



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:09 PM EDT

PDB ID : 5SCJ / pdb_00005scj
Title : Structure of liver pyruvate kinase in complex with anthraquinone derivative 106
Authors : Lulla, A.; Foller, A.; Nain-Perez, A.; Grotli, M.; Brear, P.; Hyvonen, M.
Deposited on : 2021-12-01
Resolution : 2.35 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:

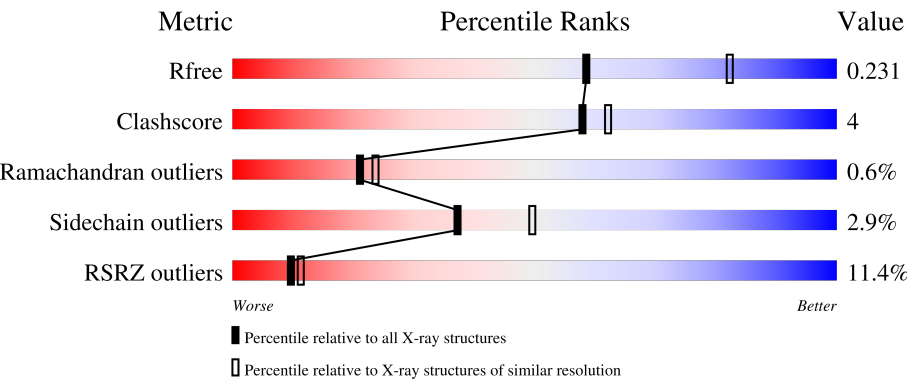
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	447	21% 82% 12% 6%
1	B	447	20% 84% 13% ..
1	C	447	10% 82% 12% • 5%
1	D	447	4% 81% 13% • 5%
1	E	447	16% 81% 12% • 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 27221 atoms, of which 87 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	422	Total	C	N	O	S	0	6	0
			3236	2034	585	597	20			
1	B	436	Total	C	N	O	S	0	4	0
			3329	2090	604	615	20			
1	C	425	Total	C	N	O	S	0	4	0
			3247	2040	585	603	19			
1	D	425	Total	C	N	O	S	0	6	0
			3252	2042	590	601	19			
1	E	419	Total	C	N	O	S	0	5	0
			3210	2018	579	593	20			
1	F	432	Total	C	N	O	S	0	7	0
			3321	2090	597	614	20			
1	G	421	Total	C	N	O	S	0	6	0
			3231	2031	581	600	19			
1	H	425	Total	C	N	O	S	0	4	0
			3251	2040	594	598	19			

There are 48 discrepancies between the modelled and reference sequences:

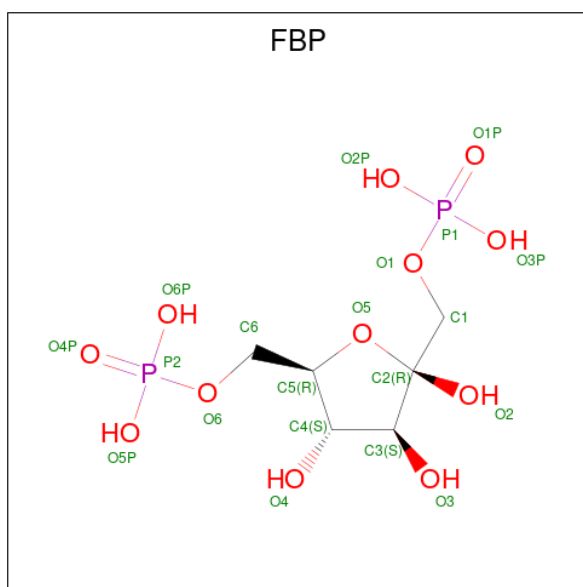
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q16716
A	0	SER	-	expression tag	UNP Q16716
A	12	ASP	SER	conflict	UNP Q16716
A	130	GLY	-	linker	UNP Q16716
A	131	SER	-	linker	UNP Q16716
A	132	GLY	-	linker	UNP Q16716
B	-1	GLY	-	expression tag	UNP Q16716
B	0	SER	-	expression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

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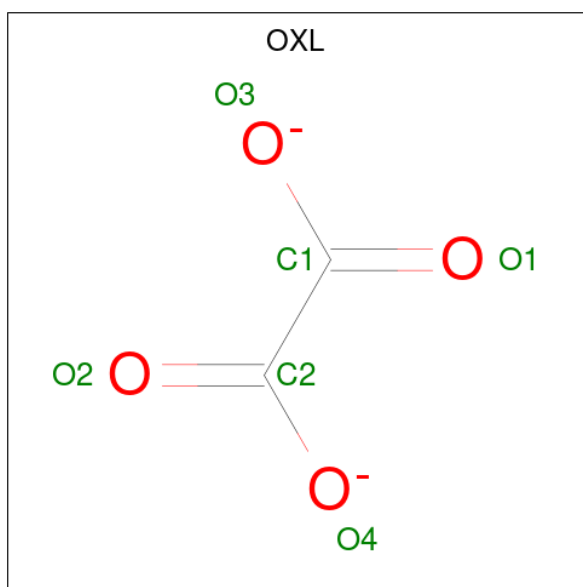
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP Q16716
C	12	ASP	SER	conflict	UNP Q16716
C	130	GLY	-	linker	UNP Q16716
C	131	SER	-	linker	UNP Q16716
C	132	GLY	-	linker	UNP Q16716
D	-1	GLY	-	expression tag	UNP Q16716
D	0	SER	-	expression tag	UNP Q16716
D	12	ASP	SER	conflict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

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



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

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



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

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

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

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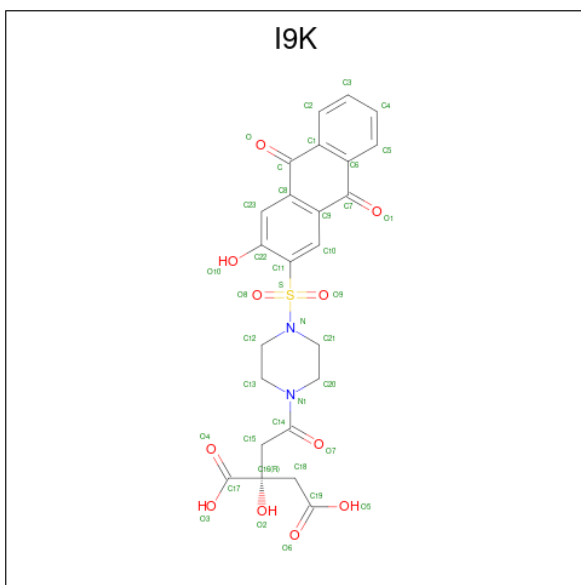
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		
4	G	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		

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

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

- Molecule 6 is (2R)-2-hydroxy-2-{2-[4-(3-hydroxy-9,10-dioxo-9,10-dihydroanthracene-2-sulfonyl)piperazin-1-yl]-2-oxoethyl}butanedioic acid (CCD ID: I9K) (formula: C₂₄H₂₂N₂O₁₁S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	A	1	Total 60	C 24	H 22	N 2	O 11	S 1	22	0
6	C	1	Total 59	C 24	H 21	N 2	O 11	S 1	21	0
6	F	1	Total 60	C 24	H 22	N 2	O 11	S 1	22	0
6	G	1	Total 60	C 24	H 22	N 2	O 11	S 1	22	0

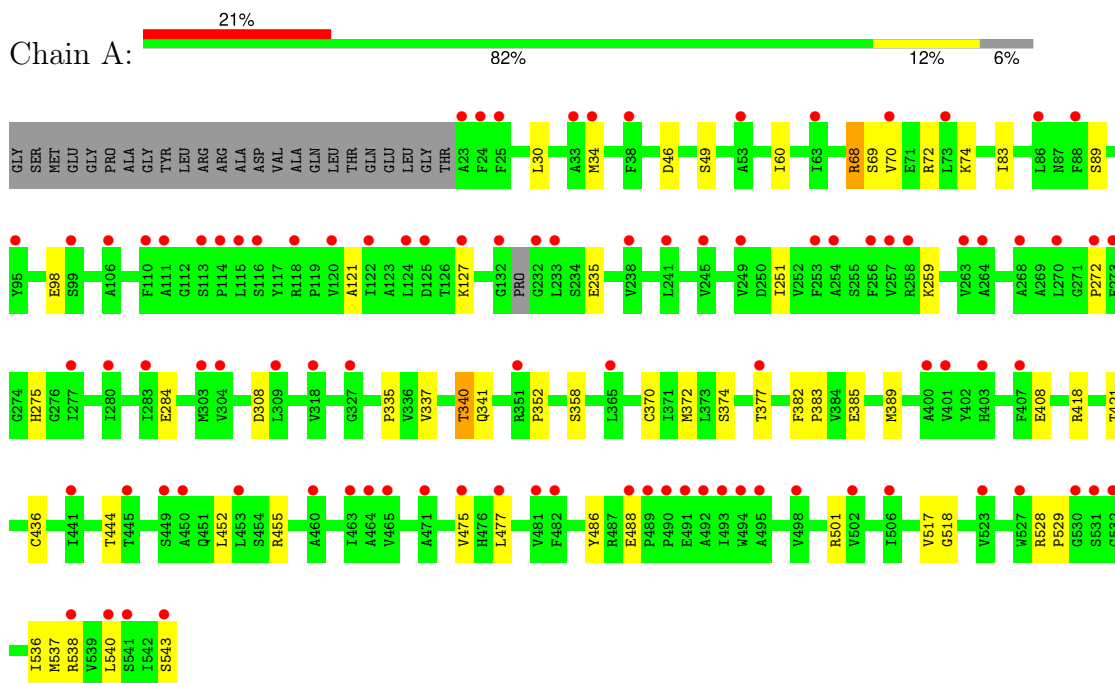
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	30	Total	O	0	0
			30	30		
7	B	44	Total	O	0	0
			44	44		
7	C	92	Total	O	0	0
			92	92		
7	D	113	Total	O	0	0
			113	113		
7	E	47	Total	O	0	0
			47	47		
7	F	94	Total	O	0	0
			94	94		
7	G	109	Total	O	0	0
			109	109		
7	H	152	Total	O	0	0
			152	152		

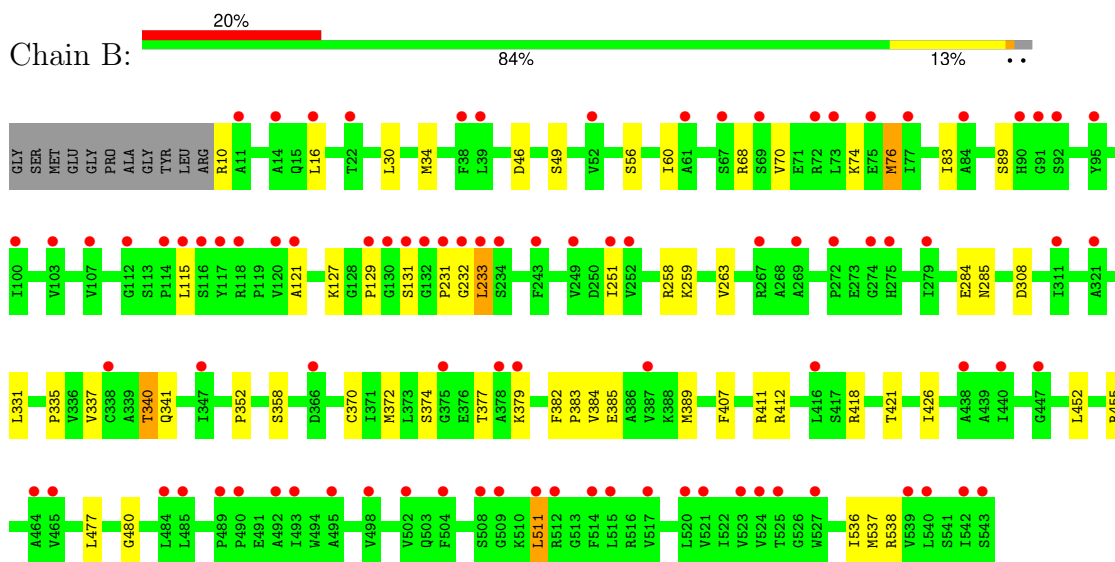
3 Residue-property plots [i](#)

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.

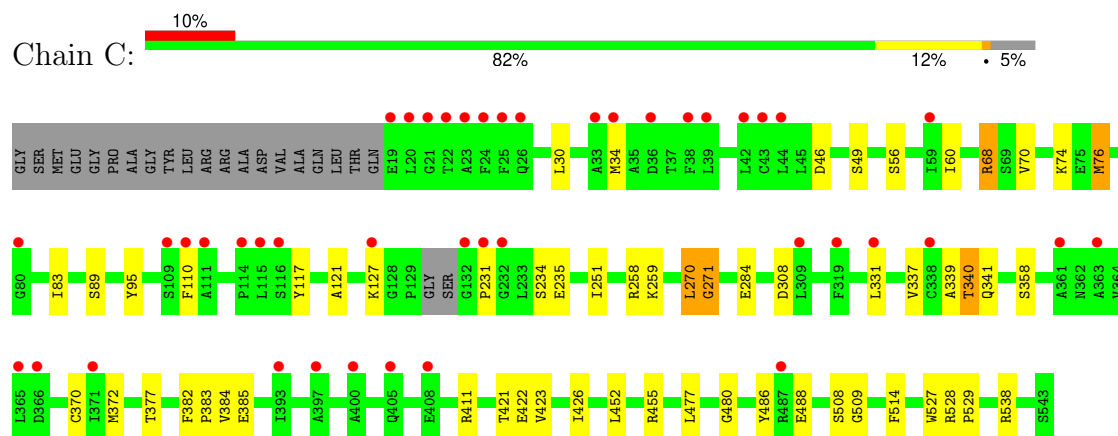
• Molecule 1: Pyruvate kinase



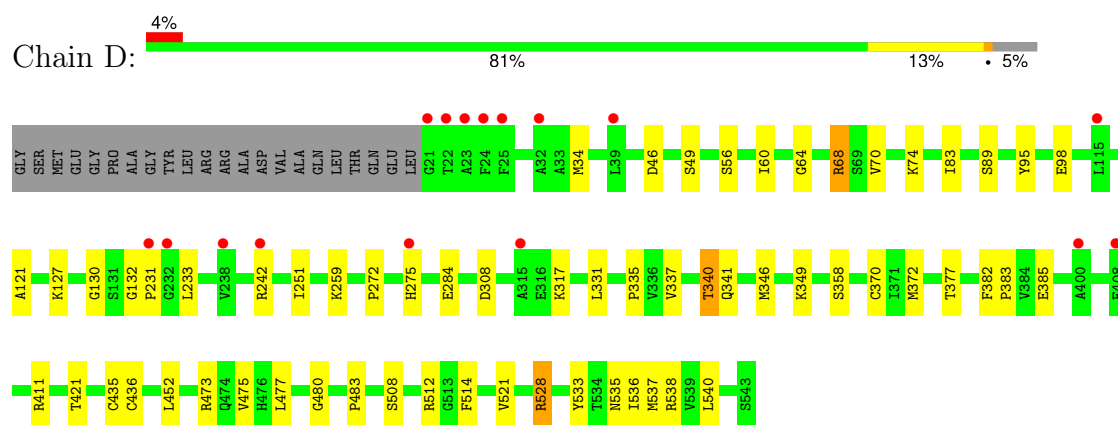
• Molecule 1: Pyruvate kinase



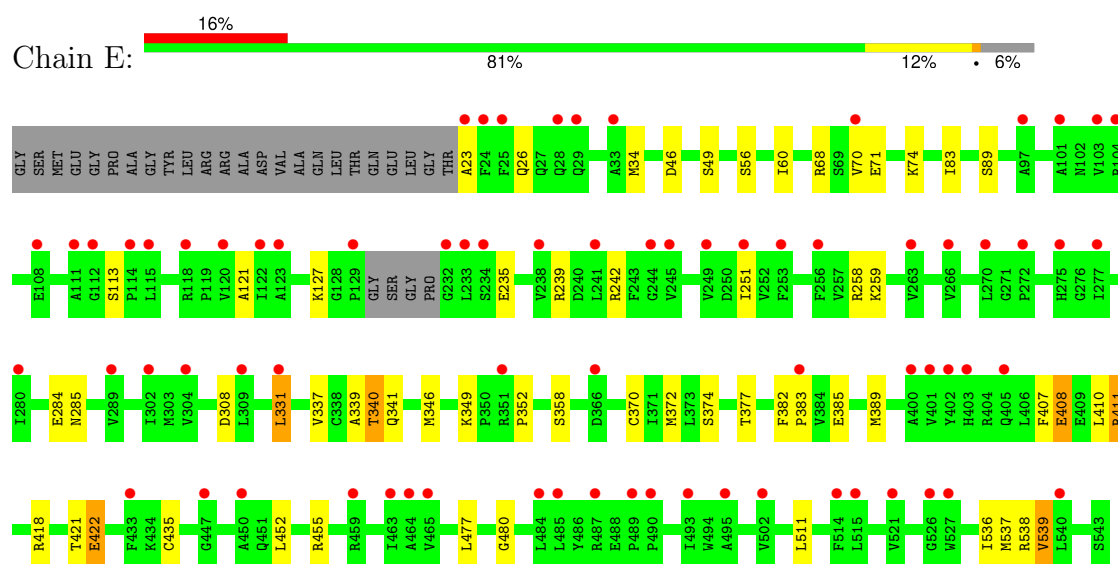
• Molecule 1: Pyruvate kinase



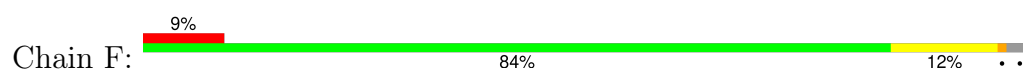
• Molecule 1: Pyruvate kinase

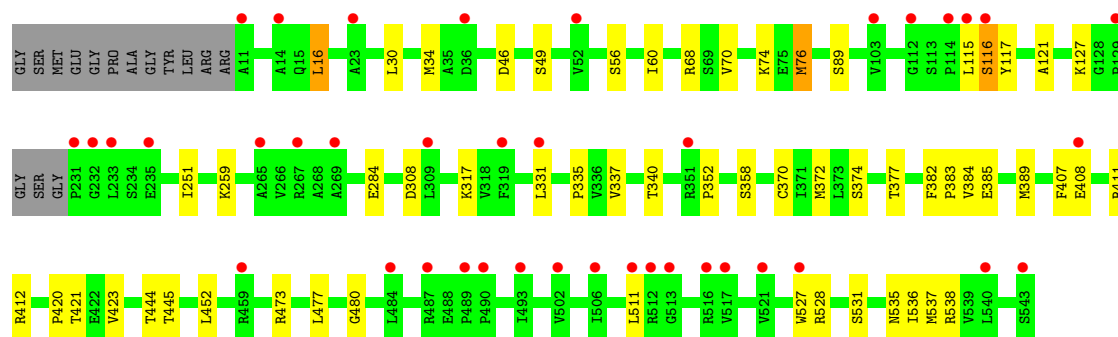


• Molecule 1: Pyruvate kinase

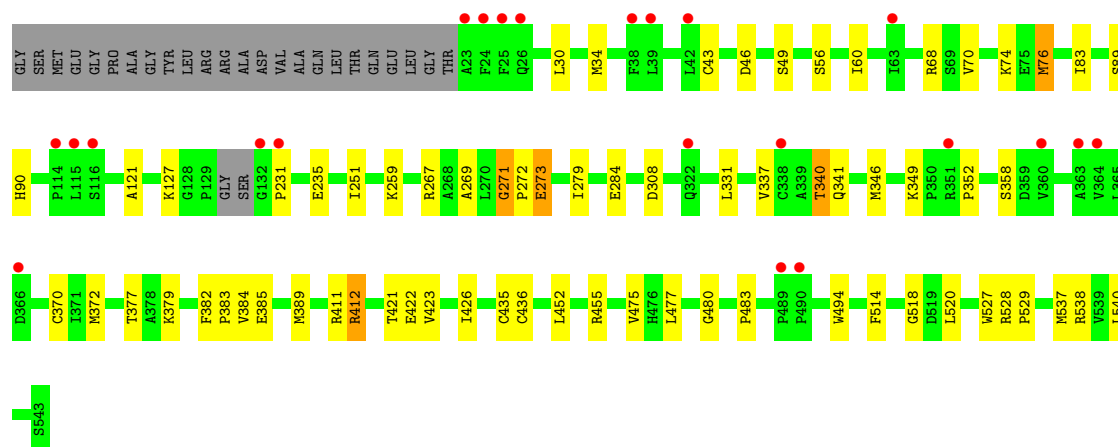
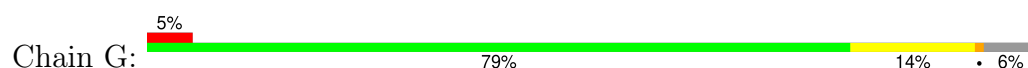


