



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:01 PM UTC

PDB ID : 7FRZ / pdb_00007frz
Title : Structure of liver pyruvate kinase in complex with allosteric modulator 7
Authors : Lulla, A.; Nilsson, O.; Brear, P.; Nain-Perez, A.; Grotli, M.; Hyvonen, M.
Deposited on : 2022-12-18
Resolution : 2.08 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

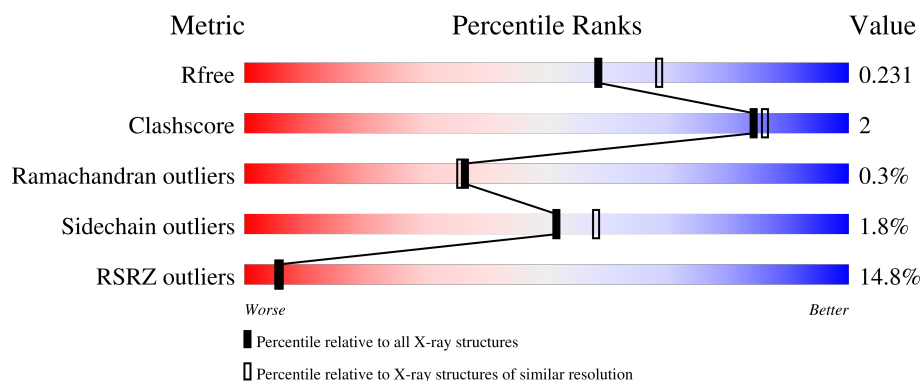
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	28% 87% 7% • 6%
1	B	447	26% 91% 6% • •
1	C	447	15% 89% 6% 5%
1	D	447	4% 90% 5% 5%
1	E	447	22% 87% 6% • 6%

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

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

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

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 27856 atoms, of which 68 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 PKLR.

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 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P30613
A	0	SER	-	expression tag	UNP P30613
A	1	MET	-	expression tag	UNP P30613
A	2	GLU	-	expression tag	UNP P30613
A	12	ASP	SER	conflict	UNP P30613
A	130	GLY	-	linker	UNP P30613
A	131	SER	-	linker	UNP P30613
A	132	GLY	-	linker	UNP P30613
B	-1	GLY	-	expression tag	UNP P30613
B	0	SER	-	expression tag	UNP P30613
B	1	MET	-	expression tag	UNP P30613
B	2	GLU	-	expression tag	UNP P30613
B	12	ASP	SER	conflict	UNP P30613

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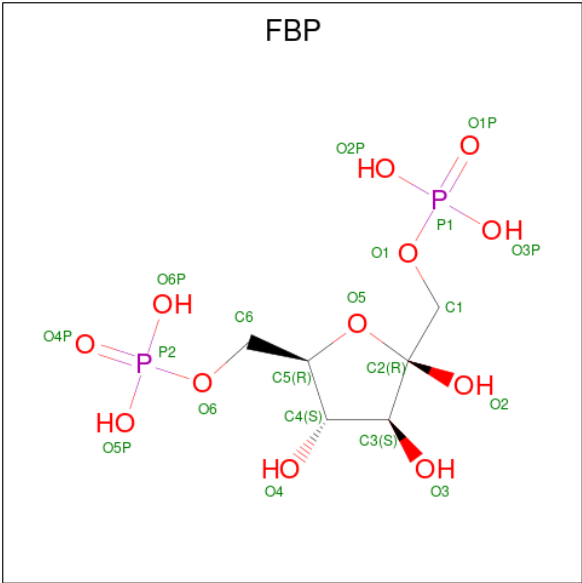
Chain	Residue	Modelled	Actual	Comment	Reference
B	130	GLY	-	linker	UNP P30613
B	131	SER	-	linker	UNP P30613
B	132	GLY	-	linker	UNP P30613
C	-1	GLY	-	expression tag	UNP P30613
C	0	SER	-	expression tag	UNP P30613
C	1	MET	-	expression tag	UNP P30613
C	2	GLU	-	expression tag	UNP P30613
C	12	ASP	SER	conflict	UNP P30613
C	130	GLY	-	linker	UNP P30613
C	131	SER	-	linker	UNP P30613
C	132	GLY	-	linker	UNP P30613
D	-1	GLY	-	expression tag	UNP P30613
D	0	SER	-	expression tag	UNP P30613
D	1	MET	-	expression tag	UNP P30613
D	2	GLU	-	expression tag	UNP P30613
D	12	ASP	SER	conflict	UNP P30613
D	130	GLY	-	linker	UNP P30613
D	131	SER	-	linker	UNP P30613
D	132	GLY	-	linker	UNP P30613
E	-1	GLY	-	expression tag	UNP P30613
E	0	SER	-	expression tag	UNP P30613
E	1	MET	-	expression tag	UNP P30613
E	2	GLU	-	expression tag	UNP P30613
E	12	ASP	SER	conflict	UNP P30613
E	228	GLY	-	linker	UNP P30613
E	229	SER	-	linker	UNP P30613
E	230	GLY	-	linker	UNP P30613
F	-1	GLY	-	expression tag	UNP P30613
F	0	SER	-	expression tag	UNP P30613
F	1	MET	-	expression tag	UNP P30613
F	2	GLU	-	expression tag	UNP P30613
F	12	ASP	SER	conflict	UNP P30613
F	228	GLY	-	linker	UNP P30613
F	229	SER	-	linker	UNP P30613
F	230	GLY	-	linker	UNP P30613
G	-1	GLY	-	expression tag	UNP P30613
G	0	SER	-	expression tag	UNP P30613
G	1	MET	-	expression tag	UNP P30613
G	2	GLU	-	expression tag	UNP P30613
G	12	ASP	SER	conflict	UNP P30613
G	130	GLY	-	linker	UNP P30613
G	131	SER	-	linker	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
G	132	GLY	-	linker	UNP P30613
H	-1	GLY	-	expression tag	UNP P30613
H	0	SER	-	expression tag	UNP P30613
H	1	MET	-	expression tag	UNP P30613
H	2	GLU	-	expression tag	UNP P30613
H	12	ASP	SER	conflict	UNP P30613
H	130	GLY	-	linker	UNP P30613
H	131	SER	-	linker	UNP P30613
H	132	GLY	-	linker	UNP P30613

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: C₆H₁₄O₁₂P₂).



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		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		

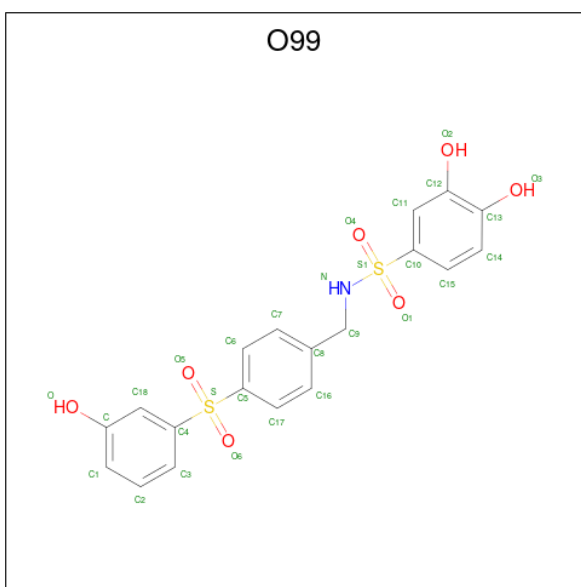
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

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

- Molecule 6 is 3,4-dihydroxy-N-{{4-(3-hydroxybenzene-1-sulfonyl)phenyl}methyl}benzene-1-sulfonamide (CCD ID: O99) (formula: C₁₉H₁₇NO₇S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total 46	C 19	H 17	N 1	O 7	S 2	17	0
6	D	1	Total 46	C 19	H 17	N 1	O 7	S 2	17	0
6	E	1	Total 46	C 19	H 17	N 1	O 7	S 2	17	0
6	F	1	Total 46	C 19	H 17	N 1	O 7	S 2	17	0

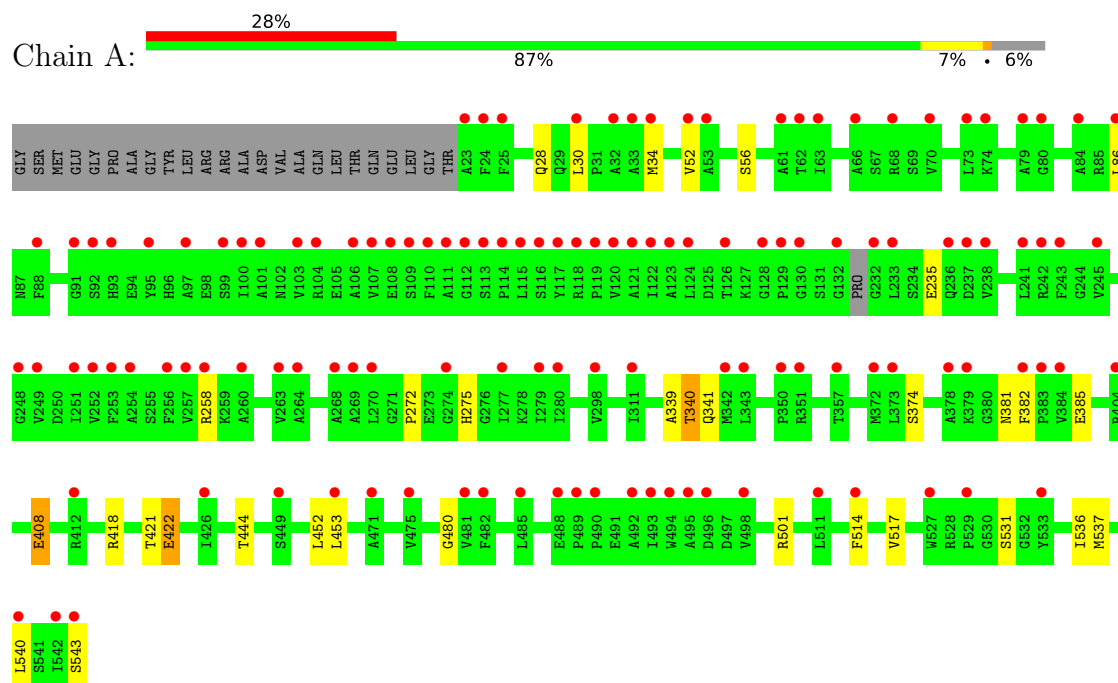
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	85	Total	O	0	0
			85	85		
7	B	117	Total	O	0	0
			117	117		
7	C	171	Total	O	0	0
			171	171		
7	D	237	Total	O	0	0
			237	237		
7	E	112	Total	O	0	0
			112	112		
7	F	178	Total	O	0	0
			178	178		
7	G	218	Total	O	0	0
			218	218		
7	H	253	Total	O	0	0
			253	253		

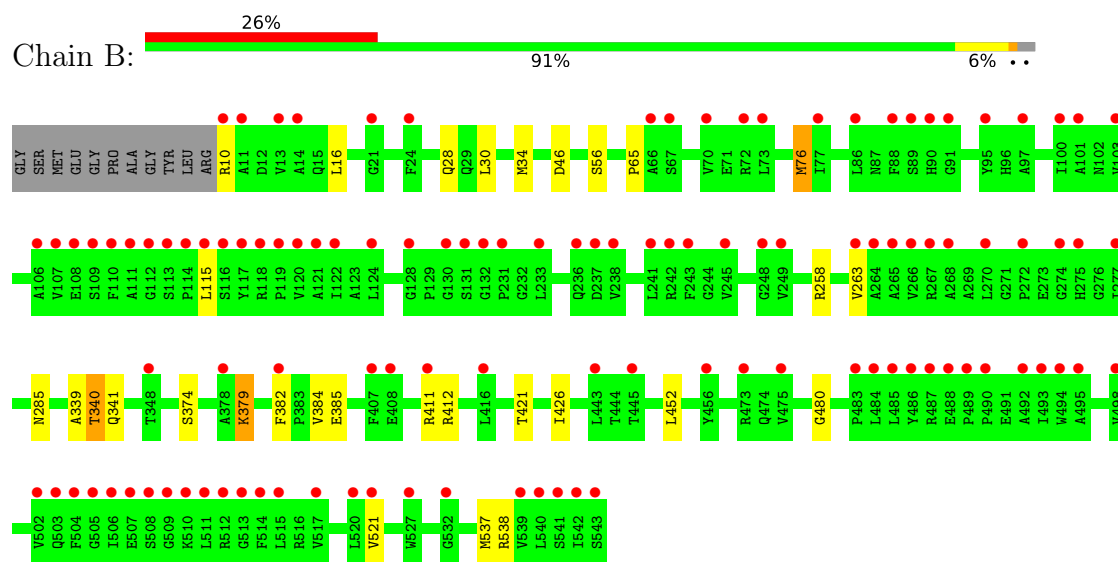
3 Residue-property plots [i](#)

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.

