



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:33 AM UTC

PDB ID : 7FS0 / pdb_00007fs0
Title : Structure of liver pyruvate kinase in complex with allosteric modulator 8
Authors : Lulla, A.; Nilsson, O.; Brear, P.; Nain-Perez, A.; Grotli, M.; Hyvonen, M.
Deposited on : 2022-12-18
Resolution : 2.41 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:

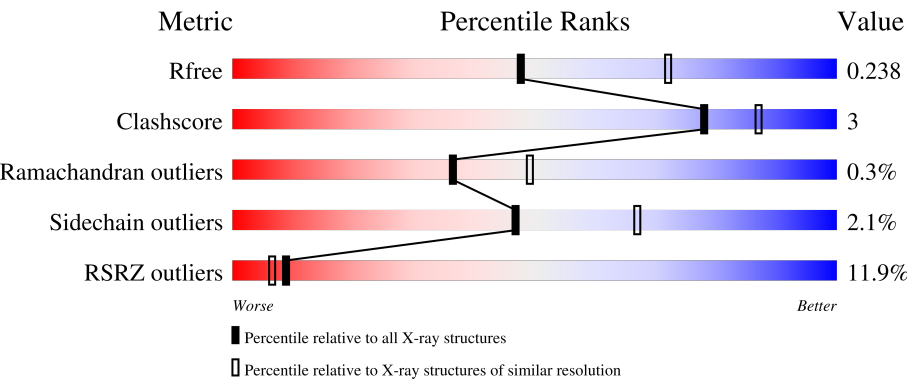
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 2.41 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	447	23% 86% 8% 6%
1	B	447	21% 89% 8% ..
1	C	447	18% 87% 8% 5%
1	D	447	2% 89% 5% 5%
1	E	447	14% 86% 7% 6%

Continued on next page...

Continued from previous page...

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

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

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

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 27561 atoms, of which 76 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

Continued on next page...

Continued from previous page...

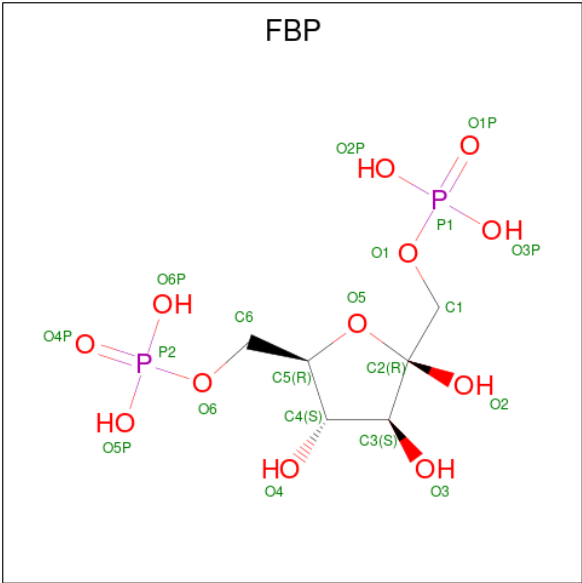
Chain	Residue	Modelled	Actual	Comment	Reference
B	130	GLY	-	linker	UNP P30613
B	131	SER	-	linker	UNP P30613
B	132	GLY	-	linker	UNP P30613
C	-1	GLY	-	expression tag	UNP P30613
C	0	SER	-	expression tag	UNP P30613
C	1	MET	-	expression tag	UNP P30613
C	2	GLU	-	expression tag	UNP P30613
C	12	ASP	SER	conflict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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

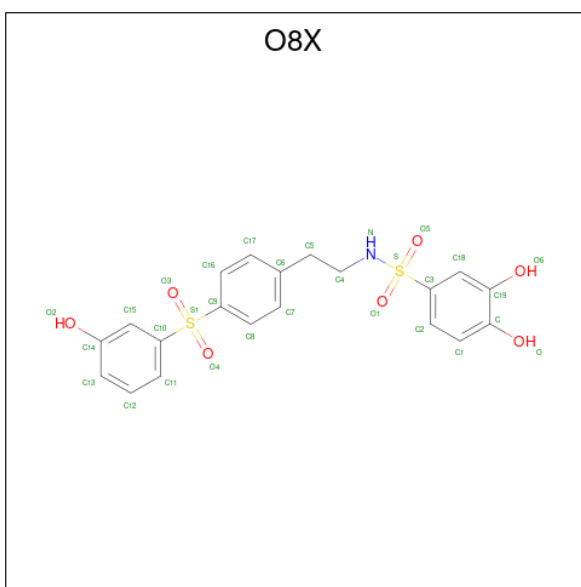
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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-{2-[4-(3-hydroxybenzene-1-sulfonyl)phenyl]ethyl}benzene-1-sulfonamide (CCD ID: O8X) (formula: C₂₀H₁₉NO₇S₂) (labeled as "Ligand of Interest" by depositor).

