:MET:HG2	2.14	0.48
1:B:56:SER:HB2	1:B:480:GLY:CA	2.43	0.48
1:E:272:PRO:HA	1:E:275[A]:HIS:CE1	2.47	0.48
1:G:412:ARG:CZ	1:H:404:ARG:HD3	2.44	0.48
1:D:30:LEU:O	1:D:34:MET:HG2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:412:ARG:NH2	1:H:404:ARG:HD3	2.28	0.48
1:H:56:SER:HB2	1:H:480:GLY:CA	2.44	0.48
1:A:404:ARG:HD3	7:B:794:HOH:O	2.13	0.48
1:C:30:LEU:O	1:C:34:MET:HG2	2.14	0.48
1:C:411:ARG:HH12	1:D:411:ARG:NH2	2.13	0.47
1:A:28:GLN:HB3	1:A:52:VAL:HG22	1.96	0.47
1:C:67:SER:HA	1:C:72:ARG:HG2	1.95	0.47
1:H:30:LEU:O	1:H:34:MET:HG2	2.14	0.47
1:A:67:SER:HA	1:A:72:ARG:HG2	1.97	0.47
1:B:30:LEU:O	1:B:34:MET:HG2	2.14	0.47
1:F:317:LYS:NZ	7:F:709:HOH:O	2.47	0.47
1:G:28:GLN:HB3	1:G:52:VAL:HG22	1.97	0.47
1:G:30:LEU:O	1:G:34:MET:HG2	2.15	0.47
1:G:100:ILE:HG23	1:G:122:ILE:HD13	1.97	0.46
1:C:118:ARG:HD2	7:C:902:HOH:O	2.16	0.46
1:C:528:ARG:NH2	1:G:233:LEU:O	2.37	0.46
1:F:86:LEU:HD11	1:F:100:ILE:HG12	1.97	0.46
1:B:115:LEU:HD21	1:B:511:LEU:HD23	1.98	0.46
1:C:100:ILE:HG23	1:C:122:ILE:HD13	1.97	0.46
1:E:55:ARG:HB2	1:E:395:ARG:HG3	1.98	0.46
1:D:28:GLN:HG3	1:D:30:LEU:HG	1.99	0.45
1:G:55:ARG:HB2	1:G:395:ARG:HG3	1.98	0.45
1:B:300:ASP:O	1:B:335:PRO:HD2	2.16	0.45
1:G:86:LEU:HD11	1:G:100:ILE:HG12	1.98	0.45
1:C:421:THR:HG22	1:C:452:LEU:HD12	1.98	0.45
1:F:28:GLN:HG3	1:F:30:LEU:HG	1.99	0.45
1:C:412:ARG:HH12	1:D:404:ARG:HH11	1.64	0.45
1:C:300:ASP:O	1:C:335:PRO:HD2	2.17	0.45
1:D:521:VAL:HG12	1:D:540:LEU:HB3	1.97	0.45
1:F:68:ARG:NH2	1:F:98:GLU:HB3	2.32	0.45
1:B:28:GLN:HG3	1:B:30:LEU:HG	1.98	0.45
1:F:300:ASP:O	1:F:335:PRO:HD2	2.17	0.45
1:D:55:ARG:HB2	1:D:395:ARG:HG3	1.99	0.45
1:E:56:SER:HB2	1:E:480:GLY:CA	2.46	0.45
1:H:300:ASP:O	1:H:335:PRO:HD2	2.17	0.45
1:C:55:ARG:HB2	1:C:395:ARG:HG3	1.99	0.44
1:C:411:ARG:HG2	1:C:426:ILE:HD11	1.99	0.44
1:D:300:ASP:O	1:D:335:PRO:HD2	2.17	0.44
1:A:300:ASP:O	1:A:335:PRO:HD2	2.17	0.44
1:C:374:SER:HB3	6:C:603:I8U:O	2.17	0.44
1:E:28:GLN:HG3	1:E:30:LEU:HG	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:ASP:OD2	1:D:448:ARG:NH2	2.50	0.44
1:C:411:ARG:NH1	1:D:411:ARG:NH2	2.66	0.44
1:H:28:GLN:HG3	1:H:30:LEU:HG	2.00	0.44
1:A:55:ARG:HB2	1:A:395:ARG:HG3	2.00	0.44
1:A:100:ILE:HG23	1:A:122:ILE:HD13	2.00	0.44
1:A:430:GLU:OE2	1:B:430[A]:GLU:OE1	2.36	0.44
1:B:115:LEU:HD11	1:B:511:LEU:CB	2.48	0.44
1:A:89:SER:HA	1:A:127:LYS:HG3	1.99	0.43
1:C:86:LEU:HD11	1:C:100:ILE:HG12	2.01	0.43
1:A:486:TYR:CZ	1:A:488[B]:GLU:HB2	2.54	0.43
1:C:28:GLN:HG3	1:C:30:LEU:HG	2.00	0.43
1:A:28:GLN:HG3	1:A:30:LEU:HG	2.01	0.43
1:C:340:THR:HG22	1:C:341:GLN:HG3	2.01	0.43
1:F:113:SER:OG	1:F:115:LEU:HD12	2.18	0.43
1:F:382:PHE:HB3	1:F:385:GLU:HB2	1.99	0.43
1:H:290:LYS:HA	1:H:290:LYS:HD2	1.87	0.43
1:D:421:THR:HG22	1:D:452:LEU:HD12	2.00	0.43
1:G:28:GLN:HG3	1:G:30:LEU:HG	2.01	0.43
1:D:56:SER:HB2	1:D:480:GLY:CA	2.47	0.43
1:H:68:ARG:HD2	1:H:95:TYR:OH	2.19	0.43
1:C:412:ARG:NH1	1:D:404:ARG:NH1	2.66	0.42
1:D:71[B]:GLU:CD	1:D:71[B]:GLU:H	2.27	0.42
1:D:312:GLU:HB3	7:D:846:HOH:O	2.18	0.42
1:G:419:ASP:OD2	1:G:448:ARG:NH2	2.51	0.42
1:B:435:CYS:HB2	1:B:520:LEU:HD12	2.00	0.42
1:B:86:LEU:HD11	1:B:100:ILE:HG12	2.01	0.42
1:F:421:THR:HG22	1:F:452:LEU:HD12	2.01	0.42
1:C:28:GLN:HB3	1:C:52:VAL:HG22	2.00	0.42
1:G:300:ASP:O	1:G:335:PRO:HD2	2.19	0.42
1:H:55:ARG:HB2	1:H:395:ARG:HG3	2.00	0.42
1:B:115:LEU:HD12	1:B:512:ARG:HG3	2.02	0.42
1:E:300:ASP:O	1:E:335:PRO:HD2	2.19	0.42
1:F:407:PHE:CZ	1:F:411:ARG:NH1	2.88	0.42
1:G:486:TYR:CE2	1:G:488:GLU:HB2	2.53	0.42
1:E:28:GLN:HB3	1:E:52:VAL:HG22	2.01	0.42
1:G:382:PHE:HB3	1:G:385:GLU:HB2	2.01	0.42
1:A:517:VAL:HG22	1:A:543:SER:HB3	2.02	0.41
1:B:43:CYS:SG	1:D:331:LEU:HD22	2.60	0.41
1:C:527:TRP:CE2	1:C:528:ARG:HG2	2.55	0.41
1:A:415:PRO:HB3	1:B:12:ASP:HA	2.02	0.41
1:E:39:LEU:HG	1:G:331:LEU:HD13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:LEU:HD12	1:B:331:LEU:HA	1.95	0.41
1:E:86:LEU:HD11	1:E:100:ILE:HG12	2.01	0.41
1:F:411:ARG:HH11	1:F:411:ARG:HB2	1.85	0.41
1:A:382:PHE:HB3	1:A:385:GLU:HB2	2.02	0.41
1:C:486:TYR:CZ	1:C:488:GLU:HB2	2.55	0.41
1:G:67:SER:HA	1:G:72:ARG:HG2	2.02	0.41
1:G:271:GLY:HA2	7:G:788:HOH:O	2.19	0.41
1:H:60:ILE:HG12	1:H:83:ILE:HB	2.02	0.41
1:D:340:THR:HG22	1:D:341:GLN:HG3	2.03	0.41
1:B:444:THR:OG1	2:B:601:FBP:O4P	2.37	0.41
1:F:55:ARG:HB2	1:F:395:ARG:HG3	2.02	0.41
1:A:407:PHE:CZ	1:A:411:ARG:NH1	2.88	0.41
1:D:317:LYS:NZ	7:D:711:HOH:O	2.52	0.41
1:D:475:VAL:CG2	1:D:483:PRO:HB3	2.51	0.41
1:E:60:ILE:HG12	1:E:83:ILE:HB	2.03	0.41
1:H:421:THR:HG22	1:H:452:LEU:HD12	2.03	0.41
1:A:412:ARG:NH1	1:B:404:ARG:HH11	2.19	0.41
1:D:68:ARG:NH2	1:D:98:GLU:HB2	2.33	0.41
1:H:258:ARG:HD3	1:H:285:ASN:HD21	1.86	0.41
1:G:435:CYS:HB2	1:G:520:LEU:HD12	2.03	0.40
1:F:258:ARG:HD3	1:F:285:ASN:HD21	1.87	0.40
1:B:55:ARG:HB2	1:B:395:ARG:HG2	2.03	0.40
1:C:270[A]:LEU:HD12	1:C:270[A]:LEU:HA	1.99	0.40
1:C:509:GLY:HA2	1:C:514:PHE:HD2	1.86	0.40
1:F:100:ILE:HG23	1:F:122:ILE:HD13	2.03	0.40
1:F:435:CYS:HB2	1:F:520:LEU:HD12	2.03	0.40
1:G:423:VAL:HG21	1:H:435:CYS:HB3	2.02	0.40
1:G:527:TRP:CD2	1:G:528:ARG:HG2	2.55	0.40
1:H:233:LEU:HD12	1:H:233:LEU:HA	1.83	0.40
1:C:337:VAL:HG22	1:C:370:CYS:HB2	2.04	0.40
1:C:486:TYR:CE2	1:C:488:GLU:HB2	2.57	0.40
1:A:56:SER:HB3	1:A:479:ARG:HG2	2.02	0.40
1:E:100:ILE:HG23	1:E:122:ILE:HD13	2.04	0.40
1:E:335:PRO:HB3	1:E:477:LEU:O	2.21	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%)	423 (99%)	3 (1%)	1 (0%)	43	37
1	B	442/447 (99%)	436 (99%)	5 (1%)	1 (0%)	43	37
1	C	428/447 (96%)	421 (98%)	6 (1%)	1 (0%)	43	37
1	D	431/447 (96%)	426 (99%)	3 (1%)	2 (0%)	24	16
1	E	429/447 (96%)	425 (99%)	2 (0%)	2 (0%)	24	16
1	F	436/447 (98%)	432 (99%)	3 (1%)	1 (0%)	43	37
1	G	426/447 (95%)	421 (99%)	4 (1%)	1 (0%)	43	37
1	H	432/447 (97%)	427 (99%)	3 (1%)	2 (0%)	24	16
All	All	3451/3576 (96%)	3411 (99%)	29 (1%)	11 (0%)	36	30

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	231	PRO
1	B	340	THR
1	D	340	THR
1	E	129	PRO
1	E	340	THR
1	F	340	THR
1	H	340	THR
1	A	340	THR
1	C	340	THR
1	G	340	THR
1	D	231	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%)	327 (95%)	18 (5%)	21	14
1	B	353/352 (100%)	337 (96%)	16 (4%)	24	18
1	C	344/352 (98%)	331 (96%)	13 (4%)	29	24
1	D	344/352 (98%)	326 (95%)	18 (5%)	21	14
1	E	346/352 (98%)	329 (95%)	17 (5%)	22	15
1	F	351/352 (100%)	338 (96%)	13 (4%)	30	25
1	G	343/352 (97%)	333 (97%)	10 (3%)	37	33
1	H	345/352 (98%)	332 (96%)	13 (4%)	29	24
All	All	2771/2816 (98%)	2653 (96%)	118 (4%)	28	20