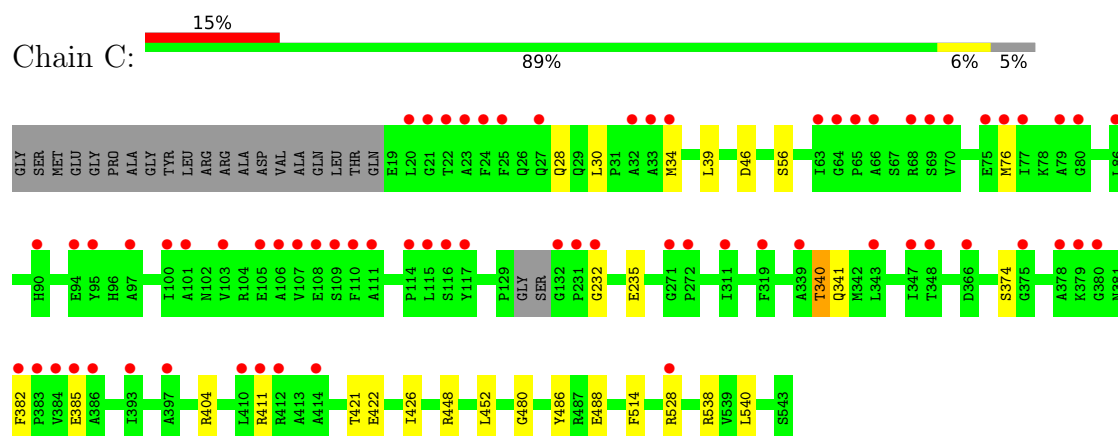
• Molecule 1: Pyruvate kinase PKLR



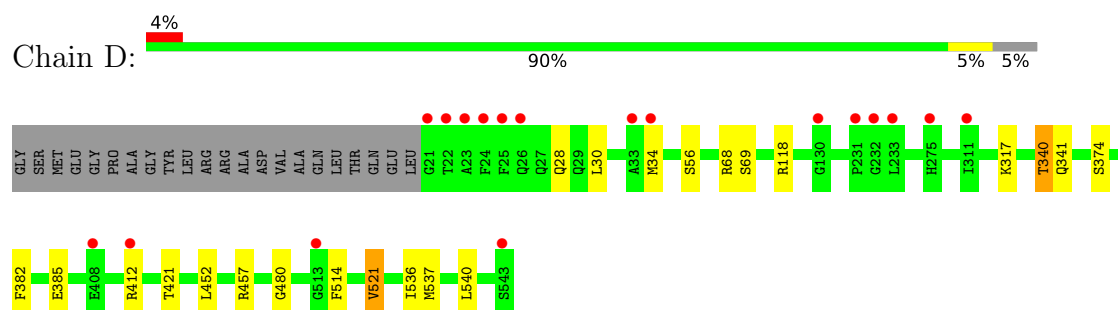
• Molecule 1: Pyruvate kinase PKLR



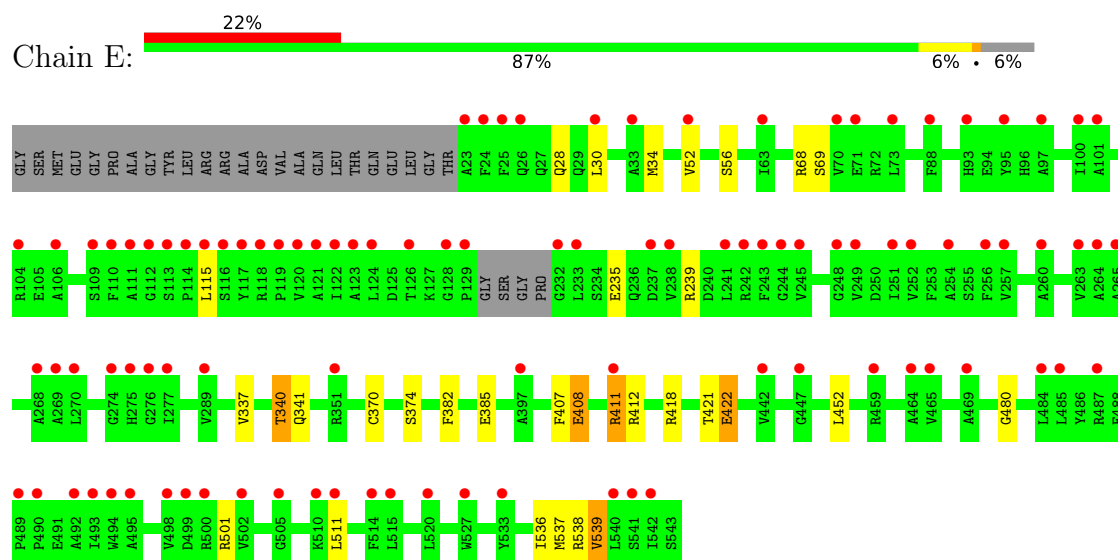
- Molecule 1: Pyruvate kinase PKLR



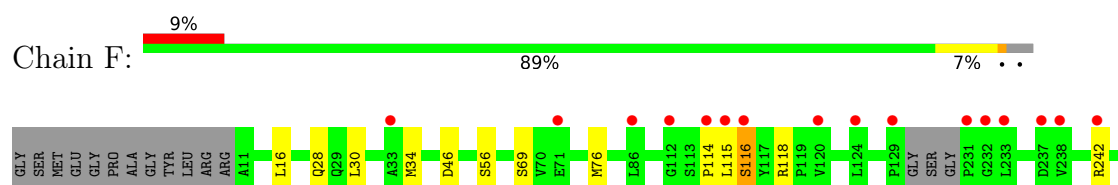
- Molecule 1: Pyruvate kinase PKLR

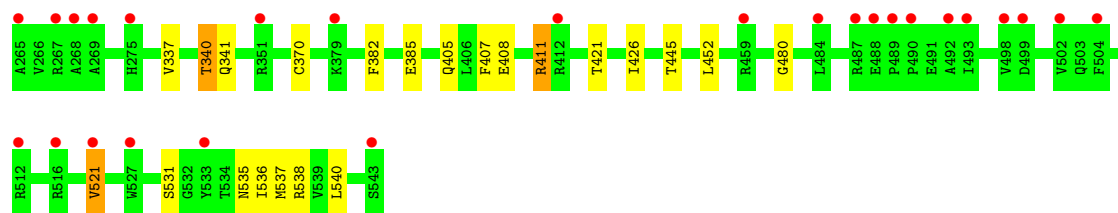


- Molecule 1: Pyruvate kinase PKLR

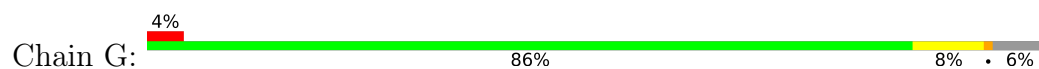


- Molecule 1: Pyruvate kinase PKLR

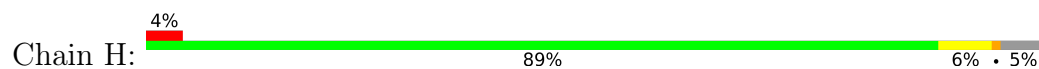




● Molecule 1: Pyruvate kinase PKLR



● Molecule 1: Pyruvate kinase PKLR



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	207.18Å 112.98Å 187.82Å 90.00° 92.26° 90.00°	Depositor
Resolution (Å)	187.67 – 2.08 187.67 – 2.08	Depositor EDS
% Data completeness (in resolution range)	65.9 (187.67-2.08) 65.9 (187.67-2.08)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.09Å)	Xtriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, R_{free}	0.212 , 0.241 (Not available) , 0.231	Depositor DCC
R_{free} test set	8150 reflections (3.17%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.020	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	0.95	EDS
Total number of atoms	27856	wwPDB-VP
Average B, all atoms (Å ²)	51.0	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 63.96 % 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 8.9152e-06. 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: MG, K, FBP, O99, OXL

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	0.67	1/3307 (0.0%)	1.01	6/4469 (0.1%)
1	B	0.69	1/3396 (0.0%)	1.00	3/4592 (0.1%)
1	C	0.74	1/3313 (0.0%)	1.01	2/4479 (0.0%)
1	D	0.76	2/3326 (0.1%)	1.02	1/4497 (0.0%)
1	E	0.67	1/3278 (0.0%)	1.01	1/4430 (0.0%)
1	F	0.73	0/3396	1.02	1/4591 (0.0%)
1	G	0.76	0/3303	1.01	1/4465 (0.0%)
1	H	0.80	0/3316	1.04	5/4483 (0.1%)
All	All	0.73	6/26635 (0.0%)	1.02	20/36006 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	374	SER	CA-C	6.28	1.55	1.52
1	D	374	SER	CA-C	5.91	1.55	1.52
1	C	374	SER	CA-C	5.85	1.55	1.52
1	D	457	ARG	CA-CB	5.81	1.56	1.52
1	E	374	SER	CA-C	5.43	1.55	1.52
1	A	374	SER	CA-C	5.43	1.55	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	422	GLU	CB-CG-CD	7.94	126.10	112.60
1	A	422	GLU	CB-CG-CD	7.25	124.92	112.60
1	G	514	PHE	CA-CB-CG	6.21	120.01	113.80
1	F	46	ASP	CA-CB-CG	5.69	118.29	112.60
1	C	514	PHE	CA-CB-CG	5.66	119.46	113.80
1	D	514	PHE	CA-CB-CG	5.46	119.27	113.80
1	H	514	PHE	CA-CB-CG	5.38	119.18	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	530	GLY	CA-C-N	5.25	128.67	120.75
1	H	530	GLY	C-N-CA	5.25	128.67	120.75
1	A	453	LEU	CA-C-N	5.24	127.30	120.28
1	A	453	LEU	C-N-CA	5.24	127.30	120.28
1	B	46	ASP	CA-CB-CG	5.17	117.77	112.60
1	H	453	LEU	CA-C-N	5.11	127.13	120.28
1	H	453	LEU	C-N-CA	5.11	127.13	120.28
1	A	339	ALA	CA-C-N	5.08	131.25	121.54
1	A	339	ALA	C-N-CA	5.08	131.25	121.54
1	A	514	PHE	CA-CB-CG	5.08	118.88	113.80
1	C	46	ASP	CA-CB-CG	5.02	117.62	112.60
1	B	339	ALA	CA-C-N	5.01	131.12	121.54
1	B	339	ALA	C-N-CA	5.01	131.12	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3236	0	3299	15	0
1	B	3329	0	3394	14	0
1	C	3247	0	3299	19	0
1	D	3252	0	3310	10	0
1	E	3210	0	3270	17	0
1	F	3321	0	3393	21	0
1	G	3231	0	3284	29	0
1	H	3251	0	3306	17	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	1	0
2	F	20	0	10	0	0
2	G	20	0	10	0	0
2	H	20	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	A	29	17	0	1	0
6	D	29	17	0	0	0
6	E	29	17	0	0	0
6	F	29	17	0	1	0
7	A	85	0	0	1	0
7	B	117	0	0	0	0
7	C	171	0	0	3	0
7	D	237	0	0	1	0
7	E	112	0	0	0	0
7	F	178	0	0	1	0
7	G	218	0	0	2	0
7	H	253	0	0	1	0
All	All	27788	68	26635	123	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 2.

All (123) 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:A:408:GLU:OE2	1:B:411:ARG:NH2	1.92	1.02
1:C:411:ARG:HG3	1:C:426:ILE:HD11	1.44	0.99
1:B:411:ARG:HG3	1:B:426:ILE:HD11	1.52	0.91
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.63	0.81
1:C:422[A]:GLU:HG3	1:C:452:LEU:HD13	1.66	0.78
1:C:528:ARG:HH22	1:G:233:LEU:HB3	1.52	0.74
1:A:418[A]:ARG:HG3	1:B:16:LEU:HD11	1.72	0.70
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.73	0.70
1:E:408:GLU:OE2	1:F:411:ARG:NH2	2.24	0.70
1:G:538:ARG:HG2	1:H:536:ILE:HG12	1.72	0.70
1:F:407:PHE:CE2	1:F:411:ARG:NH1	2.63	0.67
1:C:538:ARG:HG2	1:D:536:ILE:HG12	1.79	0.64
1:E:235:GLU:O	1:E:239:ARG:HD3	2.00	0.61
1:G:340:THR:HG22	1:G:341:GLN:HG3	1.83	0.61
1:H:245:VAL:HG11	1:H:273:GLU:HG2	1.81	0.61
1:D:521:VAL:HG12	1:D:540:LEU:HB3	1.84	0.60
1:C:340:THR:HG22	1:C:341:GLN:HG3	1.85	0.59
1:A:340:THR:HG22	1:A:341:GLN:HG3	1.85	0.58
1:E:340:THR:HG22	1:E:341:GLN:HG3	1.86	0.58
1:E:536:ILE:HG12	1:F:538:ARG:HG2	1.86	0.57
1:D:340:THR:HG22	1:D:341:GLN:HG3	1.86	0.57
1:A:517:VAL:HG13	1:A:543:SER:HB3	1.88	0.56
1:G:537:MET:HE3	1:H:537:MET:HG2	1.87	0.56
1:B:340:THR:HG22	1:B:341:GLN:HG3	1.88	0.56
1:H:411:ARG:HB3	1:H:426:ILE:HD11	1.88	0.55
1:G:536:ILE:HG12	1:H:538[A]:ARG:HG2	1.86	0.55
1:F:115:LEU:O	1:F:116:SER:HB3	2.07	0.54
1:E:407:PHE:O	1:E:411:ARG:HB2	2.07	0.54
1:E:538:ARG:HG2	1:F:536:ILE:HG12	1.88	0.54
1:C:235:GLU:HG3	1:G:529:PRO:HG3	1.90	0.53
1:H:340:THR:HG22	1:H:341:GLN:HG3	1.89	0.53
1:F:411:ARG:HG2	1:F:426:ILE:HD11	1.90	0.53
1:B:411:ARG:CG	1:B:426:ILE:HD11	2.34	0.53
1:F:340:THR:HG22	1:F:341:GLN:HG3	1.90	0.53
1:D:30:LEU:O	1:D:34:MET:HG3	2.10	0.52
1:F:411:ARG:CG	1:F:426:ILE:HD11	2.40	0.52
1:G:245:VAL:CG1	1:G:273:GLU:HG2	2.40	0.52
1:E:539:VAL:HG13	1:F:535:ASN:HB2	1.91	0.51
1:F:114:PRO:HA	7:F:769:HOH:O	2.10	0.51
1:E:30:LEU:O	1:E:34:MET:HG3	2.10	0.51
1:C:486:TYR:CZ	1:C:488:GLU:HB2	2.46	0.50
1:G:269:ALA:C	1:G:271:GLY:H	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:411:ARG:CG	1:G:426:ILE:HD11	2.42	0.50
1:C:382:PHE:HB3	1:C:385:GLU:HB2	1.95	0.49
1:F:382:PHE:HB3	1:F:385:GLU:HB2	1.93	0.49
1:B:30:LEU:O	1:B:34:MET:HG2	2.14	0.48
1:G:56:SER:HB2	1:G:480:GLY:HA2	1.94	0.48
1:H:30:LEU:O	1:H:34:MET:HG2	2.13	0.48
1:C:538:ARG:HD3	7:C:765:HOH:O	2.13	0.48
1:A:382:PHE:HB3	1:A:385:GLU:HB2	1.96	0.48
1:B:258:ARG:HD3	1:B:285:ASN:HD21	1.78	0.48
1:D:382:PHE:HB3	1:D:385:GLU:HB2	1.95	0.48
1:F:30:LEU:O	1:F:34:MET:HG2	2.14	0.48
1:B:382:PHE:HB3	1:B:385:GLU:HB2	1.96	0.47
1:B:421:THR:HG22	1:B:452:LEU:HD12	1.97	0.47
1:C:30:LEU:O	1:C:34:MET:HG2	2.15	0.47
1:C:411:ARG:CG	1:C:426:ILE:HD11	2.30	0.47
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.97	0.46
1:H:56:SER:HB2	1:H:480:GLY:HA2	1.97	0.46
1:E:382:PHE:HB3	1:E:385:GLU:HB2	1.97	0.46
1:F:56:SER:HB2	1:F:480:GLY:HA2	1.98	0.46
1:F:407:PHE:CD2	1:F:411:ARG:NH1	2.84	0.46
1:G:30:LEU:O	1:G:34:MET:HG2	2.15	0.46
1:C:421:THR:HG22	1:C:452:LEU:HD12	1.96	0.46
1:A:56:SER:HB3	1:A:480:GLY:HA2	1.98	0.46
1:E:501:ARG:NH1	2:E:601:FBP:O1P	2.43	0.46
1:E:421:THR:HG22	1:E:452:LEU:HD12	1.97	0.45
1:A:421:THR:HG22	1:A:452:LEU:HD12	1.99	0.45
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.97	0.45
1:G:412:ARG:NH2	1:H:404:ARG:HH11	2.15	0.45
1:C:232:GLY:HA3	7:C:793:HOH:O	2.17	0.45
1:D:421:THR:HG22	1:D:452:LEU:HD12	1.99	0.45
1:G:382:PHE:HB3	1:G:385:GLU:HB2	1.98	0.45
1:B:28:GLN:HG3	1:B:30:LEU:HG	1.99	0.45
1:E:418:ARG:HD3	1:F:16:LEU:HD11	1.99	0.45
1:F:421:THR:HG22	1:F:452:LEU:HD12	1.99	0.45
1:D:317:LYS:NZ	7:D:711:HOH:O	2.50	0.45
1:G:272:PRO:HD2	1:G:273:GLU:OE1	2.17	0.45
1:A:30:LEU:O	1:A:34:MET:HG2	2.17	0.44
1:F:28:GLN:HG3	1:F:30:LEU:HG	1.99	0.44
1:H:421:THR:HG22	1:H:452:LEU:HD12	2.00	0.44
1:H:475:VAL:CG2	1:H:483:PRO:HB3	2.48	0.44
6:A:605:O99:O	1:C:39:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.99	0.44
1:F:405:GLN:HB3	6:F:605:O99:O6	2.18	0.43
1:H:28:GLN:HG3	1:H:30:LEU:HG	2.00	0.43
1:C:404:ARG:HD3	1:D:412:ARG:NH2	2.33	0.43
1:G:412:ARG:CZ	1:H:404:ARG:HD3	2.49	0.43
1:G:411:ARG:HG2	1:G:426:ILE:HD11	2.00	0.43
1:H:382:PHE:HB3	1:H:385:GLU:HB2	2.01	0.43
1:G:470:GLN:NE2	7:G:703:HOH:O	2.41	0.42
1:D:28:GLN:HG3	1:D:30:LEU:HG	2.01	0.42
1:F:445:THR:HB	1:F:531:SER:OG	2.19	0.42
1:G:421:THR:HG22	1:G:452:LEU:HD12	2.01	0.42
1:A:381:ASN:ND2	7:A:703:HOH:O	2.52	0.42
1:B:65:PRO:HG2	1:B:379:LYS:HG2	2.00	0.42
1:C:28:GLN:HG3	1:C:30:LEU:HG	2.01	0.42
1:A:28:GLN:HG3	1:A:30:LEU:HG	2.01	0.42
1:G:411:ARG:HG3	1:G:426:ILE:HD11	2.00	0.42
1:G:412:ARG:NH2	1:H:404:ARG:HD3	2.34	0.42
1:A:501:ARG:NH1	2:A:601:FBP:O2P	2.37	0.42
1:A:28:GLN:HB3	1:A:52:VAL:HG22	2.02	0.41
1:G:28:GLN:HG3	1:G:30:LEU:HG	2.01	0.41
1:G:317:LYS:NZ	7:G:714:HOH:O	2.52	0.41
1:A:444:THR:OG1	2:A:601:FBP:O6P	2.32	0.41
1:C:448:ARG:HD3	7:C:754:HOH:O	2.19	0.41
1:C:528:ARG:NH2	1:G:233:LEU:HB3	2.25	0.41
1:F:521:VAL:HG12	1:F:540[B]:LEU:HB3	2.02	0.41
1:G:245:VAL:HG11	1:G:273:GLU:HG2	2.03	0.41
1:G:56:SER:HB2	1:G:480:GLY:CA	2.50	0.41
1:E:28:GLN:HG3	1:E:30:LEU:HG	2.01	0.41
1:G:486:TYR:CZ	1:G:488:GLU:HB2	2.56	0.41
1:G:352:PRO:HG3	1:G:389:MET:HG2	2.01	0.41
1:A:272:PRO:HA	1:A:275:HIS:NE2	2.35	0.41
1:E:28:GLN:HB3	1:E:52:VAL:HG22	2.03	0.41
1:E:337:VAL:HG22	1:E:370:CYS:HB2	2.03	0.41
1:H:337:VAL:HG22	1:H:370:CYS:HB2	2.03	0.41
1:B:76[A]:MET:HG2	1:B:384:VAL:HG22	2.03	0.41
1:E:56:SER:HB2	1:E:480:GLY:HA2	2.02	0.41
1:F:337:VAL:HG22	1:F:370:CYS:HB2	2.03	0.41
1:E:34:MET:HE2	1:E:34:MET:HB3	1.98	0.40
1:G:491:GLU:HB2	1:G:497:ASP:HB2	2.03	0.40
1:H:75:GLU:HG3	7:H:933:HOH: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	424/447 (95%)	420 (99%)	3 (1%)	1 (0%)	43	44
1	B	438/447 (98%)	434 (99%)	3 (1%)	1 (0%)	43	44
1	C	425/447 (95%)	418 (98%)	6 (1%)	1 (0%)	43	44
1	D	429/447 (96%)	425 (99%)	3 (1%)	1 (0%)	43	44
1	E	420/447 (94%)	416 (99%)	3 (1%)	1 (0%)	43	44
1	F	435/447 (97%)	429 (99%)	4 (1%)	2 (0%)	24	21
1	G	423/447 (95%)	415 (98%)	6 (1%)	2 (0%)	24	21
1	H	427/447 (96%)	421 (99%)	5 (1%)	1 (0%)	43	44
All	All	3421/3576 (96%)	3378 (99%)	33 (1%)	10 (0%)	36	36