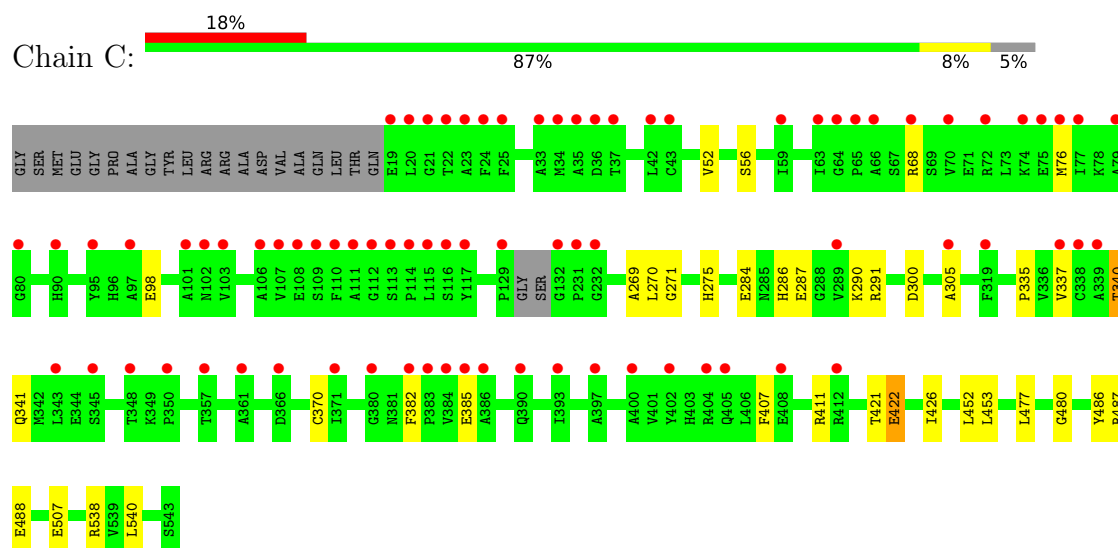


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total 49	C 20	H 19	N 1	O 7	S 2	19	0
6	D	1	Total 49	C 20	H 19	N 1	O 7	S 2	19	0
6	G	1	Total 49	C 20	H 19	N 1	O 7	S 2	19	0
6	H	1	Total 49	C 20	H 19	N 1	O 7	S 2	19	0

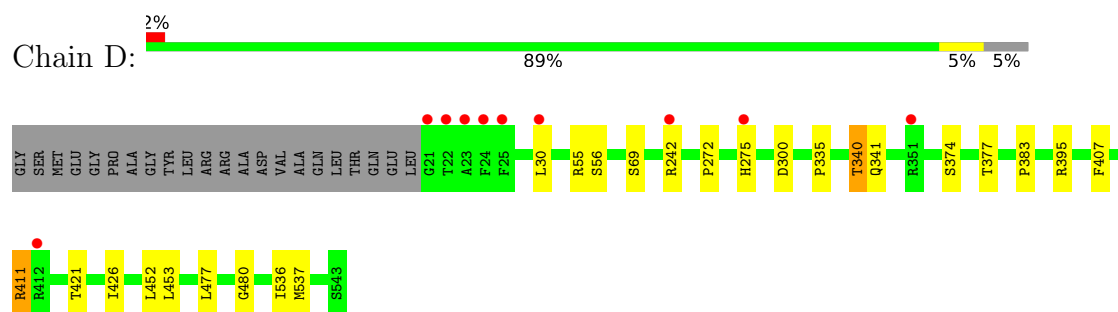
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	52	Total	O	0	0
			52	52		
7	B	48	Total	O	0	0
			48	48		
7	C	116	Total	O	0	0
			116	116		
7	D	186	Total	O	0	0
			186	186		
7	E	76	Total	O	0	0
			76	76		
7	F	144	Total	O	0	0
			144	144		
7	G	177	Total	O	0	0
			177	177		
7	H	265	Total	O	0	0
			265	265		