• Molecule 1: Pyruvate kinase

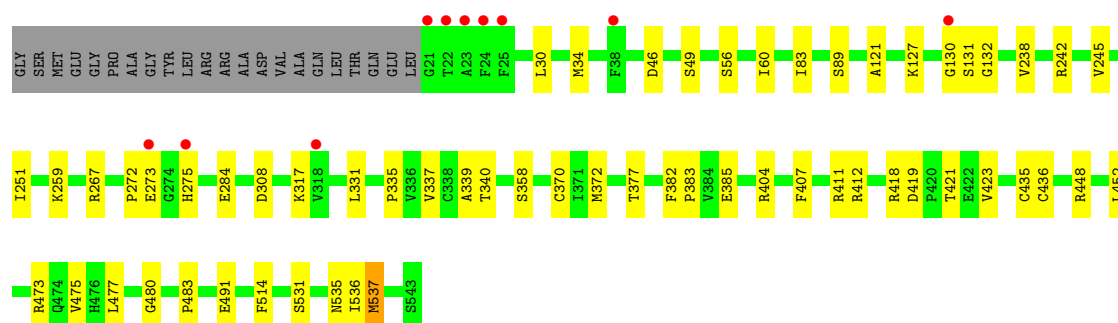
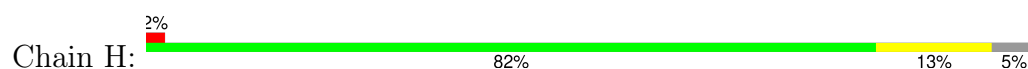




• Molecule 1: Pyruvate kinase



• 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	208.14Å 113.06Å 188.96Å 90.00° 91.54° 90.00°	Depositor
Resolution (Å)	188.89 – 2.35 188.89 – 2.35	Depositor EDS
% Data completeness (in resolution range)	56.7 (188.89-2.35) 56.7 (188.89-2.35)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.34Å)	Xtriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, R_{free}	0.218 , 0.253 0.206 , 0.231	Depositor DCC
R_{free} test set	4891 reflections (2.70%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27221	wwPDB-VP
Average B, all atoms (Å ²)	58.0	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 56.13 % 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 2.8637e-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: K, MG, OXL, FBP, I9K

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	0.68	1/3307 (0.0%)	1.06	0/4469
1	B	0.74	1/3396 (0.0%)	1.06	0/4592
1	C	0.76	0/3313	1.11	5/4479 (0.1%)
1	D	0.79	1/3326 (0.0%)	1.10	1/4497 (0.0%)
1	E	0.69	1/3278 (0.0%)	1.06	3/4430 (0.1%)
1	F	0.76	1/3396 (0.0%)	1.08	3/4591 (0.1%)
1	G	0.77	0/3303	1.08	1/4465 (0.0%)
1	H	0.79	0/3316	1.07	3/4483 (0.1%)
All	All	0.75	5/26635 (0.0%)	1.08	16/36006 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	374	SER	CA-C	8.62	1.56	1.52
1	E	374	SER	CA-C	6.88	1.55	1.52
1	F	374	SER	CA-C	5.70	1.55	1.52
1	A	374	SER	CA-C	5.69	1.55	1.52
1	D	68	ARG	CA-C	-5.33	1.45	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	422	GLU	CB-CG-CD	6.62	123.86	112.60
1	E	410	LEU	CA-C-N	6.26	128.99	120.54
1	E	410	LEU	C-N-CA	6.26	128.99	120.54
1	C	270	LEU	CA-C-N	5.84	131.04	121.87
1	C	270	LEU	C-N-CA	5.84	131.04	121.87
1	F	117	TYR	N-CA-C	-5.51	100.25	109.24
1	C	514	PHE	CA-CB-CG	5.51	119.31	113.80
1	F	116	SER	CA-C-N	5.31	130.05	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	116	SER	C-N-CA	5.31	130.05	122.72
1	G	514	PHE	CA-CB-CG	5.26	119.06	113.80
1	C	509	GLY	CA-C-N	5.14	127.12	120.44
1	C	509	GLY	C-N-CA	5.14	127.12	120.44
1	H	514	PHE	CA-CB-CG	5.09	118.89	113.80
1	H	339	ALA	CA-C-N	5.08	131.24	121.54
1	H	339	ALA	C-N-CA	5.08	131.24	121.54
1	D	514	PHE	CA-CB-CG	5.04	118.84	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3236	0	3299	31	0
1	B	3329	0	3394	29	1
1	C	3247	0	3299	34	0
1	D	3252	0	3311	34	0
1	E	3210	0	3270	32	0
1	F	3321	0	3393	29	0
1	G	3231	0	3284	44	0
1	H	3251	0	3306	35	0
2	A	20	0	10	2	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	0	0
2	F	20	0	10	1	0
2	G	20	0	10	0	0
2	H	20	0	10	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
3	E	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	A	38	22	0	0	0
6	C	38	21	0	1	0
6	F	38	22	0	0	0
6	G	38	22	0	2	0
7	A	30	0	0	0	0
7	B	44	0	0	0	1
7	C	92	0	0	0	0
7	D	113	0	0	1	0
7	E	47	0	0	1	0
7	F	94	0	0	1	0
7	G	109	0	0	1	0
7	H	152	0	0	2	0
All	All	27134	87	26636	239	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (239) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:537:MET:HE3	1:H:537:MET:HG2	1.42	0.99
1:C:422[A]:GLU:HG3	1:C:452:LEU:HD13	1.56	0.85

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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	1.60	0.84
1:G:538:ARG:HG2	1:H:536:ILE:HG12	1.66	0.77
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.70	0.72
1:E:408:GLU:OE2	1:F:411:ARG:NH2	2.23	0.71
1:C:270:LEU:O	1:C:271:GLY:O	2.13	0.67
1:E:235:GLU:O	1:E:239:ARG:HD3	1.95	0.66
1:D:64:GLY:O	1:D:68:ARG:HG3	1.96	0.65
1:E:407:PHE:O	1:E:411:ARG:HB2	1.97	0.65
1:E:538:ARG:HG2	1:F:536:ILE:HG12	1.77	0.64
1:F:407:PHE:CE2	1:F:411:ARG:NH1	2.66	0.64
7:G:718:HOH:O	1:H:411:ARG:HD2	1.97	0.64
1:D:317:LYS:NZ	7:D:701:HOH:O	2.28	0.64
1:A:501:ARG:NH1	2:A:601:FBP:O2P	2.28	0.63
1:A:272:PRO:HA	1:A:275:HIS:NE2	2.15	0.62
1:A:528:ARG:HD2	1:A:529:PRO:O	2.00	0.61
1:E:539:VAL:HG13	1:F:535:ASN:HB2	1.83	0.60
1:E:536:ILE:HG12	1:F:538:ARG:HG2	1.84	0.60
1:H:272:PRO:HA	1:H:275[A]:HIS:CE1	2.38	0.58
1:D:382:PHE:HB3	1:D:385:GLU:HB2	1.84	0.58
1:G:267:ARG:HG2	1:G:279:ILE:CD1	2.34	0.58
1:G:272:PRO:HD2	1:G:273:GLU:OE1	2.03	0.58
1:C:411:ARG:HH12	1:D:411:ARG:NH2	2.02	0.57
1:C:538:ARG:HG2	1:D:536:ILE:HG12	1.85	0.57
1:D:130:GLY:C	1:D:132:GLY:H	2.12	0.57
1:D:528:ARG:HD2	1:D:533:TYR:CD2	2.40	0.57
1:H:382:PHE:HB3	1:H:385:GLU:HB2	1.86	0.57
1:C:411:ARG:HG3	1:C:426:ILE:HD11	1.86	0.57
1:A:421:THR:HG22	1:A:452:LEU:HD12	1.86	0.56
1:A:418[A]:ARG:HG3	1:B:16:LEU:HD11	1.88	0.55
1:A:337:VAL:HG22	1:A:370:CYS:HB2	1.88	0.55
1:A:68:ARG:HH22	1:A:98:GLU:HB3	1.71	0.55
1:C:337:VAL:HG22	1:C:370:CYS:HB2	1.88	0.55
1:D:68:ARG:HH22	1:D:98:GLU:HB2	1.70	0.55
1:G:421:THR:HG22	1:G:452:LEU:HD12	1.88	0.55
1:F:382:PHE:HB3	1:F:385:GLU:HB2	1.89	0.55
1:B:411:ARG:HD2	1:B:426:ILE:HD11	1.87	0.55
1:H:337:VAL:HG22	1:H:370:CYS:HB2	1.89	0.55
1:A:69:SER:OG	1:A:72:ARG:HB2	2.08	0.54
1:G:267:ARG:HG2	1:G:279:ILE:HD12	1.89	0.54
1:E:421:THR:HG22	1:E:452:LEU:HD12	1.90	0.54
1:A:382:PHE:HB3	1:A:385:GLU:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:56:SER:HB2	1:G:480:GLY:HA2	1.88	0.54
1:H:56:SER:HB2	1:H:480:GLY:HA2	1.90	0.54
1:E:337:VAL:HG22	1:E:370:CYS:HB2	1.89	0.53
1:F:56:SER:HB2	1:F:480:GLY:HA2	1.90	0.53
1:H:130:GLY:C	1:H:132:GLY:H	2.16	0.53
1:D:337:VAL:HG22	1:D:370:CYS:HB2	1.90	0.53
1:B:337:VAL:HG22	1:B:370:CYS:HB2	1.91	0.53
1:D:521:VAL:HG13	1:D:540:LEU:HB3	1.91	0.53
1:G:382:PHE:HB3	1:G:385:GLU:HB2	1.90	0.53
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.91	0.53
1:D:340:THR:HG22	1:D:341:GLN:HG3	1.91	0.53
1:G:537:MET:HE3	1:H:537:MET:CG	2.29	0.53
1:B:421:THR:HG22	1:B:452:LEU:HD12	1.91	0.52
1:E:60:ILE:HB	1:E:372:MET:HG3	1.90	0.52
1:F:421:THR:HG22	1:F:452:LEU:HD12	1.91	0.52
1:H:30:LEU:O	1:H:34:MET:HG2	2.10	0.52
1:A:538:ARG:HG3	1:B:536:ILE:HG12	1.92	0.52
1:G:337:VAL:HG22	1:G:370:CYS:HB2	1.92	0.52
1:H:238:VAL:O	1:H:242:ARG:HG3	2.10	0.52
1:H:421:THR:HG22	1:H:452:LEU:HD12	1.91	0.52
1:A:444:THR:HA	2:A:601:FBP:H61	1.92	0.51
1:E:422:GLU:HG2	1:E:452:LEU:HD13	1.91	0.51
1:B:382:PHE:HB3	1:B:385:GLU:HB2	1.92	0.51
1:C:411:ARG:HH12	1:D:411:ARG:HH21	1.57	0.51
1:D:60:ILE:HB	1:D:372:MET:HG3	1.92	0.51
1:C:60:ILE:HB	1:C:372:MET:HG3	1.93	0.51
1:F:30:LEU:O	1:F:34:MET:HG2	2.11	0.51
1:B:30:LEU:O	1:B:34:MET:HG2	2.11	0.51
1:B:232:GLY:O	1:B:233:LEU:C	2.53	0.51
1:D:421:THR:HG22	1:D:452:LEU:HD12	1.93	0.51
1:E:418:ARG:HD3	1:F:16:LEU:HD11	1.92	0.51
1:G:518:GLY:O	1:H:418:ARG:NH2	2.44	0.51
1:F:337:VAL:HG22	1:F:370:CYS:HB2	1.92	0.50
1:C:382:PHE:HB3	1:C:385:GLU:HB2	1.92	0.50
1:E:382:PHE:HB3	1:E:385:GLU:HB2	1.92	0.50
1:H:317:LYS:NZ	7:H:702:HOH:O	2.38	0.50
1:E:56:SER:HB2	1:E:480:GLY:HA2	1.92	0.50
1:C:421:THR:HG22	1:C:452:LEU:HD12	1.94	0.50
1:F:60:ILE:HB	1:F:372:MET:HG3	1.92	0.50
1:G:538:ARG:HH11	1:G:540:LEU:HD21	1.77	0.50
1:A:60:ILE:HB	1:A:372:MET:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:PRO:HA	1:D:275[A]:HIS:CE1	2.47	0.49
1:B:60:ILE:HB	1:B:372:MET:HG3	1.93	0.49
1:H:89:SER:HA	1:H:127:LYS:HG3	1.94	0.49
1:H:60:ILE:HB	1:H:372:MET:HG3	1.93	0.49
1:E:113:SER:HB3	7:E:744:HOH:O	2.10	0.49
1:D:89:SER:HA	1:D:127:LYS:HG3	1.95	0.49
1:H:251:ILE:HG12	1:H:477:LEU:HD11	1.95	0.49
1:G:30:LEU:O	1:G:34:MET:HG2	2.13	0.48
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.94	0.48
1:A:517:VAL:HG13	1:A:543:SER:HB3	1.95	0.48
1:G:346:MET:HA	1:G:349:LYS:O	2.13	0.48
1:G:60:ILE:HB	1:G:372:MET:HG3	1.96	0.48
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.95	0.48
1:B:407:PHE:CZ	1:B:411:ARG:HD3	2.49	0.48
1:G:423:VAL:HG21	1:H:435:CYS:HB3	1.96	0.48
1:H:46:ASP:HB3	1:H:49:SER:HB2	1.96	0.47
1:A:518:GLY:O	1:B:418:ARG:NH2	2.43	0.47
1:C:30:LEU:O	1:C:34:MET:HG2	2.14	0.47
1:E:23:ALA:HB3	1:E:26:GLN:HG2	1.96	0.47
1:A:30:LEU:O	1:A:34:MET:HG2	2.13	0.47
1:C:251:ILE:HG12	1:C:477:LEU:HD11	1.96	0.47
1:C:529:PRO:HG2	1:G:235:GLU:HG2	1.96	0.47
1:E:83:ILE:HG12	1:E:121:ALA:HB3	1.96	0.47
1:B:284:GLU:HB3	1:B:308:ASP:HB2	1.96	0.47
1:G:284:GLU:HB3	1:G:308:ASP:HB2	1.97	0.47
1:D:46:ASP:HB3	1:D:49:SER:HB2	1.97	0.47
1:F:89:SER:HA	1:F:127:LYS:HG3	1.96	0.47
1:E:46:ASP:HB3	1:E:49:SER:HB2	1.96	0.47
1:A:89:SER:HA	1:A:127:LYS:HG3	1.97	0.46
1:A:46:ASP:HB3	1:A:49:SER:HB2	1.97	0.46
1:B:89:SER:HA	1:B:127:LYS:HG3	1.97	0.46
1:H:56:SER:HB2	1:H:480:GLY:CA	2.46	0.46
1:F:46:ASP:HB3	1:F:49:SER:HB2	1.98	0.46
1:G:83:ILE:HG12	1:G:121:ALA:HB3	1.97	0.46
1:D:83:ILE:HG12	1:D:121:ALA:HB3	1.96	0.46
1:G:56:SER:HB2	1:G:480:GLY:CA	2.45	0.46
1:G:527:TRP:CE2	1:G:528:ARG:HG2	2.51	0.46
1:D:130:GLY:C	1:D:132:GLY:N	2.70	0.46
1:E:89:SER:HA	1:E:127:LYS:HG3	1.98	0.46
1:E:539:VAL:HG13	1:F:420:PRO:HB3	1.98	0.46
1:F:284:GLU:HB3	1:F:308:ASP:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:ALA:HB1	1:C:372:MET:HE2	1.99	0.46
1:C:95:TYR:CE2	6:C:605:I9K:C3	2.99	0.45
1:B:83:ILE:HG12	1:B:121:ALA:HB3	1.98	0.45
1:D:284:GLU:HB3	1:D:308:ASP:HB2	1.98	0.45
1:H:83:ILE:HG12	1:H:121:ALA:HB3	1.98	0.45
1:C:83:ILE:HG12	1:C:121:ALA:HB3	1.97	0.45
1:C:284:GLU:HB3	1:C:308:ASP:HB2	1.98	0.45
1:A:83:ILE:HG12	1:A:121:ALA:HB3	1.98	0.45
1:C:46:ASP:HB3	1:C:49:SER:HB2	1.98	0.45
1:F:56:SER:HB2	1:F:480:GLY:CA	2.47	0.45
1:G:46:ASP:HB3	1:G:49:SER:HB2	1.97	0.45
1:B:251:ILE:HG12	1:B:477:LEU:HD11	1.99	0.45
1:F:70:VAL:HG12	1:F:74:LYS:HE3	1.99	0.45
1:A:284:GLU:HB3	1:A:308:ASP:HB2	1.99	0.44
1:B:76[A]:MET:HG2	1:B:384:VAL:HG22	1.99	0.44
1:C:70:VAL:HG12	1:C:74:LYS:HE3	1.99	0.44
1:D:508:SER:O	1:D:512:ARG:HG3	2.17	0.44
1:B:258:ARG:HD3	1:B:285:ASN:HD21	1.82	0.44
1:G:452:LEU:O	1:G:455:ARG:HG2	2.18	0.44
1:E:346:MET:HA	1:E:349:LYS:O	2.17	0.44
1:H:245:VAL:HG11	1:H:273:GLU:HG2	1.99	0.44
1:C:377:THR:HA	1:C:383:PRO:HB3	1.98	0.44
1:E:284:GLU:HB3	1:E:308:ASP:HB2	2.00	0.44
1:E:340:THR:HG22	1:E:341:GLN:HG3	2.00	0.44
1:E:377:THR:HA	1:E:383:PRO:HB3	1.99	0.44
1:C:340:THR:HG22	1:C:341:GLN:HG3	2.00	0.44
1:G:251:ILE:HG12	1:G:477:LEU:HD11	1.98	0.44
1:A:377:THR:HA	1:A:383:PRO:HB3	2.00	0.44
1:E:339:ALA:HB1	1:E:372:MET:HE2	1.99	0.44
1:E:435:CYS:HB3	1:F:423:VAL:HG21	2.00	0.44
1:G:377:THR:HA	1:G:383:PRO:HB3	2.00	0.44
1:G:412:ARG:CZ	1:H:404:ARG:HD3	2.48	0.44
1:G:352:PRO:HG3	1:G:389:MET:HG2	2.00	0.44
1:C:56:SER:HB2	1:C:480:GLY:CA	2.48	0.43
1:G:90:HIS:HB2	6:G:605:I9K:C	2.48	0.43
1:A:70:VAL:HG12	1:A:74:LYS:HE3	2.00	0.43
1:A:538:ARG:CG	1:B:536:ILE:HG12	2.47	0.43
1:F:76[A]:MET:HG2	1:F:384:VAL:HG22	2.00	0.43
1:F:251:ILE:HG12	1:F:477:LEU:HD11	2.00	0.43
1:H:121:ALA:HA	1:H:473:ARG:HB3	2.00	0.43
1:H:377:THR:HA	1:H:383:PRO:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:76[A]:MET:HG2	1:G:384:VAL:HG22	2.00	0.43
1:B:377:THR:HA	1:B:383:PRO:HB3	2.01	0.43
1:D:56:SER:HB2	1:D:480:GLY:CA	2.49	0.43
1:F:377:THR:HA	1:F:383:PRO:HB3	2.00	0.43
1:F:444:THR:OG1	2:F:601:FBP:O6P	2.33	0.43
1:C:486:TYR:CZ	1:C:488:GLU:HB2	2.53	0.43
1:F:445:THR:HB	1:F:531:SER:OG	2.18	0.43
1:B:56:SER:HB2	1:B:480:GLY:CA	2.49	0.43
1:C:527:TRP:CD2	1:C:528:ARG:HG2	2.54	0.43
1:E:56:SER:HB2	1:E:480:GLY:CA	2.49	0.43
1:C:110:PHE:O	1:C:117:TYR:HB2	2.19	0.43
1:E:251:ILE:HG12	1:E:477:LEU:HD11	2.00	0.43
1:G:435:CYS:HB3	1:H:423:VAL:HG21	2.01	0.42
1:D:121:ALA:HA	1:D:473:ARG:HB3	2.01	0.42
1:A:352:PRO:HG3	1:A:389:MET:HG2	2.01	0.42
1:F:317:LYS:NZ	7:F:703:HOH:O	2.46	0.42
1:H:407:PHE:O	1:H:411:ARG:HG2	2.20	0.42
1:A:340:THR:HG22	1:A:341:GLN:HG3	1.99	0.42
1:D:68:ARG:NH2	1:D:95:TYR:O	2.52	0.42
1:B:407:PHE:O	1:B:411:ARG:HG3	2.20	0.42
1:G:89:SER:HA	1:G:127:LYS:HG3	2.02	0.42
1:H:267[B]:ARG:HA	1:H:267[B]:ARG:HD3	1.92	0.42
1:H:475:VAL:CG2	1:H:483:PRO:HB3	2.50	0.42
1:A:251:ILE:HG12	1:A:477:LEU:HD11	2.00	0.42
1:D:70:VAL:HG12	1:D:74:LYS:HE3	2.01	0.42
1:D:251:ILE:HG12	1:D:477:LEU:HD11	2.02	0.42
1:E:258:ARG:HD3	1:E:285:ASN:HD21	1.84	0.42
1:A:517:VAL:HG22	1:A:543:SER:HB3	2.01	0.41
1:C:89:SER:HA	1:C:127:LYS:HG3	2.02	0.41
1:D:335:PRO:HB3	1:D:477:LEU:O	2.19	0.41
1:H:284:GLU:HB3	1:H:308:ASP:HB2	2.01	0.41
1:H:491:GLU:HB3	7:H:767:HOH:O	2.19	0.41
1:A:452:LEU:O	1:A:455:ARG:HG2	2.21	0.41
1:A:486:TYR:CZ	1:A:488[B]:GLU:HB2	2.55	0.41
1:B:70:VAL:HG12	1:B:74:LYS:HE3	2.02	0.41
1:C:76[A]:MET:HG2	1:C:384:VAL:HG22	2.01	0.41
1:D:233:LEU:HD12	1:D:233:LEU:HA	1.88	0.41
1:E:331:LEU:HD23	1:G:43:CYS:SG	2.60	0.41
1:F:121:ALA:HA	1:F:473:ARG:HB3	2.02	0.41
1:G:527:TRP:CD2	1:G:528:ARG:HG2	2.55	0.41
1:C:411:ARG:NH1	1:D:411:ARG:NH2	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:352:PRO:HG3	1:F:389:MET:HG2	2.03	0.41
1:F:527:TRP:CE2	1:F:528:ARG:HG2	2.55	0.41
1:G:70:VAL:HG12	1:G:74:LYS:HE3	2.01	0.41
1:G:269:ALA:C	1:G:271:GLY:H	2.28	0.41
1:H:419:ASP:OD2	1:H:448:ARG:NH2	2.53	0.41
1:B:46:ASP:HB3	1:B:49:SER:HB2	2.03	0.41
1:C:423:VAL:HG21	1:D:435:CYS:HB3	2.02	0.41
1:D:346:MET:HA	1:D:349:LYS:O	2.21	0.41
1:A:517:VAL:HG22	1:A:543:SER:CB	2.51	0.41
1:C:452:LEU:O	1:C:455:ARG:HG2	2.20	0.41
1:E:70:VAL:HG12	1:E:74:LYS:HE3	2.02	0.41
1:B:452:LEU:O	1:B:455:ARG:HG2	2.21	0.41
1:C:68:ARG:NE	1:C:95:TYR:CZ	2.89	0.41
1:G:379:LYS:HD3	6:G:605:I9K:O9	2.20	0.41
1:G:475:VAL:CG2	1:G:483:PRO:HB3	2.51	0.41
1:G:411:ARG:HG2	1:G:426:ILE:HD11	2.02	0.41
1:B:340:THR:HG22	1:B:341:GLN:HG3	2.01	0.40
1:G:340:THR:HG22	1:G:341:GLN:HG3	2.03	0.40
1:C:235:GLU:HG3	1:G:529:PRO:HG3	2.04	0.40
1:C:235:GLU:OE1	1:G:494:TRP:HB2	2.20	0.40
1:E:352:PRO:HG3	1:E:389:MET:HG2	2.03	0.40
1:F:335:PRO:HB3	1:F:477:LEU:O	2.21	0.40
1:D:377:THR:HA	1:D:383:PRO:HB3	2.04	0.40
1:A:335:PRO:HB3	1:A:477:LEU:O	2.21	0.40
1:B:352:PRO:HG3	1:B:389:MET:HG2	2.03	0.40
1:D:475:VAL:CG2	1:D:483:PRO:HB3	2.52	0.40
1:E:452:LEU:O	1:E:455:ARG:HG2	2.21	0.40
1:G:520:LEU:HD23	1:G:520:LEU:HA	1.98	0.40
1:H:335:PRO:HB3	1:H:477:LEU:O	2.22	0.40
1:B:335:PRO:HB3	1:B:477:LEU:O	2.21	0.40
1:G:435:CYS:HB3	1:H:423:VAL:CG2	2.52	0.40
1:H:273:GLU:H	1:H:273:GLU:CD	2.30	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:744:HOH:O	7:B:744:HOH:O[2_555]	1.86	0.34
1:B:511:LEU:O	1:B:511:LEU:O[2_555]	2.09	0.11