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	116	SER
1	G	271	GLY
1	A	340	THR
1	B	340	THR
1	C	340	THR
1	D	340	THR
1	E	340	THR
1	F	340	THR
1	G	340	THR
1	H	340	THR

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	340/352 (97%)	331 (97%)	9 (3%)	40	45
1	B	349/352 (99%)	339 (97%)	10 (3%)	37	40
1	C	341/352 (97%)	338 (99%)	3 (1%)	70	77
1	D	342/352 (97%)	337 (98%)	5 (2%)	57	64
1	E	338/352 (96%)	327 (97%)	11 (3%)	33	35
1	F	350/352 (99%)	340 (97%)	10 (3%)	37	40
1	G	340/352 (97%)	335 (98%)	5 (2%)	57	64
1	H	340/352 (97%)	336 (99%)	4 (1%)	63	70
All	All	2740/2816 (97%)	2683 (98%)	57 (2%)	51	52

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	235	GLU
1	A	258	ARG
1	A	408	GLU
1	A	422	GLU
1	A	531	SER
1	A	537[A]	MET
1	A	537[B]	MET
1	A	540	LEU
1	B	10	ARG
1	B	76[A]	MET
1	B	76[B]	MET
1	B	115	LEU
1	B	263	VAL
1	B	379	LYS
1	B	412	ARG
1	B	521	VAL
1	B	537[A]	MET
1	B	537[B]	MET
1	C	76[A]	MET
1	C	76[B]	MET
1	C	540	LEU
1	D	68	ARG
1	D	69	SER

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Mol	Chain	Res	Type
1	D	118	ARG
1	D	521	VAL
1	D	537	MET
1	E	68	ARG
1	E	69	SER
1	E	115	LEU
1	E	408	GLU
1	E	411	ARG
1	E	412	ARG
1	E	422	GLU
1	E	511	LEU
1	E	537[A]	MET
1	E	537[B]	MET
1	E	539	VAL
1	F	69	SER
1	F	76[A]	MET
1	F	76[B]	MET
1	F	118	ARG
1	F	242	ARG
1	F	408	GLU
1	F	411	ARG
1	F	521	VAL
1	F	537[A]	MET
1	F	537[B]	MET
1	G	76[A]	MET
1	G	76[B]	MET
1	G	273	GLU
1	G	331	LEU
1	G	540	LEU
1	H	69	SER
1	H	242	ARG
1	H	411	ARG
1	H	537	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	A	405	GLN
1	B	90	HIS
1	B	405	GLN
1	C	90	HIS

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Mol	Chain	Res	Type
1	C	275	HIS
1	C	405	GLN
1	D	90	HIS
1	D	405	GLN
1	E	27	GLN
1	E	90	HIS
1	E	405	GLN
1	F	27	GLN
1	F	90	HIS
1	F	405	GLN
1	G	90	HIS
1	G	405	GLN
1	H	27	GLN
1	H	90	HIS
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	A	602	4	5,5,5	2.04	2 (40%)	6,6,6	2.10	3 (50%)
2	FBP	H	601	-	18,20,20	0.88	1 (5%)	21,32,32	1.00	2 (9%)
3	OXL	F	602	4	5,5,5	2.82	4 (80%)	6,6,6	2.85	3 (50%)
6	O99	F	605	-	31,31,31	0.31	0	44,46,46	0.64	0
2	FBP	D	601	-	18,20,20	0.71	0	21,32,32	1.00	1 (4%)
3	OXL	B	602	4	5,5,5	2.34	2 (40%)	6,6,6	1.67	2 (33%)
3	OXL	C	602	4	5,5,5	2.25	3 (60%)	6,6,6	1.91	2 (33%)
3	OXL	D	602	4	5,5,5	2.56	3 (60%)	6,6,6	2.43	2 (33%)
2	FBP	C	601	-	18,20,20	0.70	1 (5%)	21,32,32	0.78	1 (4%)
2	FBP	B	601	-	18,20,20	0.66	0	21,32,32	0.86	1 (4%)
3	OXL	E	602	4	5,5,5	2.39	2 (40%)	6,6,6	1.45	2 (33%)
6	O99	E	605	-	31,31,31	0.21	0	44,46,46	0.57	0
6	O99	D	605	-	31,31,31	0.24	0	44,46,46	0.43	0
3	OXL	G	602	4	5,5,5	2.30	2 (40%)	6,6,6	1.90	2 (33%)
2	FBP	A	601	-	18,20,20	0.66	1 (5%)	21,32,32	0.68	0
2	FBP	G	601	-	18,20,20	0.67	1 (5%)	21,32,32	0.84	1 (4%)
2	FBP	F	601	-	18,20,20	0.52	0	21,32,32	0.70	1 (4%)
3	OXL	H	602	4	5,5,5	2.07	2 (40%)	6,6,6	1.35	1 (16%)
6	O99	A	605	-	31,31,31	0.19	0	44,46,46	0.75	1 (2%)
2	FBP	E	601	-	18,20,20	0.56	0	21,32,32	0.74	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OXL	A	602	4	-	4/4/4/4	-
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1
3	OXL	F	602	4	-	4/4/4/4	-
6	O99	F	605	-	-	3/24/24/24	0/3/3/3
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
3	OXL	B	602	4	-	4/4/4/4	-
3	OXL	C	602	4	-	4/4/4/4	-
3	OXL	D	602	4	-	4/4/4/4	-
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
3	OXL	E	602	4	-	4/4/4/4	-
6	O99	E	605	-	-	0/24/24/24	0/3/3/3
6	O99	D	605	-	-	0/24/24/24	0/3/3/3
3	OXL	G	602	4	-	4/4/4/4	-
2	FBP	A	601	-	-	6/13/32/32	0/1/1/1
2	FBP	G	601	-	-	2/13/32/32	0/1/1/1
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
3	OXL	H	602	4	-	4/4/4/4	-
6	O99	A	605	-	-	4/24/24/24	0/3/3/3
2	FBP	E	601	-	-	2/13/32/32	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	OXL	O1-C1	4.29	1.33	1.22
3	B	602	OXL	O2-C2	4.25	1.33	1.22
3	G	602	OXL	O1-C1	4.08	1.32	1.22
3	D	602	OXL	O2-C2	3.76	1.31	1.22
3	A	602	OXL	O2-C2	3.76	1.31	1.22
3	C	602	OXL	O1-C1	3.70	1.31	1.22
3	F	602	OXL	O2-C2	3.60	1.31	1.22
3	F	602	OXL	O3-C1	-3.47	1.21	1.30
3	H	602	OXL	O2-C2	3.35	1.30	1.22
3	D	602	OXL	C2-C1	3.04	1.59	1.54
3	D	602	OXL	O4-C2	-2.87	1.22	1.30
3	F	602	OXL	O1-C1	2.86	1.29	1.22
3	G	602	OXL	O3-C1	-2.83	1.22	1.30
3	H	602	OXL	O4-C2	-2.71	1.23	1.30
3	B	602	OXL	O4-C2	-2.61	1.23	1.30
3	E	602	OXL	O3-C1	-2.53	1.23	1.30
3	A	602	OXL	O4-C2	-2.47	1.23	1.30
3	F	602	OXL	O4-C2	-2.46	1.23	1.30
3	C	602	OXL	O3-C1	-2.44	1.23	1.30
2	C	601	FBP	P1-O3P	-2.32	1.46	1.54
3	C	602	OXL	C2-C1	2.25	1.58	1.54
2	H	601	FBP	P1-O1	-2.23	1.53	1.60
2	A	601	FBP	P2-O6P	-2.15	1.46	1.54
2	G	601	FBP	P2-O6P	-2.13	1.46	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	602	OXL	O4-C2-C1	4.31	121.19	112.83
3	F	602	OXL	O3-C1-C2	4.27	121.12	112.83
3	D	602	OXL	O3-C1-C2	3.83	120.25	112.83
3	A	602	OXL	O4-C2-C1	3.81	120.22	112.83
3	D	602	OXL	O4-C2-C1	3.75	120.10	112.83
3	C	602	OXL	O3-C1-C2	3.70	120.00	112.83
2	D	601	FBP	O5P-P2-O6	3.38	115.49	106.67
6	A	605	O99	C8-C9-N	3.28	119.22	112.08
3	G	602	OXL	O3-C1-C2	3.18	118.99	112.83
3	B	602	OXL	O4-C2-C1	2.95	118.56	112.83
3	H	602	OXL	O4-C2-C1	2.92	118.50	112.83
2	H	601	FBP	O5P-P2-O6	2.88	114.19	106.67
3	F	602	OXL	O2-C2-C1	-2.73	114.93	120.63
3	E	602	OXL	O3-C1-C2	2.67	118.00	112.83
3	G	602	OXL	O4-C2-C1	2.63	117.93	112.83
3	A	602	OXL	O3-C1-C2	2.54	117.75	112.83
3	B	602	OXL	O3-C1-C2	2.44	117.56	112.83
2	B	601	FBP	O3P-P1-O2P	2.43	116.91	107.80
2	E	601	FBP	O3P-P1-O2P	2.30	116.43	107.80
3	A	602	OXL	O2-C2-C1	-2.23	115.98	120.63
2	C	601	FBP	O6-P2-O4P	2.14	112.22	106.44
2	G	601	FBP	O3P-P1-O2P	2.14	115.82	107.80
3	C	602	OXL	O4-C2-C1	2.13	116.95	112.83
2	H	601	FBP	O2P-P1-O1	2.09	112.11	106.67
3	E	602	OXL	O4-C2-C1	2.05	116.81	112.83
2	F	601	FBP	O3P-P1-O1P	2.04	118.78	110.83

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FBP	O1-C1-C2-C3
2	A	601	FBP	O1-C1-C2-O5
2	A	601	FBP	C4-C5-C6-O6
2	B	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6
2	E	601	FBP	C4-C5-C6-O6
2	F	601	FBP	C4-C5-C6-O6
2	G	601	FBP	C4-C5-C6-O6
2	H	601	FBP	C4-C5-C6-O6
2	A	601	FBP	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	D	601	FBP	C4-C5-C6-O6
6	A	605	O99	C9-N-S1-O1
6	A	605	O99	C9-N-S1-O4
2	C	601	FBP	O5-C5-C6-O6
6	A	605	O99	C9-N-S1-C10
2	B	601	FBP	O5-C5-C6-O6
2	D	601	FBP	O5-C5-C6-O6
2	E	601	FBP	O5-C5-C6-O6
2	F	601	FBP	O5-C5-C6-O6
2	H	601	FBP	O5-C5-C6-O6
2	G	601	FBP	O5-C5-C6-O6
3	A	602	OXL	O3-C1-C2-O4
3	F	602	OXL	O3-C1-C2-O4
3	B	602	OXL	O3-C1-C2-O4
3	C	602	OXL	O3-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O4
3	G	602	OXL	O3-C1-C2-O4
6	F	605	O99	C9-N-S1-O1
3	A	602	OXL	O1-C1-C2-O2
3	B	602	OXL	O1-C1-C2-O2
3	F	602	OXL	O1-C1-C2-O2
3	D	602	OXL	O3-C1-C2-O4
3	H	602	OXL	O3-C1-C2-O4
3	D	602	OXL	O1-C1-C2-O2
3	G	602	OXL	O1-C1-C2-O2
2	A	601	FBP	O1-C1-C2-O2
3	E	602	OXL	O1-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O2
6	F	605	O99	C9-N-S1-O4
3	C	602	OXL	O1-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	O1-C1-C2-O4
3	F	602	OXL	O3-C1-C2-O2
3	G	602	OXL	O3-C1-C2-O2
6	F	605	O99	C9-N-S1-C10
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	G	602	OXL	O1-C1-C2-O4

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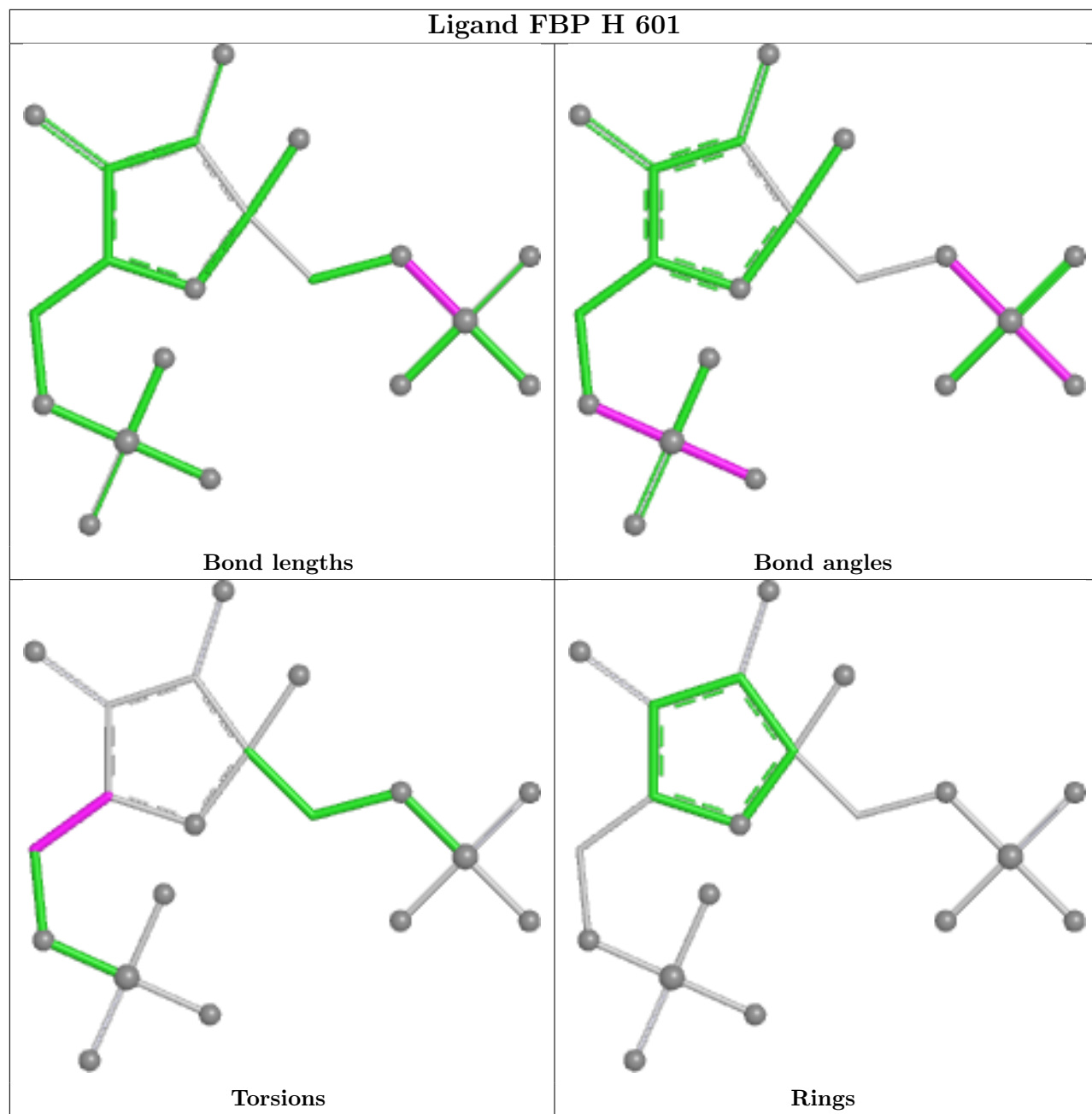
Mol	Chain	Res	Type	Atoms
3	C	602	OXL	O1-C1-C2-O4
3	C	602	OXL	O3-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O4
3	H	602	OXL	O1-C1-C2-O4
2	A	601	FBP	C1-O1-P1-O2P
3	H	602	OXL	O3-C1-C2-O2
6	A	605	O99	C17-C5-S-O6