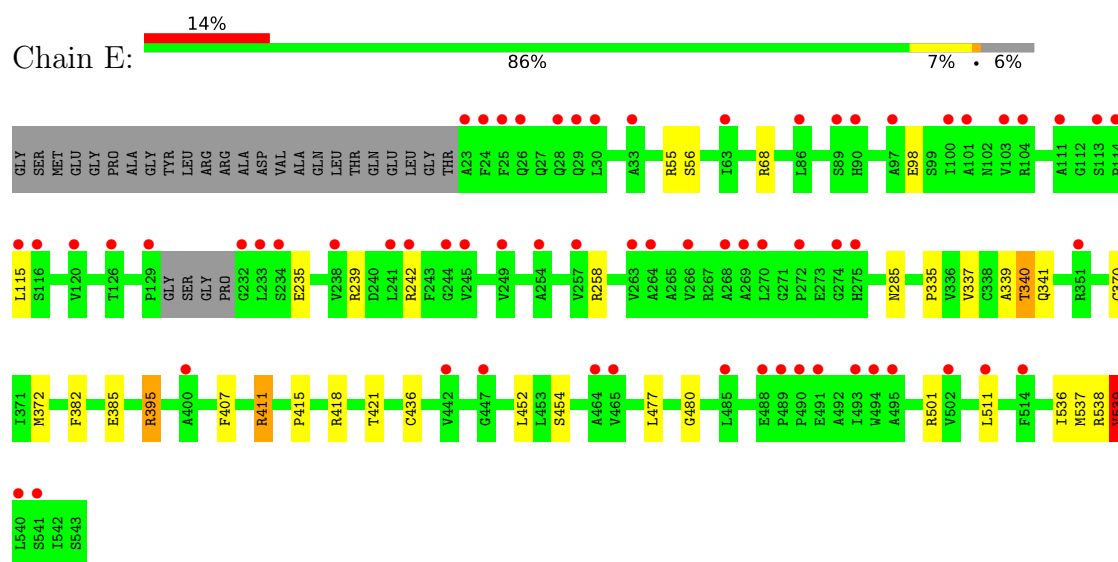
- Molecule 1: Pyruvate kinase PKLR



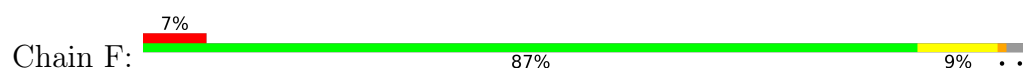
- Molecule 1: Pyruvate kinase PKLR

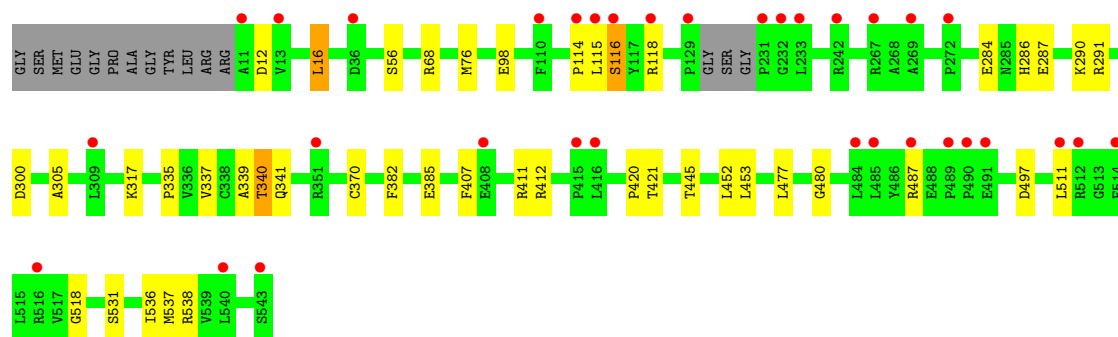


- Molecule 1: Pyruvate kinase PKLR

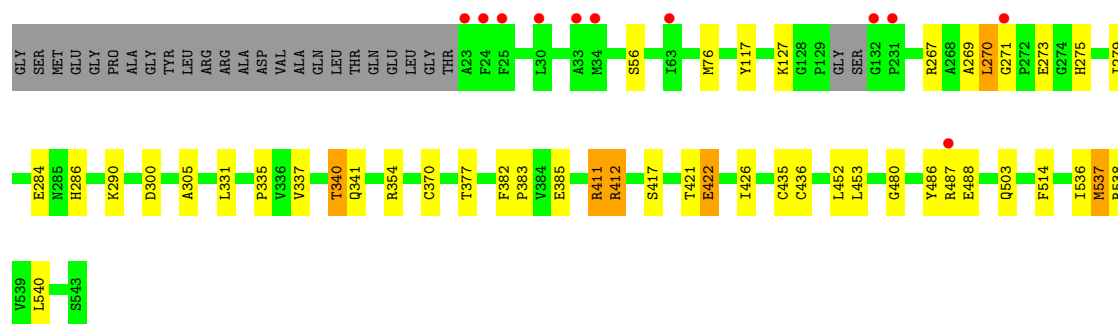
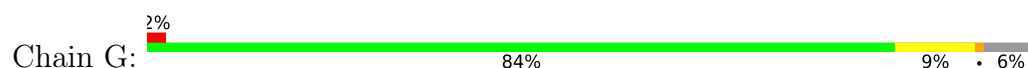


- Molecule 1: Pyruvate kinase PKLR

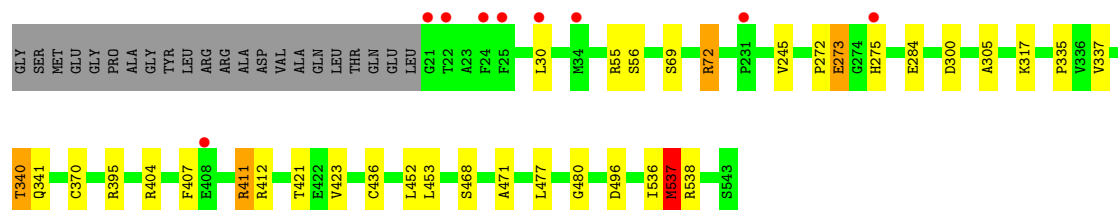
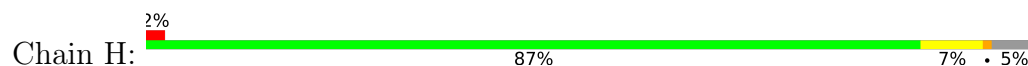