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	118	ARG
1	A	235	GLU
1	A	258	ARG
1	A	259	LYS
1	A	273	GLU
1	A	284	GLU
1	A	358	SER
1	A	395	ARG
1	A	412	ARG
1	A	422	GLU
1	A	436	CYS
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	68	ARG
1	B	76[A]	MET
1	B	76[B]	MET
1	B	115	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	259	LYS
1	B	263	VAL
1	B	284	GLU
1	B	358	SER
1	B	379	LYS
1	B	412	ARG
1	B	511	LEU
1	B	516	ARG
1	B	537[A]	MET
1	B	537[B]	MET
1	C	76[A]	MET
1	C	76[B]	MET
1	C	118	ARG
1	C	259	LYS
1	C	270[A]	LEU
1	C	270[B]	LEU
1	C	284	GLU
1	C	358	SER
1	C	395	ARG
1	C	412	ARG
1	C	487	ARG
1	C	541[A]	SER
1	C	541[B]	SER
1	D	68	ARG
1	D	69	SER
1	D	118	ARG
1	D	242[A]	ARG
1	D	242[B]	ARG
1	D	259	LYS
1	D	284	GLU
1	D	358	SER
1	D	395	ARG
1	D	411	ARG
1	D	412	ARG
1	D	436	CYS
1	D	511	LEU
1	D	521	VAL
1	D	528	ARG
1	D	537	MET
1	D	538	ARG
1	D	541	SER
1	E	34	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	68	ARG
1	E	115	LEU
1	E	118	ARG
1	E	259	LYS
1	E	273	GLU
1	E	284	GLU
1	E	358	SER
1	E	395	ARG
1	E	422	GLU
1	E	436	CYS
1	E	500	ARG
1	E	508	SER
1	E	511	LEU
1	E	537[A]	MET
1	E	537[B]	MET
1	E	539	VAL
1	F	16	LEU
1	F	76[A]	MET
1	F	76[B]	MET
1	F	94	GLU
1	F	115	LEU
1	F	259	LYS
1	F	284	GLU
1	F	358	SER
1	F	395	ARG
1	F	408	GLU
1	F	511	LEU
1	F	537[A]	MET
1	F	537[B]	MET
1	G	76[A]	MET
1	G	76[B]	MET
1	G	113	SER
1	G	259	LYS
1	G	273	GLU
1	G	284	GLU
1	G	358	SER
1	G	395	ARG
1	G	436	CYS
1	G	475	VAL
1	H	118	ARG
1	H	242[A]	ARG
1	H	242[B]	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	259	LYS
1	H	273	GLU
1	H	284	GLU
1	H	331	LEU
1	H	358	SER
1	H	395	ARG
1	H	411	ARG
1	H	511	LEU
1	H	537	MET
1	H	541	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	405	GLN
1	B	236	GLN
1	B	405	GLN
1	C	275	HIS
1	C	405	GLN
1	D	27	GLN
1	D	390	GLN
1	D	405	GLN
1	D	535	ASN
1	E	405	GLN
1	F	236	GLN
1	F	405	GLN
1	G	405	GLN
1	G	503	GLN
1	H	390	GLN
1	H	405	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 37 ligands modelled in this entry, 16 are monoatomic - leaving 21 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	E	601	-	18,20,20	0.48	0	21,32,32	0.76	1 (4%)
3	OXL	D	602	4	5,5,5	2.18	2 (40%)	6,6,6	2.59	4 (66%)
6	I8U	G	603	-	23,23,23	0.43	0	35,36,36	0.41	0
3	OXL	C	602	4	5,5,5	1.86	2 (40%)	6,6,6	1.26	1 (16%)
3	OXL	H	602	4	5,5,5	1.96	2 (40%)	6,6,6	1.36	1 (16%)
2	FBP	D	601	-	18,20,20	0.63	0	21,32,32	0.89	1 (4%)
2	FBP	F	601	-	18,20,20	0.35	0	21,32,32	0.57	0
2	FBP	C	601	-	18,20,20	0.78	1 (5%)	21,32,32	0.76	0
2	FBP	A	601	-	18,20,20	0.60	0	21,32,32	0.79	0
6	I8U	C	603	-	23,23,23	0.59	1 (4%)	35,36,36	0.35	0
6	I8U	E	603	-	23,23,23	0.62	1 (4%)	35,36,36	0.40	0
6	I8U	B	603	-	23,23,23	0.68	1 (4%)	35,36,36	0.40	0
2	FBP	G	601	-	18,20,20	0.71	1 (5%)	21,32,32	0.67	0
3	OXL	A	602	4	5,5,5	2.08	2 (40%)	6,6,6	2.43	3 (50%)
2	FBP	B	601	-	18,20,20	0.72	0	21,32,32	0.82	2 (9%)
2	FBP	H	601	-	18,20,20	0.73	0	21,32,32	0.84	1 (4%)
3	OXL	F	602	4	5,5,5	2.78	4 (80%)	6,6,6	2.86	3 (50%)
3	OXL	E	602	4	5,5,5	2.35	2 (40%)	6,6,6	1.54	2 (33%)
3	OXL	G	602	4	5,5,5	2.29	3 (60%)	6,6,6	2.99	4 (66%)
6	I8U	F	603	-	23,23,23	0.41	0	35,36,36	0.48	0
3	OXL	B	602	4	5,5,5	2.56	2 (40%)	6,6,6	1.07	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	E	601	-	-	5/13/32/32	0/1/1/1
3	OXL	D	602	4	-	4/4/4/4	-
6	I8U	G	603	-	-	0/6/22/22	0/3/3/3
3	OXL	C	602	4	-	4/4/4/4	-
3	OXL	H	602	4	-	4/4/4/4	-
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
6	I8U	C	603	-	-	4/6/22/22	0/3/3/3
6	I8U	E	603	-	-	4/6/22/22	0/3/3/3
6	I8U	B	603	-	-	4/6/22/22	0/3/3/3
2	FBP	G	601	-	-	2/13/32/32	0/1/1/1
3	OXL	A	602	4	-	4/4/4/4	-
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1
3	OXL	F	602	4	-	4/4/4/4	-
3	OXL	E	602	4	-	4/4/4/4	-
3	OXL	G	602	4	-	4/4/4/4	-
6	I8U	F	603	-	-	3/6/22/22	0/3/3/3
3	OXL	B	602	4	-	4/4/4/4	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	OXL	O2-C2	4.78	1.34	1.22
3	E	602	OXL	O1-C1	4.43	1.33	1.22
3	A	602	OXL	O2-C2	4.02	1.32	1.22
3	D	602	OXL	O2-C2	3.74	1.31	1.22
3	F	602	OXL	O3-C1	-3.58	1.20	1.30
3	F	602	OXL	O2-C2	3.55	1.31	1.22
3	H	602	OXL	O2-C2	3.24	1.30	1.22
6	B	603	I8U	C-S	-3.09	1.69	1.77
3	G	602	OXL	O1-C1	3.05	1.30	1.22
3	C	602	OXL	O1-C1	3.01	1.30	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	602	OXL	O3-C1	-2.94	1.22	1.30
3	H	602	OXL	O4-C2	-2.86	1.22	1.30
6	E	603	I8U	C-S	-2.85	1.70	1.77
3	B	602	OXL	O4-C2	-2.84	1.22	1.30
3	D	602	OXL	O4-C2	-2.80	1.23	1.30
3	F	602	OXL	O1-C1	2.79	1.29	1.22
3	C	602	OXL	O3-C1	-2.71	1.23	1.30
6	C	603	I8U	C-S	-2.70	1.70	1.77
3	G	602	OXL	C2-C1	-2.56	1.50	1.54
3	E	602	OXL	O3-C1	-2.49	1.23	1.30
2	C	601	FBP	P1-O3P	-2.47	1.45	1.54
3	F	602	OXL	O4-C2	-2.36	1.24	1.30
3	A	602	OXL	O4-C2	-2.30	1.24	1.30
2	G	601	FBP	P2-O6P	-2.10	1.47	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	602	OXL	O3-C1-C2	4.75	122.05	112.83
3	F	602	OXL	O4-C2-C1	4.44	121.44	112.83
3	A	602	OXL	O4-C2-C1	4.13	120.84	112.83
3	F	602	OXL	O3-C1-C2	4.04	120.66	112.83
3	D	602	OXL	O4-C2-C1	3.79	120.17	112.83
3	D	602	OXL	O3-C1-C2	3.67	119.95	112.83
3	G	602	OXL	O4-C2-C1	3.47	119.57	112.83
3	G	602	OXL	O1-C1-C2	-3.47	113.40	120.63
2	D	601	FBP	O5P-P2-O6	3.33	115.35	106.67
3	F	602	OXL	O2-C2-C1	-3.04	114.29	120.63
3	A	602	OXL	O3-C1-C2	3.03	118.71	112.83
3	H	602	OXL	O4-C2-C1	2.86	118.39	112.83
3	E	602	OXL	O3-C1-C2	2.76	118.18	112.83
3	C	602	OXL	O3-C1-C2	2.73	118.13	112.83
3	A	602	OXL	O2-C2-C1	-2.71	114.99	120.63
3	G	602	OXL	O2-C2-C1	-2.57	115.29	120.63
3	D	602	OXL	O1-C1-C2	-2.53	115.36	120.63
2	H	601	FBP	O5P-P2-O6	2.47	113.11	106.67
3	D	602	OXL	O2-C2-C1	-2.46	115.51	120.63
2	E	601	FBP	O3P-P1-O2P	2.36	116.67	107.80
3	E	602	OXL	O4-C2-C1	2.19	117.07	112.83
2	B	601	FBP	O5P-P2-O6	2.05	112.03	106.67
2	B	601	FBP	O3P-P1-O2P	2.03	115.40	107.80

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	601	FBP	C1-O1-P1-O1P
2	E	601	FBP	C6-O6-P2-O4P
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	D	601	FBP	C4-C5-C6-O6
2	F	601	FBP	C4-C5-C6-O6
2	H	601	FBP	C4-C5-C6-O6
2	E	601	FBP	C4-C5-C6-O6
2	G	601	FBP	C4-C5-C6-O6
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	F	601	FBP	O5-C5-C6-O6
2	H	601	FBP	O5-C5-C6-O6
2	C	601	FBP	O5-C5-C6-O6
6	B	603	I8U	C1-C-S-O5
6	B	603	I8U	C1-C-S-O
6	C	603	I8U	C1-C-S-O5
6	E	603	I8U	C1-C-S-O5
6	E	603	I8U	C1-C-S-O
2	E	601	FBP	O5-C5-C6-O6
3	A	602	OXL	O3-C1-C2-O4
3	B	602	OXL	O3-C1-C2-O4
3	D	602	OXL	O3-C1-C2-O4
3	E	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
6	B	603	I8U	C3-C-S-O5
6	E	603	I8U	C3-C-S-O5
6	F	603	I8U	C3-C-S-O5
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	E	602	OXL	O1-C1-C2-O2
3	H	602	OXL	O3-C1-C2-O4
6	C	603	I8U	C1-C-S-O
3	C	602	OXL	O1-C1-C2-O2
3	F	602	OXL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	G	602	OXL	O1-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O2
6	F	603	I8U	C3-C-S-O4
2	G	601	FBP	O5-C5-C6-O6
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	B	602	OXL	O3-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O4
3	D	602	OXL	O3-C1-C2-O2
3	E	602	OXL	O1-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O2
3	F	602	OXL	O3-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O4
3	C	602	OXL	O3-C1-C2-O2
3	G	602	OXL	O3-C1-C2-O2
3	C	602	OXL	O1-C1-C2-O4
3	F	602	OXL	O1-C1-C2-O4
3	G	602	OXL	O1-C1-C2-O4
2	E	601	FBP	C6-O6-P2-O5P
3	H	602	OXL	O3-C1-C2-O2
6	C	603	I8U	C3-C-S-O5
6	F	603	I8U	C1-C-S-O5
6	B	603	I8U	C3-C-S-O4
6	C	603	I8U	C3-C-S-O4
6	E	603	I8U	C3-C-S-O4

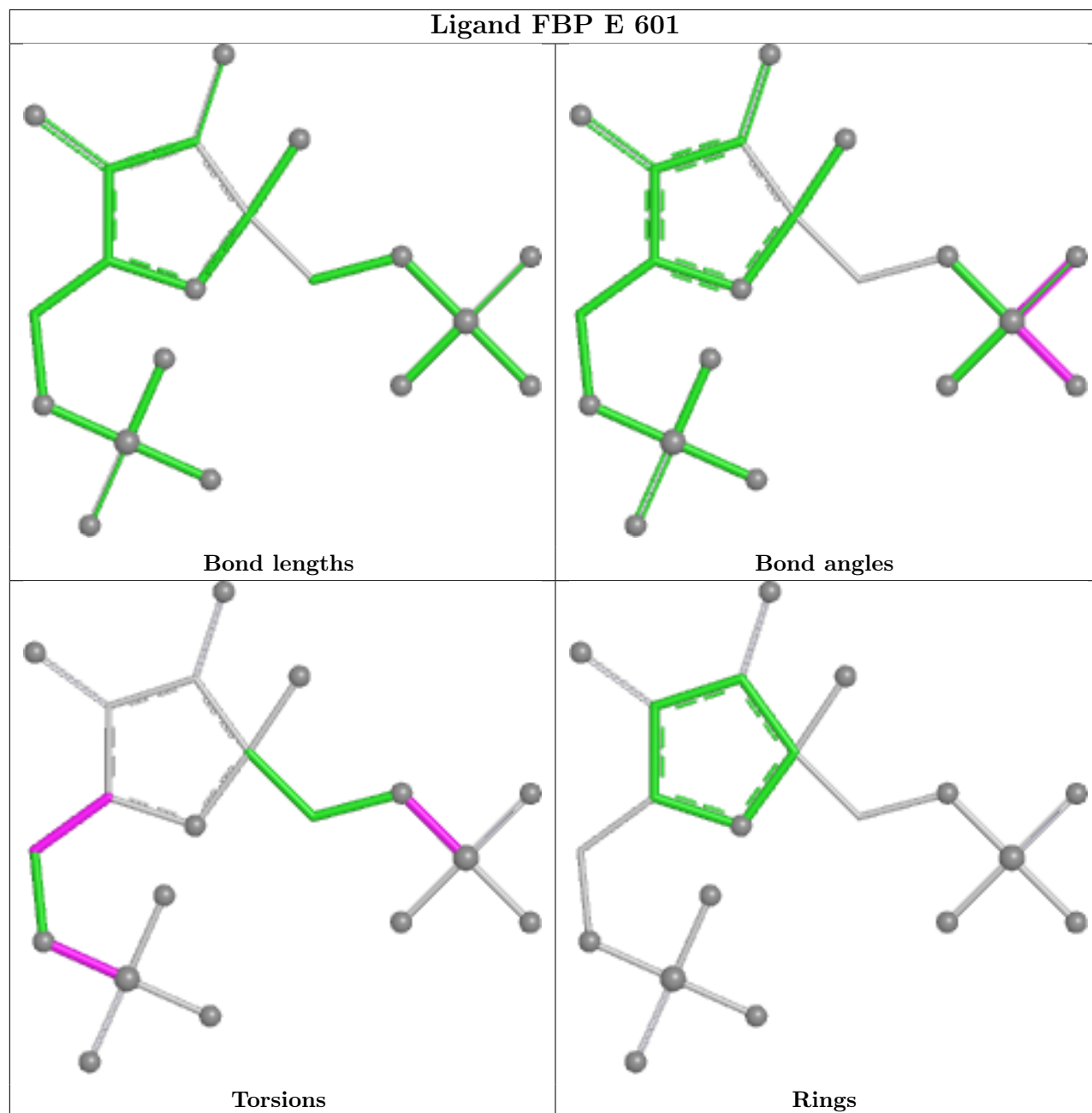
There are no ring outliers.