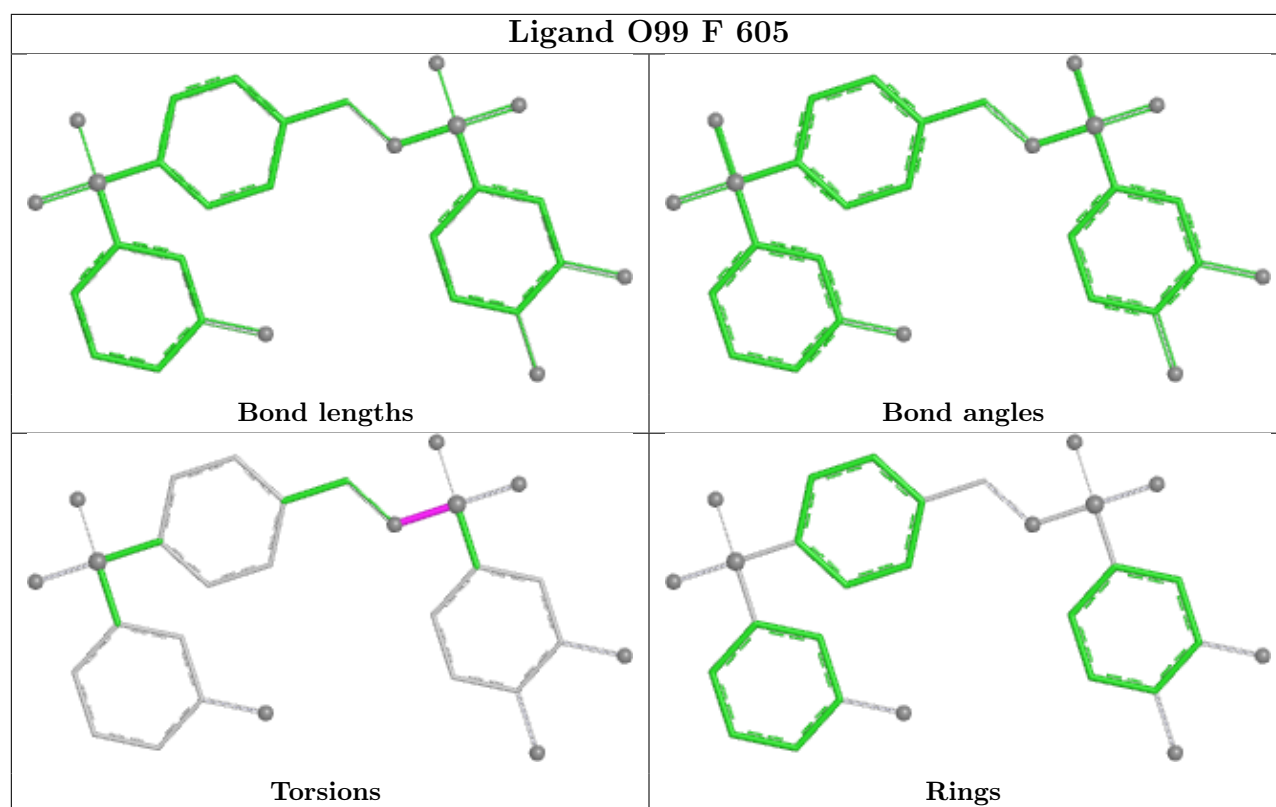
There are no ring outliers.

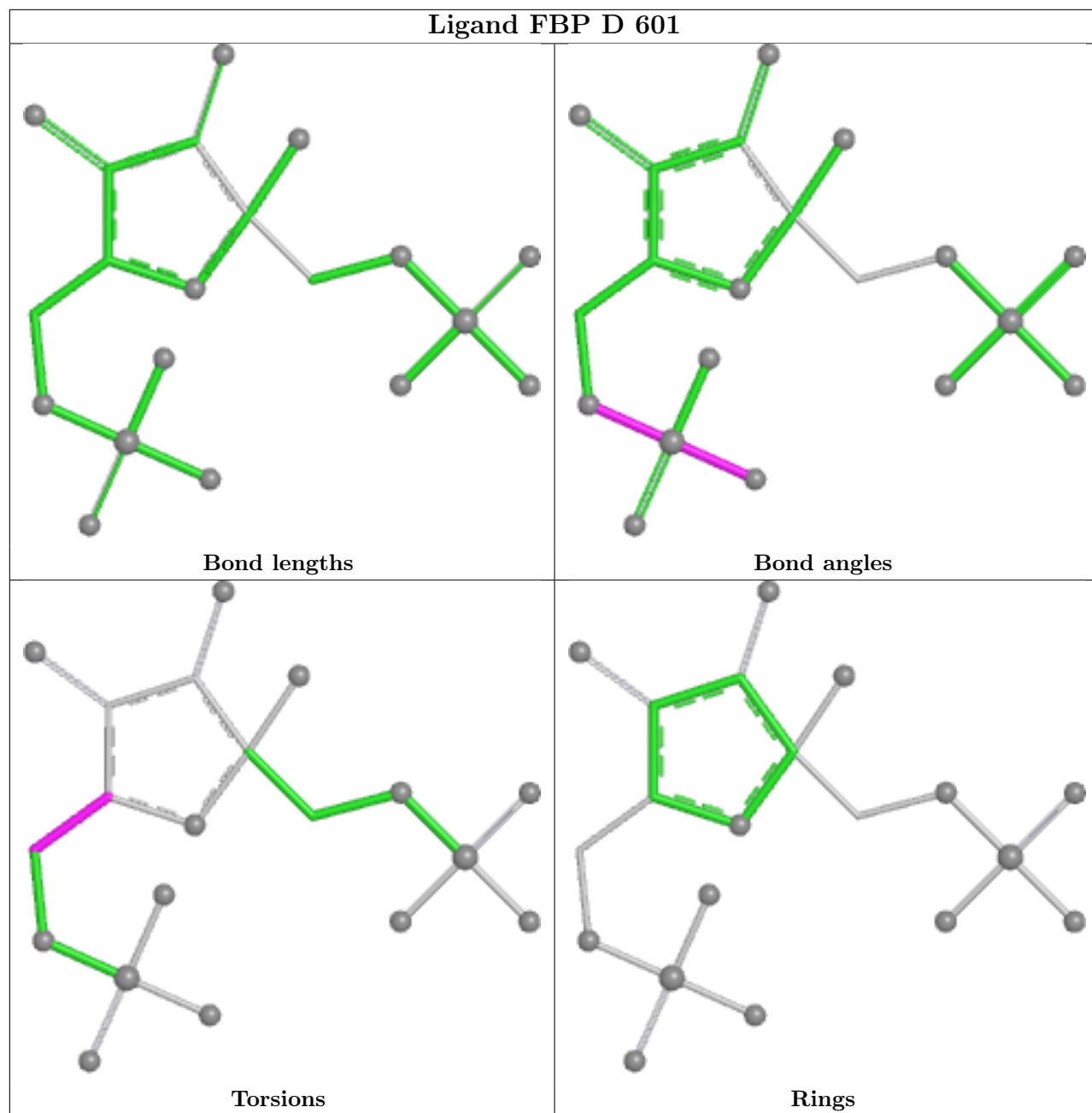
4 monomers are involved in 5 short contacts:

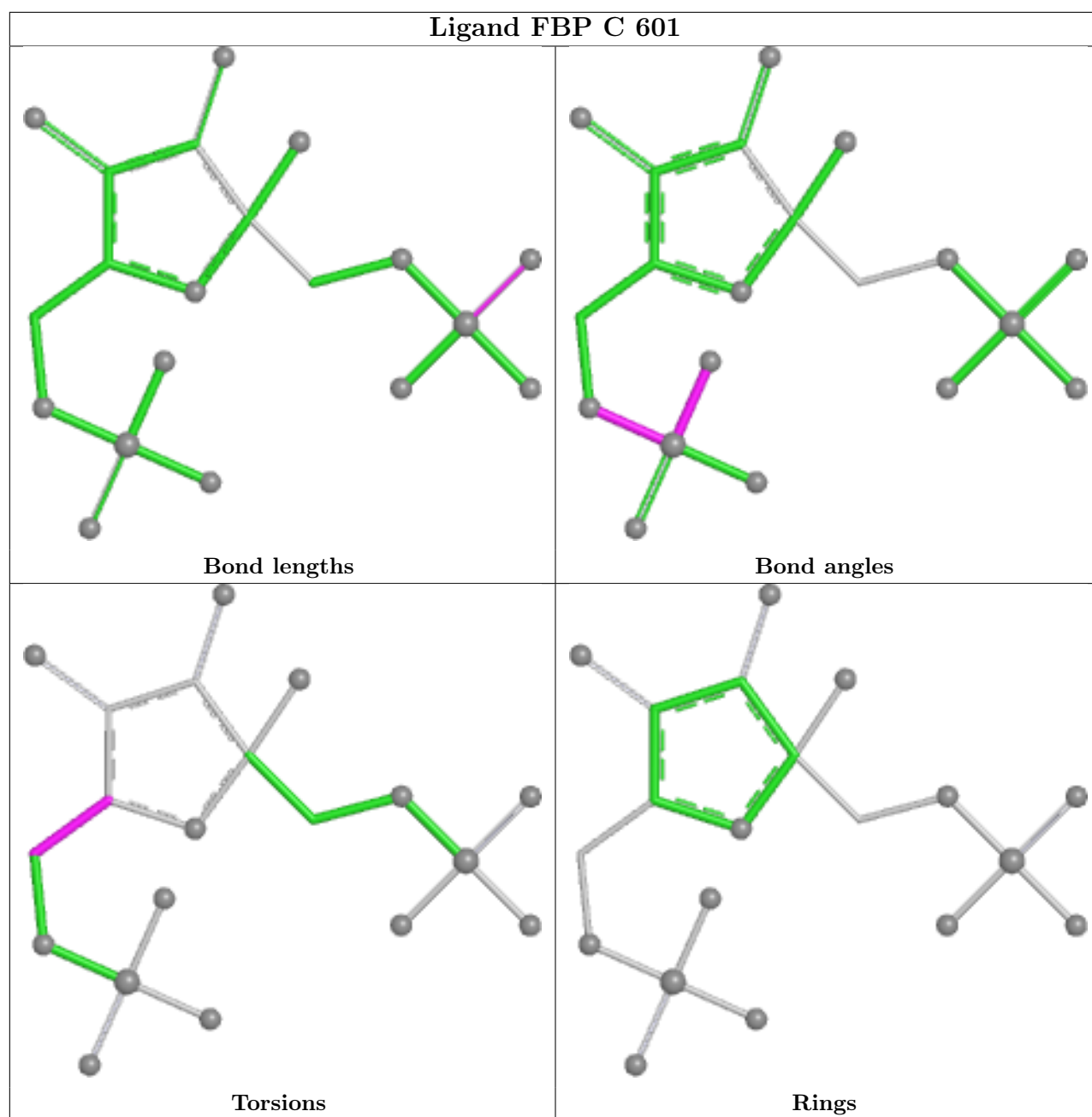
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	605	O99	1	0
2	A	601	FBP	2	0
6	A	605	O99	1	0
2	E	601	FBP	1	0

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.