• Molecule 1: Pyruvate kinase PKLR



• 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	209.00Å 113.34Å 189.48Å 90.00° 91.12° 90.00°	Depositor
Resolution (Å)	189.45 – 2.41 189.45 – 2.41	Depositor EDS
% Data completeness (in resolution range)	80.0 (189.45-2.41) 80.0 (189.45-2.41)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.43Å)	Xtriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, R_{free}	0.219 , 0.253 0.208 , 0.238	Depositor DCC
R_{free} test set	6799 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27561	wwPDB-VP
Average B, all atoms (Å ²)	61.0	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 64.76 % 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 7.8799e-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: FBP, O8X, MG, K, 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	0.69	0/3307	1.05	2/4469 (0.0%)
1	B	0.70	0/3396	1.05	2/4592 (0.0%)
1	C	0.76	0/3313	1.08	5/4479 (0.1%)
1	D	0.78	1/3326 (0.0%)	1.06	2/4497 (0.0%)
1	E	0.67	0/3278	1.04	1/4430 (0.0%)
1	F	0.75	1/3396 (0.0%)	1.06	6/4591 (0.1%)
1	G	0.79	2/3303 (0.1%)	1.07	5/4465 (0.1%)
1	H	0.81	1/3316 (0.0%)	1.08	3/4483 (0.1%)
All	All	0.75	5/26635 (0.0%)	1.06	26/36006 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	116	SER	CA-C	6.16	1.61	1.52
1	D	374	SER	CA-C	6.12	1.55	1.52
1	G	537	MET	SD-CE	-5.47	1.65	1.79
1	H	537	MET	SD-CE	-5.12	1.66	1.79
1	G	417	SER	CA-C	-5.11	1.46	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	507	GLU	CB-CG-CD	6.88	124.30	112.60
1	C	270	LEU	CA-C-N	6.04	131.36	121.87
1	C	270	LEU	C-N-CA	6.04	131.36	121.87
1	C	453	LEU	CA-C-N	5.77	128.01	120.28
1	C	453	LEU	C-N-CA	5.77	128.01	120.28
1	A	453	LEU	CA-C-N	5.67	127.88	120.28
1	A	453	LEU	C-N-CA	5.67	127.88	120.28
1	G	514	PHE	CA-CB-CG	5.67	119.47	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	453	LEU	CA-C-N	5.66	127.86	120.28
1	B	453	LEU	C-N-CA	5.66	127.86	120.28
1	G	270	LEU	CA-C-N	5.60	130.66	121.87
1	G	270	LEU	C-N-CA	5.60	130.66	121.87
1	F	453	LEU	CA-C-N	5.58	127.75	120.28
1	F	453	LEU	C-N-CA	5.58	127.75	120.28
1	G	453	LEU	CA-C-N	5.46	127.87	120.38
1	G	453	LEU	C-N-CA	5.46	127.87	120.38
1	E	539	VAL	N-CA-CB	5.26	117.36	111.21
1	F	339	ALA	CA-C-N	5.26	131.58	121.54
1	F	339	ALA	C-N-CA	5.26	131.58	121.54
1	H	453	LEU	CA-C-N	5.23	127.29	120.28
1	H	453	LEU	C-N-CA	5.23	127.29	120.28
1	F	497	ASP	CA-C-N	5.18	127.08	120.56
1	F	497	ASP	C-N-CA	5.18	127.08	120.56
1	D	453	LEU	CA-C-N	5.17	127.21	120.28
1	D	453	LEU	C-N-CA	5.17	127.21	120.28
1	H	496	ASP	CA-CB-CG	5.07	117.67	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3236	0	3300	22	0
1	B	3329	0	3394	23	1
1	C	3247	0	3300	21	0
1	D	3252	0	3310	12	0
1	E	3210	0	3270	21	0
1	F	3321	0	3393	23	0
1	G	3231	0	3285	28	0
1	H	3251	0	3306	22	0
2	A	20	0	10	0	0
2	B	20	0	10	0	0
2	C	20	0	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	20	0	10	0	0
2	E	20	0	10	1	0
2	F	20	0	10	0	0
2	G	20	0	10	0	0
2	H	20	0	10	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0
3	G	6	0	0	0	0
3	H	6	0	0	0	0
4	A	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	30	19	0	0	0
6	D	30	19	0	0	0
6	G	30	19	0	0	0
6	H	30	19	0	0	0
7	A	52	0	0	0	0
7	B	48	0	0	3	0
7	C	116	0	0	1	0
7	D	186	0	0	0	0
7	E	76	0	0	0	0
7	F	144	0	0	1	0
7	G	177	0	0	1	0
7	H	265	0	0	1	0
All	All	27485	76	26638	149	1