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	424/447 (95%)	418 (99%)	5 (1%)	1 (0%)	43	52
1	B	438/447 (98%)	430 (98%)	4 (1%)	4 (1%)	14	14
1	C	425/447 (95%)	419 (99%)	3 (1%)	3 (1%)	18	20
1	D	429/447 (96%)	420 (98%)	6 (1%)	3 (1%)	18	20
1	E	420/447 (94%)	416 (99%)	3 (1%)	1 (0%)	43	52
1	F	435/447 (97%)	429 (99%)	5 (1%)	1 (0%)	43	52
1	G	423/447 (95%)	415 (98%)	5 (1%)	3 (1%)	18	20
1	H	427/447 (96%)	420 (98%)	4 (1%)	3 (1%)	18	20
All	All	3421/3576 (96%)	3367 (98%)	35 (1%)	19 (1%)	21	24

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	271	GLY
1	B	129	PRO
1	B	231	PRO
1	C	231	PRO
1	G	271	GLY
1	B	233	LEU
1	G	231	PRO
1	H	131	SER
1	D	535	ASN
1	E	340	THR
1	H	535	ASN
1	A	340	THR
1	B	340	THR
1	C	340	THR
1	D	340	THR
1	F	340	THR
1	G	340	THR

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Mol	Chain	Res	Type
1	H	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	340/352 (97%)	330 (97%)	10 (3%)	37	49
1	B	349/352 (99%)	334 (96%)	15 (4%)	26	34
1	C	341/352 (97%)	332 (97%)	9 (3%)	40	54
1	D	342/352 (97%)	332 (97%)	10 (3%)	37	49
1	E	338/352 (96%)	325 (96%)	13 (4%)	29	39
1	F	350/352 (99%)	336 (96%)	14 (4%)	28	37
1	G	340/352 (97%)	331 (97%)	9 (3%)	40	54
1	H	340/352 (97%)	333 (98%)	7 (2%)	47	61
All	All	2740/2816 (97%)	2653 (97%)	87 (3%)	37	46

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ARG
1	A	235	GLU
1	A	259	LYS
1	A	358	SER
1	A	408	GLU
1	A	436	CYS
1	A	475	VAL
1	A	537[A]	MET
1	A	537[B]	MET
1	A	540	LEU
1	B	10	ARG
1	B	68	ARG
1	B	76[A]	MET

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Mol	Chain	Res	Type
1	B	76[B]	MET
1	B	115	LEU
1	B	131	SER
1	B	259	LYS
1	B	263	VAL
1	B	331	LEU
1	B	358	SER
1	B	379	LYS
1	B	412	ARG
1	B	511	LEU
1	B	537[A]	MET
1	B	537[B]	MET
1	C	68	ARG
1	C	76[A]	MET
1	C	76[B]	MET
1	C	234	SER
1	C	258	ARG
1	C	259	LYS
1	C	331	LEU
1	C	358	SER
1	C	508	SER
1	D	34	MET
1	D	242[A]	ARG
1	D	242[B]	ARG
1	D	259	LYS
1	D	331	LEU
1	D	358	SER
1	D	436	CYS
1	D	528	ARG
1	D	537	MET
1	D	538	ARG
1	E	34	MET
1	E	68	ARG
1	E	71	GLU
1	E	242	ARG
1	E	259	LYS
1	E	331	LEU
1	E	358	SER
1	E	408	GLU
1	E	411	ARG
1	E	511	LEU
1	E	537[A]	MET

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Mol	Chain	Res	Type
1	E	537[B]	MET
1	E	539	VAL
1	F	16	LEU
1	F	68	ARG
1	F	76[A]	MET
1	F	76[B]	MET
1	F	115	LEU
1	F	116	SER
1	F	259	LYS
1	F	331	LEU
1	F	358	SER
1	F	408	GLU
1	F	412	ARG
1	F	511	LEU
1	F	537[A]	MET
1	F	537[B]	MET
1	G	68	ARG
1	G	76[A]	MET
1	G	76[B]	MET
1	G	259	LYS
1	G	273	GLU
1	G	331	LEU
1	G	358	SER
1	G	412	ARG
1	G	436	CYS
1	H	259	LYS
1	H	331	LEU
1	H	358	SER
1	H	412	ARG
1	H	436	CYS
1	H	531	SER
1	H	537	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	405	GLN
1	B	285	ASN
1	B	405	GLN
1	C	405	GLN
1	D	405	GLN
1	E	405	GLN

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Mol	Chain	Res	Type
1	F	405	GLN
1	G	275	HIS
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 36 ligands modelled in this entry, 16 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	OXL	F	602	4	5,5,5	2.75	4 (80%)	6,6,6	3.27	4 (66%)
2	FBP	H	601	-	18,20,20	0.86	0	21,32,32	0.91	1 (4%)
3	OXL	C	602	4	5,5,5	1.94	2 (40%)	6,6,6	1.58	1 (16%)
3	OXL	D	602	4	5,5,5	2.54	3 (60%)	6,6,6	2.79	3 (50%)
2	FBP	G	601	-	18,20,20	0.63	0	21,32,32	0.89	0
2	FBP	E	601	-	18,20,20	0.65	0	21,32,32	0.74	1 (4%)
6	I9K	C	605	-	41,41,41	0.32	0	62,63,63	0.66	0
2	FBP	A	601	-	18,20,20	0.69	0	21,32,32	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FBP	D	601	-	18,20,20	0.67	1 (5%)	21,32,32	1.14	2 (9%)
2	FBP	F	601	-	18,20,20	0.66	1 (5%)	21,32,32	0.67	0
2	FBP	C	601	-	18,20,20	0.58	0	21,32,32	1.15	3 (14%)
3	OXL	A	602	4	5,5,5	1.85	2 (40%)	6,6,6	2.89	3 (50%)
6	I9K	F	605	-	41,41,41	0.35	0	62,63,63	0.74	2 (3%)
2	FBP	B	601	-	18,20,20	0.55	0	21,32,32	1.02	2 (9%)
3	OXL	H	602	4	5,5,5	2.07	2 (40%)	6,6,6	1.54	1 (16%)
3	OXL	G	602	4	5,5,5	2.32	2 (40%)	6,6,6	1.53	2 (33%)
6	I9K	A	605	-	41,41,41	0.27	0	62,63,63	0.62	1 (1%)
3	OXL	B	602	4	5,5,5	2.31	2 (40%)	6,6,6	1.49	1 (16%)
3	OXL	E	602	4	5,5,5	2.39	2 (40%)	6,6,6	1.49	2 (33%)
6	I9K	G	605	-	41,41,41	0.34	0	62,63,63	0.47	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
3	OXL	F	602	4	-	4/4/4/4	-
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1
3	OXL	C	602	4	-	4/4/4/4	-
3	OXL	D	602	4	-	4/4/4/4	-
2	FBP	G	601	-	-	2/13/32/32	0/1/1/1
2	FBP	E	601	-	-	4/13/32/32	0/1/1/1
6	I9K	C	605	-	-	8/32/58/58	0/4/4/4
2	FBP	A	601	-	-	5/13/32/32	0/1/1/1
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
3	OXL	A	602	4	-	4/4/4/4	-
6	I9K	F	605	-	-	12/32/58/58	0/4/4/4
2	FBP	B	601	-	-	4/13/32/32	0/1/1/1
3	OXL	H	602	4	-	4/4/4/4	-
3	OXL	G	602	4	-	4/4/4/4	-
6	I9K	A	605	-	-	4/32/58/58	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OXL	B	602	4	-	4/4/4/4	-
3	OXL	E	602	4	-	4/4/4/4	-
6	I9K	G	605	-	-	8/32/58/58	0/4/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	OXL	O2-C2	4.67	1.34	1.22
3	E	602	OXL	O1-C1	4.37	1.33	1.22
3	D	602	OXL	O2-C2	4.18	1.32	1.22
3	G	602	OXL	O3-C1	-3.75	1.20	1.30
3	H	602	OXL	O2-C2	3.52	1.31	1.22
3	A	602	OXL	O2-C2	3.41	1.31	1.22
3	F	602	OXL	O1-C1	3.30	1.30	1.22
3	G	602	OXL	O1-C1	3.26	1.30	1.22
3	F	602	OXL	O2-C2	3.15	1.30	1.22
3	F	602	OXL	O3-C1	-3.15	1.22	1.30
3	C	602	OXL	O1-C1	3.04	1.30	1.22
3	C	602	OXL	O3-C1	-2.93	1.22	1.30
3	H	602	OXL	O4-C2	-2.77	1.23	1.30
3	E	602	OXL	O3-C1	-2.74	1.23	1.30
3	D	602	OXL	O4-C2	-2.62	1.23	1.30
3	F	602	OXL	O4-C2	-2.59	1.23	1.30
3	D	602	OXL	C2-C1	2.46	1.58	1.54
2	F	601	FBP	P2-O4P	2.39	1.57	1.50
3	A	602	OXL	O4-C2	-2.34	1.24	1.30
2	D	601	FBP	P2-O5P	-2.18	1.46	1.54
3	B	602	OXL	O4-C2	-2.08	1.24	1.30