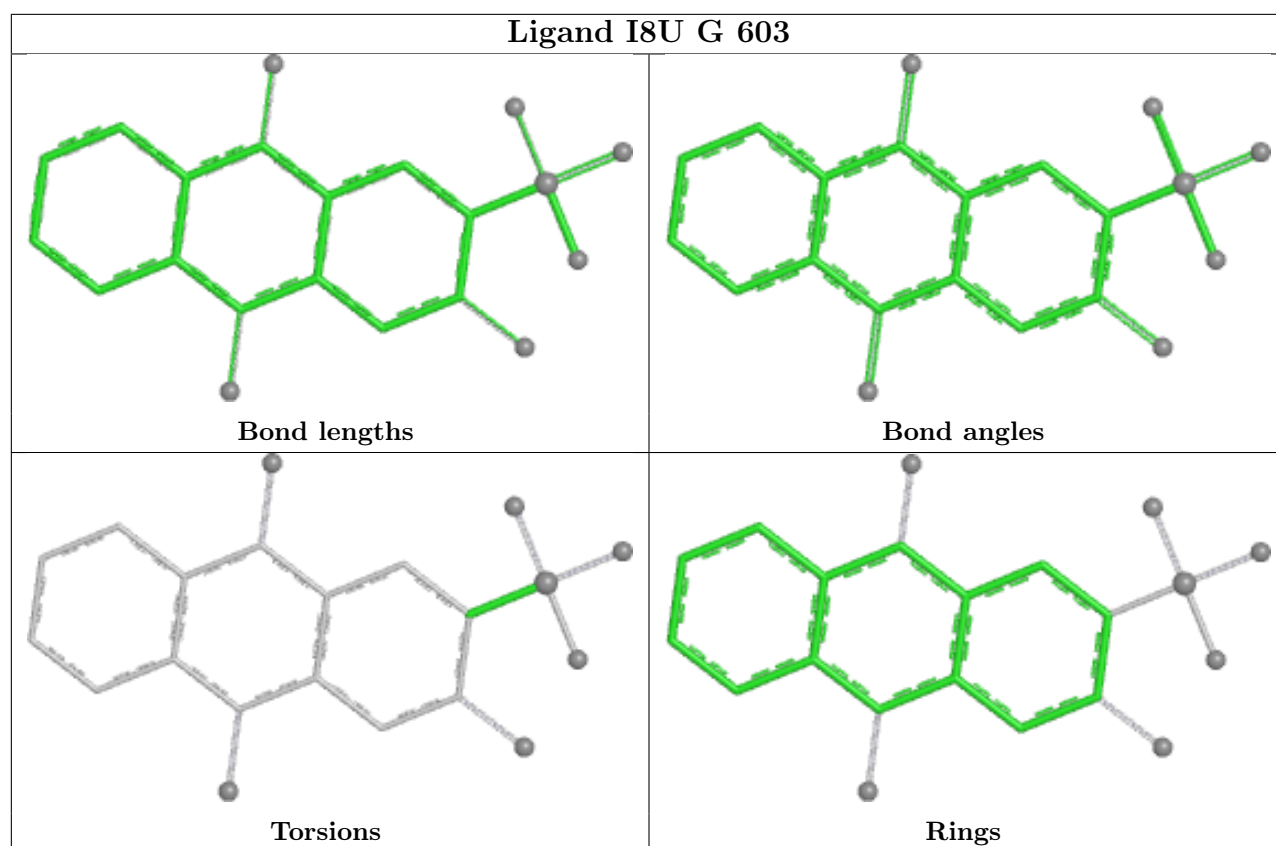
3 monomers are involved in 3 short contacts:

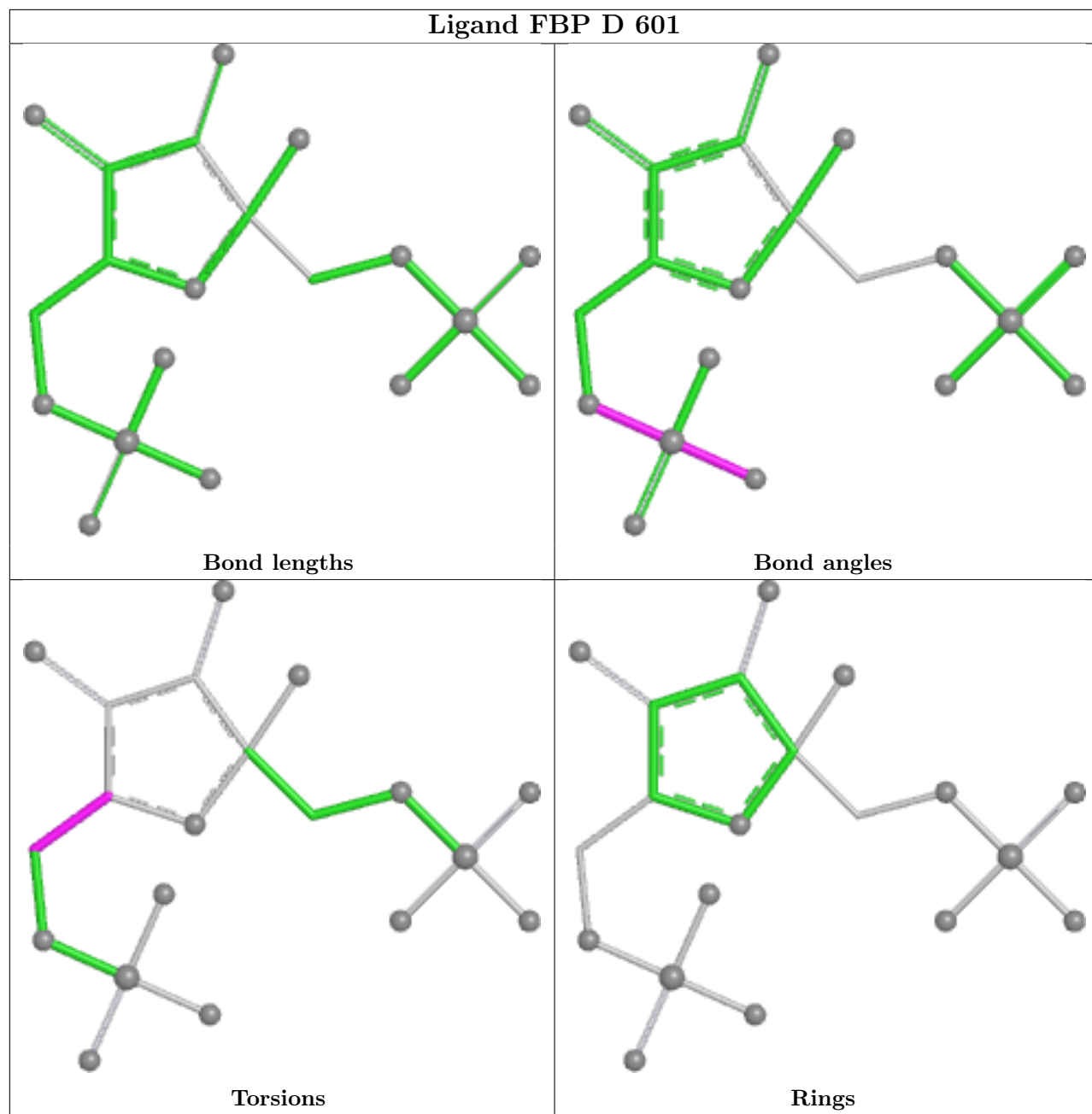
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	603	I8U	1	0
6	C	603	I8U	1	0
2	B	601	FBP	1	0

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

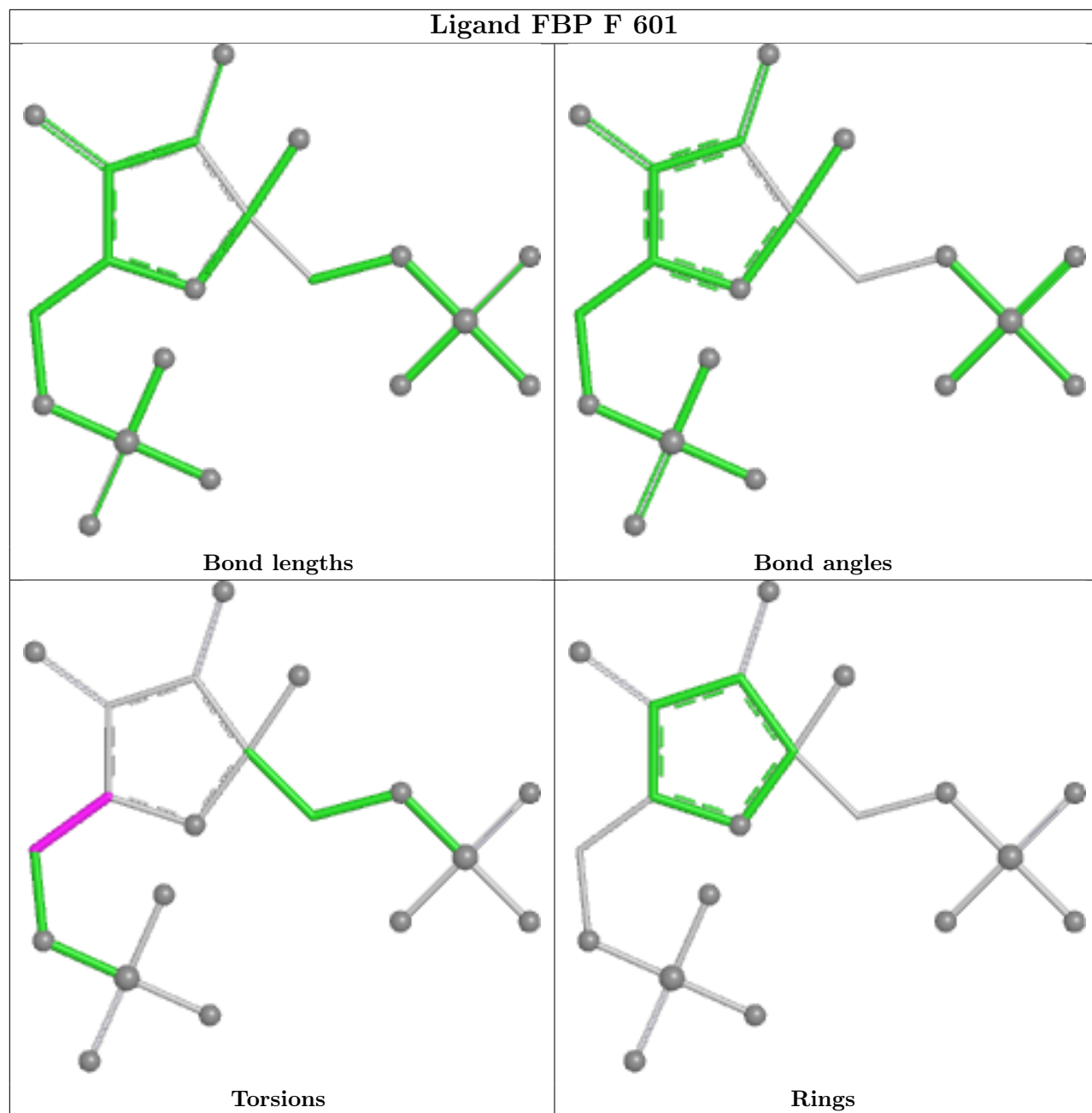
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