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

All (149) 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:272:PRO:HA	1:A:275:HIS:NE2	1.90	0.85
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.65	0.79
1:E:539:VAL:HG22	1:F:420:PRO:HB3	1.67	0.77
1:C:422[A]:GLU:HG3	1:C:452:LEU:HD13	1.75	0.69
1:F:407:PHE:CE2	1:F:411:ARG:NH1	2.62	0.66
1:H:272:PRO:HA	1:H:275[A]:HIS:CE1	2.32	0.65
1:A:408:GLU:OE2	1:B:411:ARG:NH2	2.28	0.65
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.79	0.65
1:G:538:ARG:HG2	1:H:536:ILE:HG12	1.81	0.63
1:D:272:PRO:HA	1:D:275[A]:HIS:CE1	2.34	0.63
1:E:235:GLU:O	1:E:239:ARG:HD3	1.99	0.61
1:G:486:TYR:CZ	1:G:488:GLU:HB2	2.37	0.59
1:G:56:SER:HB2	1:G:480:GLY:HA2	1.83	0.59
1:E:407:PHE:O	1:E:411:ARG:HB2	2.03	0.59
1:H:407:PHE:O	1:H:411:ARG:HG3	2.03	0.59
1:G:340:THR:HG22	1:G:341:GLN:HG3	1.85	0.59
1:C:271:GLY:O	1:C:275:HIS:CE1	2.56	0.58
1:C:340:THR:HG22	1:C:341:GLN:HG3	1.86	0.58
1:C:411:ARG:HG3	1:C:426:ILE:HD11	1.85	0.58
1:G:537:MET:HE3	1:H:537:MET:HG2	1.86	0.57
1:B:411:ARG:HG3	1:B:426:ILE:HD11	1.87	0.57
1:C:538:ARG:HD3	7:C:716:HOH:O	2.06	0.56
1:C:538:ARG:HG2	1:D:536:ILE:HG12	1.88	0.56
1:E:539:VAL:CG2	1:F:420:PRO:HB3	2.34	0.56
1:B:382:PHE:HB3	1:B:385:GLU:HB2	1.88	0.56
1:F:56:SER:HB2	1:F:480:GLY:HA2	1.87	0.56
1:H:56:SER:HB2	1:H:480:GLY:HA2	1.88	0.55
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.89	0.55
1:E:340:THR:HG22	1:E:341:GLN:HG3	1.88	0.55
1:A:418[A]:ARG:HG3	1:B:16:LEU:HD11	1.87	0.55
1:E:418:ARG:NH2	1:F:518:GLY:O	2.37	0.55
1:D:340:THR:HG22	1:D:341:GLN:HG3	1.89	0.54
1:A:340:THR:HG22	1:A:341:GLN:HG3	1.90	0.54
1:A:272:PRO:HA	1:A:275:HIS:CD2	2.42	0.54
1:C:382:PHE:HB3	1:C:385:GLU:HB2	1.90	0.53
1:F:114:PRO:HB3	1:F:487:ARG:HE	1.72	0.53
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:267:ARG:HG2	1:G:279:ILE:CD1	2.38	0.53
1:A:382:PHE:HB3	1:A:385:GLU:HB2	1.90	0.53
1:G:269:ALA:C	1:G:271:GLY:H	2.15	0.52
1:G:536:ILE:HG12	1:H:538[A]:ARG:HG2	1.90	0.52
1:G:127:LYS:NZ	7:G:702:HOH:O	2.41	0.52
1:F:382:PHE:HB3	1:F:385:GLU:HB2	1.91	0.51
1:H:340:THR:HG22	1:H:341:GLN:HG3	1.91	0.51
1:E:56:SER:HB2	1:E:480:GLY:HA2	1.91	0.51
1:E:382:PHE:HB3	1:E:385:GLU:HB2	1.93	0.51
1:E:536:ILE:HG12	1:F:538:ARG:HG2	1.92	0.51
1:H:468:SER:HB3	1:H:471:ALA:HB3	1.92	0.51
1:A:67:SER:HA	1:A:72:ARG:HG2	1.93	0.50
1:G:271:GLY:O	1:G:275:HIS:CE1	2.64	0.50
1:C:269:ALA:C	1:C:271:GLY:H	2.17	0.50
1:D:411:ARG:HG2	1:D:426:ILE:HD11	1.92	0.50
1:D:377:THR:HA	1:D:383:PRO:HB3	1.94	0.50
1:E:501:ARG:NH1	2:E:601:FBP:O1P	2.38	0.50
1:C:486:TYR:CZ	1:C:488:GLU:HB2	2.47	0.49
1:A:538:ARG:HG3	1:B:536:ILE:HG12	1.95	0.49
1:C:287:GLU:HG2	1:C:291:ARG:HD2	1.94	0.49
1:A:68:ARG:HH22	1:A:98:GLU:HB3	1.77	0.49
1:G:267:ARG:HG2	1:G:279:ILE:HD12	1.94	0.49
1:E:258:ARG:HD3	1:E:285:ASN:HD21	1.76	0.49
1:F:421:THR:HG22	1:F:452:LEU:HD12	1.95	0.49
1:B:340:THR:HG22	1:B:341:GLN:HG3	1.93	0.49
1:D:421:THR:HG22	1:D:452:LEU:HD12	1.95	0.48
1:C:421:THR:HG22	1:C:452:LEU:HD12	1.94	0.48
1:F:445:THR:HB	1:F:531:SER:OG	2.13	0.48
1:E:538:ARG:HG2	1:F:536:ILE:HG12	1.94	0.48
1:G:421:THR:HG22	1:G:452:LEU:HD12	1.95	0.48
1:A:421:THR:HG22	1:A:452:LEU:HD12	1.95	0.47
1:B:275:HIS:HB3	7:B:723:HOH:O	2.13	0.47
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.95	0.47
1:A:486:TYR:CZ	1:A:488[B]:GLU:HB2	2.50	0.47
1:H:421:THR:HG22	1:H:452:LEU:HD12	1.97	0.47