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	602	OXL	O4-C2-C1	5.37	123.24	112.83
3	A	602	OXL	O4-C2-C1	5.06	122.65	112.83
3	D	602	OXL	O3-C1-C2	4.59	121.74	112.83
3	F	602	OXL	O3-C1-C2	4.27	121.12	112.83
3	D	602	OXL	O4-C2-C1	3.74	120.09	112.83
3	A	602	OXL	O2-C2-C1	-3.49	113.36	120.63
3	F	602	OXL	O2-C2-C1	-3.42	113.51	120.63
2	D	601	FBP	O5P-P2-O6	3.25	115.15	106.67
6	F	605	I9K	C12-N-S	3.24	123.09	117.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	602	OXL	O4-C2-C1	3.20	119.04	112.83
3	A	602	OXL	O3-C1-C2	3.17	118.97	112.83
3	C	602	OXL	O3-C1-C2	3.13	118.90	112.83
2	B	601	FBP	O5P-P2-O6	3.07	114.67	106.67
6	F	605	I9K	C21-N-S	2.99	122.61	117.06
3	D	602	OXL	O1-C1-C2	-2.77	114.87	120.63
3	G	602	OXL	O4-C2-C1	2.56	117.78	112.83
2	C	601	FBP	O3-C3-C4	2.51	122.09	113.25
2	C	601	FBP	O3P-P1-O1	2.49	113.17	106.67
3	E	602	OXL	O3-C1-C2	2.47	117.62	112.83
3	B	602	OXL	O4-C2-C1	2.47	117.62	112.83
3	E	602	OXL	O4-C2-C1	2.46	117.60	112.83
3	G	602	OXL	O3-C1-C2	2.42	117.53	112.83
3	F	602	OXL	O1-C1-C2	-2.29	115.87	120.63
2	C	601	FBP	O6-P2-O4P	2.14	112.23	106.44
2	D	601	FBP	O6-P2-O4P	-2.11	100.73	106.44
2	E	601	FBP	O6-P2-O4P	2.10	112.12	106.44
2	B	601	FBP	O3P-P1-O2P	2.09	115.65	107.80
2	H	601	FBP	O6P-P2-O5P	2.07	115.57	107.80
6	A	605	I9K	C13-N1-C14	2.02	129.48	122.83

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FBP	C6-O6-P2-O4P
2	A	601	FBP	C6-O6-P2-O5P
2	A	601	FBP	C6-O6-P2-O6P
2	B	601	FBP	C1-O1-P1-O2P
2	B	601	FBP	C1-O1-P1-O3P
2	E	601	FBP	C1-O1-P1-O2P
2	E	601	FBP	O1-C1-C2-O5
6	G	605	I9K	N1-C14-C15-C16
6	G	605	I9K	O7-C14-C15-C16
6	G	605	I9K	C14-C15-C16-O2
6	G	605	I9K	C14-C15-C16-C17
6	G	605	I9K	C14-C15-C16-C18
2	B	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6
2	D	601	FBP	C4-C5-C6-O6
2	E	601	FBP	C4-C5-C6-O6
2	F	601	FBP	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	H	601	FBP	C4-C5-C6-O6
6	G	605	I9K	C21-N-S-O8
6	C	605	I9K	C14-C15-C16-O2
6	C	605	I9K	C14-C15-C16-C18
6	C	605	I9K	C14-C15-C16-C17
2	E	601	FBP	O5-C5-C6-O6
2	H	601	FBP	O5-C5-C6-O6
6	F	605	I9K	C12-N-S-O9
6	F	605	I9K	C12-N-S-O8
6	G	605	I9K	C21-N-S-C11
2	D	601	FBP	O5-C5-C6-O6
6	C	605	I9K	C21-N-S-O8
2	A	601	FBP	O5-C5-C6-O6
2	B	601	FBP	O5-C5-C6-O6
2	F	601	FBP	O5-C5-C6-O6
2	G	601	FBP	C4-C5-C6-O6
6	A	605	I9K	O2-C16-C18-C19
6	A	605	I9K	C17-C16-C18-C19
6	F	605	I9K	O2-C16-C18-C19
6	F	605	I9K	C17-C16-C18-C19
2	A	601	FBP	C4-C5-C6-O6
2	C	601	FBP	O5-C5-C6-O6
3	D	602	OXL	O3-C1-C2-O4
6	A	605	I9K	C15-C16-C18-C19
3	H	602	OXL	O3-C1-C2-O4
6	F	605	I9K	C12-N-S-C11
6	C	605	I9K	C21-N-S-C11
6	F	605	I9K	C15-C16-C18-C19
6	F	605	I9K	C21-N-S-O8
3	C	602	OXL	O3-C1-C2-O4
6	F	605	I9K	C21-N-S-O9
3	A	602	OXL	O3-C1-C2-O4
3	B	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
6	A	605	I9K	C22-C11-S-O8
6	F	605	I9K	C22-C11-S-O8
6	G	605	I9K	C22-C11-S-O8
3	A	602	OXL	O1-C1-C2-O2
3	B	602	OXL	O1-C1-C2-O2
3	H	602	OXL	O3-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	C	602	OXL	O1-C1-C2-O2
3	F	602	OXL	O1-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O2
3	E	602	OXL	O1-C1-C2-O2
3	G	602	OXL	O1-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O4
3	D	602	OXL	O3-C1-C2-O2
6	C	605	I9K	C12-N-S-O9
6	C	605	I9K	C12-N-S-O8
6	C	605	I9K	C22-C11-S-O9
2	G	601	FBP	O5-C5-C6-O6
3	C	602	OXL	O3-C1-C2-O2
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	F	602	OXL	O3-C1-C2-O2
3	G	602	OXL	O3-C1-C2-O2
6	F	605	I9K	C21-N-S-C11
3	C	602	OXL	O1-C1-C2-O4
3	E	602	OXL	O1-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O2
3	F	602	OXL	O1-C1-C2-O4
3	G	602	OXL	O1-C1-C2-O4
6	F	605	I9K	N1-C14-C15-C16
3	H	602	OXL	O1-C1-C2-O4
6	F	605	I9K	O7-C14-C15-C16

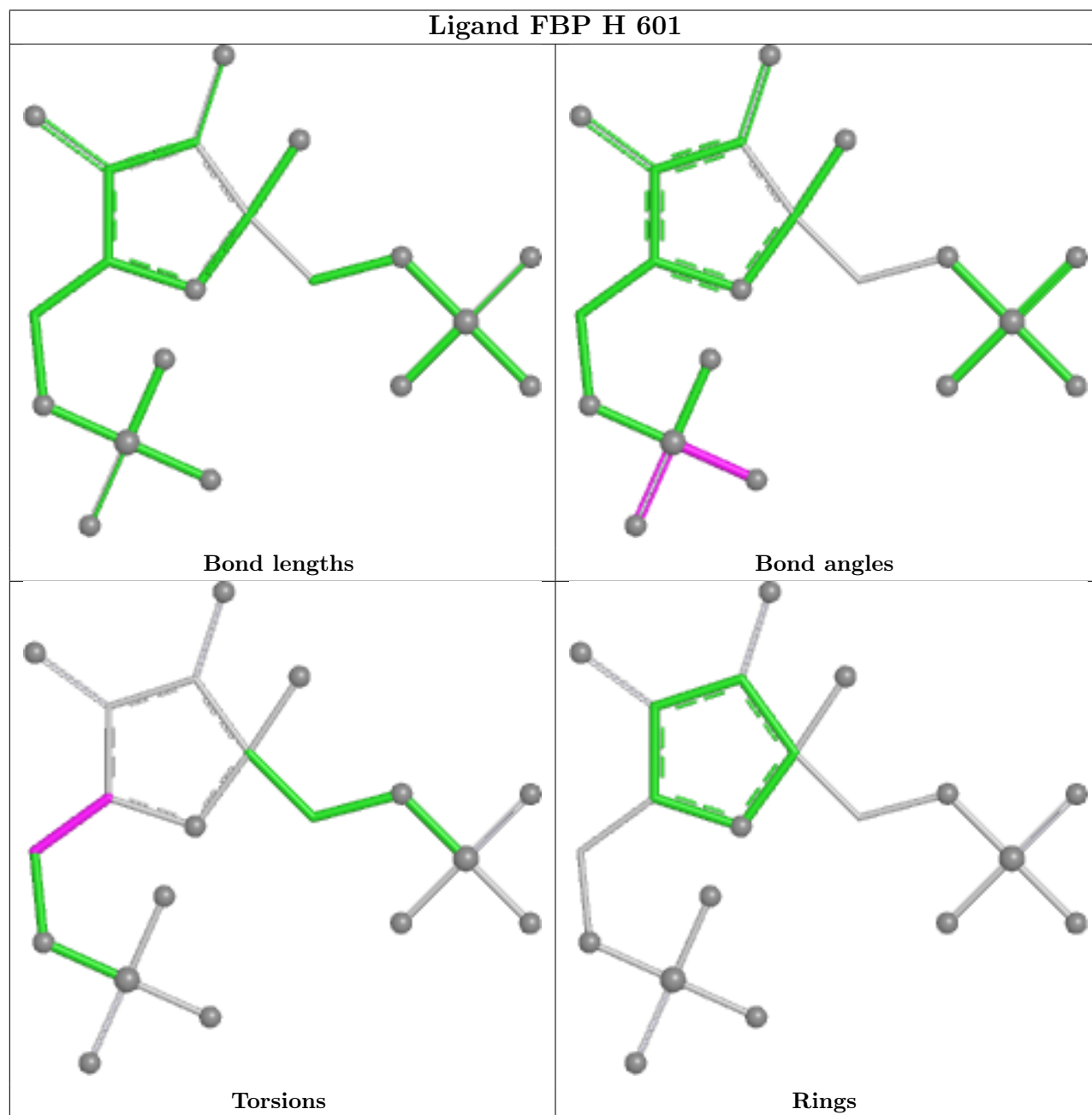
There are no ring outliers.

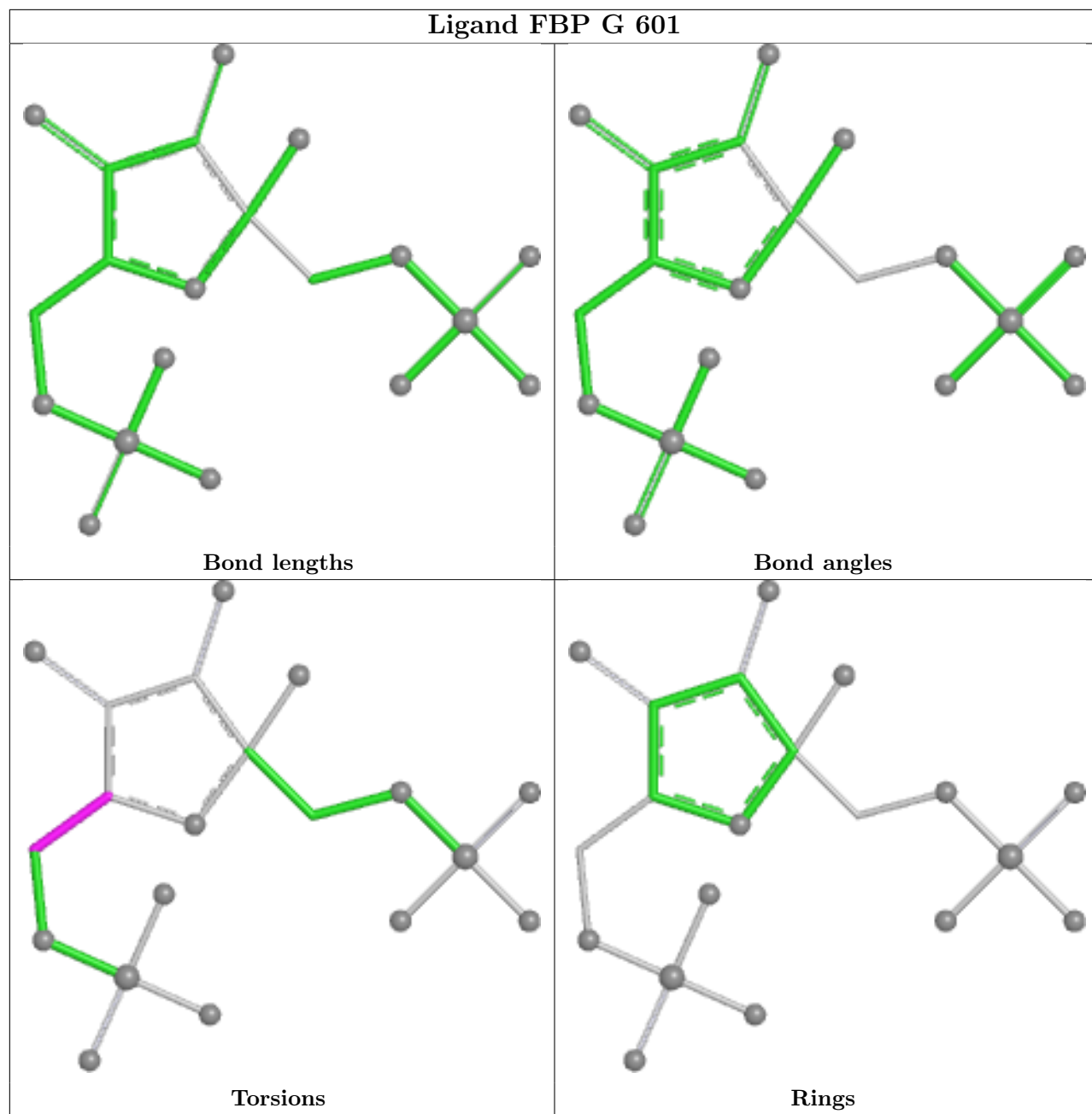
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	605	I9K	1	0
2	A	601	FBP	2	0
2	F	601	FBP	1	0
6	G	605	I9K	2	0

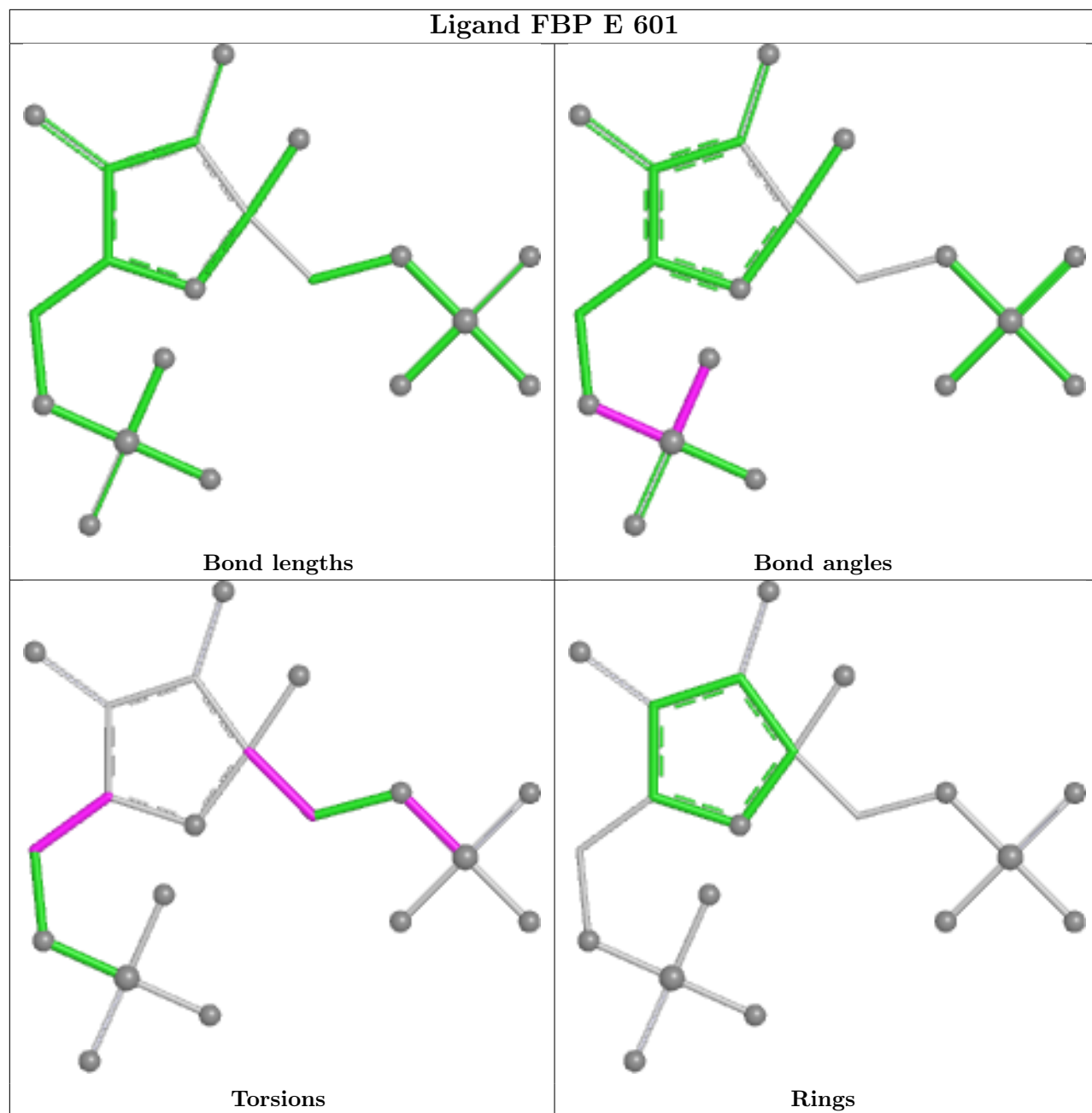
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