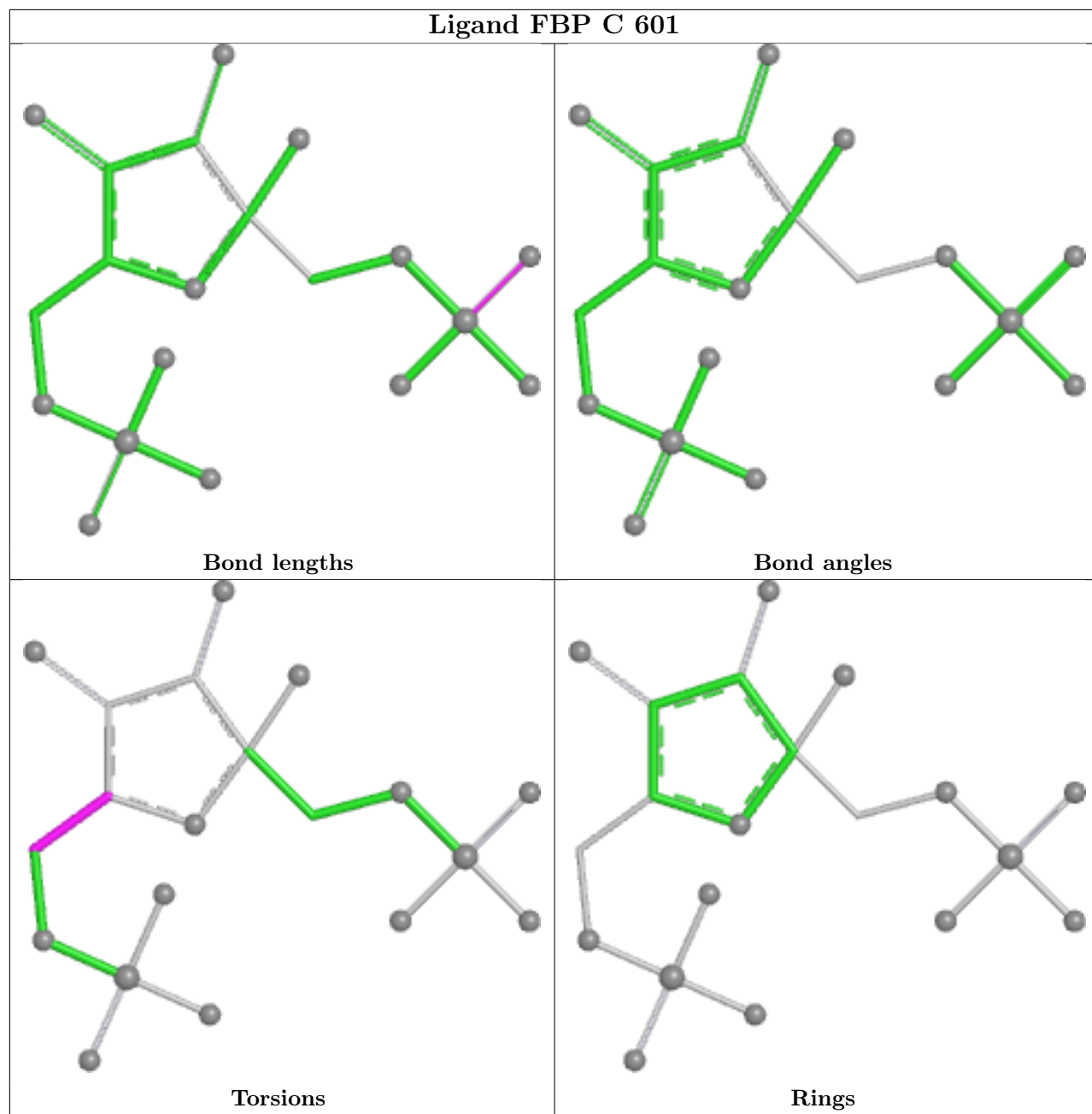


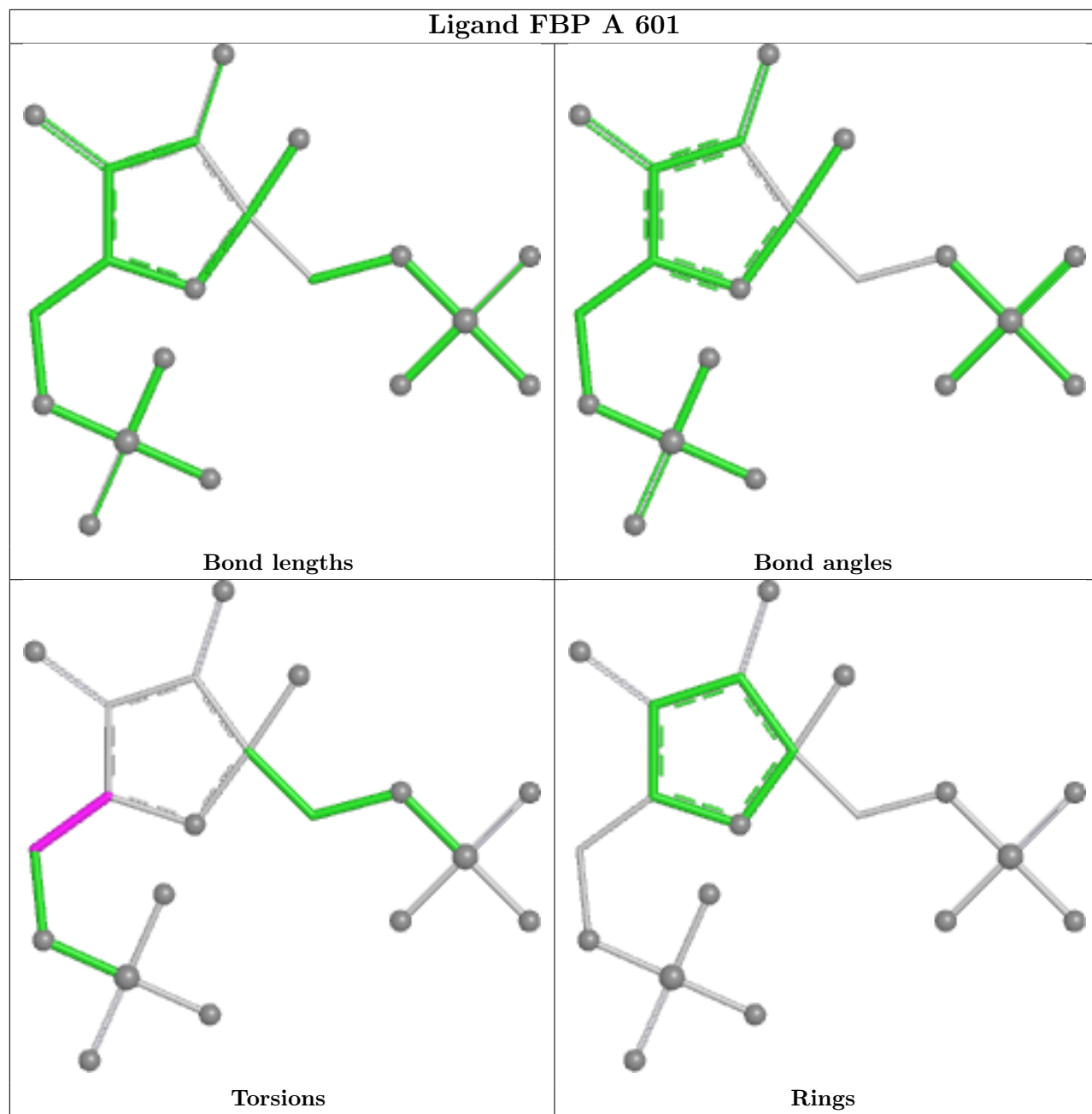




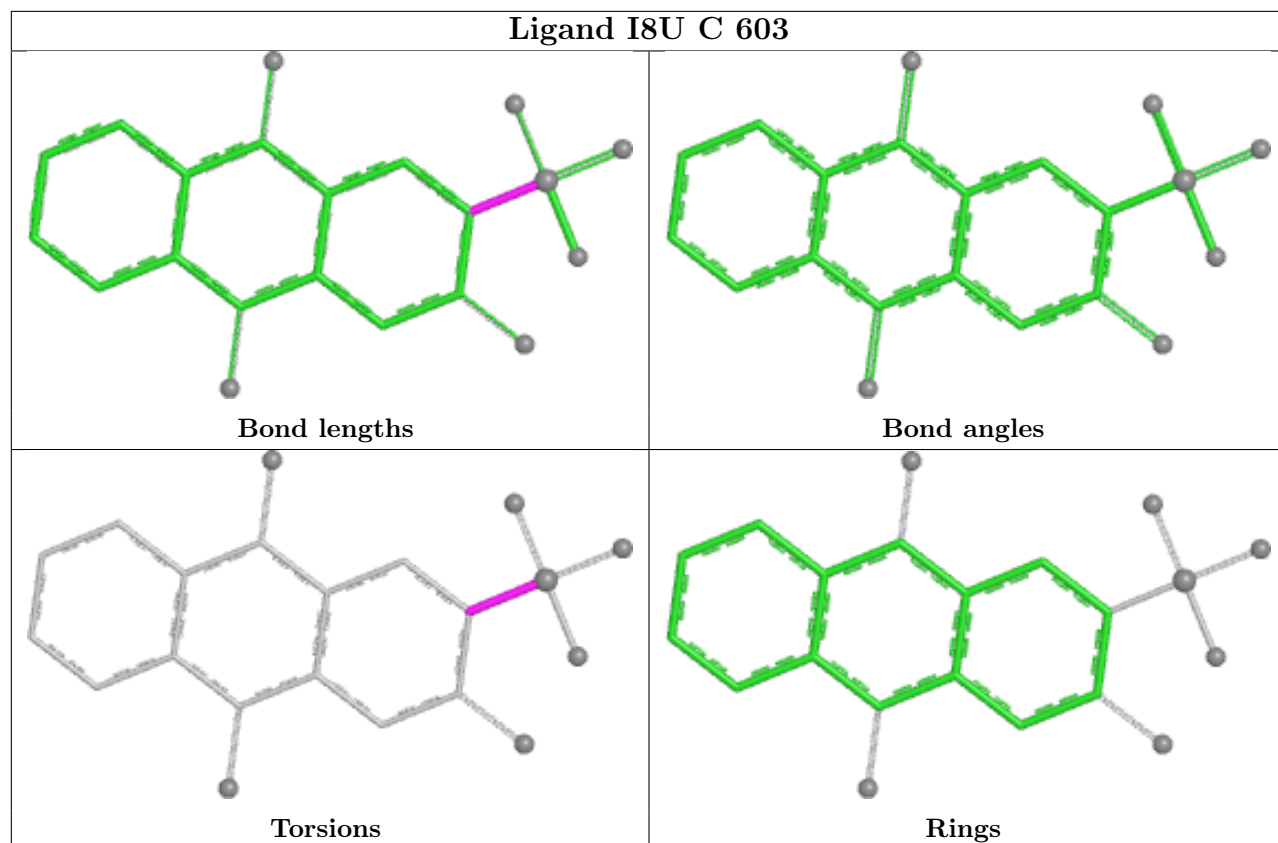
Ligand FBP F 601



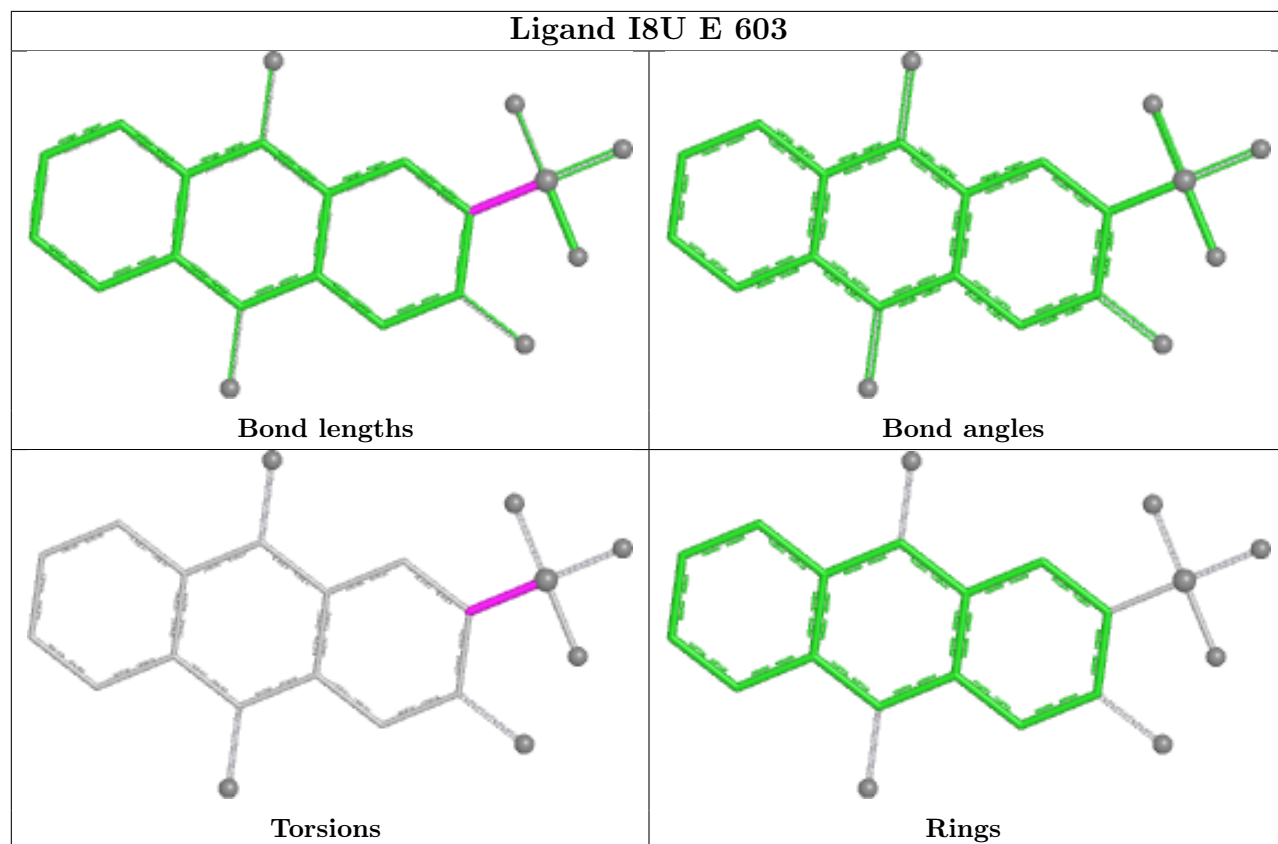


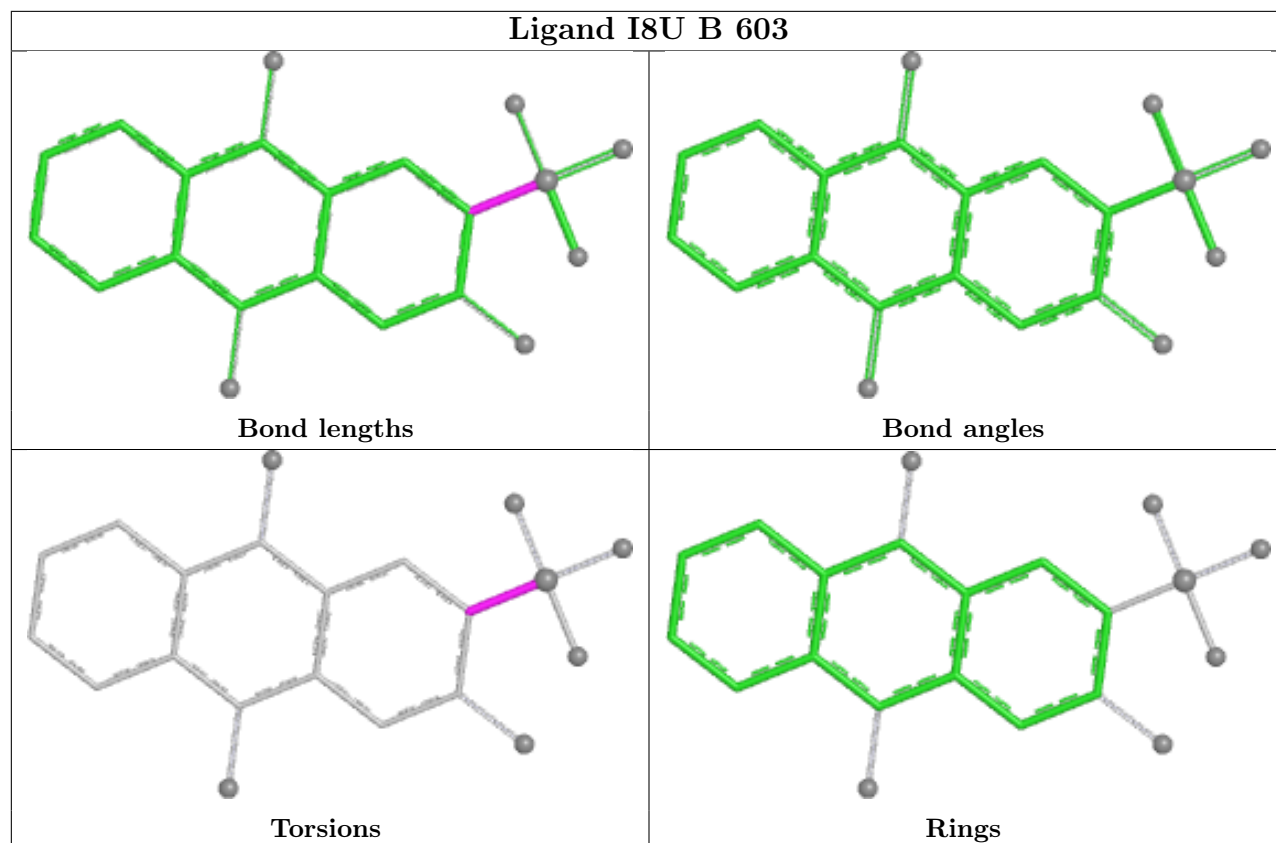


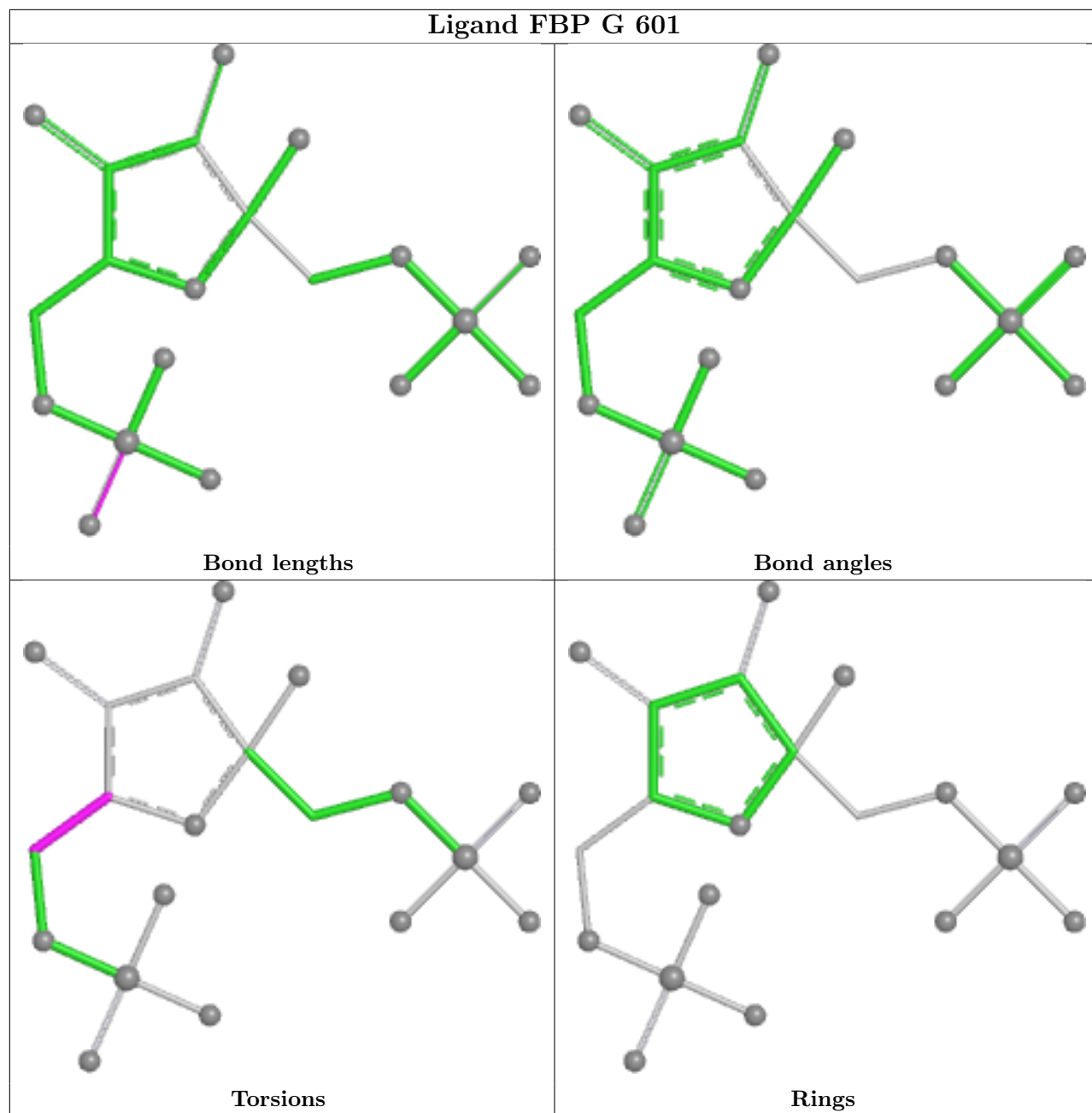
Ligand I8U C 603

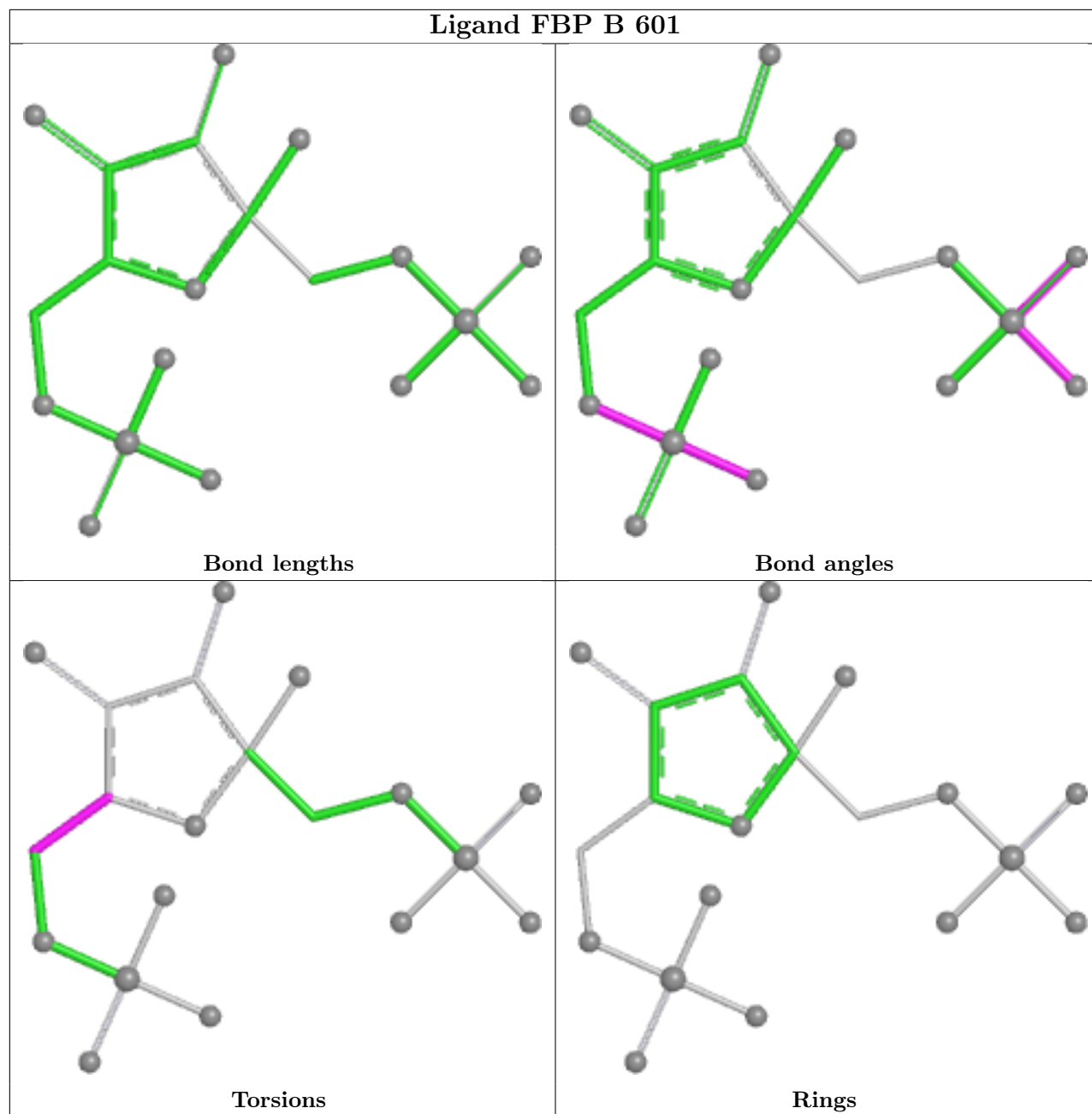


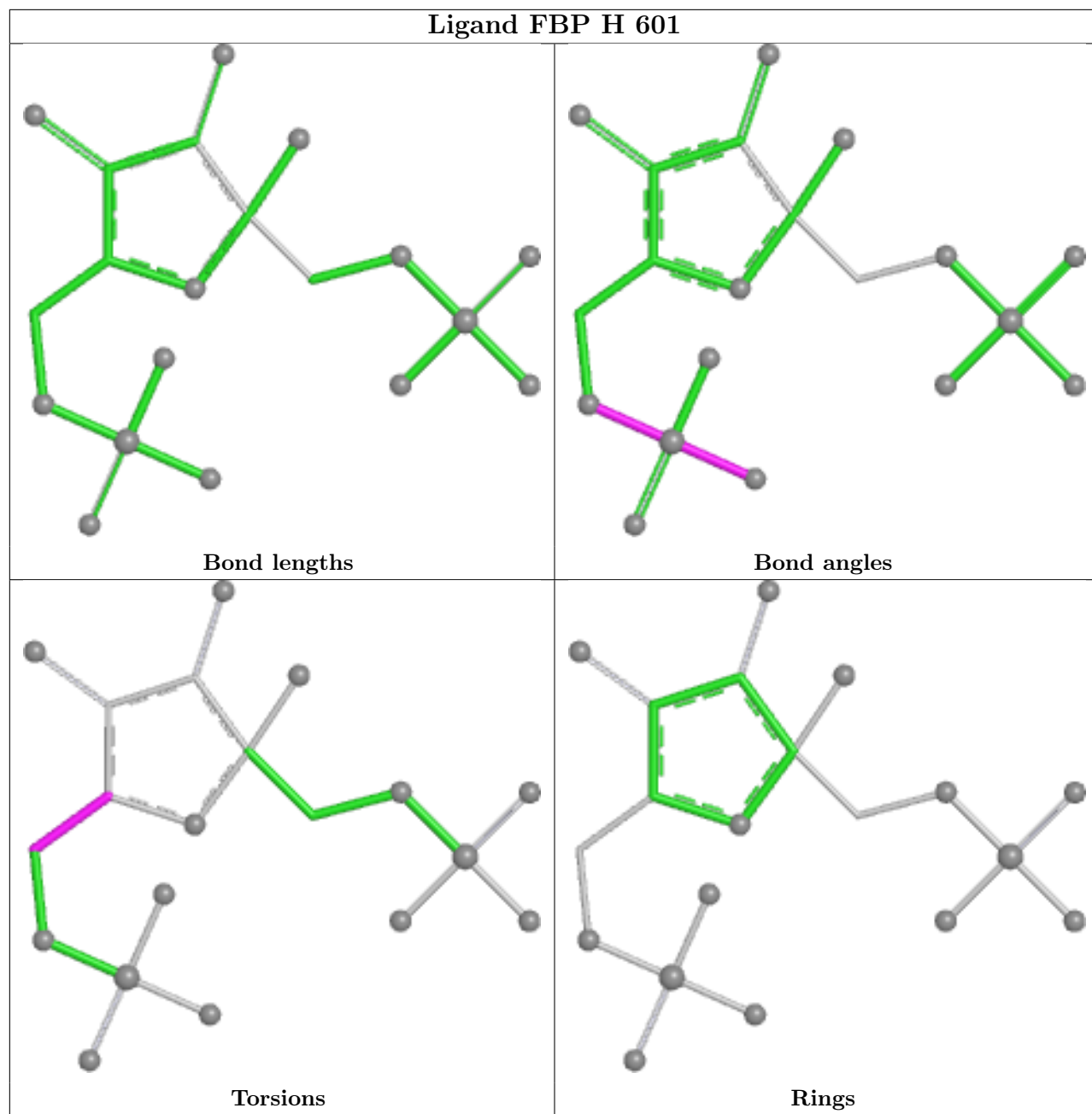
Ligand I8U E 603

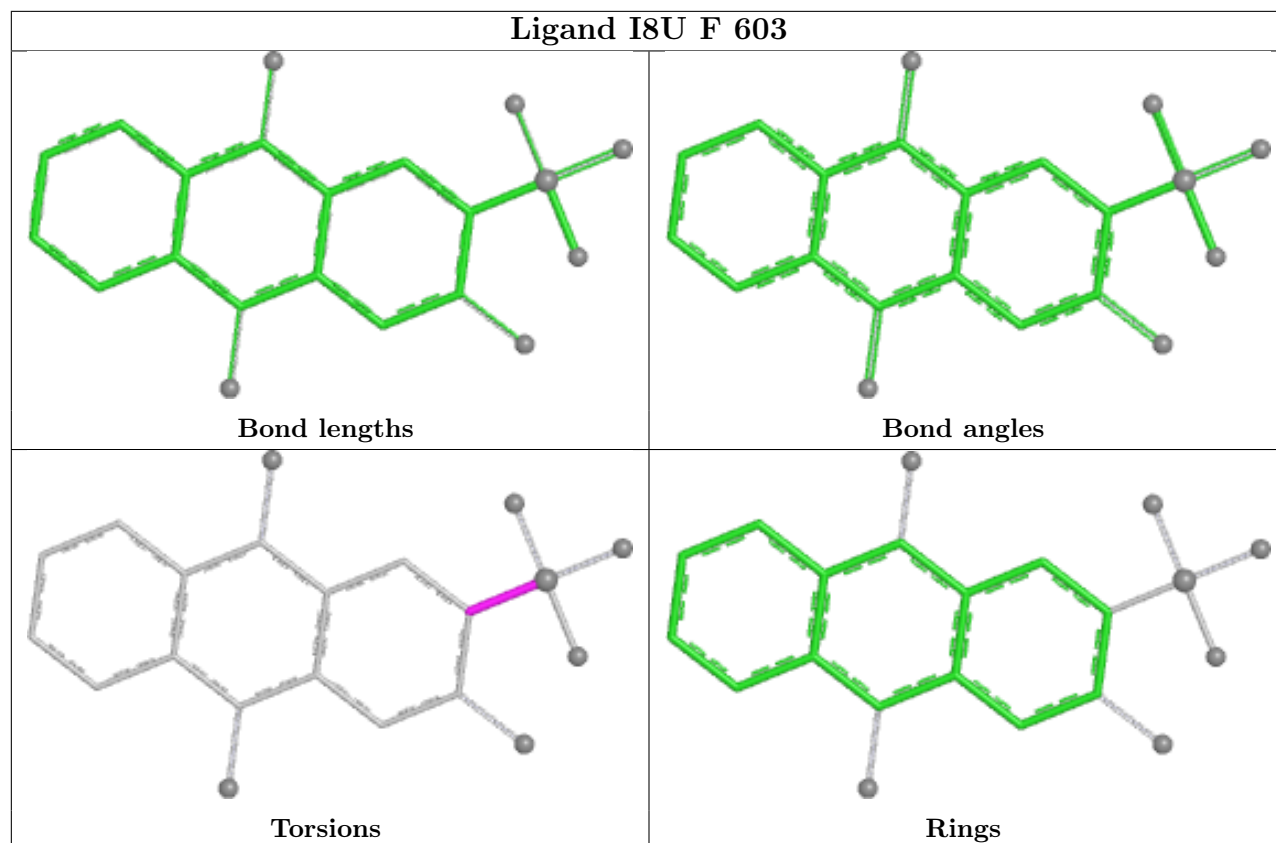












5.7 Other polymers [i](#)

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%)	0.90	51 (12%)	8 7	30, 59, 87, 102	13 (3%)
1	B	436/447 (97%)	0.80	39 (8%)	15 15	29, 55, 86, 103	8 (1%)
1	C	425/447 (95%)	0.42	23 (5%)	31 31	26, 46, 74, 133	7 (1%)
1	D	425/447 (95%)	0.20	18 (4%)	40 40	21, 40, 68, 127	8 (1%)
1	E	420/447 (93%)	1.14	70 (16%)	4 4	30, 62, 95, 113	13 (3%)
1	F	432/447 (96%)	0.58	28 (6%)	25 24	29, 51, 79, 98	8 (1%)
1	G	422/447 (94%)	0.16	18 (4%)	40 40	22, 41, 67, 119	9 (2%)
1	H	425/447 (95%)	0.01	15 (3%)	47 48	20, 38, 65, 113	9 (2%)
All	All	3403/3576 (95%)	0.53	262 (7%)	19 20	20, 50, 84, 133	75 (2%)

All (262) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	231	PRO	7.6
1	E	275[A]	HIS	6.2
1	D	130	GLY	6.0
1	D	25	PHE	5.9
1	D	131	SER	5.8
1	C	20	LEU	5.8
1	D	24	PHE	5.2
1	C	132	GLY	4.8
1	G	271	GLY	4.7
1	G	25	PHE	4.5
1	E	130	GLY	4.5
1	E	495	ALA	4.4
1	D	132	GLY	4.4
1	F	231	PRO	4.4
1	E	115	LEU	4.3
1	B	527	TRP	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	25	PHE	4.2
1	H	21	GLY	4.1
1	E	490	PRO	4.1
1	B	13	VAL	4.1
1	G	22	THR	4.1
1	B	379	LYS	4.1
1	C	115	LEU	4.1
1	H	25	PHE	4.1
1	B	490	PRO	4.1
1	E	114	PRO	4.1
1	G	231	PRO	4.1
1	C	271	GLY	4.0
1	F	484	LEU	4.0
1	D	23	ALA	3.9
1	A	543	SER	3.9
1	A	30	LEU	3.9
1	B	267[A]	ARG	3.9
1	E	249	VAL	3.8
1	A	500	ARG	3.8
1	E	30	LEU	3.8
1	H	24	PHE	3.8
1	G	24	PHE	3.8
1	E	23	ALA	3.7
1	E	400	ALA	3.7
1	C	22	THR	3.7
1	C	25	PHE	3.7
1	F	11	ALA	3.7
1	C	23	ALA	3.6
1	G	23	ALA	3.6
1	F	13	VAL	3.6
1	D	22	THR	3.6
1	C	514	PHE	3.5
1	E	269	ALA	3.5
1	F	512	ARG	3.4
1	E	257	VAL	3.4
1	B	231	PRO	3.4
1	D	232	GLY	3.4
1	E	502	VAL	3.4
1	H	232	GLY	3.4
1	D	21	GLY	3.3
1	G	21	GLY	3.3
1	A	238	VAL	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	514	PHE	3.3
1	F	267[A]	ARG	3.3
1	E	504	PHE	3.3
1	A	33	ALA	3.2
1	G	232	GLY	3.2
1	H	231	PRO	3.2
1	C	66	ALA	3.2
1	A	115	LEU	3.2
1	E	485	LEU	3.2
1	F	489	PRO	3.2
1	A	527	TRP	3.1