1:E:415:PRO:HB3	1:F:12:ASP:HA	1.96	0.47
1:E:421:THR:HG22	1:E:452:LEU:HD12	1.96	0.47
1:F:317:LYS:NZ	7:F:704:HOH:O	2.47	0.47
1:G:382:PHE:HB3	1:G:385:GLU:HB2	1.95	0.47
1:G:411:ARG:HG2	1:G:426:ILE:HD11	1.97	0.46
1:B:300:ASP:O	1:B:335:PRO:HD2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:ASP:O	1:C:335:PRO:HD2	2.16	0.46
1:G:117:TYR:CD2	1:G:487:ARG:NH2	2.83	0.46
1:G:412:ARG:CZ	1:H:404:ARG:HD3	2.46	0.46
1:G:435:CYS:HB3	1:H:423:VAL:HG21	1.97	0.46
1:E:335:PRO:HB3	1:E:477:LEU:O	2.16	0.45
1:H:317:LYS:NZ	7:H:703:HOH:O	2.43	0.45
1:G:56:SER:HB2	1:G:480:GLY:CA	2.44	0.45
1:H:69:SER:HB3	1:H:72:ARG:HB3	1.98	0.45
1:B:335:PRO:HB3	1:B:477:LEU:O	2.17	0.45
1:G:300:ASP:O	1:G:335:PRO:HD2	2.16	0.45
1:B:421:THR:HG22	1:B:452:LEU:HD12	1.99	0.45
1:A:300:ASP:O	1:A:335:PRO:HD2	2.17	0.44
1:A:335:PRO:HB3	1:A:477:LEU:O	2.17	0.44
1:A:337:VAL:HG22	1:A:370:CYS:HB2	1.98	0.44
1:F:340:THR:HG22	1:F:341:GLN:HG3	1.99	0.44
1:B:68:ARG:NH2	1:B:98:GLU:HB3	2.32	0.44
1:D:407:PHE:CE2	1:D:411:ARG:HD3	2.53	0.44
1:F:56:SER:HB2	1:F:480:GLY:CA	2.48	0.44
1:D:335:PRO:HB3	1:D:477:LEU:O	2.17	0.44
1:C:68:ARG:NH2	1:C:98:GLU:HB3	2.33	0.44
1:C:337:VAL:HG22	1:C:370:CYS:HB2	1.99	0.44
1:B:114:PRO:HA	7:B:709:HOH:O	2.17	0.44
1:G:537:MET:HE3	1:H:537:MET:CG	2.48	0.44
1:H:55:ARG:HB2	1:H:395:ARG:HG3	2.00	0.44
1:D:300:ASP:O	1:D:335:PRO:HD2	2.18	0.44
1:E:337:VAL:HG22	1:E:370:CYS:HB2	2.00	0.44
1:H:300:ASP:O	1:H:335:PRO:HD2	2.17	0.44
1:E:68:ARG:NH2	1:E:98:GLU:HB3	2.32	0.43
1:F:68:ARG:NH2	1:F:98:GLU:HB3	2.33	0.43
1:A:538:ARG:CG	1:B:536:ILE:HG12	2.48	0.43
1:H:56:SER:HB2	1:H:480:GLY:CA	2.49	0.43
1:H:337:VAL:HG22	1:H:370:CYS:HB2	2.01	0.43
1:E:418:ARG:HD3	1:F:16:LEU:HD11	2.01	0.43
1:E:341:GLN:OE1	1:G:354:ARG:HG2	2.18	0.42
1:B:337:VAL:HG22	1:B:370:CYS:HB2	2.00	0.42
1:F:335:PRO:HB3	1:F:477:LEU:O	2.19	0.42
1:B:116:SER:HB3	7:B:731:HOH:O	2.19	0.42
1:C:335:PRO:HB3	1:C:477:LEU:O	2.19	0.42
1:C:407:PHE:O	1:C:411:ARG:HB2	2.19	0.42
1:G:377:THR:HA	1:G:383:PRO:HB3	2.01	0.42
1:B:56:SER:HB2	1:B:480:GLY:CA	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:245:VAL:HG11	1:H:273:GLU:HG2	2.02	0.42
1:G:286:HIS:CE1	1:G:290:LYS:HG3	2.55	0.42
1:G:337:VAL:HG22	1:G:370:CYS:HB2	2.02	0.42
1:A:423:VAL:HG21	1:B:435:CYS:HB3	2.01	0.41
1:H:335:PRO:HB3	1:H:477:LEU:O	2.20	0.41
1:A:55:ARG:HB2	1:A:395:ARG:HG3	2.01	0.41
1:A:411:ARG:NH2	1:B:411:ARG:HH12	2.18	0.41
1:B:55:ARG:HB2	1:B:395:ARG:HG2	2.03	0.41
1:C:286:HIS:CE1	1:C:290:LYS:HG3	2.55	0.41
1:H:284:GLU:HG2	1:H:305:ALA:HB3	2.02	0.41
1:C:486:TYR:CE2	1:C:488:GLU:HB2	2.55	0.41
1:B:284:GLU:HG2	1:B:305:ALA:HB3	2.03	0.41
1:D:55:ARG:HB2	1:D:395:ARG:HG3	2.02	0.41
1:F:300:ASP:O	1:F:335:PRO:HD2	2.20	0.41
1:E:339:ALA:HB1	1:E:372:MET:HE2	2.01	0.41
1:A:235:GLU:HB3	1:A:239:ARG:HH21	1.84	0.41
1:E:55:ARG:HB2	1:E:395:ARG:HG3	2.01	0.41
1:F:286:HIS:CE1	1:F:290:LYS:HG3	2.56	0.41
1:C:56:SER:HB2	1:C:480:GLY:CA	2.49	0.41
1:F:337:VAL:HG22	1:F:370:CYS:HB2	2.03	0.41
1:G:117:TYR:CE2	1:G:487:ARG:NH2	2.88	0.41
1:G:284:GLU:HG2	1:G:305:ALA:HB3	2.03	0.41
1:A:517:VAL:HG13	1:A:543:SER:HB3	2.01	0.41
1:F:284:GLU:HG2	1:F:305:ALA:HB3	2.03	0.41
1:F:287:GLU:OE2	1:F:291:ARG:NH1	2.54	0.41
1:A:415:PRO:HB3	1:B:12:ASP:HA	2.03	0.40
1:C:284:GLU:HG2	1:C:305:ALA:HB3	2.03	0.40
1:H:30:LEU:HD23	1:H:30:LEU:HA	1.99	0.40
1:G:486:TYR:CE2	1:G:488:GLU:HB2	2.56	0.40
1:D:30:LEU:HD23	1:D:30:LEU:HA	1.99	0.40