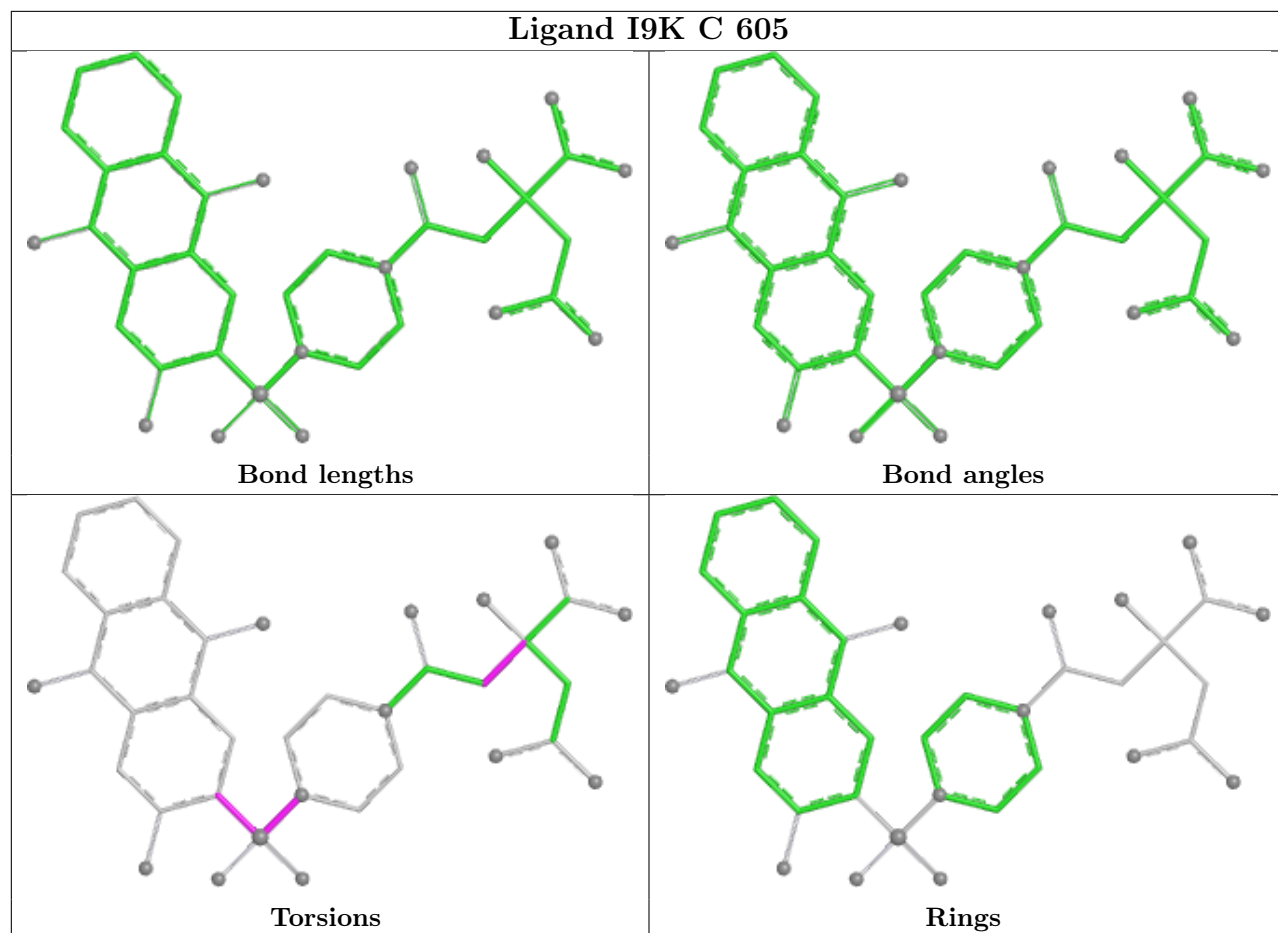




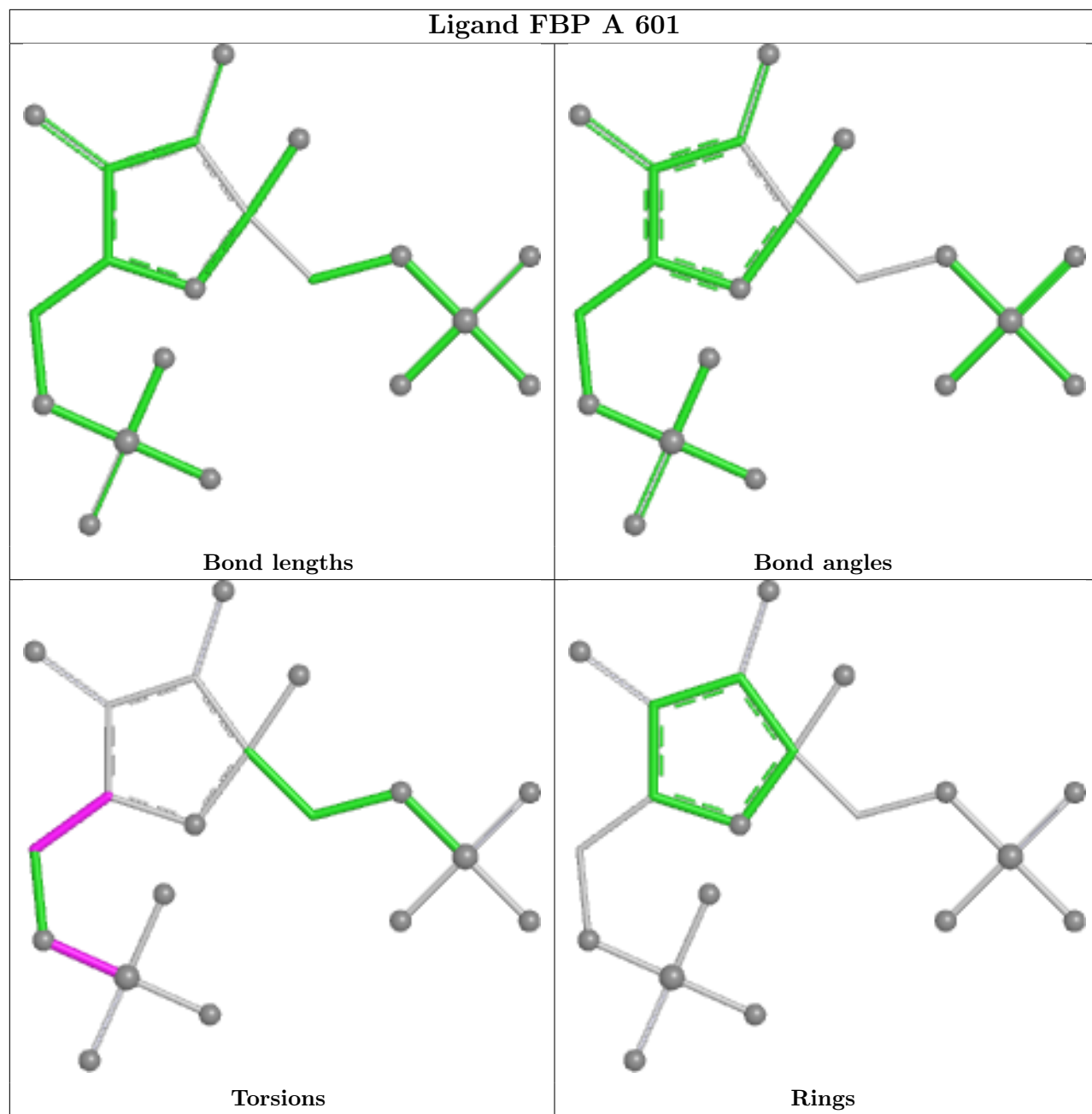
Ligand FBP E 601

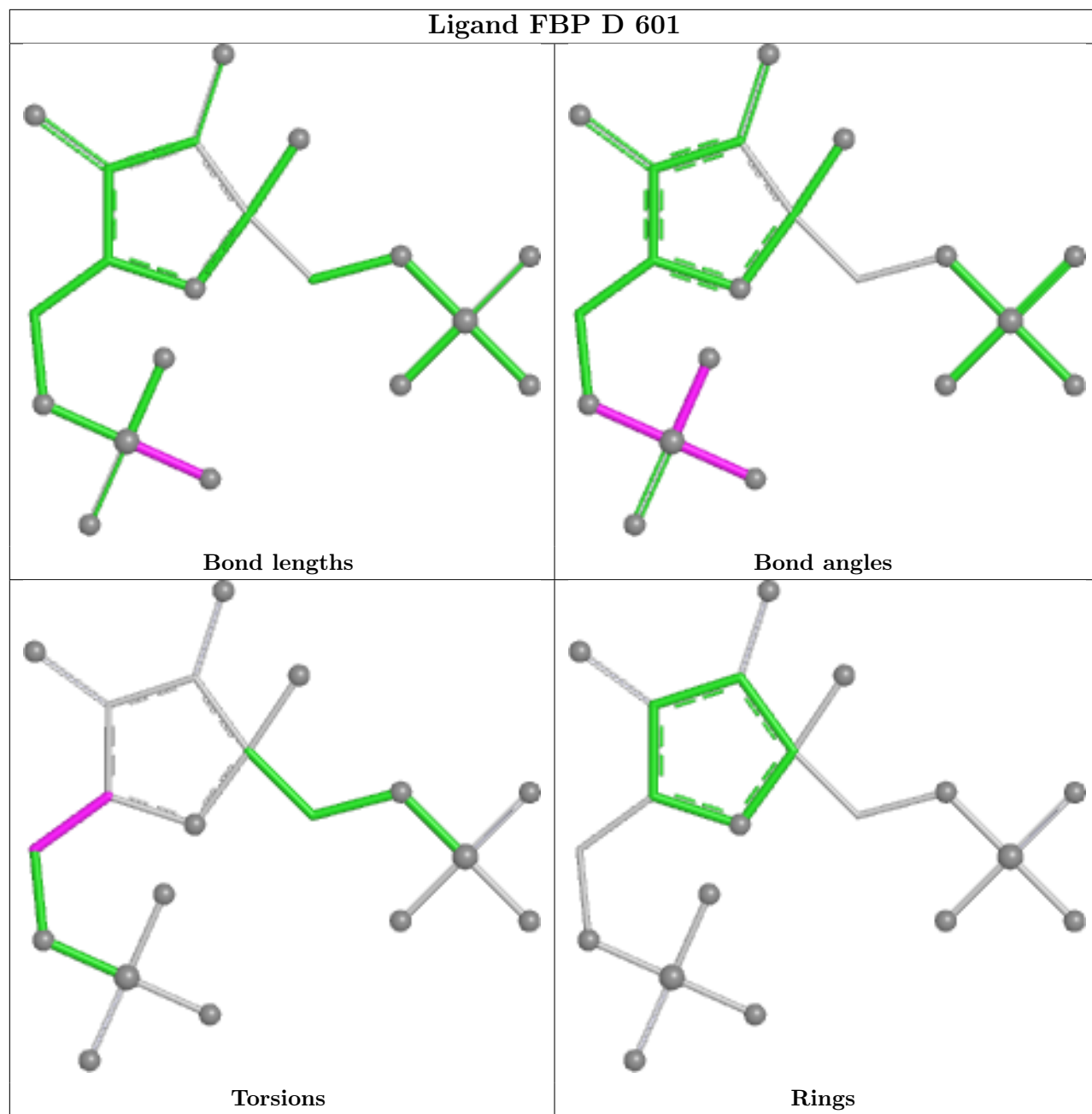


Ligand I9K C 605

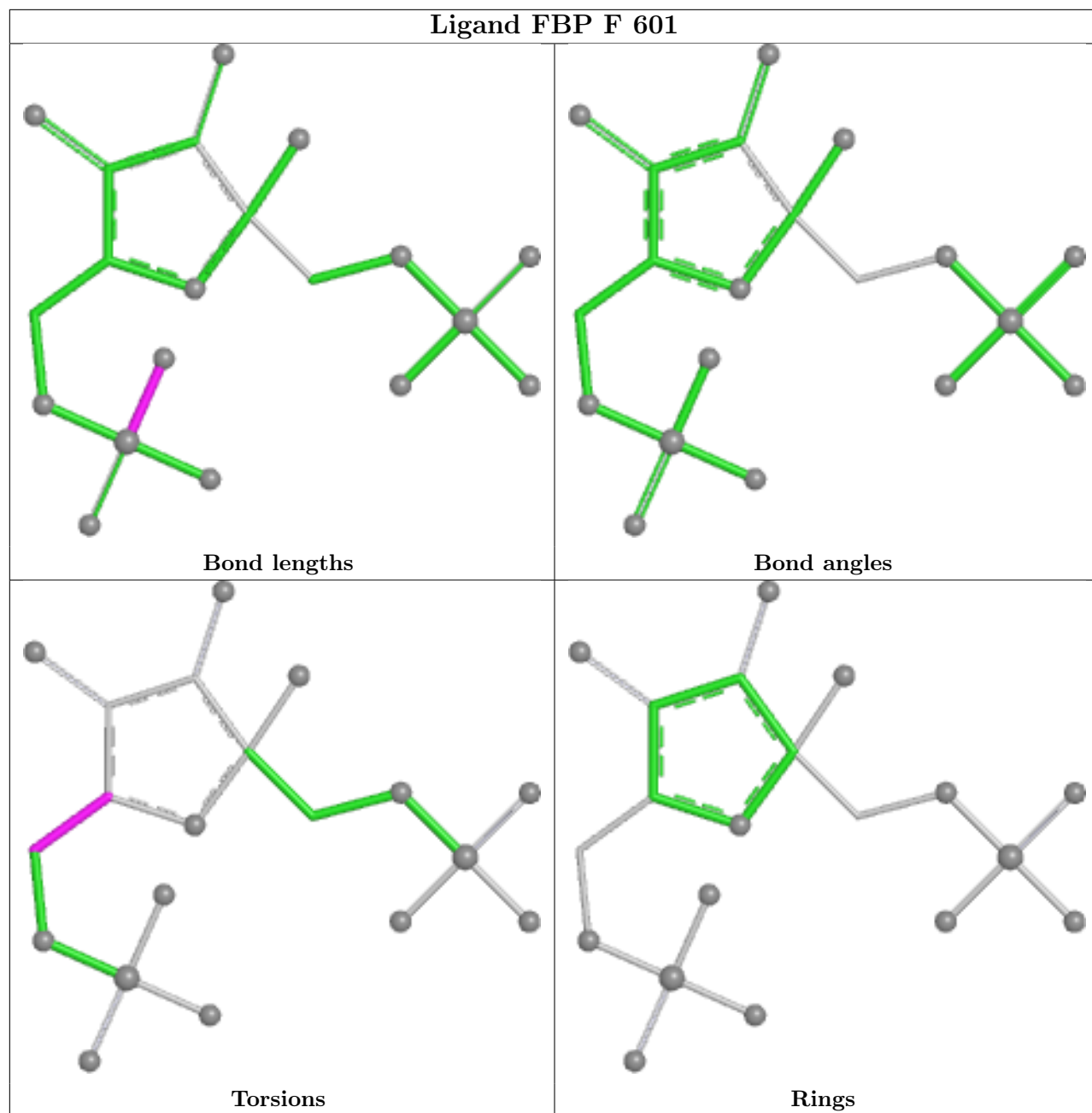


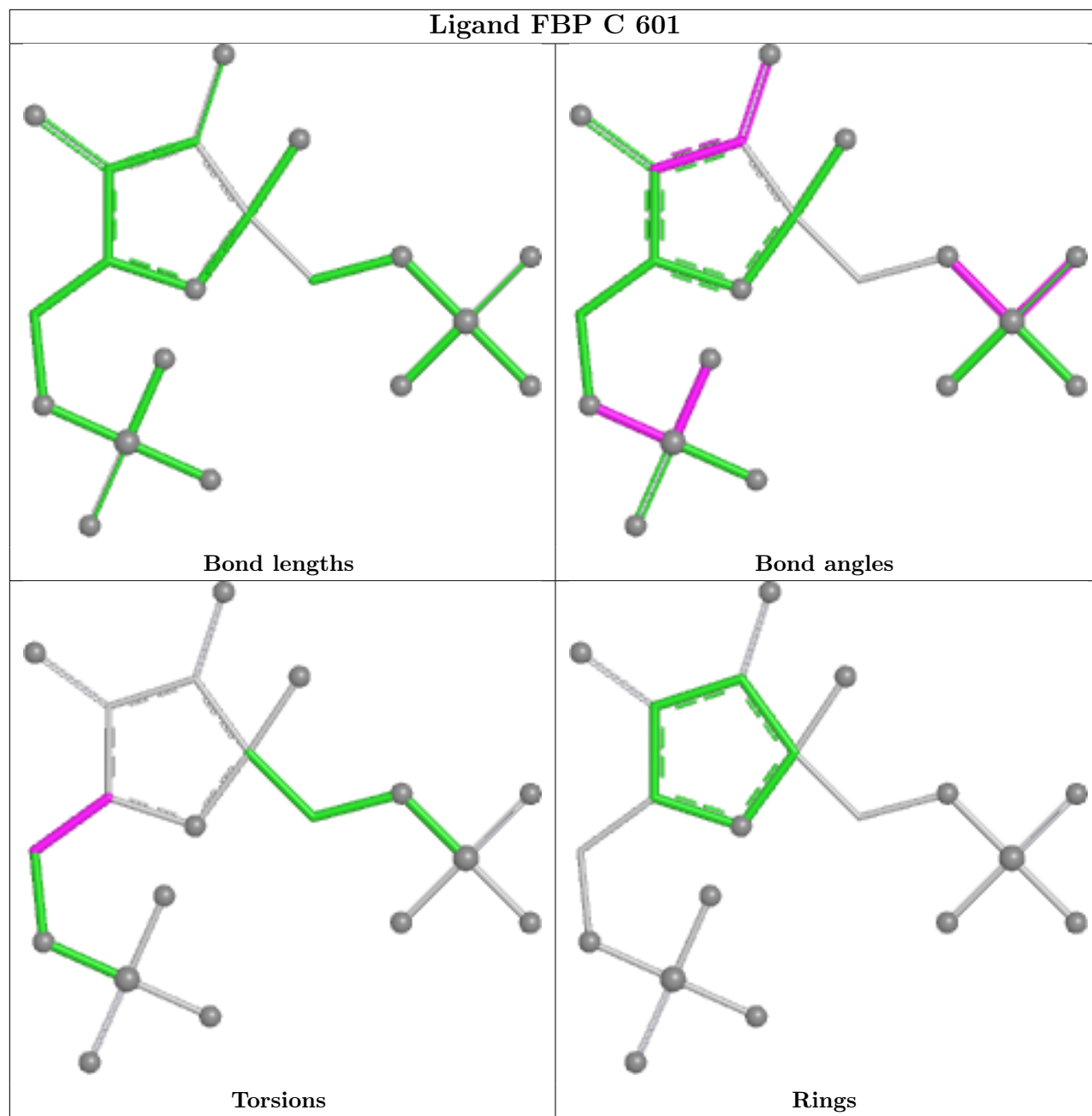
Ligand FBP A 601



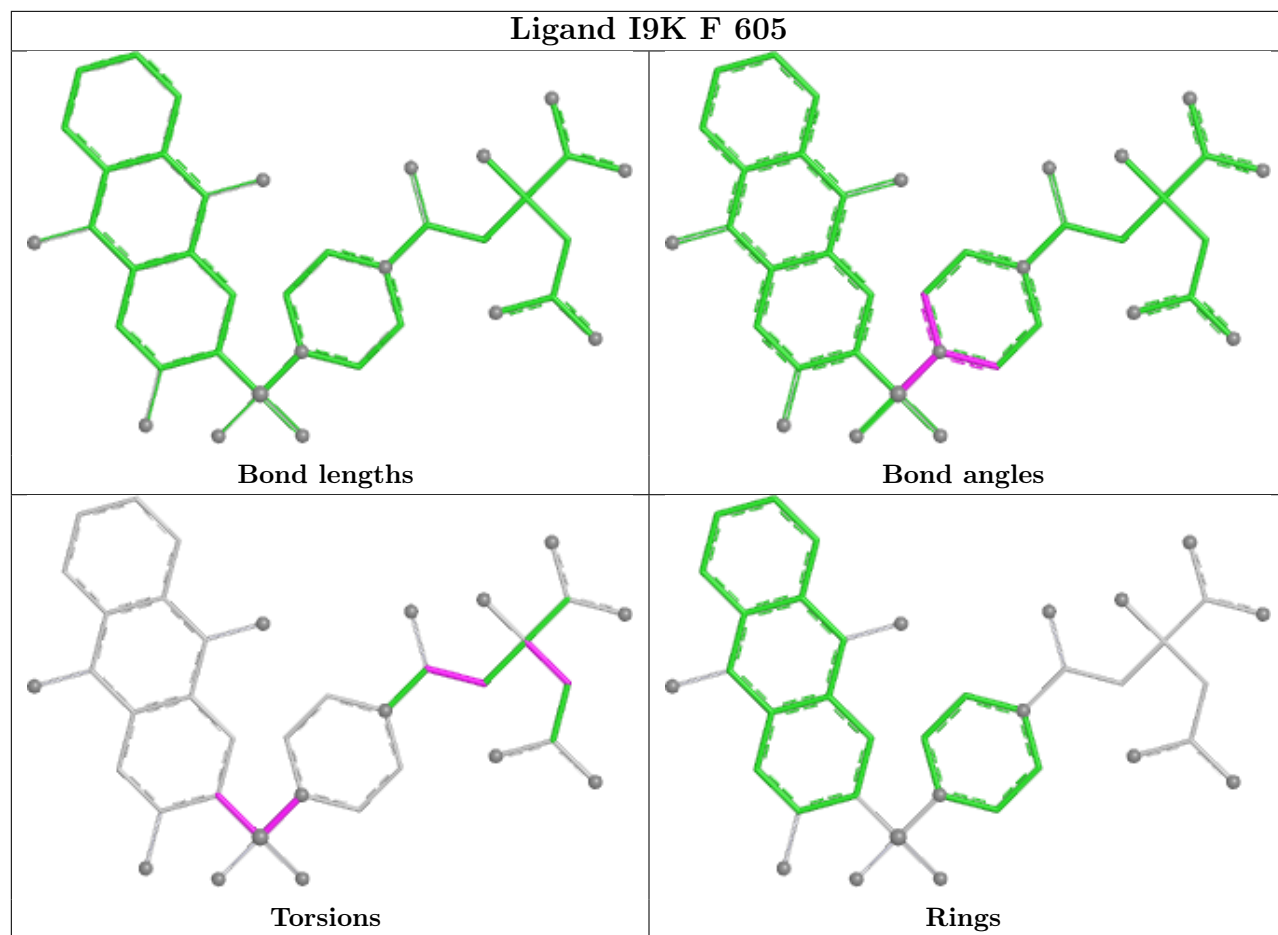


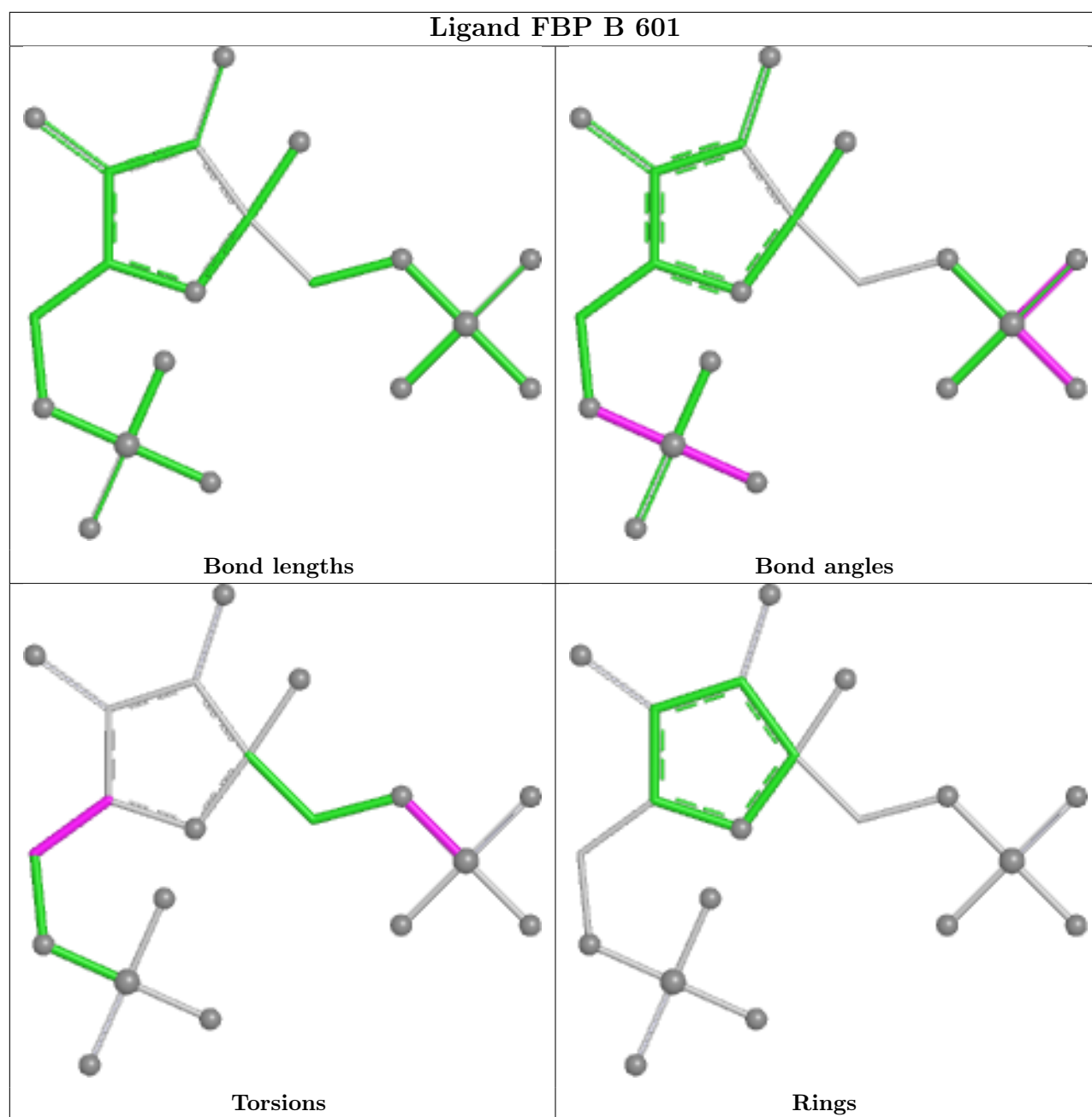
Ligand FBP F 601



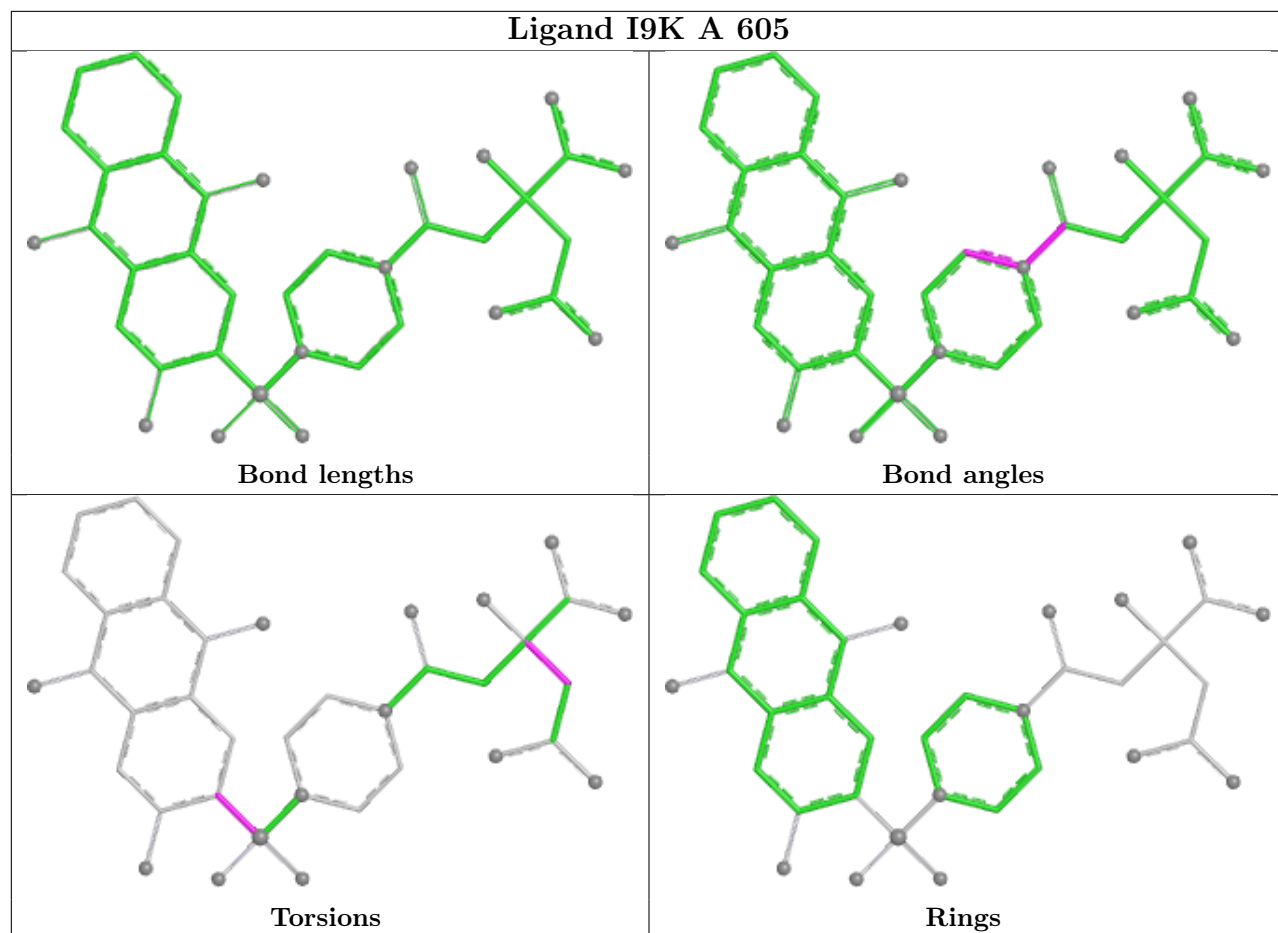


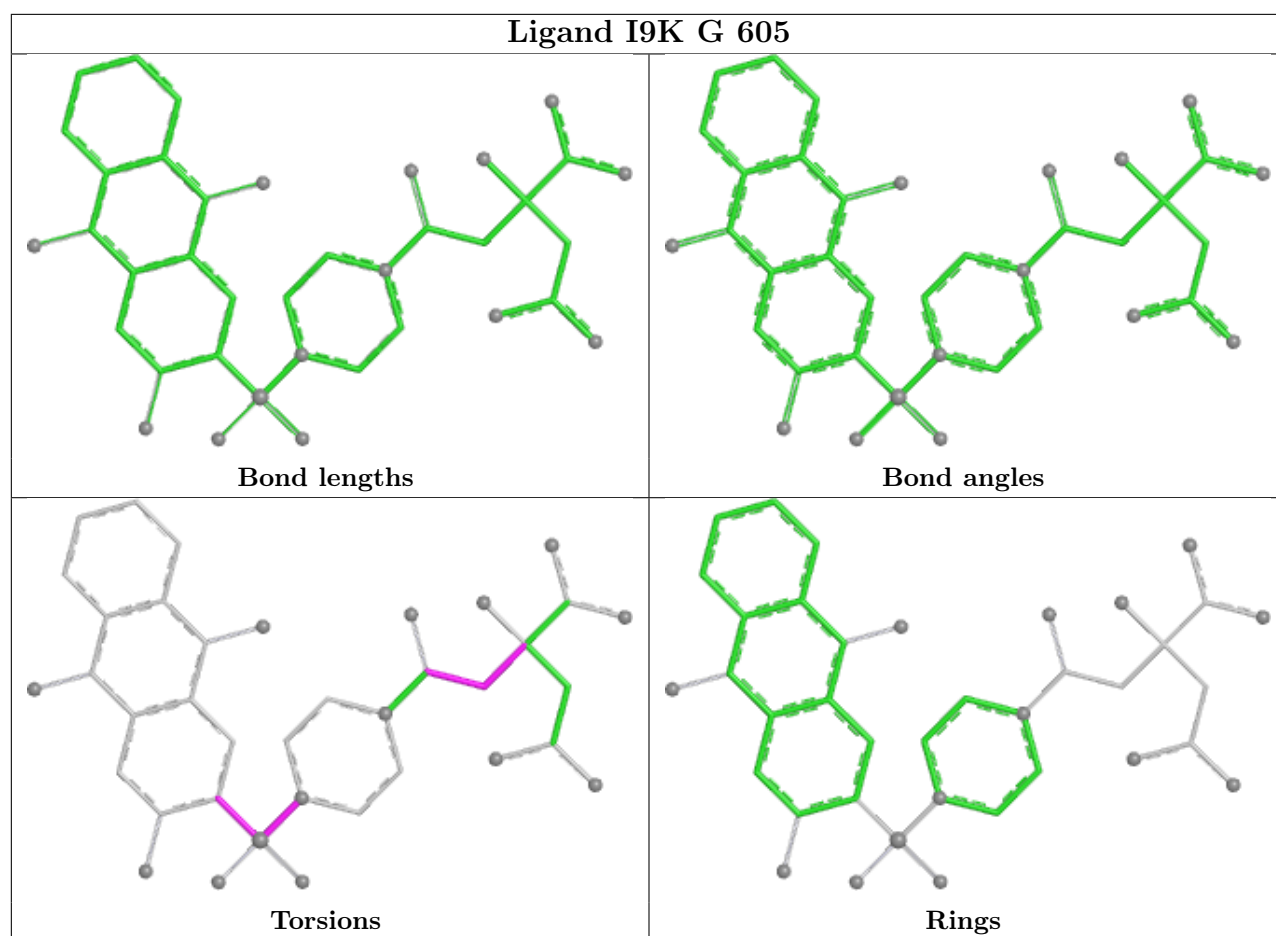
Ligand I9K F 605





Ligand I9K A 605





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	422/447 (94%)	1.40	94 (22%)	2 2	40, 75, 107, 120	6 (1%)
1	B	436/447 (97%)	1.26	90 (20%)	2 2	30, 64, 98, 108	4 (0%)
1	C	425/447 (95%)	0.66	43 (10%)	12 14	28, 52, 81, 133	4 (0%)
1	D	425/447 (95%)	0.25	16 (3%)	44 50	21, 41, 73, 122	6 (1%)
1	E	419/447 (93%)	1.14	73 (17%)	4 4	33, 67, 97, 117	5 (1%)
1	F	432/447 (96%)	0.69	40 (9%)	14 17	32, 53, 84, 100	7 (1%)
1	G	421/447 (94%)	0.44	22 (5%)	33 38	24, 46, 73, 106	7 (1%)
1	H	425/447 (95%)	0.06	10 (2%)	59 66	20, 39, 67, 116	4 (0%)
All	All	3405/3576 (95%)	0.74	388 (11%)	10 11	20, 54, 94, 133	43 (1%)