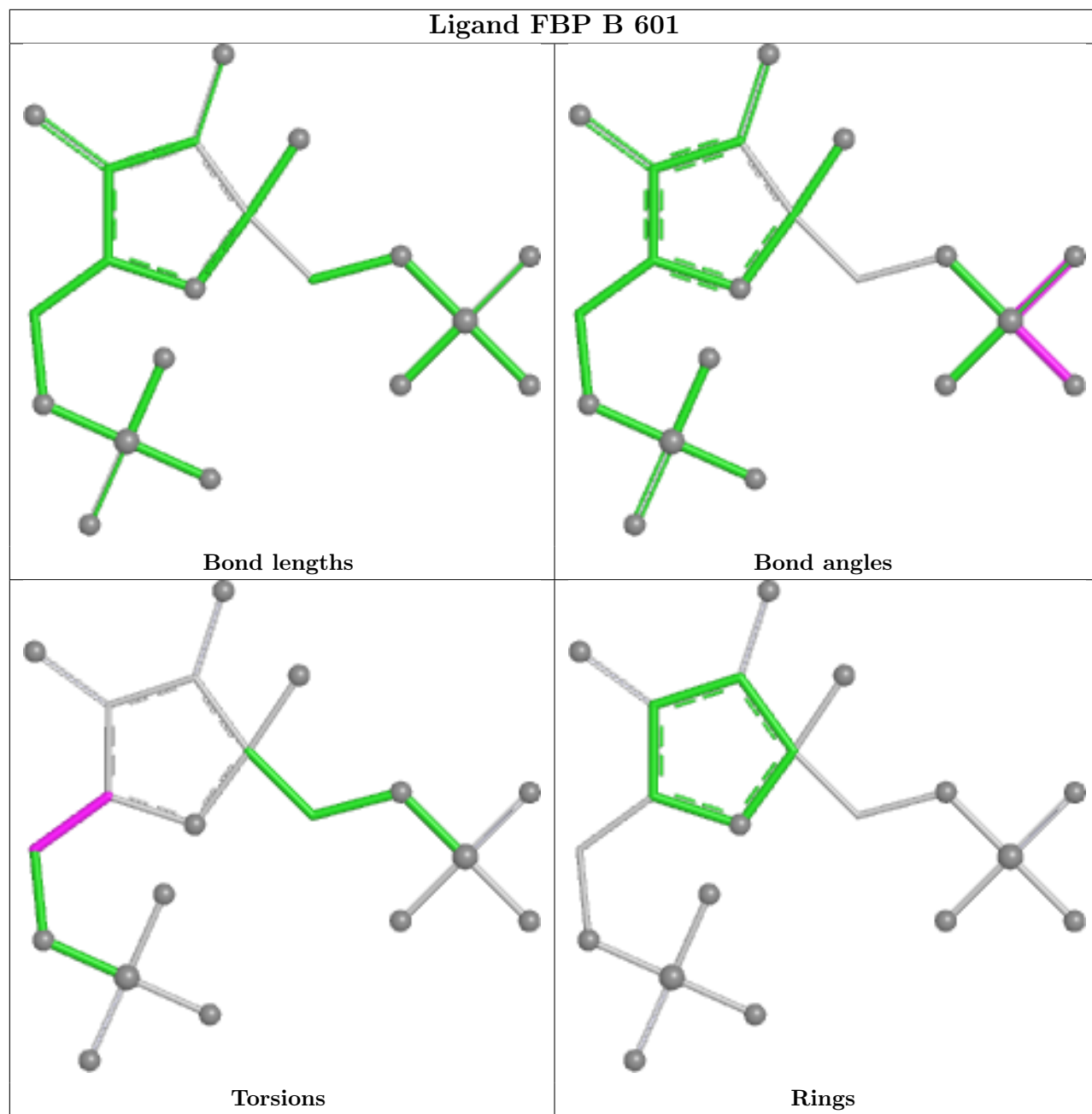




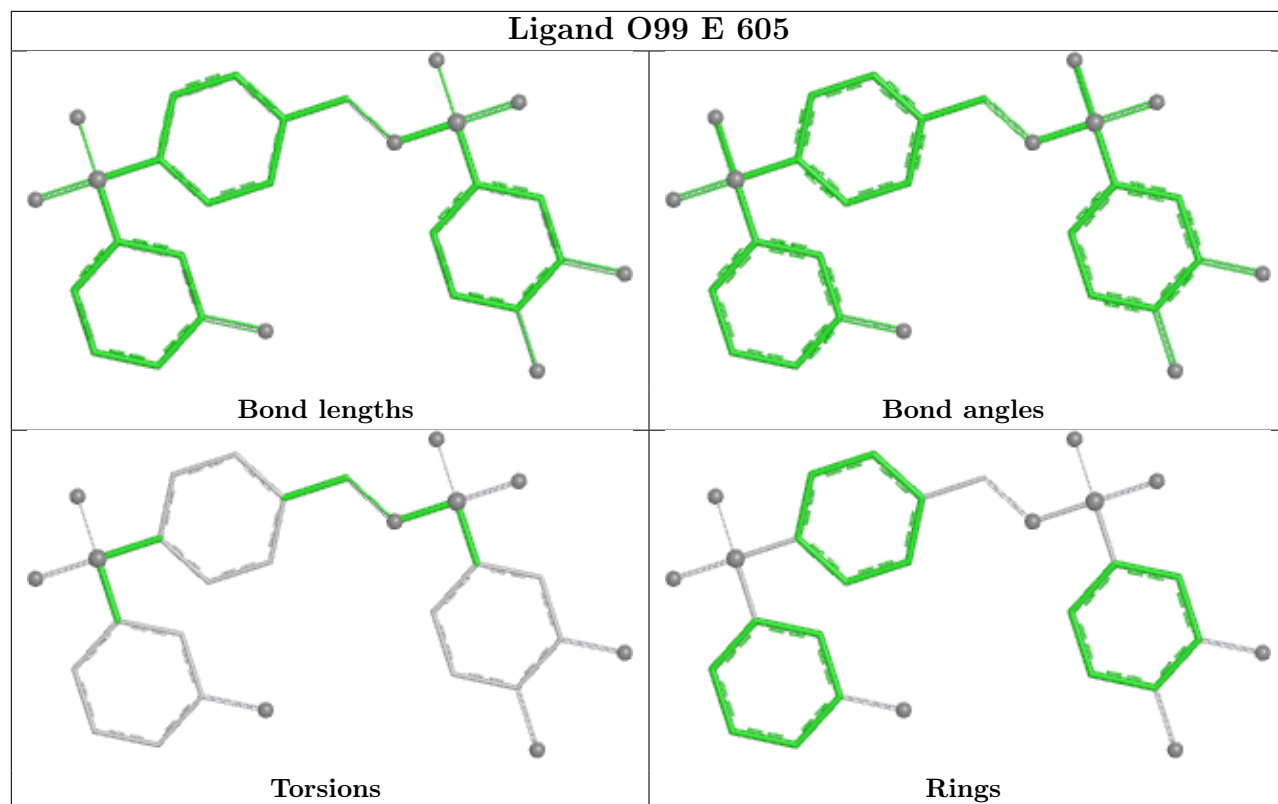




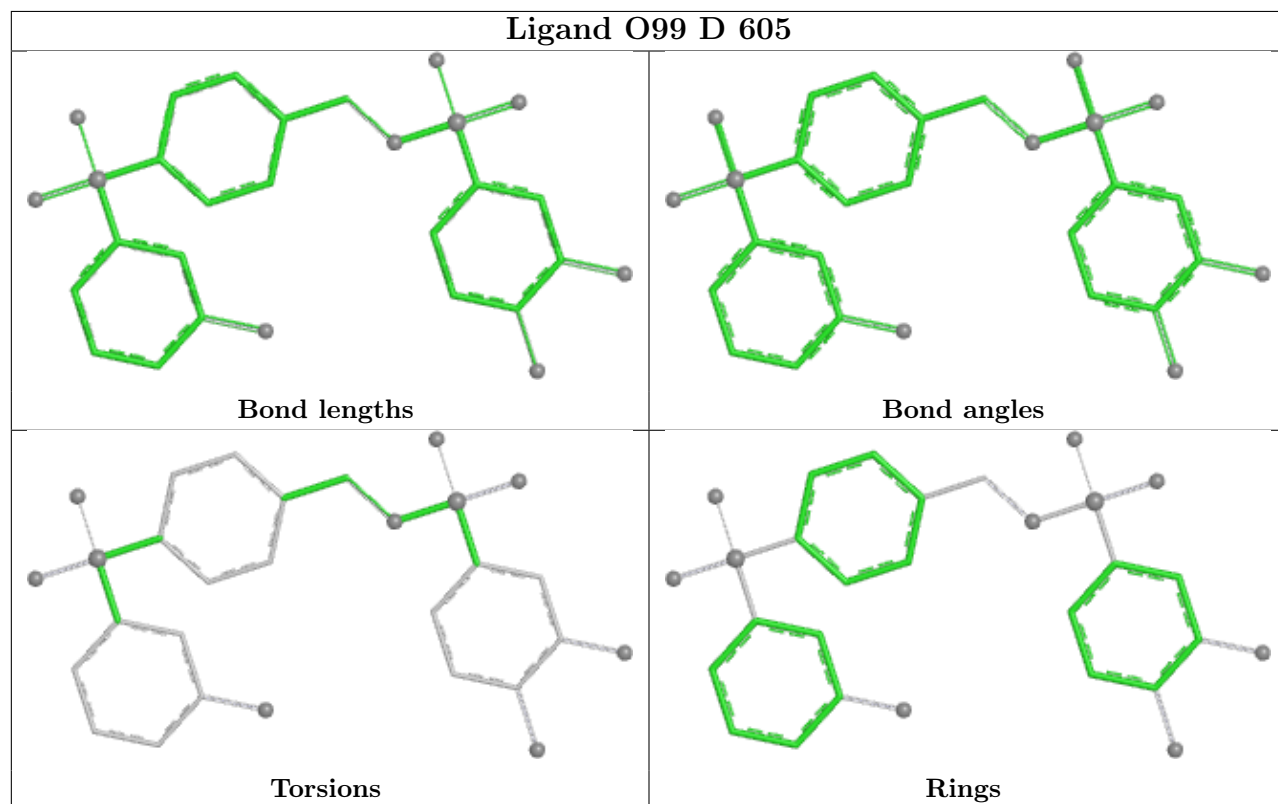
Ligand FBP B 601

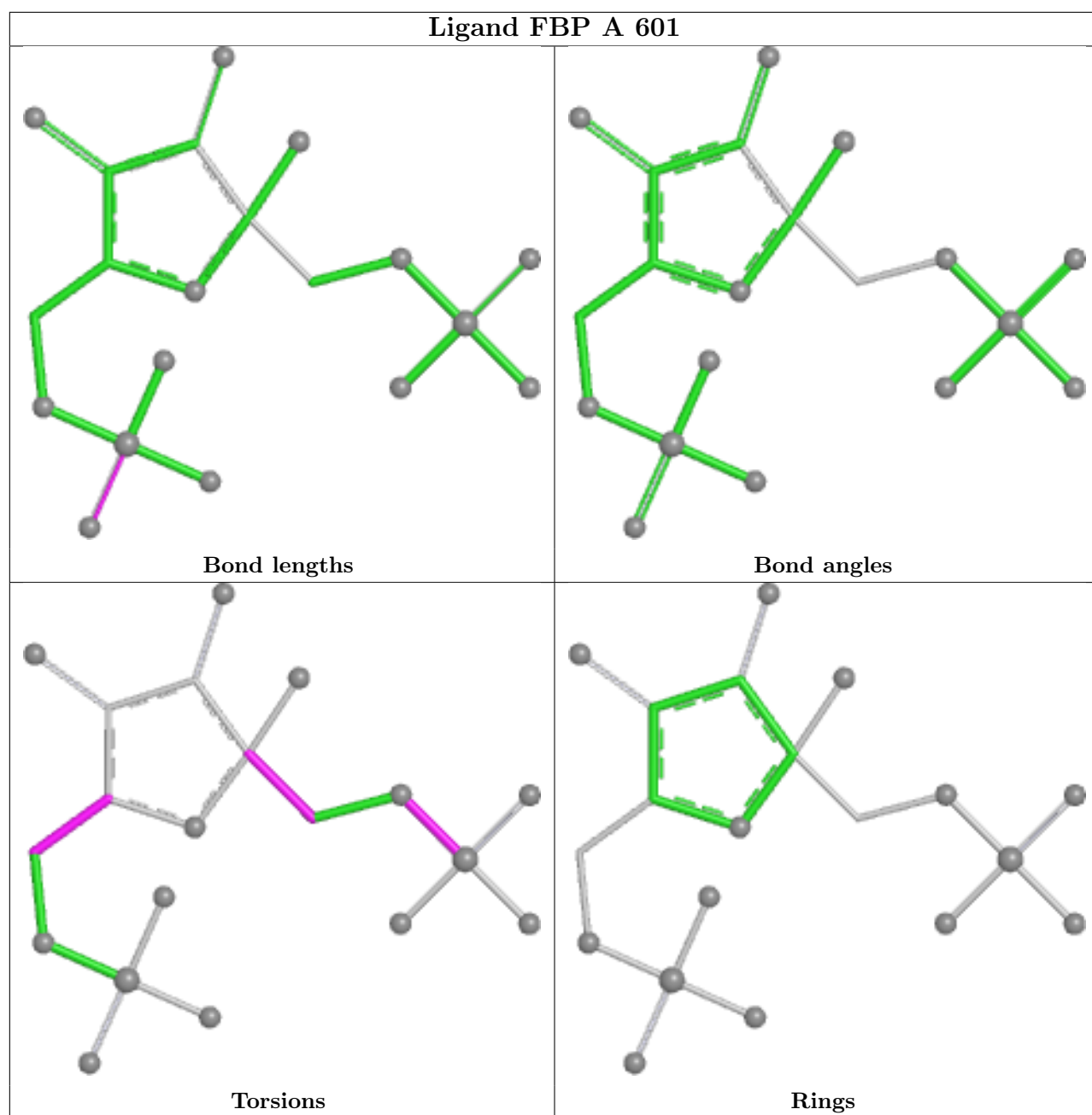


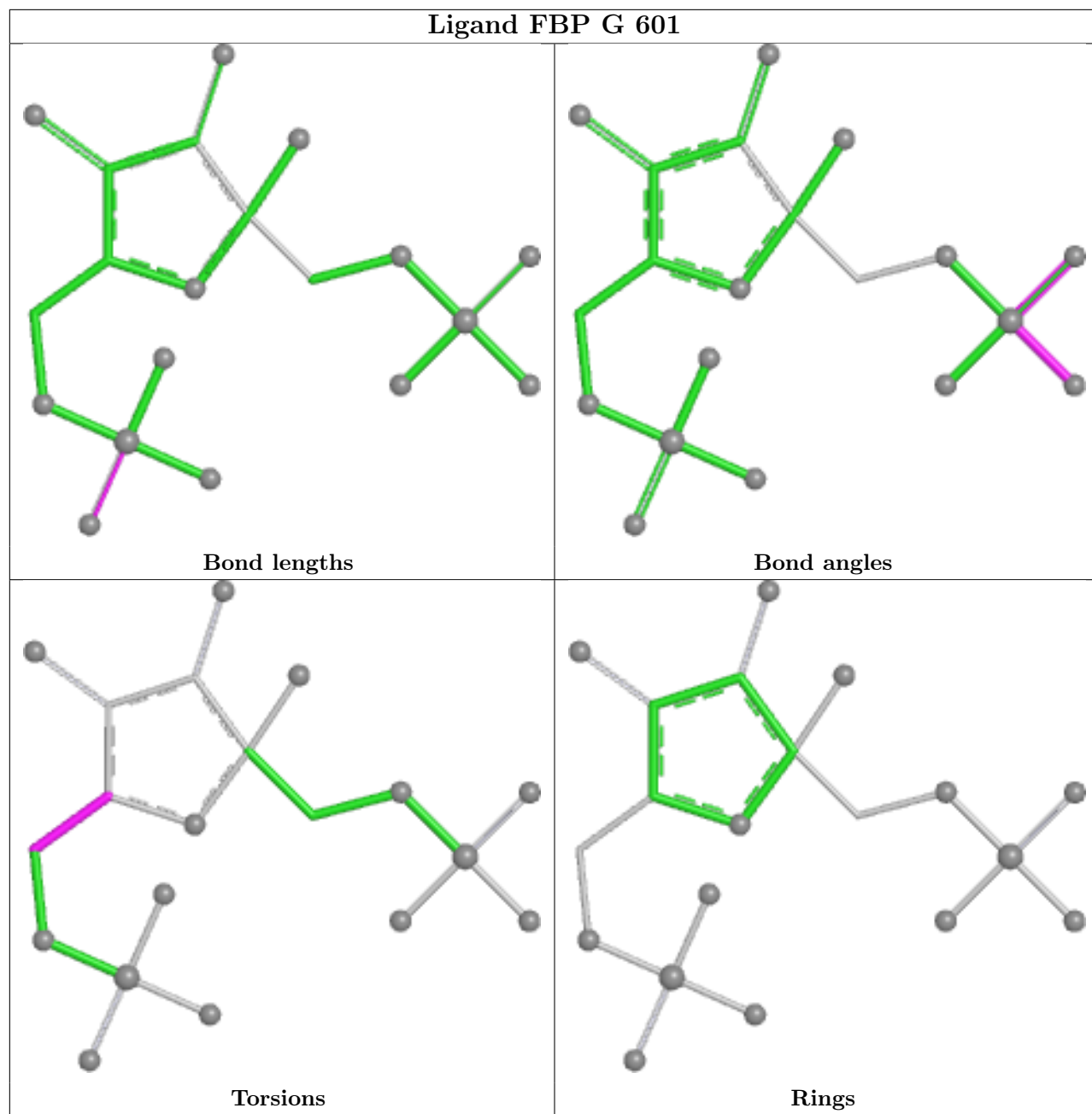
Ligand O99 E 605



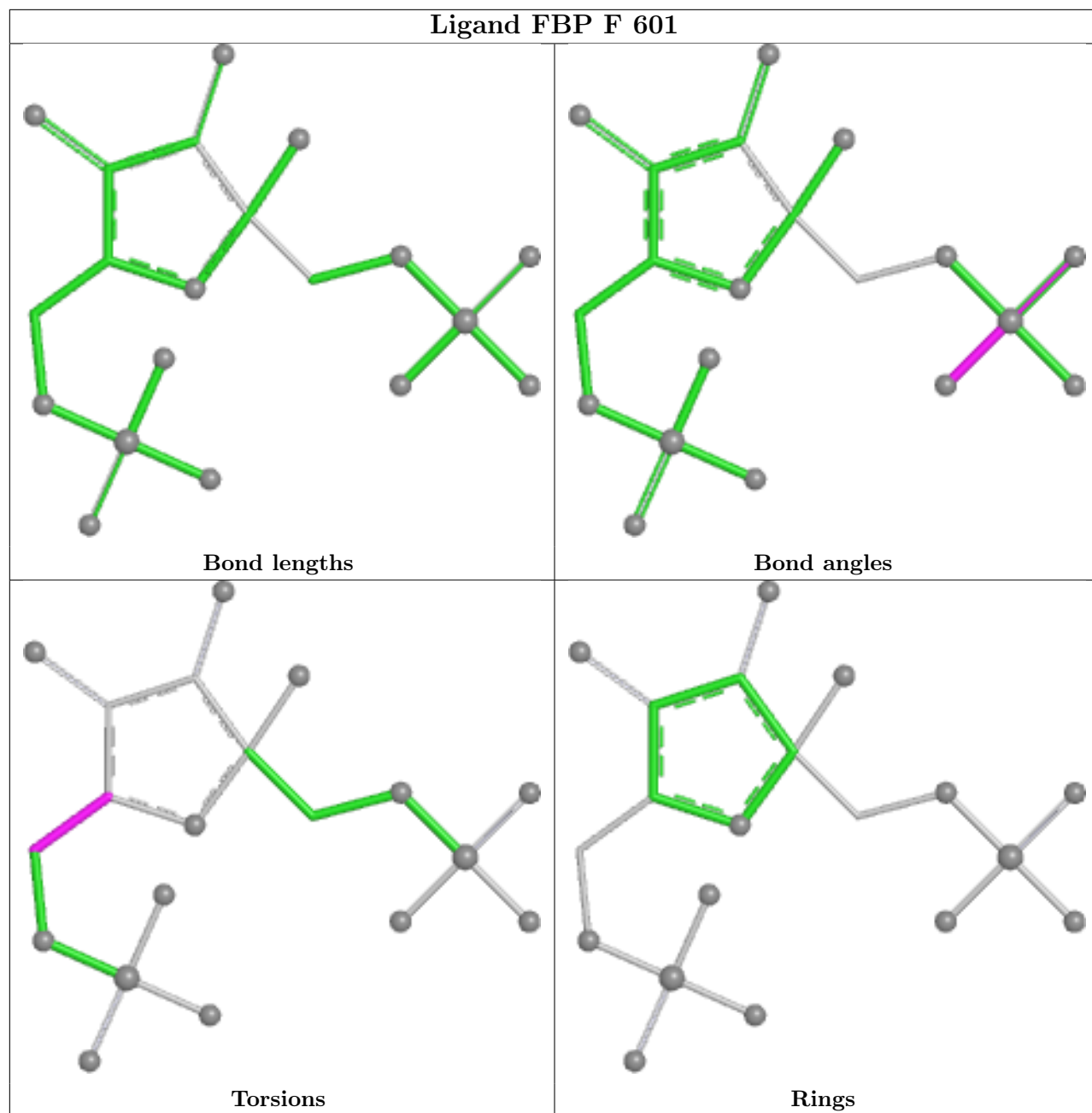
Ligand O99 D 605

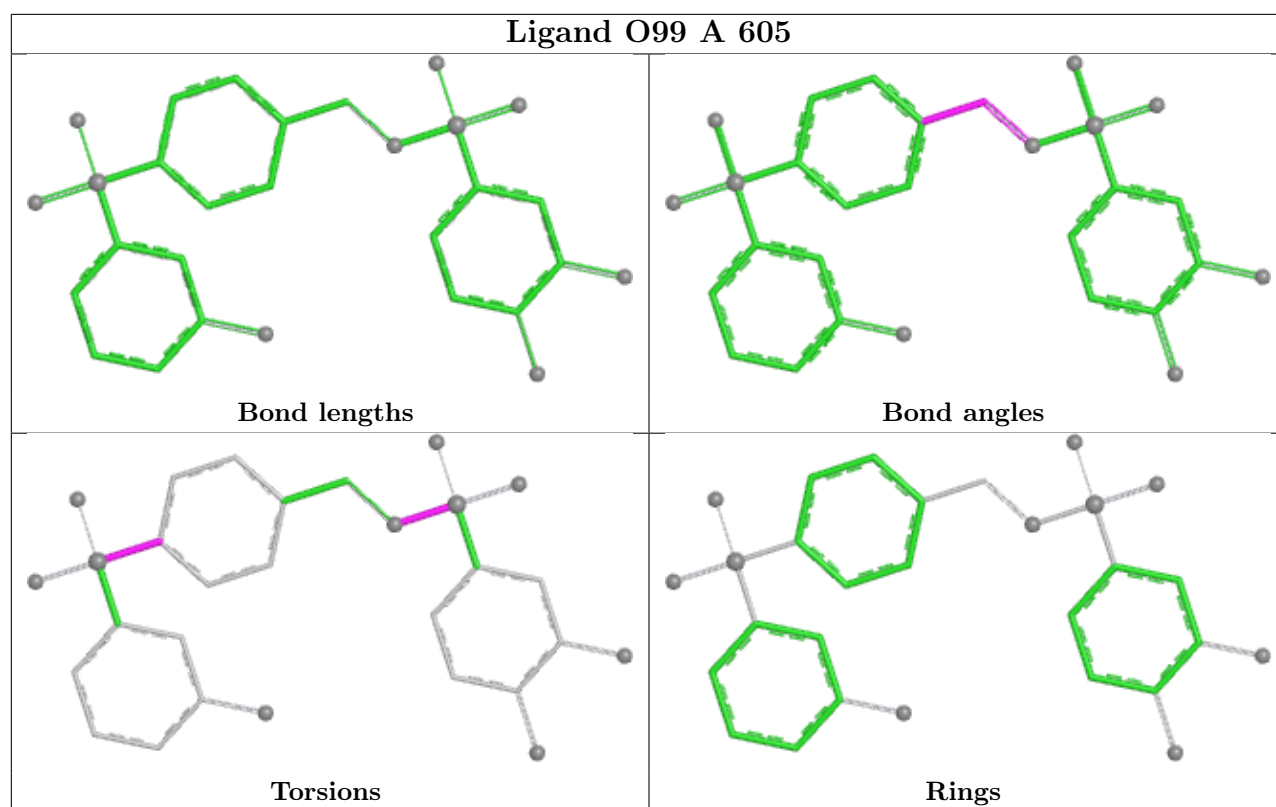


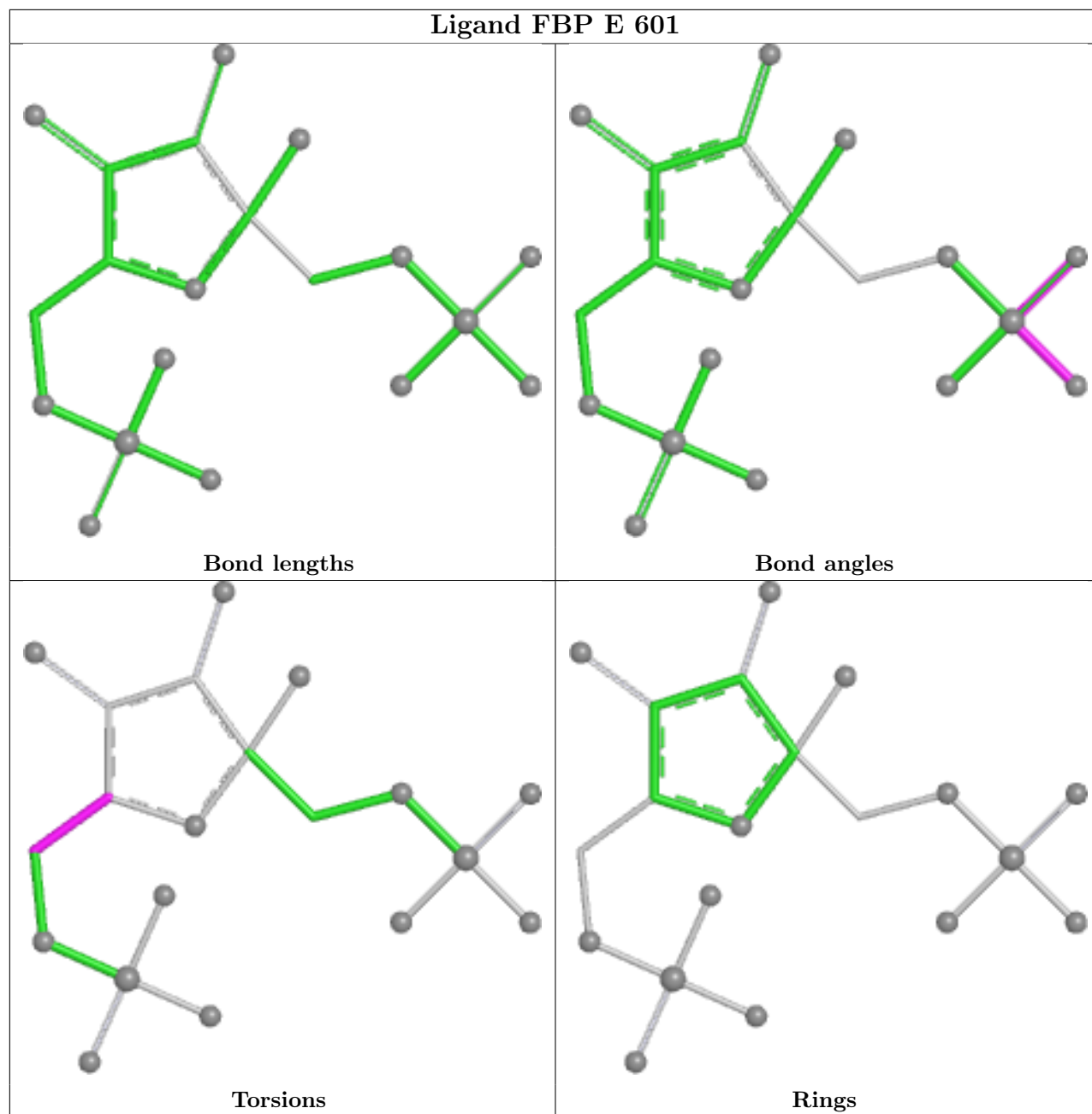




Ligand FBP F 601







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	422/447 (94%)	1.65	125 (29%) 1 1	32, 65, 100, 117	6 (1%)
1	B	436/447 (97%)	1.42	115 (26%) 1 1	30, 55, 93, 101	4 (0%)
1	C	425/447 (95%)	0.95	69 (16%) 4 5	23, 49, 76, 112	4 (0%)
1	D	425/447 (95%)	0.19	18 (4%) 40 42	17, 35, 62, 103	6 (1%)
1	E	419/447 (93%)	1.36	99 (23%) 2 2	26, 58, 91, 107	5 (1%)
1	F	432/447 (96%)	0.80	42 (9%) 13 14	28, 45, 72, 94	7 (1%)
1	G	421/447 (94%)	0.41	20 (4%) 35 37	21, 41, 61, 84	7 (1%)
1	H	425/447 (95%)	0.02	16 (3%) 44 46	17, 32, 54, 94	4 (0%)
All	All	3405/3576 (95%)	0.85	504 (14%) 5 6	17, 47, 86, 117	43 (1%)

All (504) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	115	LEU	8.6
1	B	511	LEU	8.3
1	F	114	PRO	6.9
1	A	238	VAL	6.9
1	F	115	LEU	6.6
1	A	25	PHE	6.3
1	H	21	GLY	6.1
1	E	114	PRO	5.8
1	A	132	GLY	5.6
1	E	238	VAL	5.4
1	D	24	PHE	5.2
1	D	25	PHE	5.2
1	B	543	SER	5.2
1	B	517	VAL	5.1
1	B	114	PRO	5.1
1	C	20	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	F	116	SER	5.0
1	F	231	PRO	5.0
1	G	271	GLY	5.0
1	D	22	THR	4.9
1	G	33	ALA	4.9
1	D	21	GLY	4.8
1	E	115	LEU	4.7
1	E	25	PHE	4.6
1	A	30	LEU	4.6
1	A	33	ALA	4.5
1	A	232	GLY	4.5
1	C	271	GLY	4.5
1	B	502	VAL	4.5
1	D	23	ALA	4.5
1	B	506	ILE	4.5
1	E	23	ALA	4.5
1	B	490	PRO	4.4
1	A	124	LEU	4.4
1	A	95	TYR	4.4
1	A	115	LEU	4.4
1	A	112	GLY	4.3
1	B	267[A]	ARG	4.3
1	E	129	PRO	4.3
1	B	116	SER	4.3
1	E	495	ALA	4.3
1	B	493	ILE	4.3
1	G	24	PHE	4.2
1	B	542	ILE	4.2
1	A	269	ALA	4.2
1	C	63	ILE	4.2
1	B	485	LEU	4.2
1	C	103	VAL	4.2
1	A	241	LEU	4.1
1	A	249	VAL	4.1
1	B	110	PHE	4.1
1	B	504	PHE	4.1
1	B	508	SER	4.1
1	A	114	PRO	4.0
1	E	245	VAL	4.0
1	E	122	ILE	4.0
1	B	495	ALA	4.0
1	A	24	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	257	VAL	4.0
1	A	23	ALA	3.9
1	F	512	ARG	3.9
1	C	66	ALA	3.9
1	A	543	SER	3.9
1	C	115	LEU	3.9
1	E	485	LEU	3.9
1	B	489	PRO	3.9
1	C	80	GLY	3.9
1	A	34	MET	3.9
1	B	527	TRP	3.8
1	F	484	LEU	3.8
1	A	489	PRO	3.8
1	C	231	PRO	3.8
1	F	112	GLY	3.8
1	F	267[A]	ARG	3.8
1	H	22	THR	3.8
1	B	249	VAL	3.8
1	B	512	ARG	3.8
1	H	24	PHE	3.8
1	A	32	ALA	3.7
1	B	11	ALA	3.7
1	E	33	ALA	3.7
1	C	22	THR	3.7
1	A	243	PHE	3.7
1	A	471	ALA	3.7
1	A	116	SER	3.7
1	B	498	VAL	3.7
1	E	251	ILE	3.7
1	B	509	GLY	3.6
1	E	493	ILE	3.6
1	C	117	TYR	3.6
1	A	120	VAL	3.6
1	B	521	VAL	3.6
1	A	100	ILE	3.6
1	E	269	ALA	3.6
1	A	270	LEU	3.6
1	C	114	PRO	3.6
1	B	117	TYR	3.6
1	B	70	VAL	3.6
1	G	25	PHE	3.6
1	B	507	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	65	PRO	3.5
1	E	120	VAL	3.5
1	B	505	GLY	3.5
1	A	70	VAL	3.5
1	A	357	THR	3.5
1	E	244	GLY	3.5
1	A	496	ASP	3.5
1	H	516	ARG	3.5
1	E	490	PRO	3.4
1	F	489	PRO	3.4
1	E	233	LEU	3.4
1	A	263	VAL	3.4
1	A	475	VAL	3.4
1	C	111	ALA	3.4
1	E	101	ALA	3.4
1	B	118	ARG	3.4
1	A	63	ILE	3.4
1	F	499	ASP	3.4
1	G	116	SER	3.4
1	G	23	ALA	3.4
1	B	86	LEU	3.4
1	B	484	LEU	3.4
1	E	124	LEU	3.4
1	E	540	LEU	3.4
1	F	516	ARG	3.4
1	B	513	GLY	3.4
1	A	111	ALA	3.4
1	E	111	ALA	3.4
1	F	233	LEU	3.4
1	C	385	GLU	3.3
1	C	23	ALA	3.3
1	C	311	ILE	3.3
1	H	23	ALA	3.3
1	A	73	LEU	3.3
1	B	411	ARG	3.3
1	F	543	SER	3.3
1	C	21	GLY	3.3
1	A	378	ALA	3.3
1	E	97	ALA	3.3
1	A	233	LEU	3.3
1	H	25	PHE	3.3
1	B	128	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	232	GLY	3.3
1	E	257	VAL	3.3
1	E	502	VAL	3.3
1	C	75	GLU	3.3
1	A	482	PHE	3.3
1	A	514	PHE	3.3
1	E	116	SER	3.2
1	C	79	ALA	3.2
1	E	264	ALA	3.2
1	E	256	PHE	3.2
1	G	351	ARG	3.2
1	A	384	VAL	3.2
1	A	117	TYR	3.2
1	B	241	LEU	3.2
1	E	241	LEU	3.2
1	C	25	PHE	3.2
1	E	109	SER	3.2
1	E	489	PRO	3.2
1	B	107	VAL	3.2
1	C	107	VAL	3.2
1	E	498	VAL	3.2
1	C	347	ILE	3.2
1	E	110	PHE	3.2
1	A	113	SER	3.2
1	E	26	GLN	3.2
1	A	123	ALA	3.1
1	E	249	VAL	3.1
1	F	351	ARG	3.1
1	A	88	PHE	3.1
1	C	382	PHE	3.1
1	A	93	HIS	3.1
1	B	95	TYR	3.1
1	C	380	GLY	3.1
1	A	106	ALA	3.1
1	C	70	VAL	3.1
1	E	70	VAL	3.1
1	A	251	ILE	3.1
1	B	67	SER	3.1
1	C	110	PHE	3.1
1	A	101	ALA	3.1
1	B	111	ALA	3.1
1	E	123	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	130	GLY	3.0
1	B	348	THR	3.0
1	A	53	ALA	3.0
1	A	495	ALA	3.0
1	A	245	VAL	3.0
1	B	124	LEU	3.0
1	B	270	LEU	3.0
1	B	100	ILE	3.0
1	E	447	GLY	3.0
1	E	527	TRP	3.0
1	A	119	PRO	3.0
1	A	490	PRO	3.0
1	E	442	VAL	3.0
1	E	118	ARG	3.0
1	A	527	TRP	3.0
1	B	486	TYR	3.0
1	B	514	PHE	3.0
1	C	24	PHE	3.0
1	B	492	ALA	3.0
1	C	397	ALA	3.0
1	B	233	LEU	3.0
1	B	515	LEU	3.0
1	A	110	PHE	3.0
1	E	24	PHE	3.0
1	F	527	TRP	3.0
1	A	99	SER	2.9
1	A	103	VAL	2.9
1	E	112	GLY	2.9
1	E	248	GLY	2.9
1	E	63	ILE	2.9
1	B	119	PRO	2.9
1	B	88	PHE	2.9
1	E	514	PHE	2.9
1	B	540[A]	LEU	2.9
1	C	343	LEU	2.9
1	B	120	VAL	2.9
1	A	122	ILE	2.9
1	A	277	ILE	2.9
1	E	542	ILE	2.9