All (1) 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)
1:B:511:LEU:O	1:B:511:LEU:O[2_555]	2.15	0.05

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	57
1	B	438/447 (98%)	432 (99%)	5 (1%)	1 (0%)	43	57
1	C	425/447 (95%)	418 (98%)	6 (1%)	1 (0%)	43	57
1	D	429/447 (96%)	424 (99%)	4 (1%)	1 (0%)	43	57
1	E	420/447 (94%)	415 (99%)	4 (1%)	1 (0%)	43	57
1	F	435/447 (97%)	430 (99%)	3 (1%)	2 (0%)	24	35
1	G	423/447 (95%)	414 (98%)	7 (2%)	2 (0%)	24	35
1	H	427/447 (96%)	423 (99%)	3 (1%)	1 (0%)	43	57
All	All	3421/3576 (96%)	3376 (99%)	35 (1%)	10 (0%)	36	49

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	116	SER
1	G	270	LEU
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%)	333 (98%)	7 (2%)	47	67
1	B	349/352 (99%)	337 (97%)	12 (3%)	32	52
1	C	341/352 (97%)	334 (98%)	7 (2%)	47	67
1	D	342/352 (97%)	337 (98%)	5 (2%)	57	75
1	E	338/352 (96%)	327 (97%)	11 (3%)	33	53
1	F	350/352 (99%)	341 (97%)	9 (3%)	40	61
1	G	340/352 (97%)	329 (97%)	11 (3%)	34	54
1	H	340/352 (97%)	334 (98%)	6 (2%)	51	71
All	All	2740/2816 (97%)	2672 (98%)	68 (2%)	47	62

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	395	ARG
1	A	436	CYS
1	A	531	SER
1	A	537[A]	MET
1	A	537[B]	MET
1	A	540	LEU
1	B	10	ARG
1	B	16	LEU
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	511	LEU
1	B	516	ARG
1	B	537[A]	MET
1	B	537[B]	MET
1	C	52	VAL
1	C	76[A]	MET
1	C	76[B]	MET
1	C	422[A]	GLU
1	C	422[B]	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	487	ARG
1	C	540	LEU
1	D	69	SER
1	D	242[A]	ARG
1	D	242[B]	ARG
1	D	411	ARG
1	D	537	MET
1	E	115	LEU
1	E	242	ARG
1	E	395	ARG
1	E	411	ARG
1	E	436	CYS
1	E	454[A]	SER
1	E	454[B]	SER
1	E	511	LEU
1	E	537[A]	MET
1	E	537[B]	MET
1	E	539	VAL
1	F	16	LEU
1	F	76[A]	MET
1	F	76[B]	MET
1	F	115	LEU
1	F	118	ARG
1	F	412	ARG
1	F	511	LEU
1	F	537[A]	MET
1	F	537[B]	MET
1	G	76[A]	MET
1	G	76[B]	MET
1	G	273	GLU
1	G	331	LEU
1	G	411	ARG
1	G	412	ARG
1	G	422[A]	GLU
1	G	422[B]	GLU
1	G	436	CYS
1	G	503	GLN
1	G	540	LEU
1	H	72	ARG
1	H	273	GLU
1	H	411	ARG
1	H	412	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	436	CYS
1	H	537	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	A	236	GLN
1	A	390	GLN
1	A	405	GLN
1	B	90	HIS
1	B	390	GLN
1	B	405	GLN
1	C	90	HIS
1	C	275	HIS
1	C	390	GLN
1	C	405	GLN
1	D	90	HIS
1	D	390	GLN
1	D	405	GLN
1	E	90	HIS
1	E	390	GLN
1	E	405	GLN
1	F	90	HIS
1	F	390	GLN
1	F	405	GLN
1	G	90	HIS
1	G	275	HIS
1	G	381	ASN
1	G	390	GLN
1	G	405	GLN
1	H	90	HIS
1	H	390	GLN
1	H	405	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [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	E	602	4	5,5,5	2.25	2 (40%)	6,6,6	1.57	2 (33%)
2	FBP	C	601	-	18,20,20	0.70	1 (5%)	21,32,32	0.71	0
2	FBP	B	601	-	18,20,20	0.70	0	21,32,32	0.82	2 (9%)
2	FBP	A	601	-	18,20,20	0.53	0	21,32,32	0.68	0
3	OXL	H	602	4	5,5,5	1.92	2 (40%)	6,6,6	1.59	1 (16%)
2	FBP	G	601	-	18,20,20	0.61	0	21,32,32	0.96	1 (4%)
2	FBP	D	601	-	18,20,20	0.68	0	21,32,32	0.92	1 (4%)
3	OXL	B	602	4	5,5,5	2.35	2 (40%)	6,6,6	1.41	2 (33%)
3	OXL	F	602	4	5,5,5	2.76	4 (80%)	6,6,6	2.53	3 (50%)
2	FBP	H	601	-	18,20,20	0.97	0	21,32,32	0.84	0
6	O8X	A	605	-	32,32,32	2.06	5 (15%)	45,47,47	1.90	14 (31%)
3	OXL	C	602	4	5,5,5	2.13	2 (40%)	6,6,6	1.15	1 (16%)
3	OXL	A	602	4	5,5,5	2.12	2 (40%)	6,6,6	1.81	1 (16%)
6	O8X	D	605	-	32,32,32	2.17	4 (12%)	45,47,47	2.22	20 (44%)
6	O8X	G	605	-	32,32,32	2.40	6 (18%)	45,47,47	1.85	13 (28%)
3	OXL	D	602	4	5,5,5	2.22	2 (40%)	6,6,6	2.67	4 (66%)
2	FBP	F	601	-	18,20,20	0.36	0	21,32,32	0.66	0
3	OXL	G	602	4	5,5,5	2.33	2 (40%)	6,6,6	1.91	2 (33%)
2	FBP	E	601	-	18,20,20	0.37	0	21,32,32	0.73	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	O8X	H	605	-	32,32,32	2.13	6 (18%)	45,47,47	2.18	17 (37%)