1	A	130	GLY	3.1
1	C	114	PRO	3.1
1	E	119	PRO	3.1
1	G	33	ALA	3.1
1	F	516	ARG	3.1
1	F	233	LEU	3.1
1	E	24	PHE	3.1
1	E	120	VAL	3.1
1	A	63	ILE	3.1
1	C	21	GLY	3.1
1	F	232	GLY	3.1
1	A	482	PHE	3.1
1	E	489	PRO	3.1
1	E	493	ILE	3.1
1	E	464	ALA	3.0
1	B	489	PRO	3.0
1	A	488[A]	GLU	3.0
1	D	32	ALA	3.0
1	A	116	SER	2.9
1	A	453	LEU	2.9
1	E	245	VAL	2.9
1	E	272	PRO	2.9
1	A	378	ALA	2.9
1	E	33	ALA	2.9
1	E	244	GLY	2.9
1	C	231	PRO	2.9
1	B	14	ALA	2.9
1	A	514	PHE	2.8
1	D	33	ALA	2.8
1	H	23	ALA	2.8
1	A	26	GLN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	132	GLY	2.8
1	B	115	LEU	2.8
1	H	275[A]	HIS	2.7
1	A	270	LEU	2.7
1	B	11	ALA	2.7
1	D	30	LEU	2.7
1	A	28	GLN	2.7
1	G	272	PRO	2.7
1	B	131	SER	2.7
1	A	269	ALA	2.7
1	A	241	LEU	2.7
1	F	490	PRO	2.7
1	E	232	GLY	2.7
1	F	276	GLY	2.7
1	F	527	TRP	2.7
1	F	23	ALA	2.6
1	D	275[A]	HIS	2.6
1	F	12	ASP	2.6
1	B	252	VAL	2.6
1	E	238	VAL	2.6
1	E	487	ARG	2.6
1	C	111	ALA	2.6
1	A	86	LEU	2.6
1	F	253	PHE	2.6
1	E	494	TRP	2.6
1	E	418[A]	ARG	2.6
1	E	111	ALA	2.6
1	A	233	LEU	2.6
1	H	22	THR	2.5
1	E	129	PRO	2.5
1	B	270	LEU	2.5
1	F	270	LEU	2.5
1	B	12	ASP	2.5
1	E	270	LEU	2.5
1	A	253	PHE	2.5
1	E	123	ALA	2.5
1	H	416	LEU	2.5
1	C	310	GLY	2.5
1	E	527	TRP	2.5
1	A	257	VAL	2.4
1	B	249	VAL	2.4
1	E	264	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	86	LEU	2.4
1	A	411	ARG	2.4
1	B	88	PHE	2.4
1	E	271	GLY	2.4
1	A	70	VAL	2.4
1	E	122	ILE	2.4
1	E	498	VAL	2.4
1	B	411	ARG	2.4
1	A	515	LEU	2.4
1	B	251	ILE	2.4
1	E	251	ILE	2.4
1	B	269	ALA	2.4
1	B	86	LEU	2.4
1	E	241	LEU	2.4
1	F	86	LEU	2.4
1	F	511	LEU	2.4
1	E	524	VAL	2.4
1	E	126	THR	2.4
1	B	484	LEU	2.3
1	B	511	LEU	2.3
1	E	511	LEU	2.3
1	A	112	GLY	2.3
1	A	118	ARG	2.3
1	B	10	ARG	2.3
1	C	24	PHE	2.3
1	H	411	ARG	2.3
1	B	543	SER	2.3
1	E	52	VAL	2.3
1	A	114	PRO	2.3
1	B	84	ALA	2.3
1	E	268	ALA	2.3
1	B	241	LEU	2.3
1	E	233	LEU	2.3
1	F	274	GLY	2.3
1	A	418[A]	ARG	2.3
1	H	242[A]	ARG	2.3
1	G	514	PHE	2.3
1	A	120	VAL	2.3
1	C	33	ALA	2.3
1	D	499	ASP	2.3
1	H	516	ARG	2.3
1	A	407	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	94	GLU	2.3
1	B	517	VAL	2.3
1	D	489	PRO	2.3
1	A	495	ALA	2.3
1	C	232	GLY	2.3
1	C	233	LEU	2.3
1	A	131	SER	2.2
1	A	80	GLY	2.2
1	A	305	ALA	2.2
1	A	513	GLY	2.2
1	E	437	ALA	2.2
1	B	416	LEU	2.2
1	B	507	GLU	2.2
1	H	273	GLU	2.2
1	G	236	GLN	2.2
1	E	243	PHE	2.2
1	E	256	PHE	2.2
1	A	475	VAL	2.2
1	B	70	VAL	2.2
1	C	70	VAL	2.2
1	D	31	PRO	2.2
1	E	513	GLY	2.2