1	E	119	PRO	2.9
1	A	84	ALA	2.9
1	F	232	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	104	ARG	2.9
1	E	487	ARG	2.9
1	A	350	PRO	2.9
1	E	113	SER	2.9
1	A	79	ALA	2.9
1	A	494	TRP	2.9
1	B	13	VAL	2.8
1	F	490	PRO	2.8
1	A	449	SER	2.8
1	E	275	HIS	2.8
1	F	459	ARG	2.8
1	E	106	ALA	2.8
1	A	108	GLU	2.8
1	B	238	VAL	2.8
1	F	498	VAL	2.8
1	A	351	ARG	2.8
1	E	128	GLY	2.8
1	A	254	ALA	2.8
1	A	488[A]	GLU	2.8
1	C	108	GLU	2.8
1	F	269	ALA	2.8
1	B	231	PRO	2.8
1	C	77	ILE	2.8
1	F	493	ILE	2.8
1	C	68	ARG	2.8
1	C	69	SER	2.8
1	G	34	MET	2.8
1	C	232	GLY	2.8
1	E	30	LEU	2.8
1	G	115	LEU	2.8
1	B	272	PRO	2.8
1	A	52	VAL	2.8
1	C	384	VAL	2.8
1	A	280	ILE	2.8
1	G	118	ARG	2.7
1	B	382	PHE	2.7
1	C	319	PHE	2.7
1	E	126	THR	2.7
1	A	118	ARG	2.7
1	E	263	VAL	2.7
1	C	116	SER	2.7
1	A	80	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	66	ALA	2.7
1	A	253	PHE	2.7
1	A	256	PHE	2.7
1	B	243	PHE	2.7
1	A	62	THR	2.7
1	A	540	LEU	2.7
1	E	511	LEU	2.7
1	F	412	ARG	2.7
1	C	95	TYR	2.7
1	A	311	ILE	2.7
1	A	404	ARG	2.7
1	C	528	ARG	2.7
1	C	101	ALA	2.7
1	E	95	TYR	2.7
1	B	541	SER	2.7
1	D	543	SER	2.7
1	D	311	ILE	2.7
1	E	121	ALA	2.6
1	A	343	LEU	2.6
1	E	270	LEU	2.6
1	H	231	PRO	2.6
1	E	237	ASP	2.6
1	A	298	VAL	2.6
1	G	63	ILE	2.6
1	A	412	ARG	2.6
1	F	487	ARG	2.6
1	C	27	GLN	2.6
1	C	132	GLY	2.6
1	D	232	GLY	2.6
1	C	33	ALA	2.6
1	E	265	ALA	2.6
1	B	416	LEU	2.6
1	C	86	LEU	2.6
1	B	113	SER	2.6
1	G	487	ARG	2.6
1	A	279	ILE	2.6
1	E	510	LYS	2.6
1	B	121	ALA	2.6
1	E	499	ASP	2.6
1	E	515	LEU	2.6
1	B	103	VAL	2.5
1	E	465	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	274	GLY	2.5
1	C	383	PRO	2.5
1	D	33	ALA	2.5
1	F	33	ALA	2.5
1	A	511	LEU	2.5
1	B	73	LEU	2.5
1	D	233	LEU	2.5
1	F	488	GLU	2.5
1	E	243	PHE	2.5
1	A	107	VAL	2.5
1	A	274	GLY	2.5
1	D	275[A]	HIS	2.5
1	F	533	TYR	2.5
1	C	412	ARG	2.5
1	E	464	ALA	2.5
1	F	275	HIS	2.5
1	F	237	ASP	2.5
1	A	61	ALA	2.5
1	A	97	ALA	2.5
1	C	386	ALA	2.5
1	F	268	ALA	2.5
1	G	411	ARG	2.5
1	B	122	ILE	2.5
1	B	108	GLU	2.4
1	E	73	LEU	2.4
1	B	90	HIS	2.4
1	B	275	HIS	2.4
1	C	90	HIS	2.4
1	E	351	ARG	2.4
1	E	88	PHE	2.4
1	F	71	GLU	2.4
1	E	52	VAL	2.4
1	E	494	TRP	2.4
1	E	117	TYR	2.4
1	F	129	PRO	2.4
1	G	272	PRO	2.4
1	B	264	ALA	2.4
1	F	492	ALA	2.4
1	E	520	LEU	2.4
1	E	276	GLY	2.4
1	C	105	GLU	2.4
1	B	475	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	126	THR	2.4
1	B	10	ARG	2.4
1	A	129	PRO	2.4
1	A	529	PRO	2.4
1	B	97	ALA	2.4
1	B	408	GLU	2.4
1	A	130	GLY	2.4
1	B	112	GLY	2.4
1	A	372	MET	2.4
1	B	109	SER	2.4
1	H	543	SER	2.4
1	A	121	ALA	2.3
1	B	265	ALA	2.3
1	F	265	ALA	2.3
1	A	373	LEU	2.3
1	A	453	LEU	2.3
1	B	237	ASP	2.3
1	A	382	PHE	2.3
1	G	412	ARG	2.3
1	A	493	ILE	2.3
1	A	542	ILE	2.3
1	A	252	VAL	2.3
1	E	252	VAL	2.3
1	F	238	VAL	2.3
1	G	231	PRO	2.3
1	C	106	ALA	2.3
1	E	268	ALA	2.3
1	F	242	ARG	2.3
1	A	92	SER	2.3
1	G	109	SER	2.3
1	E	289	VAL	2.3
1	F	521	VAL	2.3
1	A	264	ALA	2.3
1	B	14	ALA	2.3
1	H	351	ARG	2.3
1	H	34	MET	2.3
1	B	131	SER	2.3
1	C	109	SER	2.3
1	G	543	SER	2.3
1	A	236	GLN	2.3
1	B	277	ILE	2.3
1	B	263	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	231	PRO	2.3
1	C	378	ALA	2.3
1	E	492	ALA	2.3
1	G	132	GLY	2.3
1	B	520	LEU	2.3
1	E	484	LEU	2.3
1	A	426	ILE	2.2
1	C	393	ILE	2.2
1	E	277	ILE	2.2
1	A	498	VAL	2.2
1	F	502	VAL	2.2
1	B	72	ARG	2.2
1	B	487	ARG	2.2
1	B	510	LYS	2.2
1	B	132	GLY	2.2
1	A	104	ARG	2.2
1	E	242	ARG	2.2
1	H	412	ARG	2.2
1	C	272	PRO	2.2
1	C	348	THR	2.2
1	C	76[A]	MET	2.2
1	C	64	GLY	2.2
1	E	505	GLY	2.2
1	H	130	GLY	2.2
1	B	66	ALA	2.2
1	E	260	ALA	2.2
1	F	124	LEU	2.2
1	E	93	HIS	2.2
1	A	242	ARG	2.2
1	B	494	TRP	2.2
1	D	412	ARG	2.2
1	C	379	LYS	2.2
1	C	34	MET	2.2
1	A	260	ALA	2.2
1	A	268	ALA	2.2
1	C	32	ALA	2.2
1	H	275[A]	HIS	2.2
1	A	109	SER	2.2
1	B	456	TYR	2.2
1	E	533	TYR	2.2
1	C	100	ILE	2.1
1	B	266	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	397	ALA	2.1
1	A	258	ARG	2.1
1	C	411	ARG	2.1
1	E	541[A]	SER	2.1
1	A	342	MET	2.1
1	D	34	MET	2.1
1	B	236	GLN	2.1
1	D	26	GLN	2.1
1	E	274	GLY	2.1
1	B	242	ARG	2.1
1	A	492	ALA	2.1
1	B	268	ALA	2.1
1	C	339	ALA	2.1
1	E	254	ALA	2.1
1	A	86	LEU	2.1
1	C	410	LEU	2.1
1	E	71	GLU	2.1
1	H	273	GLU	2.1
1	A	383	PRO	2.1
1	B	503	GLN	2.1
1	G	114	PRO	2.1
1	A	68	ARG	2.1
1	A	248	GLY	2.1
1	B	91	GLY	2.1
1	B	248	GLY	2.1
1	C	375	GLY	2.1
1	H	232	GLY	2.1
1	B	407	PHE	2.1
1	B	245	VAL	2.1
1	B	539	VAL	2.1
1	B	378	ALA	2.1
1	E	469	ALA	2.1
1	B	443	LEU	2.1
1	F	86	LEU	2.1
1	C	94	GLU	2.1
1	B	445	THR	2.1
1	B	483	PRO	2.1
1	B	21	GLY	2.1
1	D	130	GLY	2.1
1	B	77	ILE	2.1
1	E	100	ILE	2.1
1	B	24	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	504	PHE	2.1
1	B	101	ALA	2.1
1	B	106	ALA	2.1
1	B	488	GLU	2.0
1	C	97	ALA	2.1
1	A	485	LEU	2.0
1	A	237	ASP	2.0
1	E	411	ARG	2.0
1	F	379	LYS	2.0
1	B	532	GLY	2.0
1	A	481	VAL	2.0
1	D	408	GLU	2.0
1	F	120	VAL	2.0
1	B	89	SER	2.0
1	C	414	ALA	2.0
1	C	366	ASP	2.0
1	B	473	ARG	2.0
1	E	459	ARG	2.0
1	E	500	ARG	2.0
1	H	242	ARG	2.0
1	A	74	LYS	2.0
1	A	379	LYS	2.0
1	A	91	GLY	2.0
1	A	128	GLY	2.0
1	D	513	GLY	2.0
1	A	533	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