All (388) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	543	SER	6.2
1	F	231	PRO	6.1
1	C	20	LEU	6.1
1	A	232	GLY	6.0
1	A	490	PRO	6.0
1	A	241	LEU	5.7
1	G	23	ALA	5.7
1	B	231	PRO	5.5
1	H	21	GLY	5.4
1	D	21	GLY	5.3
1	E	400	ALA	5.2
1	A	489	PRO	5.0
1	B	517	VAL	4.9
1	A	23	ALA	4.8
1	E	23	ALA	4.8
1	A	482	PHE	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	249	VAL	4.6
1	B	132	GLY	4.6
1	D	25	PHE	4.6
1	G	115	LEU	4.6
1	A	132	GLY	4.5
1	G	25	PHE	4.5
1	C	366	ASP	4.5
1	A	63	ILE	4.5
1	A	463	ILE	4.5
1	G	363	ALA	4.5
1	C	23	ALA	4.5
1	E	25	PHE	4.4
1	B	115	LEU	4.4
1	B	511	LEU	4.4
1	A	475	VAL	4.3
1	E	103	VAL	4.3
1	C	400	ALA	4.3
1	A	253	PHE	4.3
1	E	120	VAL	4.3
1	C	22	THR	4.3
1	E	540	LEU	4.3
1	A	238	VAL	4.2
1	E	238	VAL	4.2
1	E	244	GLY	4.2
1	D	23	ALA	4.1
1	C	132	GLY	4.1
1	E	129	PRO	4.1
1	D	24	PHE	4.0
1	E	232	GLY	4.0
1	A	493	ILE	4.0
1	G	42	LEU	4.0
1	A	531	SER	4.0
1	B	543	SER	4.0
1	B	379	LYS	3.9
1	A	25	PHE	3.9
1	A	530	GLY	3.9
1	E	447	GLY	3.9
1	E	24	PHE	3.9
1	G	24	PHE	3.9
1	A	464	ALA	3.8
1	A	495	ALA	3.8
1	B	490	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	242[A]	ARG	3.8
1	A	492	ALA	3.8
1	C	21	GLY	3.7
1	F	233	LEU	3.7
1	H	23	ALA	3.7
1	F	36	ASP	3.7
1	G	132	GLY	3.6
1	E	233	LEU	3.6
1	B	114	PRO	3.6
1	C	338	CYS	3.6
1	B	95	TYR	3.5
1	F	511	LEU	3.5
1	A	114	PRO	3.5
1	B	116	SER	3.5
1	D	22	THR	3.5
1	H	25	PHE	3.5
1	A	465	VAL	3.5
1	F	115	LEU	3.5
1	H	24	PHE	3.5
1	B	520	LEU	3.4
1	B	540[A]	LEU	3.4
1	G	322	GLN	3.4
1	G	38	PHE	3.4
1	B	515	LEU	3.4
1	A	33	ALA	3.4
1	A	471	ALA	3.4
1	C	115	LEU	3.3
1	C	25	PHE	3.3
1	A	453	LEU	3.3
1	F	540[A]	LEU	3.3
1	A	280	ILE	3.3
1	B	120	VAL	3.3
1	E	101	ALA	3.3
1	C	42	LEU	3.3
1	D	275[A]	HIS	3.3
1	C	19	GLU	3.3
1	D	238	VAL	3.3
1	E	495	ALA	3.2
1	H	22	THR	3.2
1	E	272	PRO	3.2
1	E	489	PRO	3.2
1	C	371	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	514	PHE	3.2
1	B	267[A]	ARG	3.2
1	C	397	ALA	3.2
1	A	532	GLY	3.2
1	E	275	HIS	3.2
1	C	231	PRO	3.2
1	A	88	PHE	3.2
1	A	441	ILE	3.1
1	A	124	LEU	3.1
1	F	351	ARG	3.1
1	B	279	ILE	3.1
1	C	39	LEU	3.1
1	A	24	PHE	3.0
1	B	489	PRO	3.0
1	E	266	VAL	3.0
1	E	277	ILE	3.0
1	C	487	ARG	3.0
1	C	24	PHE	3.0
1	A	115	LEU	3.0
1	B	498	VAL	3.0
1	E	463	ILE	3.0
1	F	493	ILE	3.0
1	E	490	PRO	3.0
1	E	304	VAL	2.9
1	B	509	GLY	2.9
1	F	114	PRO	2.9
1	G	39	LEU	2.9
1	A	498	VAL	2.9
1	A	523	VAL	2.9
1	E	114	PRO	2.9
1	E	123	ALA	2.9
1	F	459	ARG	2.9
1	B	107	VAL	2.9
1	B	502	VAL	2.9
1	A	110	PHE	2.9
1	A	309	LEU	2.9
1	B	495	ALA	2.9
1	G	26	GLN	2.9
1	A	502	VAL	2.9
1	B	523	VAL	2.9
1	C	109	SER	2.8
1	E	234	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	543	SER	2.8
1	A	365	LEU	2.8
1	E	33	ALA	2.8
1	E	245	VAL	2.8
1	B	338	CYS	2.8
1	F	232	GLY	2.8
1	F	516	ARG	2.8
1	G	351	ARG	2.8
1	E	403	HIS	2.8
1	C	331	LEU	2.8
1	E	450	ALA	2.8
1	H	318	VAL	2.8
1	B	272	PRO	2.8
1	C	111	ALA	2.8
1	C	361	ALA	2.8
1	F	11	ALA	2.8
1	B	514	PHE	2.8
1	B	52	VAL	2.8
1	G	366	ASP	2.8
1	B	100	ILE	2.7
1	E	493	ILE	2.7
1	A	450	ALA	2.7
1	B	14	ALA	2.7
1	E	111	ALA	2.7
1	B	387	VAL	2.7
1	F	517	VAL	2.7
1	B	233	LEU	2.7
1	B	61	ALA	2.7
1	B	38	PHE	2.7
1	B	22	THR	2.7
1	F	267[A]	ARG	2.7
1	A	233	LEU	2.7
1	B	485	LEU	2.7
1	D	400	ALA	2.6
1	E	28	GLN	2.6
1	A	488[A]	GLU	2.6
1	B	524	VAL	2.6
1	B	375	GLY	2.6
1	F	487	ARG	2.6
1	A	263	VAL	2.6
1	B	84	ALA	2.6
1	E	97	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	512	ARG	2.6
1	A	38	PHE	2.6
1	B	103	VAL	2.6
1	B	249	VAL	2.6
1	D	231	PRO	2.6
1	E	502	VAL	2.6
1	F	489	PRO	2.6
1	G	231	PRO	2.6
1	C	393	ILE	2.6
1	F	408	GLU	2.5
1	C	363	ALA	2.5
1	B	232	GLY	2.5
1	B	504	PHE	2.5
1	E	521	VAL	2.5
1	F	521	VAL	2.5
1	B	493	ILE	2.5
1	C	309	LEU	2.5
1	E	270	LEU	2.5
1	A	125	ASP	2.5
1	D	32	ALA	2.5
1	A	113	SER	2.5
1	B	92	SER	2.5
1	B	539	VAL	2.5
1	E	263	VAL	2.5
1	E	331	LEU	2.5
1	F	269	ALA	2.5
1	A	538	ARG	2.5
1	A	73	LEU	2.5
1	E	241	LEU	2.5
1	E	526	GLY	2.5
1	A	118	ARG	2.4
1	A	70	VAL	2.4
1	A	257	VAL	2.4
1	B	440	ILE	2.4
1	B	542	ILE	2.4
1	E	402	TYR	2.4
1	C	34	MET	2.4
1	A	254	ALA	2.4
1	A	268	ALA	2.4
1	A	460	ALA	2.4
1	C	43	CYS	2.4
1	A	245	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	77	ILE	2.4
1	B	243	PHE	2.4
1	C	365	LEU	2.4
1	E	485	LEU	2.4
1	F	484	LEU	2.4
1	C	26	GLN	2.4
1	E	108	GLU	2.4
1	F	129	PRO	2.4
1	B	130	GLY	2.4
1	C	80	GLY	2.4
1	F	513	GLY	2.4
1	C	319	PHE	2.4
1	A	86	LEU	2.4
1	A	270	LEU	2.4
1	B	39	LEU	2.4
1	E	487	ARG	2.4
1	C	36	ASP	2.4
1	A	327	GLY	2.4
1	B	11	ALA	2.4
1	A	449	SER	2.4
1	F	506	ILE	2.4
1	B	73	LEU	2.4
1	E	115	LEU	2.4
1	F	512	ARG	2.4
1	A	491	GLU	2.4
1	C	114	PRO	2.3
1	A	256	PHE	2.3
1	A	318	VAL	2.3
1	C	59	ILE	2.3
1	E	465	VAL	2.3
1	D	232	GLY	2.3
1	B	378	ALA	2.3
1	A	34	MET	2.3
1	B	508	SER	2.3
1	G	116	SER	2.3
1	A	122	ILE	2.3
1	A	273	GLU	2.3
1	B	252	VAL	2.3
1	B	275	HIS	2.3
1	E	251	ILE	2.3
1	E	280	ILE	2.3
1	B	521	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	39	LEU	2.3
1	B	366	ASP	2.3
1	A	95	TYR	2.3
1	A	403	HIS	2.3
1	H	275[A]	HIS	2.3
1	B	465	VAL	2.3
1	G	364	VAL	2.3
1	A	127	LYS	2.3
1	B	129	PRO	2.3
1	B	91	GLY	2.3
1	B	112	GLY	2.3
1	B	269	ALA	2.3
1	F	527	TRP	2.3
1	A	541	SER	2.3
1	C	408	GLU	2.3
1	F	235	GLU	2.3
1	B	251	ILE	2.3
1	A	407	PHE	2.2
1	C	44	LEU	2.2
1	E	515	LEU	2.2
1	G	489	PRO	2.2
1	A	258	ARG	2.2
1	A	120	VAL	2.2
1	A	540	LEU	2.2
1	B	484	LEU	2.2
1	F	52	VAL	2.2
1	B	274	GLY	2.2
1	C	232	GLY	2.2
1	H	130	GLY	2.2
1	F	116	SER	2.2
1	A	401	VAL	2.2
1	G	360	VAL	2.2
1	C	38	PHE	2.2
1	C	110	PHE	2.2
1	E	253	PHE	2.2
1	G	114	PRO	2.2
1	G	490	PRO	2.2
1	B	527	TRP	2.2
1	A	277	ILE	2.2
1	A	283	ILE	2.2
1	A	351	ARG	2.2
1	B	72	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	366	ASP	2.2
1	E	401	VAL	2.2
1	E	433	PHE	2.2
1	H	38	PHE	2.2
1	F	490	PRO	2.2
1	C	127	LYS	2.2
1	A	116	SER	2.2
1	A	377	THR	2.2
1	A	400	ALA	2.2
1	B	321	ALA	2.2
1	F	14	ALA	2.2
1	F	23	ALA	2.2
1	B	117	TYR	2.1
1	E	118	ARG	2.1
1	B	347	ILE	2.1
1	A	494	TRP	2.1
1	E	309	LEU	2.1
1	A	304	VAL	2.1
1	E	70	VAL	2.1
1	F	103	VAL	2.1
1	A	53	ALA	2.1
1	A	99	SER	2.1
1	B	121	ALA	2.1
1	E	104	ARG	2.1
1	A	477	LEU	2.1
1	B	416	LEU	2.1
1	E	122	ILE	2.1
1	E	484	LEU	2.1
1	F	309	LEU	2.1
1	A	527	TRP	2.1
1	E	289	VAL	2.1
1	E	256	PHE	2.1
1	E	383	PRO	2.1
1	F	502	VAL	2.1
1	F	319	PHE	2.1
1	A	111	ALA	2.1
1	B	67	SER	2.1
1	C	116	SER	2.1
1	D	315	ALA	2.1
1	E	464	ALA	2.1
1	B	311	ILE	2.1
1	E	302	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	405	GLN	2.1
1	A	445	THR	2.1
1	B	131	SER	2.1
1	A	106	ALA	2.1
1	B	438	ALA	2.1
1	C	33	ALA	2.1
1	B	75	GLU	2.1
1	C	405	GLN	2.1
1	E	29	GLN	2.1
1	F	331	LEU	2.1
1	G	63	ILE	2.1
1	A	481	VAL	2.1
1	B	447	GLY	2.1
1	F	112	GLY	2.1
1	E	351	ARG	2.1
1	E	459	ARG	2.1
1	E	527	TRP	2.1
1	B	69	SER	2.0
1	B	234	SER	2.0
1	B	525	THR	2.0
1	A	264	ALA	2.0
1	A	303	MET	2.0
1	D	408	GLU	2.0
1	F	265	ALA	2.0
1	D	115	LEU	2.0
1	A	506	ILE	2.0
1	A	272	PRO	2.0
1	A	249	VAL	2.0
1	E	112	GLY	2.0
1	H	273	GLU	2.0
1	B	464	ALA	2.0
1	B	492	ALA	2.0
1	B	90	HIS	2.0
1	G	338	CYS	2.0
1	B	16	LEU	2.0
1	B	118	ARG	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	I9K	A	605	38/38	0.78	0.18	129,130,131,131	22
5	K	E	604	1/1	0.80	0.15	113,113,113,113	0
3	OXL	E	602	6/6	0.85	0.13	85,86,86,86	0
4	MG	D	603	1/1	0.85	0.18	57,57,57,57	0
6	I9K	F	605	38/38	0.85	0.15	76,79,89,89	22
6	I9K	C	605	38/38	0.86	0.14	93,94,98,99	21
4	MG	C	603	1/1	0.88	0.17	59,59,59,59	0
6	I9K	G	605	38/38	0.88	0.14	79,86,94,94	22
5	K	A	604	1/1	0.89	0.10	101,101,101,101	0
2	FBP	A	601	20/20	0.89	0.10	81,82,84,84	0
3	OXL	G	602	6/6	0.89	0.10	47,48,49,49	0
4	MG	H	603	1/1	0.90	0.17	53,53,53,53	0
5	K	C	604	1/1	0.91	0.08	77,77,77,77	0
3	OXL	C	602	6/6	0.91	0.10	51,52,53,54	0
3	OXL	A	602	6/6	0.92	0.08	76,77,77,77	0
2	FBP	E	601	20/20	0.92	0.09	69,70,73,74	0
3	OXL	D	602	6/6	0.93	0.10	43,44,45,46	0
5	K	H	604	1/1	0.93	0.07	73,73,73,73	0
2	FBP	B	601	20/20	0.93	0.08	64,65,67,67	0
2	FBP	F	601	20/20	0.94	0.08	55,60,65,65	0
5	K	B	604	1/1	0.94	0.09	80,80,80,80	0
3	OXL	H	602	6/6	0.94	0.08	48,49,49,49	0
4	MG	B	603	1/1	0.94	0.07	45,45,45,45	0
5	K	G	604	1/1	0.94	0.05	65,65,65,65	0
3	OXL	B	602	6/6	0.95	0.05	48,49,49,49	0
3	OXL	F	602	6/6	0.95	0.08	59,60,61,62	0
4	MG	A	603	1/1	0.95	0.09	73,73,73,73	0
4	MG	E	603	1/1	0.95	0.06	70,70,70,70	0
4	MG	G	603	1/1	0.95	0.14	30,30,30,30	0
5	K	F	604	1/1	0.95	0.12	79,79,79,79	0
5	K	D	604	1/1	0.97	0.10	67,67,67,67	0
4	MG	F	603	1/1	0.97	0.07	46,46,46,46	0

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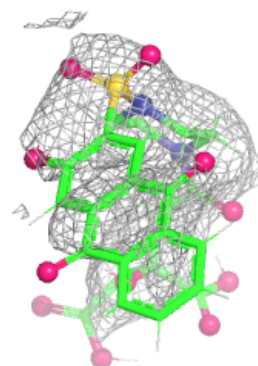
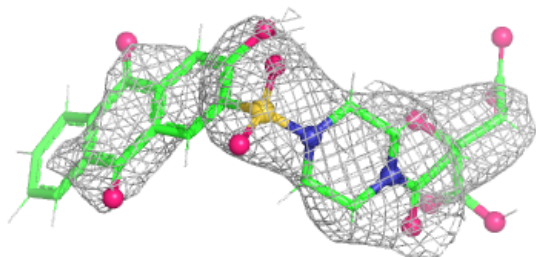
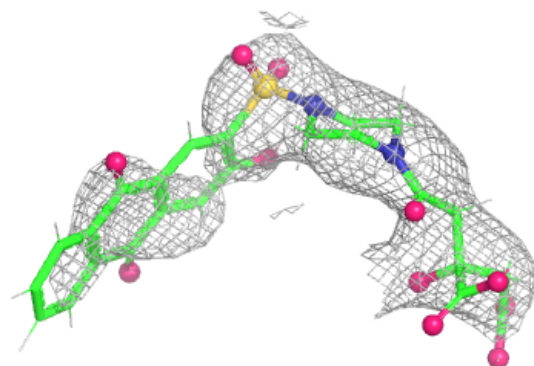
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FBP	D	601	20/20	0.97	0.06	35,37,40,40	0
2	FBP	G	601	20/20	0.98	0.05	36,40,45,45	0
2	FBP	H	601	20/20	0.98	0.06	32,35,37,39	0
2	FBP	C	601	20/20	0.98	0.05	35,37,42,42	0

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.

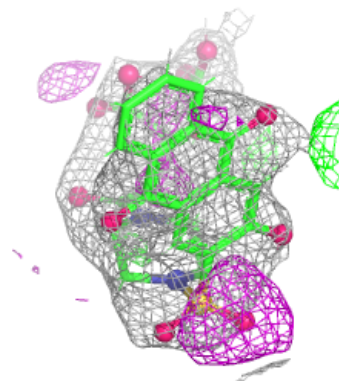
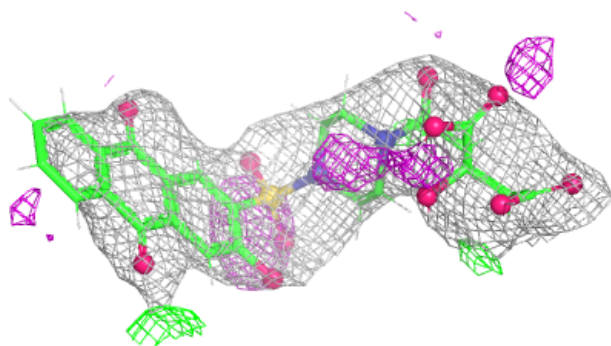
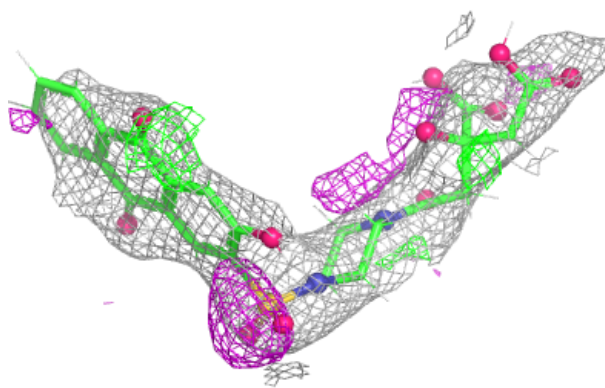
Electron density around I9K A 605:

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



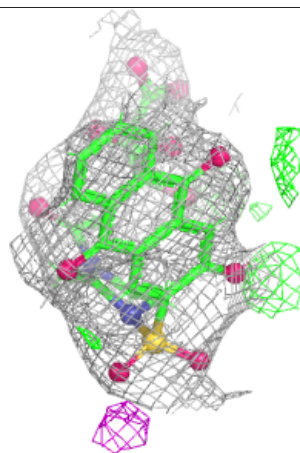
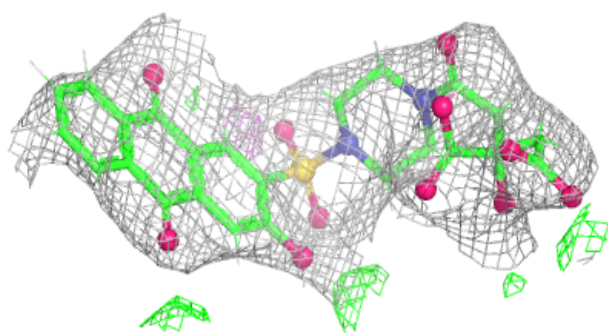
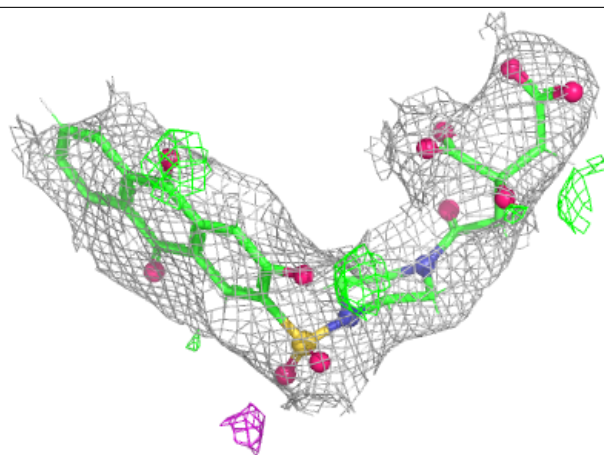
Electron density around I9K F 605:

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



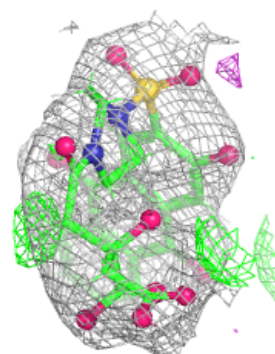
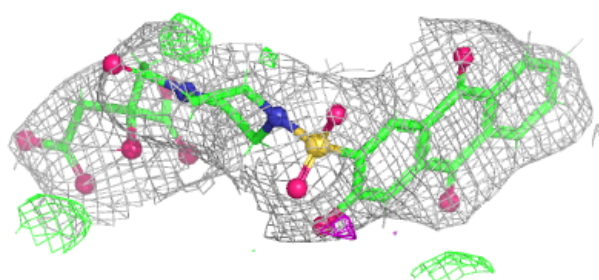
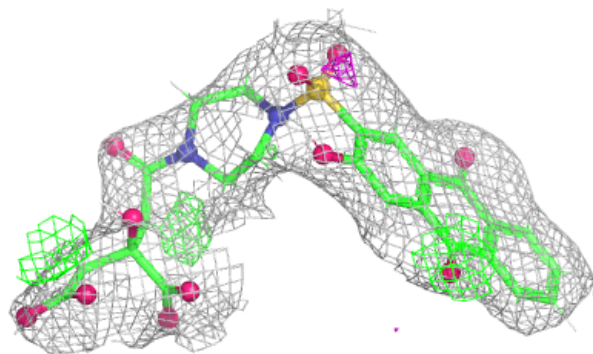
Electron density around I9K C 605:

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

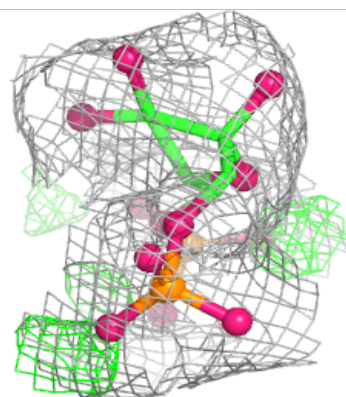
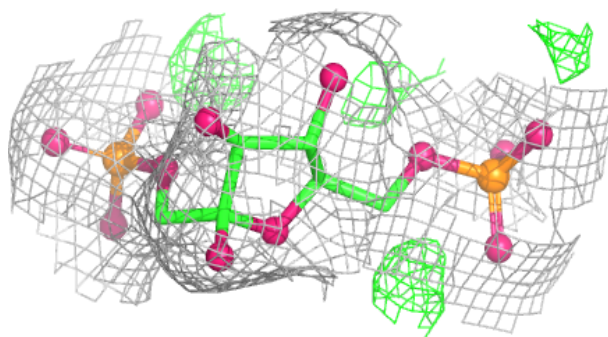
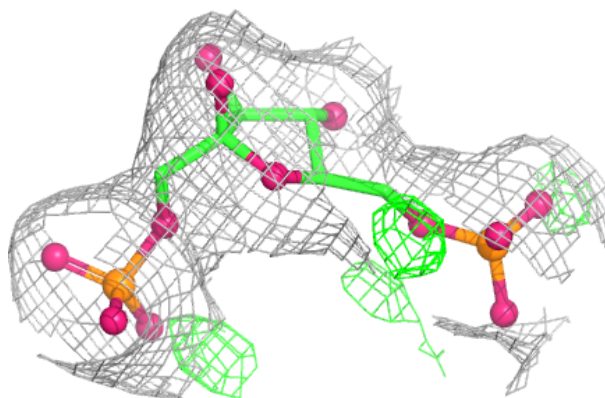


Electron density around I9K G 605:

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

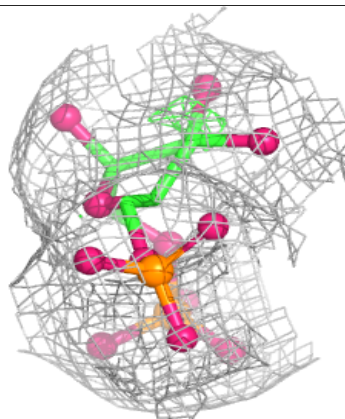
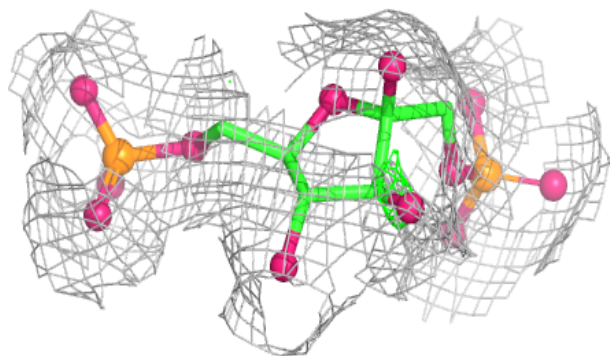
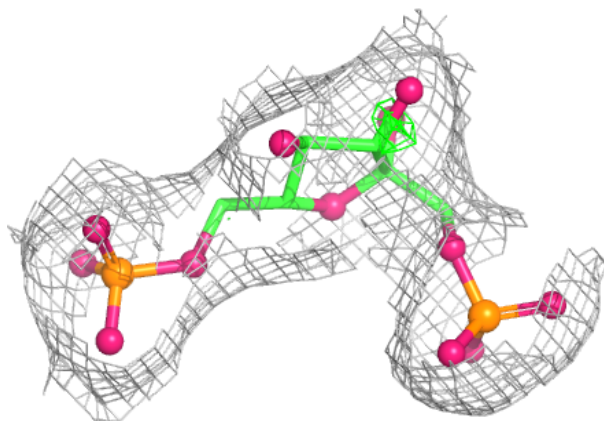
**Electron density around FBP A 601:**

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



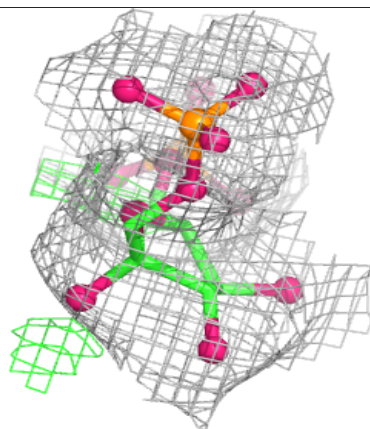
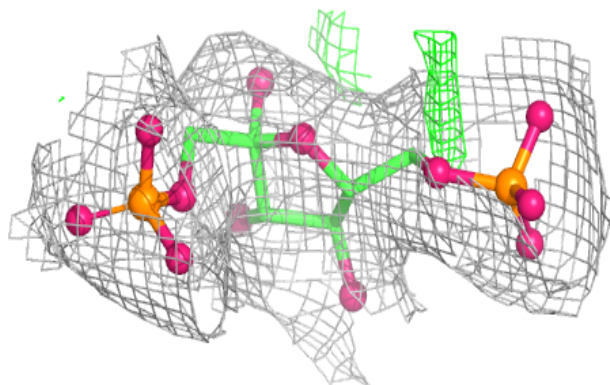
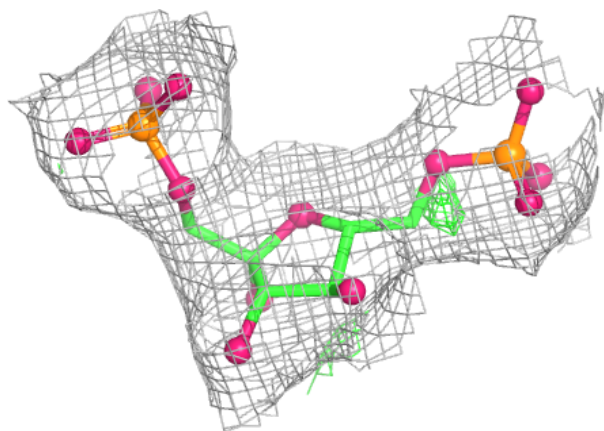
Electron density around FBP E 601:

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



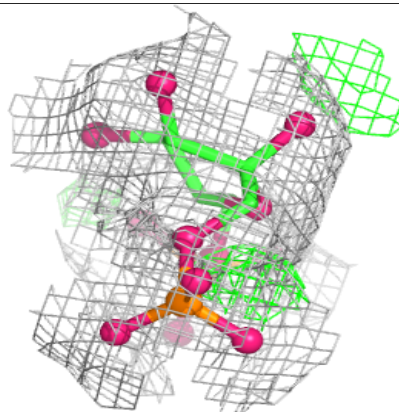
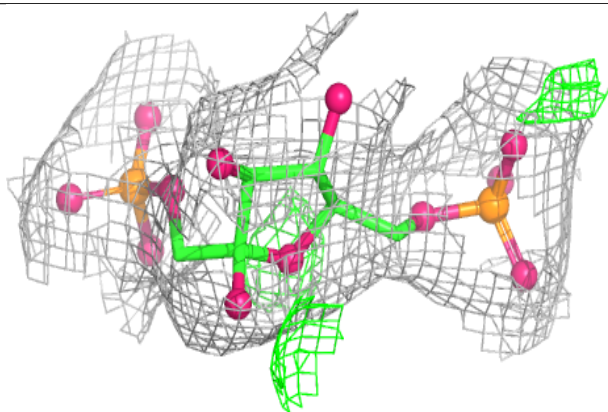
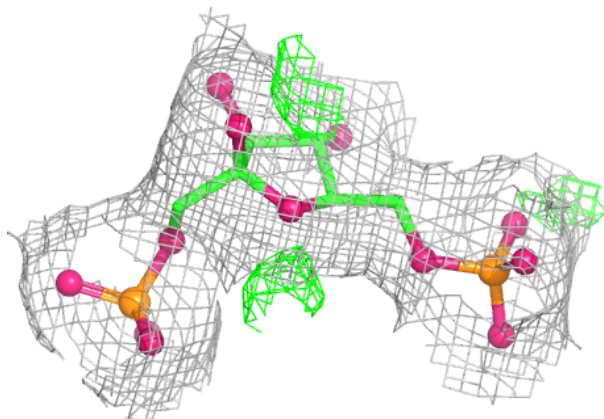
Electron density around FBP B 601:

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



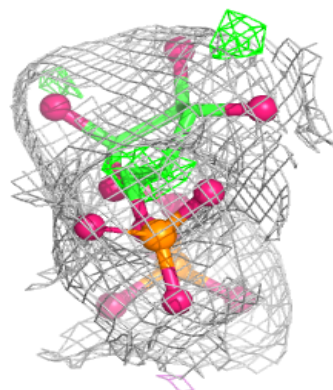
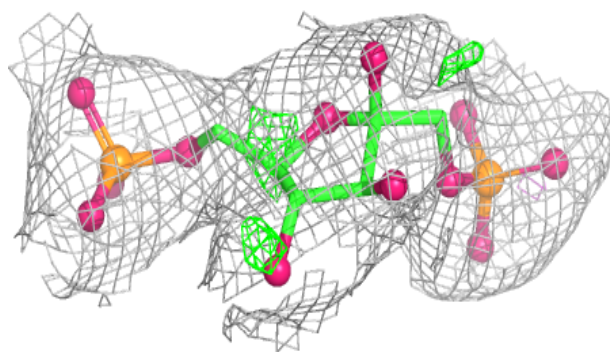
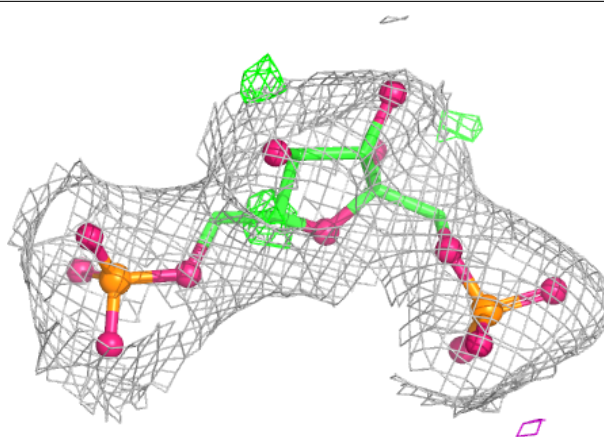
Electron density around FBP F 601:

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



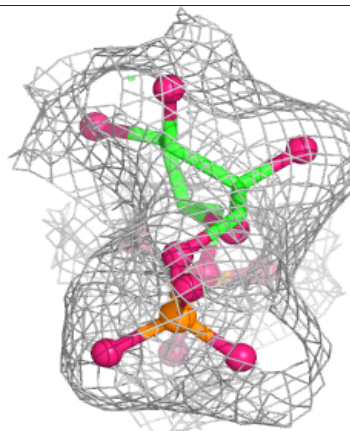
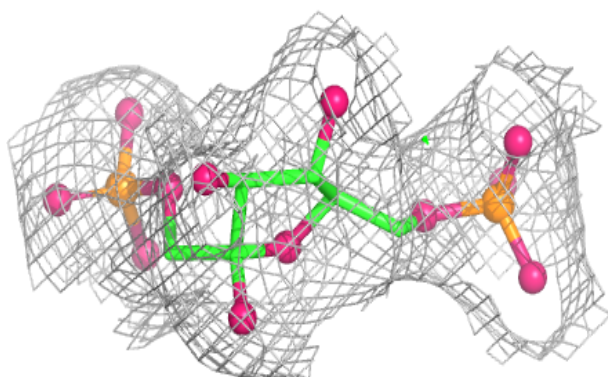
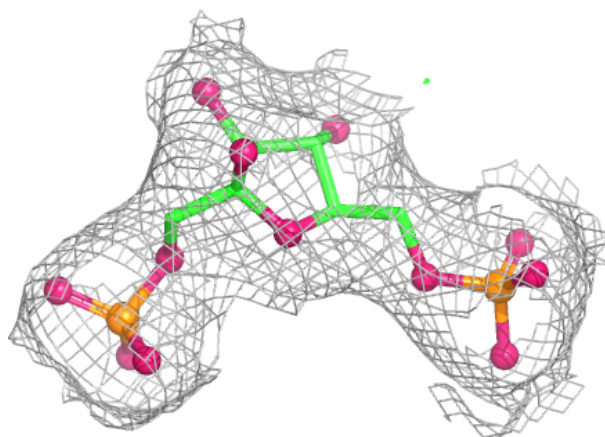
Electron density around FBP D 601:

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

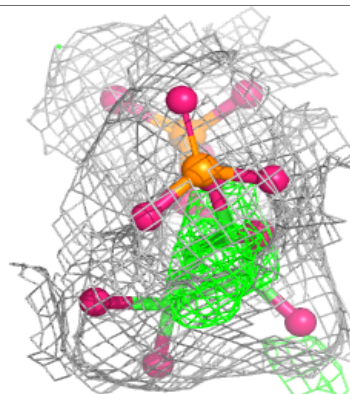
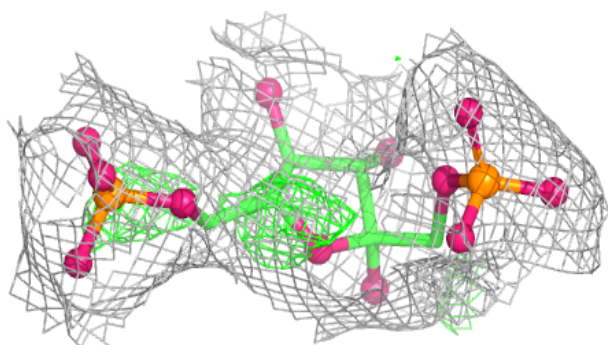
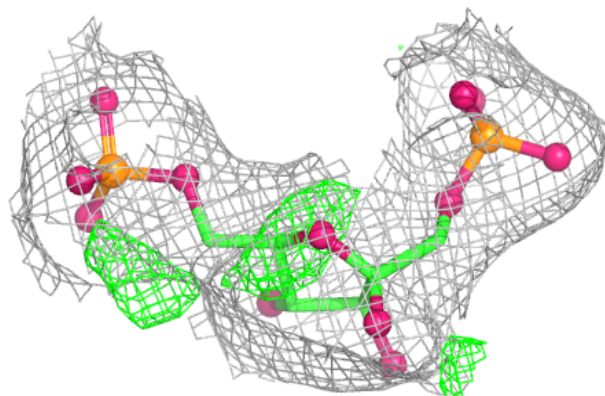


Electron density around FBP G 601:

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

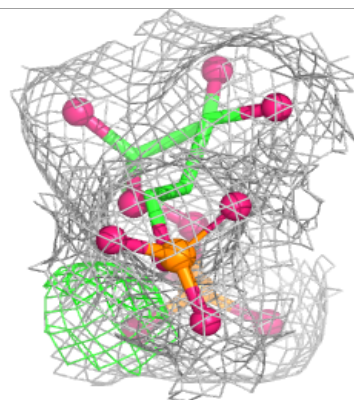
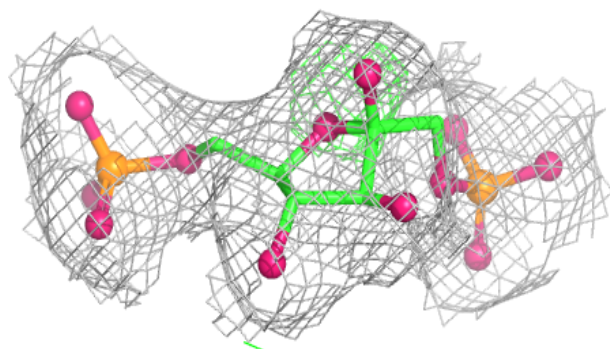
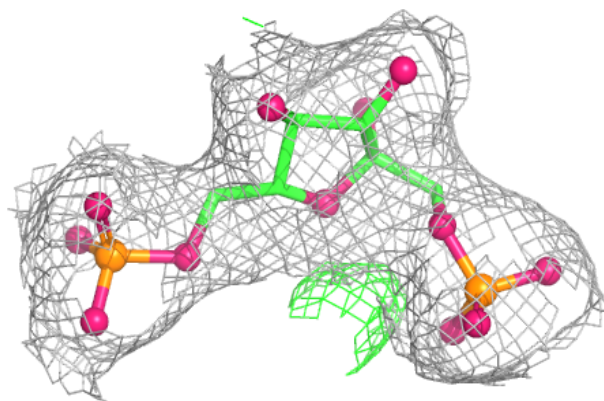
**Electron density around FBP H 601:**

$2mF_o-DF_c$ (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.