1	B	540[A]	LEU	2.2
1	E	124	LEU	2.2
1	G	115	LEU	2.2
1	E	88	PHE	2.2
1	F	129	PRO	2.2
1	E	521	VAL	2.2
1	E	428	ALA	2.2
1	F	487	ARG	2.2
1	G	411	ARG	2.2
1	A	542	ILE	2.1
1	A	460	ALA	2.1
1	E	438	ALA	2.1
1	E	469	ALA	2.1
1	B	16	LEU	2.1
1	E	540	LEU	2.1
1	C	95	TYR	2.1
1	A	237	ASP	2.1
1	B	100	ILE	2.1
1	B	242	ARG	2.1
1	F	269	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	492	ALA	2.1
1	D	39	LEU	2.1
1	B	95	TYR	2.1
1	A	31	PRO	2.1
1	C	348	THR	2.1
1	A	249	VAL	2.1
1	E	103	VAL	2.1
1	E	304	VAL	2.1
1	A	265	ALA	2.1
1	E	484	LEU	2.1
1	F	485	LEU	2.1
1	G	30	LEU	2.1
1	F	488	GLU	2.1
1	G	34	MET	2.1
1	E	26	GLN	2.1
1	G	351	ARG	2.1
1	E	536	ILE	2.1
1	E	70	VAL	2.1
1	A	69	SER	2.1
1	E	97	ALA	2.1
1	F	14	ALA	2.1
1	H	33	ALA	2.1
1	F	34	MET	2.0
1	A	124	LEU	2.0
1	C	410	LEU	2.0
1	G	28	GLN	2.0
1	E	351	ARG	2.0
1	B	493	ILE	2.0
1	E	542	ILE	2.0
1	A	110	PHE	2.0
1	A	32	ALA	2.0
1	A	111	ALA	2.0
1	B	106	ALA	2.0
1	H	267[A]	ARG	2.0
1	A	275	HIS	2.0
1	B	348	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	I8U	E	603	21/21	0.82	0.16	116,117,117,117	8
3	OXL	E	602	6/6	0.84	0.15	79,79,79,79	0
6	I8U	C	603	21/21	0.87	0.15	92,92,92,93	8
5	K	E	605	1/1	0.87	0.19	102,102,102,102	0
3	OXL	A	602	6/6	0.89	0.11	66,66,67,67	0
6	I8U	B	603	21/21	0.89	0.14	99,101,102,102	8
3	OXL	D	602	6/6	0.91	0.11	53,53,54,55	0
2	FBP	E	601	20/20	0.91	0.09	66,67,68,68	0
3	OXL	G	602	6/6	0.92	0.10	46,47,48,49	0
5	K	C	605	1/1	0.92	0.13	67,67,67,67	0
3	OXL	B	602	6/6	0.92	0.11	55,56,59,59	0
3	OXL	H	602	6/6	0.93	0.10	48,48,49,49	0
3	OXL	F	602	6/6	0.93	0.11	62,64,65,65	0
6	I8U	F	603	21/21	0.93	0.10	65,65,66,66	8
2	FBP	F	601	20/20	0.94	0.08	51,56,59,59	0
5	K	G	605	1/1	0.94	0.11	64,64,64,64	0
3	OXL	C	602	6/6	0.94	0.08	52,53,53,53	0
5	K	B	605	1/1	0.95	0.14	77,77,77,77	0
5	K	A	604	1/1	0.95	0.09	92,92,92,92	0
6	I8U	G	603	21/21	0.95	0.08	54,56,58,59	8
2	FBP	A	601	20/20	0.96	0.07	48,50,52,52	0
4	MG	D	603	1/1	0.96	0.19	29,29,29,29	0
5	K	F	605	1/1	0.96	0.06	83,83,83,83	0
5	K	D	604	1/1	0.97	0.08	60,60,60,60	0
2	FBP	B	601	20/20	0.97	0.07	51,53,57,57	0
4	MG	B	604	1/1	0.97	0.15	34,34,34,34	0
2	FBP	H	601	20/20	0.98	0.05	30,32,35,35	0
2	FBP	D	601	20/20	0.98	0.04	32,34,38,38	0
4	MG	F	604	1/1	0.98	0.12	29,29,29,29	0
2	FBP	G	601	20/20	0.98	0.04	31,33,35,35	0
4	MG	A	603	1/1	0.98	0.11	39,39,39,39	0
4	MG	H	603	1/1	0.99	0.14	21,21,21,21	0

Continued on next page...