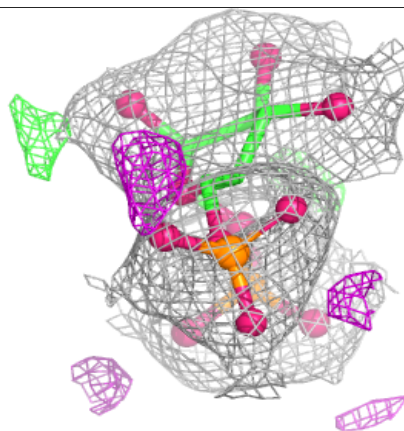
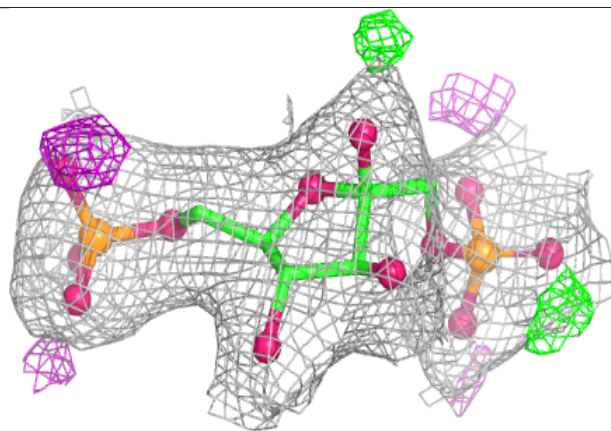
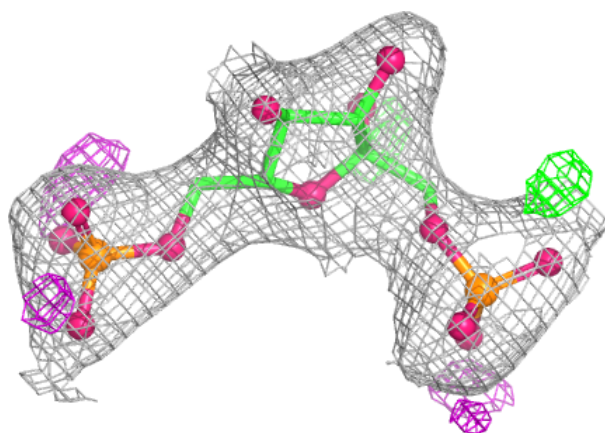
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	OXL	E	602	6/6	0.77	0.15	74,75,75,75	0
5	K	E	604	1/1	0.78	0.19	115,115,115,115	0
3	OXL	C	602	6/6	0.86	0.13	69,70,70,70	0
5	K	A	604	1/1	0.87	0.10	104,104,104,104	0
3	OXL	A	602	6/6	0.87	0.11	81,81,81,81	0
3	OXL	F	602	6/6	0.89	0.12	68,69,69,69	0
5	K	C	604	1/1	0.90	0.11	75,75,75,75	0
2	FBP	E	601	20/20	0.90	0.11	53,56,60,60	0
3	OXL	B	602	6/6	0.91	0.11	63,63,65,65	0
3	OXL	D	602	6/6	0.91	0.12	55,56,56,56	0
3	OXL	G	602	6/6	0.91	0.10	51,52,53,54	0
6	O99	F	605	29/29	0.91	0.12	40,41,42,42	17
6	O99	A	605	29/29	0.92	0.12	49,53,55,56	17
2	FBP	B	601	20/20	0.92	0.10	52,53,56,56	0
3	OXL	H	602	6/6	0.93	0.11	49,50,50,51	0
2	FBP	F	601	20/20	0.93	0.09	45,52,57,57	0
2	FBP	A	601	20/20	0.93	0.10	61,64,66,66	0
6	O99	E	605	29/29	0.94	0.10	42,45,47,47	17
6	O99	D	605	29/29	0.94	0.10	39,42,44,45	17
4	MG	B	603	1/1	0.95	0.12	45,45,45,45	0
5	K	G	604	1/1	0.95	0.08	66,66,66,66	0
4	MG	F	603	1/1	0.95	0.12	32,32,32,32	0
4	MG	E	603	1/1	0.96	0.09	49,49,49,49	0
5	K	B	604	1/1	0.96	0.12	69,69,69,69	0
4	MG	C	603	1/1	0.96	0.15	38,38,38,38	0
5	K	F	604	1/1	0.97	0.05	85,85,85,85	0
4	MG	A	603	1/1	0.97	0.10	52,52,52,52	0
5	K	D	604	1/1	0.98	0.08	51,51,51,51	0
4	MG	D	603	1/1	0.98	0.13	28,28,28,28	0
2	FBP	G	601	20/20	0.98	0.05	28,30,32,33	0
2	FBP	C	601	20/20	0.98	0.05	29,30,35,36	0
2	FBP	H	601	20/20	0.99	0.04	21,24,27,28	0
4	MG	G	603	1/1	0.99	0.08	23,23,23,23	0
2	FBP	D	601	20/20	0.99	0.04	25,26,29,30	0
5	K	H	604	1/1	0.99	0.11	51,51,51,51	0
4	MG	H	603	1/1	1.00	0.07	22,22,22,22	0

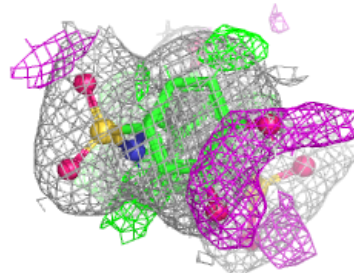
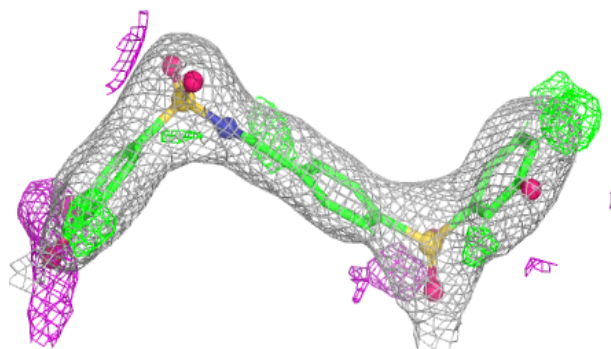
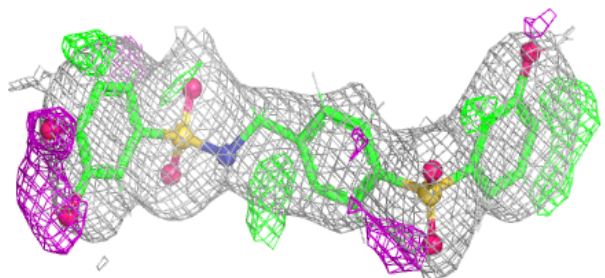
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

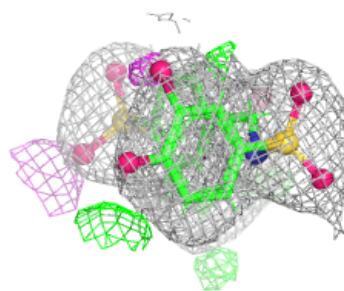
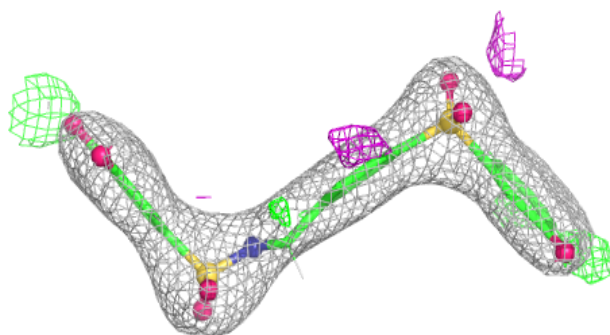
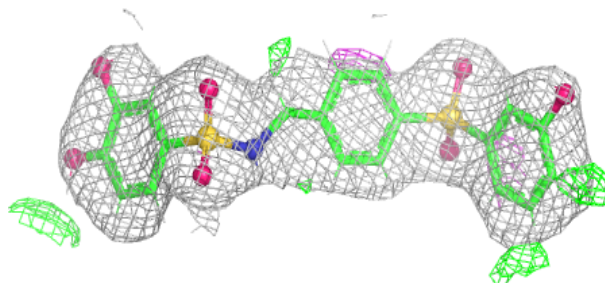
**Electron density around O99 F 605:**

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

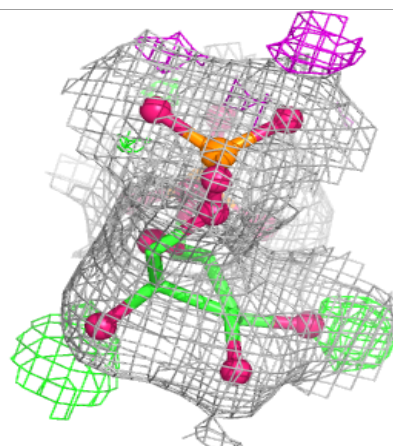
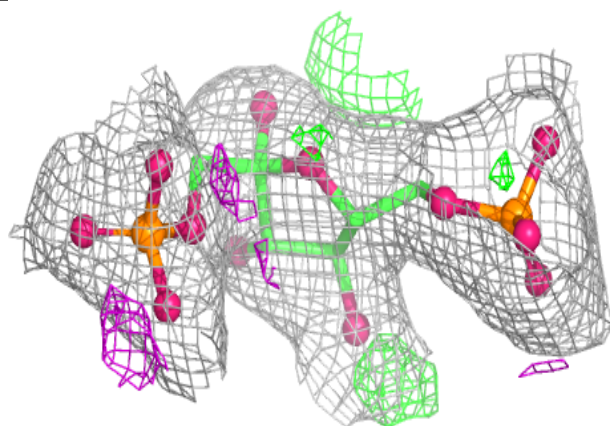
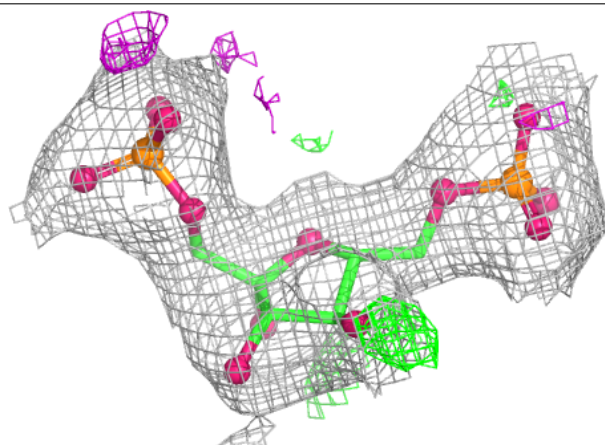


Electron density around O99 A 605:

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

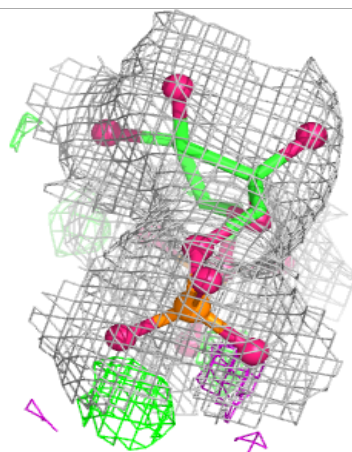
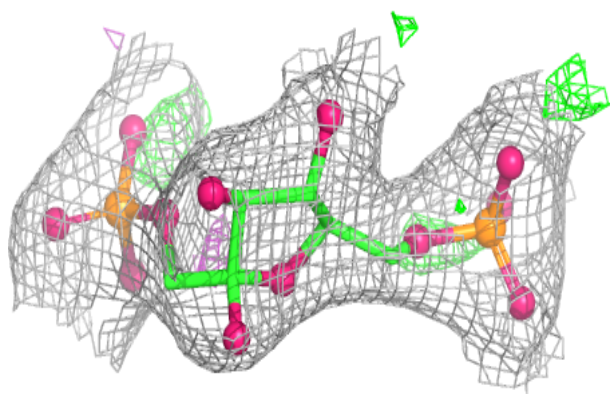
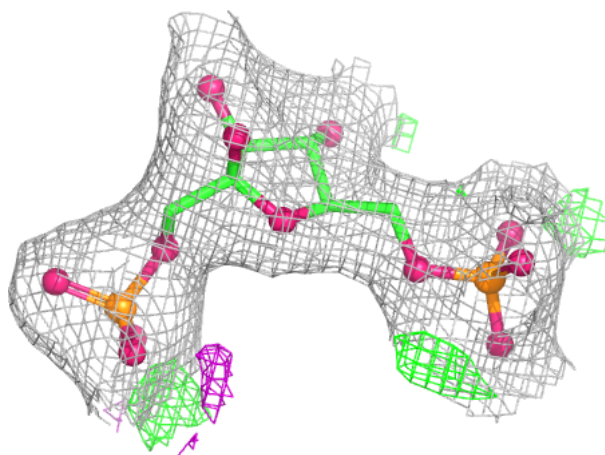
**Electron density around FBP B 601:**

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



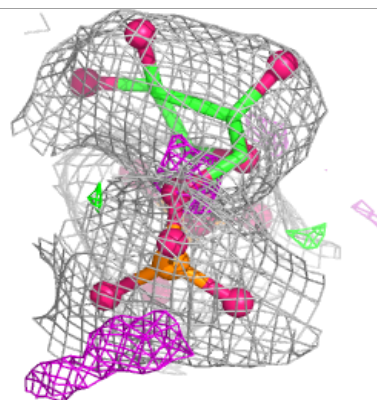
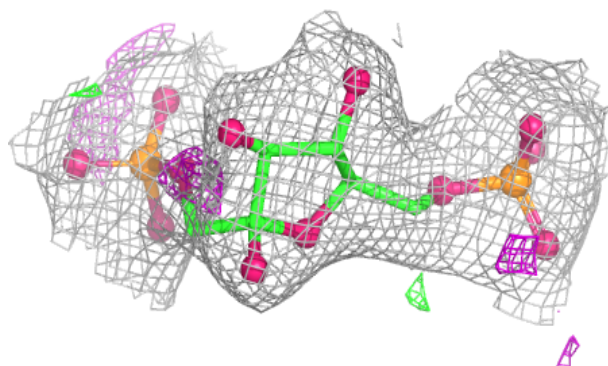
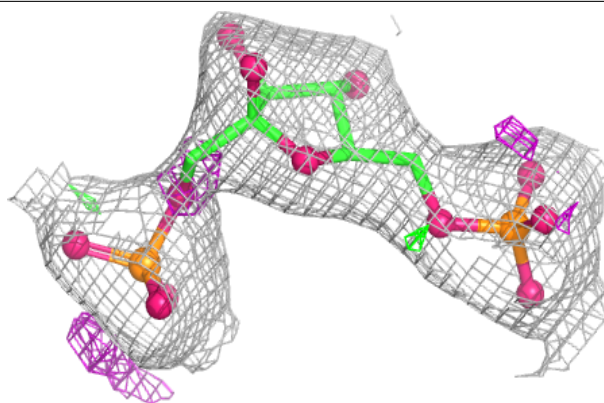
Electron density around FBP F 601:

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

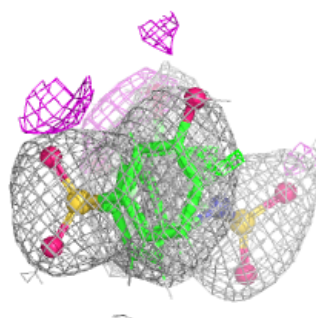
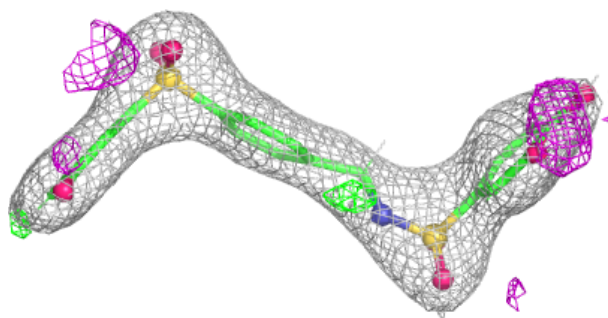
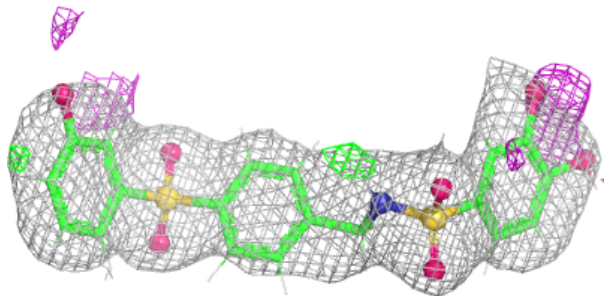


Electron density around FBP A 601:

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

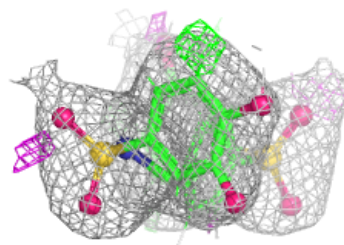
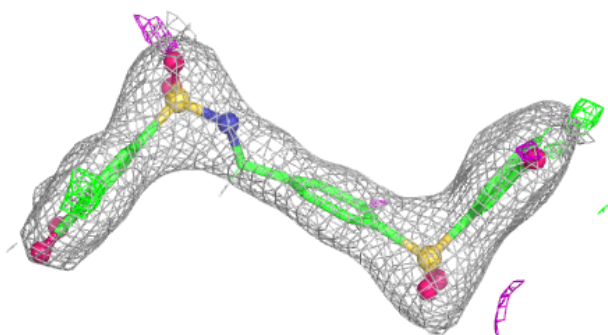
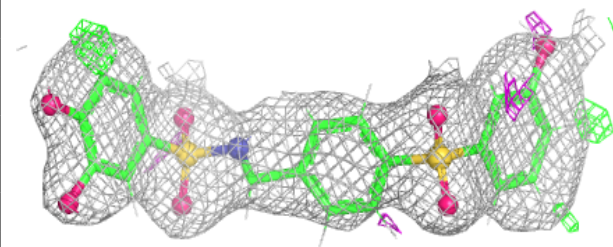
**Electron density around O99 E 605:**

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

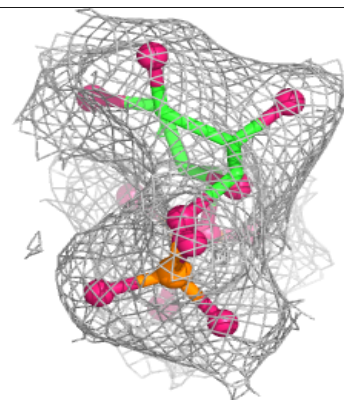
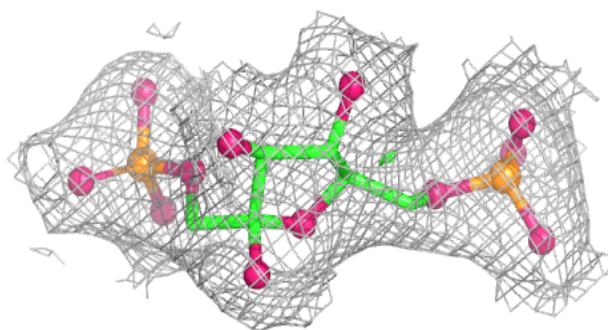
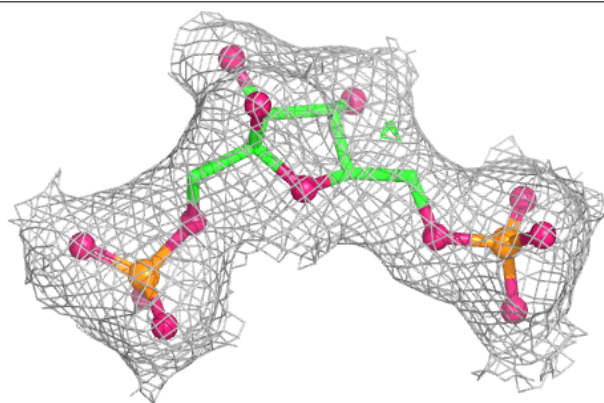


Electron density around O99 D 605:

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

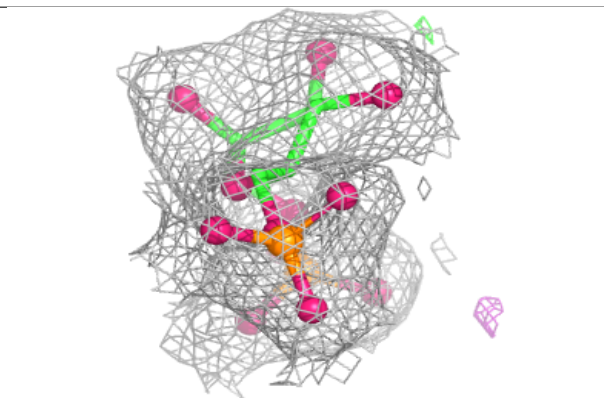
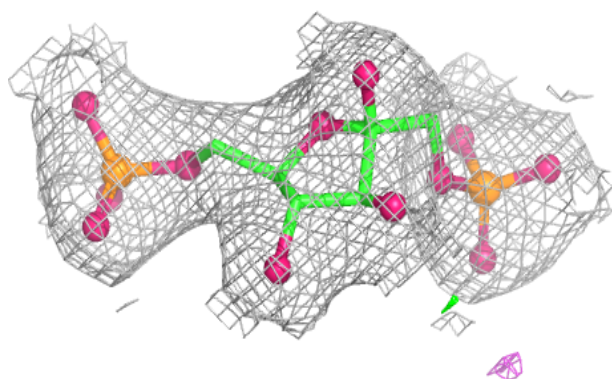
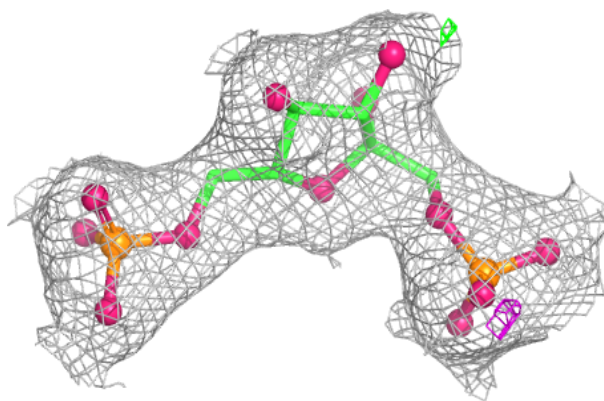
**Electron density around FBP G 601:**

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

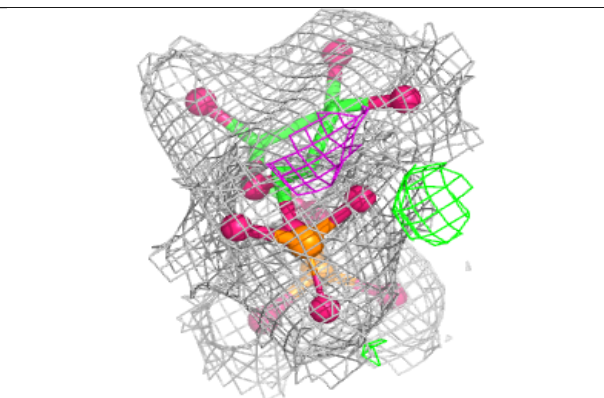
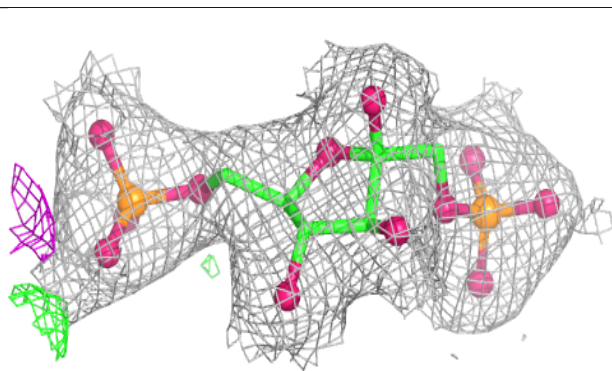
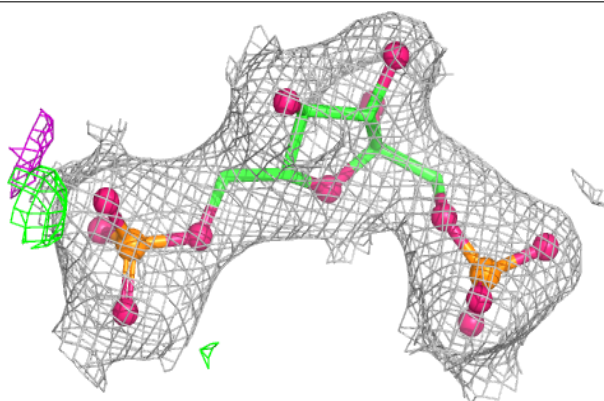


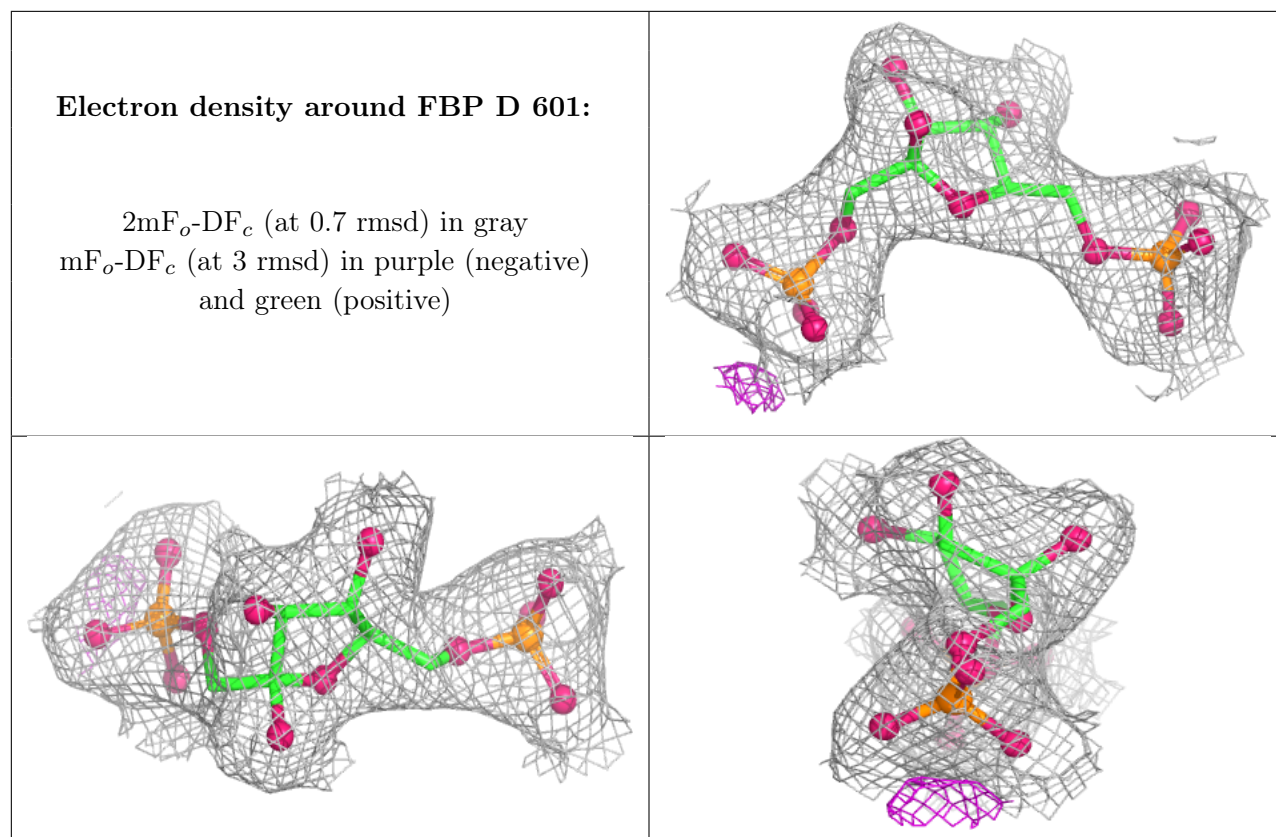
Electron density around FBP C 601:

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

**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)





6.5 Other polymers [i](#)

There are no such residues in this entry.