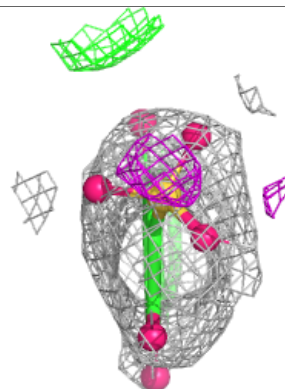
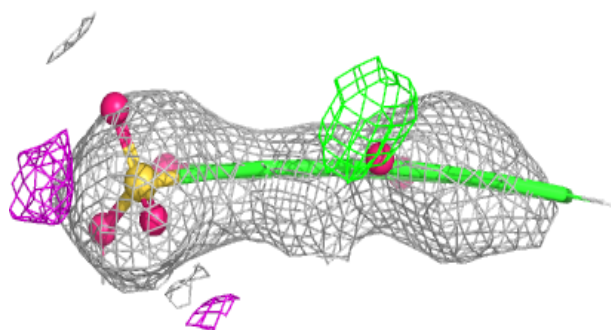
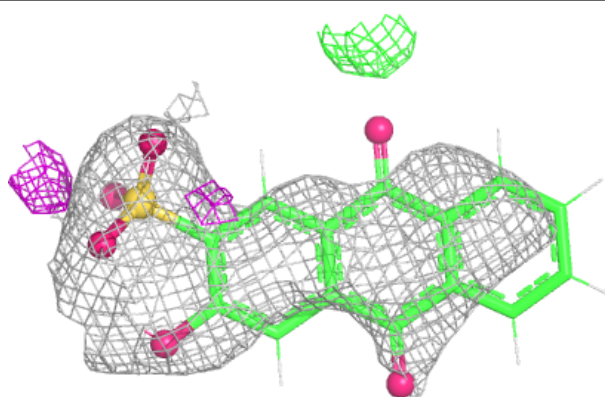
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	E	604	1/1	0.99	0.16	39,39,39,39	0
5	K	H	604	1/1	0.99	0.14	58,58,58,58	0
2	FBP	C	601	20/20	0.99	0.04	32,34,38,38	0
4	MG	C	604	1/1	1.00	0.10	26,26,26,26	0
4	MG	G	604	1/1	1.00	0.12	21,21,21,21	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.

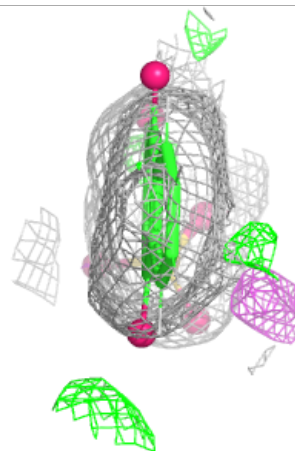
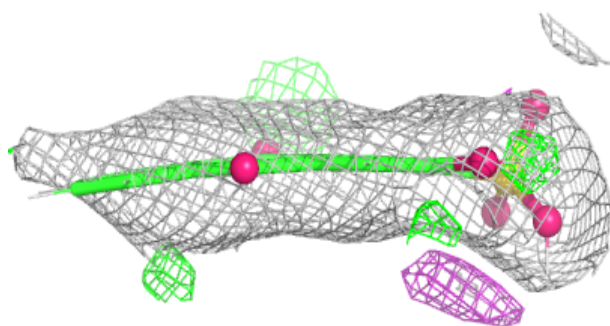
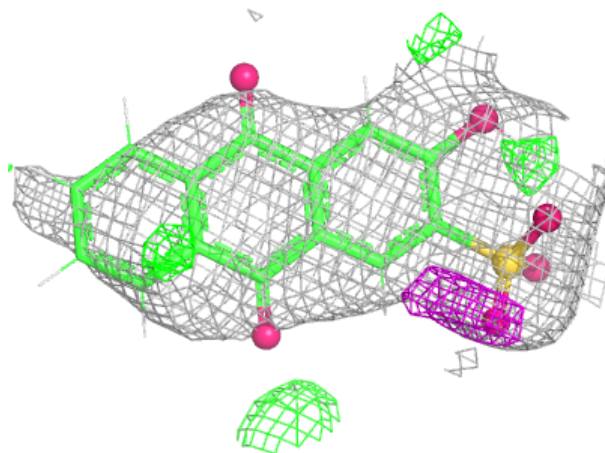
Electron density around I8U E 603:

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



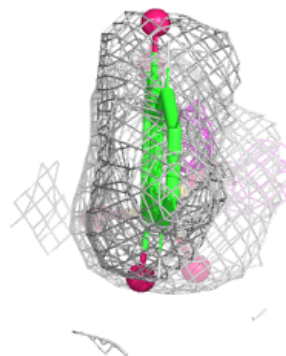
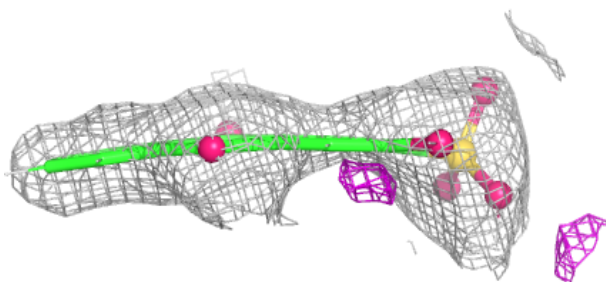
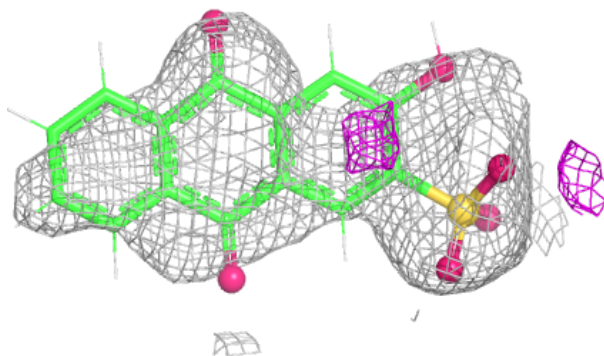
Electron density around I8U C 603:

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

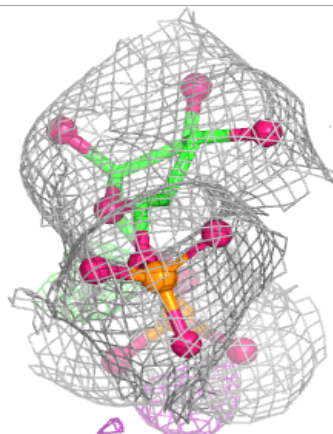
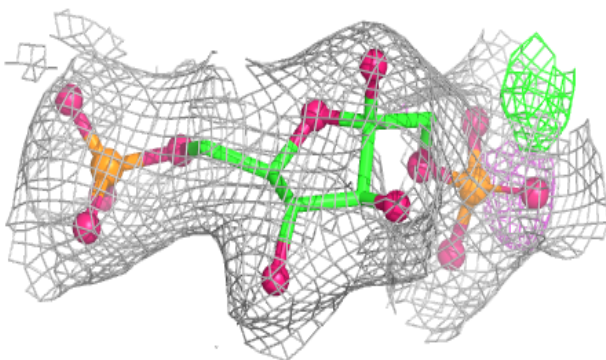
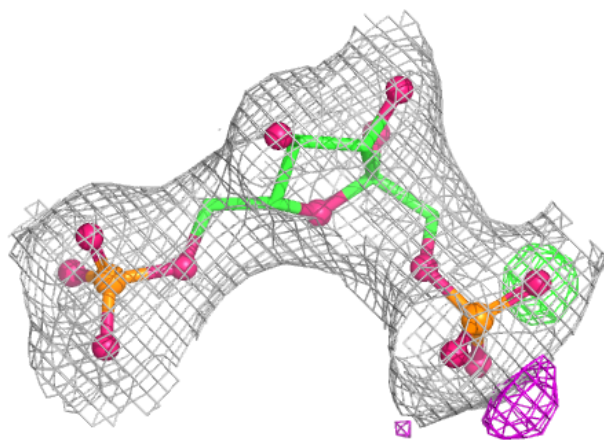


Electron density around I8U B 603:

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

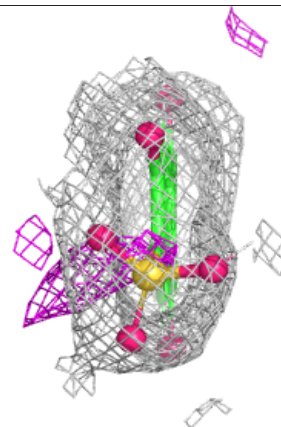
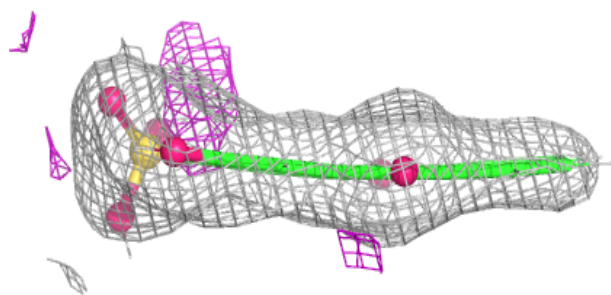
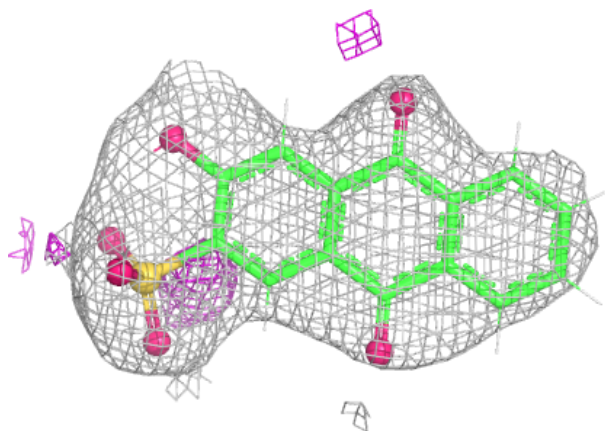
**Electron density around FBP E 601:**

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



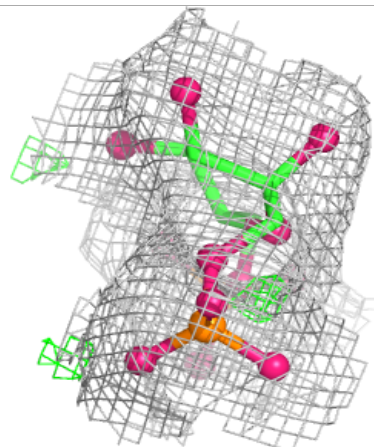
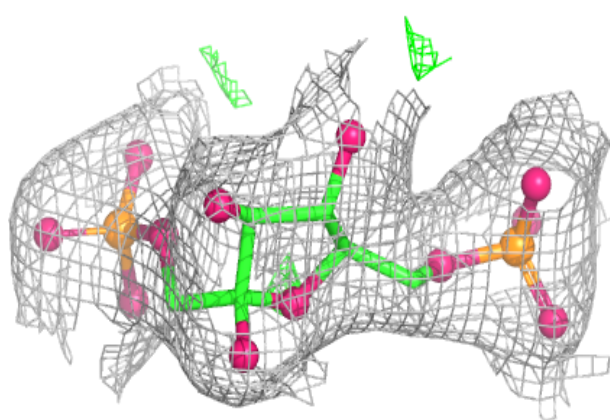
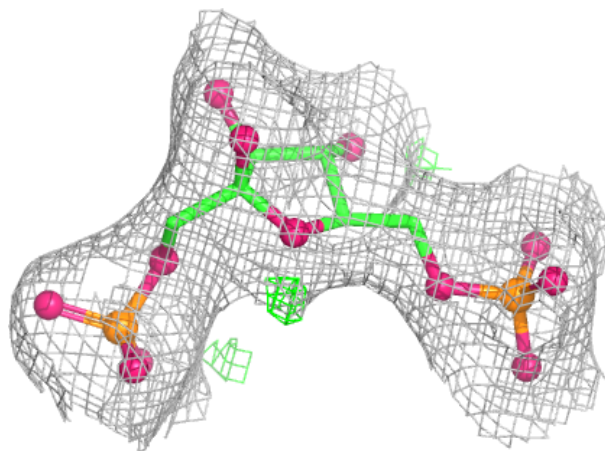
Electron density around I8U F 603:

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



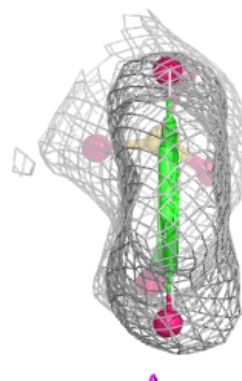
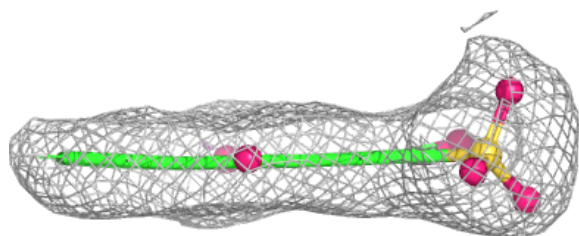
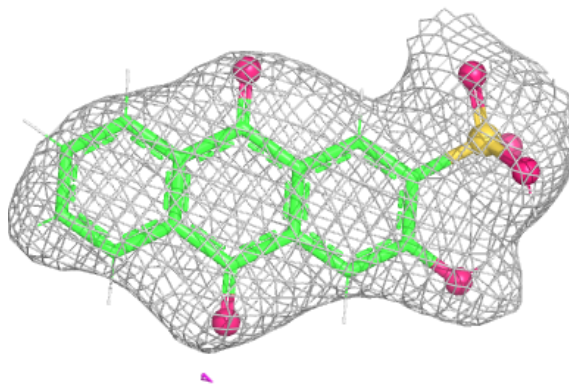
Electron density around FBP F 601:

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

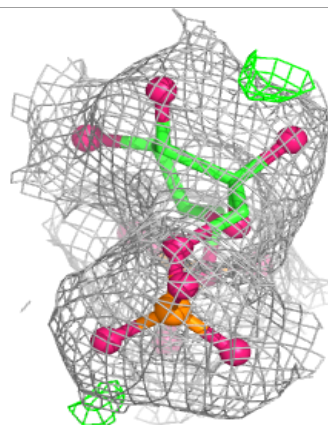
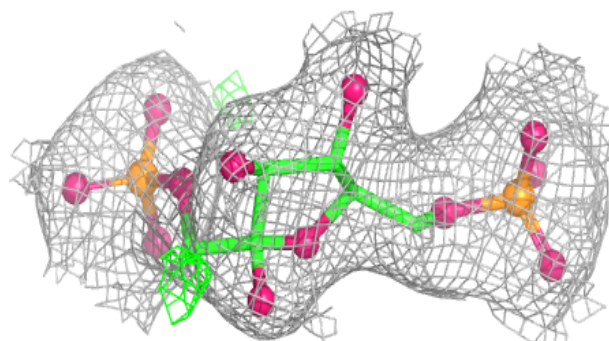
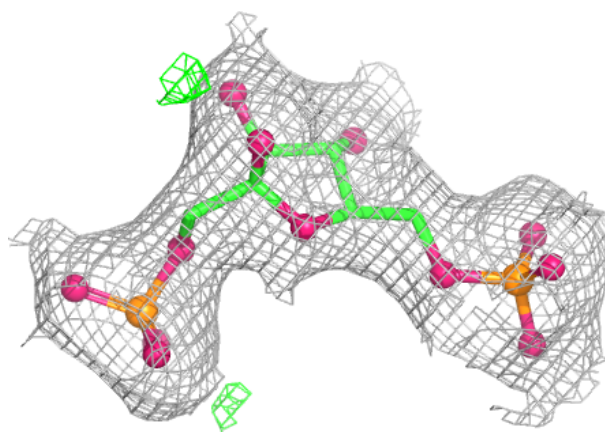


Electron density around I8U G 603:

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

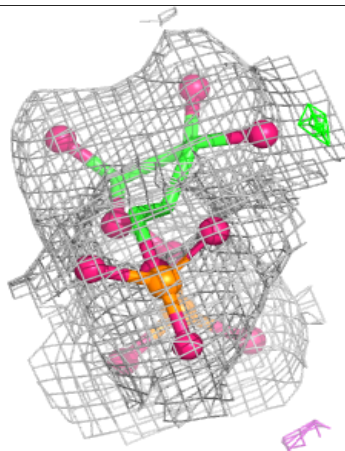
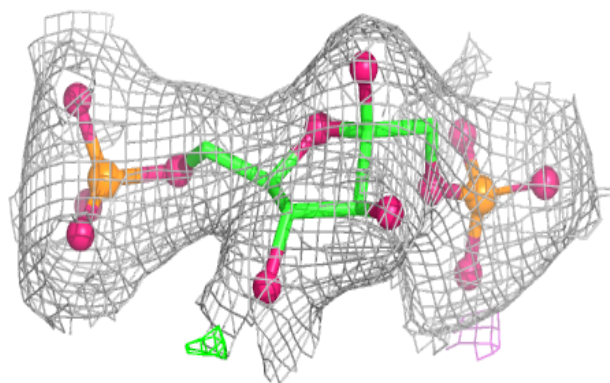
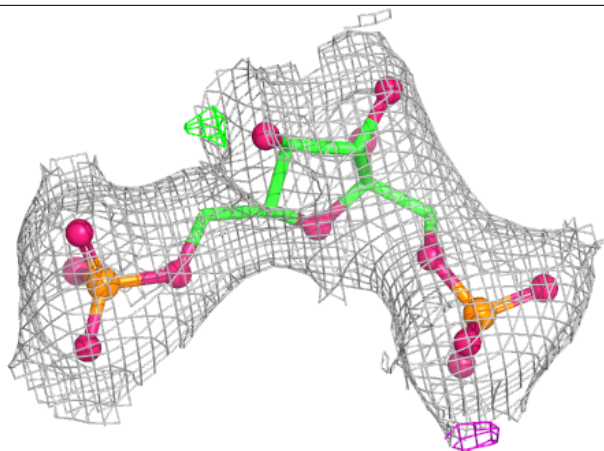
**Electron density around FBP A 601:**

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

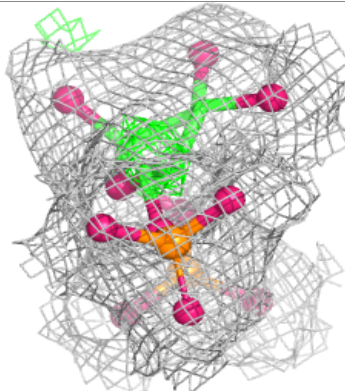
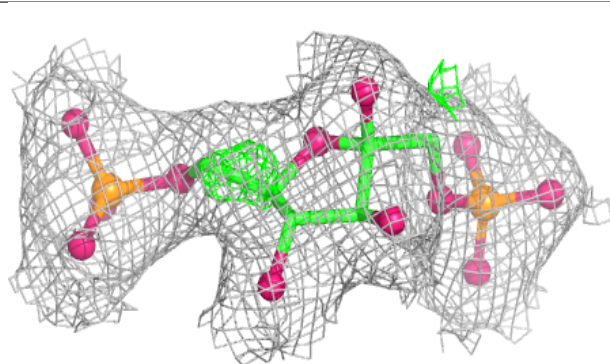
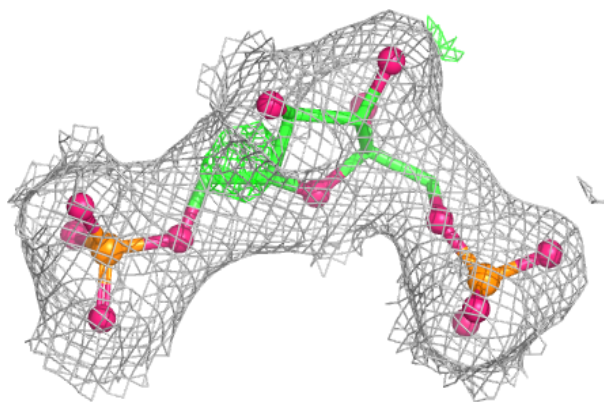


Electron density around FBP B 601:

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

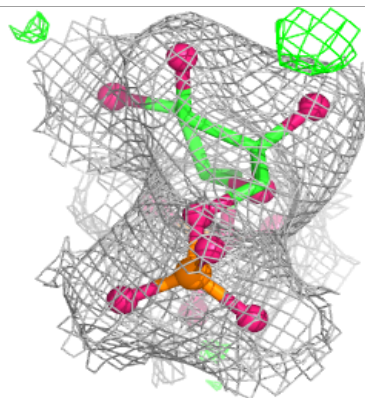
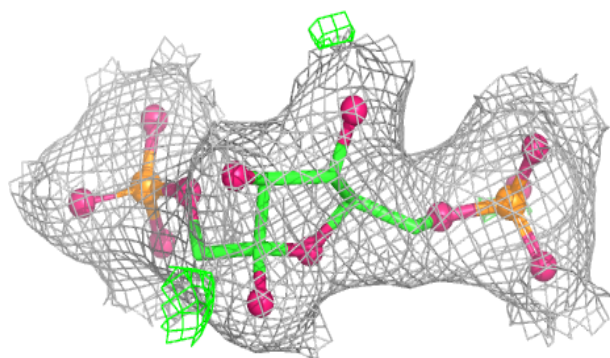
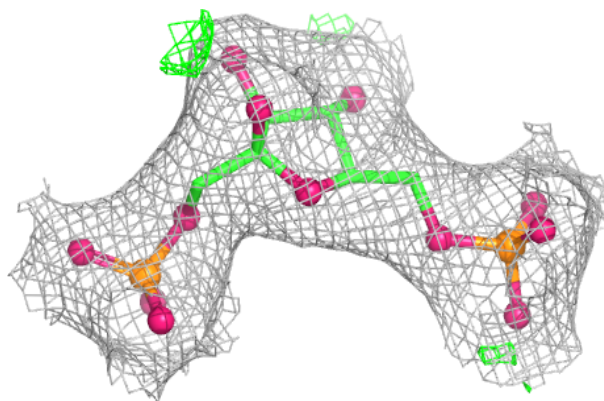
**Electron density around FBP H 601:**

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

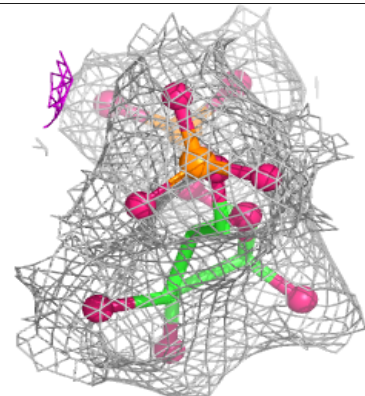
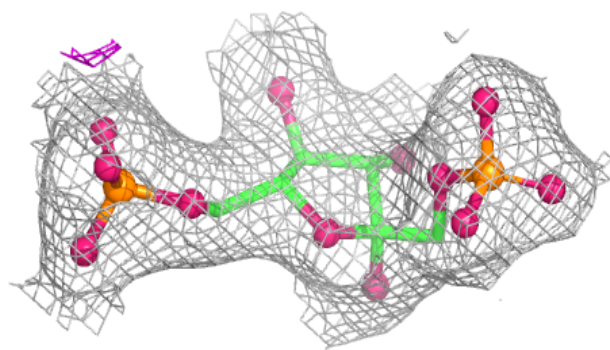
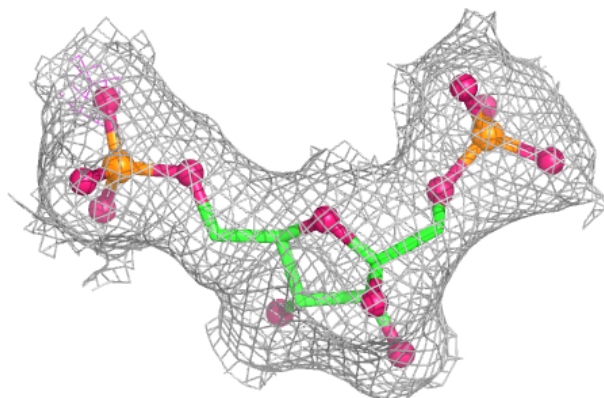


Electron density around FBP D 601:

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

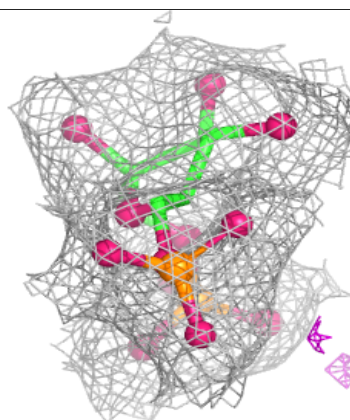
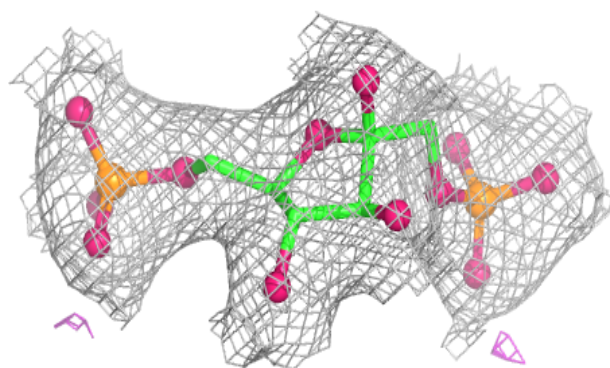
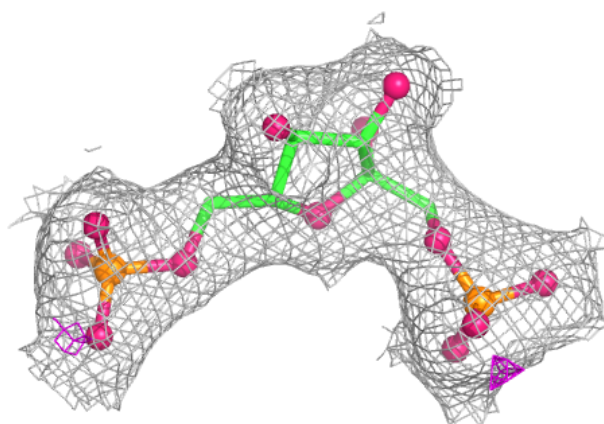
**Electron density around FBP G 601:**

$2mF_o-DF_c$ (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.