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	E	602	4	-	4/4/4/4	-
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
3	OXL	H	602	4	-	4/4/4/4	-
2	FBP	G	601	-	-	2/13/32/32	0/1/1/1
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
3	OXL	B	602	4	-	4/4/4/4	-
3	OXL	F	602	4	-	4/4/4/4	-
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1
6	O8X	A	605	-	-	2/25/25/25	0/3/3/3
3	OXL	C	602	4	-	4/4/4/4	-
3	OXL	A	602	4	-	4/4/4/4	-
6	O8X	D	605	-	-	6/25/25/25	0/3/3/3
6	O8X	G	605	-	-	2/25/25/25	0/3/3/3
3	OXL	D	602	4	-	4/4/4/4	-
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
3	OXL	G	602	4	-	4/4/4/4	-
2	FBP	E	601	-	-	2/13/32/32	0/1/1/1
6	O8X	H	605	-	-	3/25/25/25	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	605	O8X	C3-S	-9.18	1.62	1.76
6	D	605	O8X	C3-S	-7.94	1.64	1.76
6	A	605	O8X	C3-S	-7.81	1.64	1.76
6	H	605	O8X	C3-S	-7.06	1.65	1.76
6	G	605	O8X	C9-S1	-5.83	1.68	1.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	605	O8X	C10-S1	-5.49	1.68	1.77
6	D	605	O8X	C9-S1	-5.14	1.69	1.77
6	D	605	O8X	C10-S1	-5.10	1.69	1.77
6	H	605	O8X	C10-S1	-4.89	1.69	1.77
6	A	605	O8X	C9-S1	-4.84	1.69	1.77
6	H	605	O8X	C9-S1	-4.83	1.69	1.77
3	B	602	OXL	O2-C2	4.62	1.34	1.22
6	A	605	O8X	C10-S1	-4.52	1.70	1.77
3	E	602	OXL	O1-C1	4.28	1.33	1.22
3	D	602	OXL	O2-C2	4.15	1.32	1.22
3	G	602	OXL	O1-C1	3.92	1.32	1.22
3	A	602	OXL	O2-C2	3.70	1.31	1.22
3	C	602	OXL	O1-C1	3.49	1.31	1.22
3	F	602	OXL	O2-C2	3.42	1.31	1.22
6	H	605	O8X	C16-C9	3.37	1.44	1.38
3	F	602	OXL	O3-C1	-3.20	1.21	1.30
3	H	602	OXL	O2-C2	3.18	1.30	1.22
3	G	602	OXL	O3-C1	-3.16	1.22	1.30
3	F	602	OXL	O1-C1	3.08	1.30	1.22
3	C	602	OXL	O3-C1	-2.94	1.22	1.30
6	D	605	O8X	C16-C9	2.76	1.43	1.38
3	H	602	OXL	O4-C2	-2.75	1.23	1.30
3	A	602	OXL	O4-C2	-2.66	1.23	1.30
6	H	605	O8X	C11-C10	2.63	1.43	1.38
3	F	602	OXL	O4-C2	-2.60	1.23	1.30
6	G	605	O8X	C2-C1	-2.53	1.34	1.38
3	D	602	OXL	O4-C2	-2.49	1.23	1.30
3	E	602	OXL	O3-C1	-2.43	1.23	1.30
6	H	605	O8X	O5-S	2.43	1.46	1.43
3	B	602	OXL	O4-C2	-2.39	1.24	1.30
6	G	605	O8X	O-C	-2.28	1.31	1.36
6	A	605	O8X	C16-C9	2.26	1.42	1.38
6	G	605	O8X	C-C19	2.15	1.43	1.40
2	C	601	FBP	P1-O3P	-2.02	1.47	1.54
6	A	605	O8X	C2-C3	2.01	1.42	1.38

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	605	O8X	O5-S-N	-6.23	97.32	107.03
6	D	605	O8X	C3-S-N	-5.89	99.42	107.54
6	G	605	O8X	C3-S-N	-5.16	100.42	107.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	605	O8X	O3-S1-C10	4.40	113.36	107.96
6	D	605	O8X	O3-S1-C10	4.36	113.32	107.96
6	D	605	O8X	O5-S-N	-4.26	100.39	107.03
6	H	605	O8X	O5-S-O1	4.21	124.64	119.52
3	F	602	OXL	O4-C2-C1	4.08	120.74	112.83
3	D	602	OXL	O4-C2-C1	3.93	120.46	112.83
6	H	605	O8X	C3-S-N	-3.90	102.15	107.54
3	D	602	OXL	O3-C1-C2	3.80	120.20	112.83
6	A	605	O8X	C3-S-N	-3.73	102.39	107.54
6	A	605	O8X	O3-S1-C10	3.73	112.54	107.96
3	A	602	OXL	O4-C2-C1	3.53	119.67	112.83
3	F	602	OXL	O3-C1-C2	3.52	119.65	112.83
6	D	605	O8X	O1-S-N	3.45	112.40	107.03
6	H	605	O8X	C17-C16-C9	3.43	122.78	119.44
6	D	605	O8X	C5-C4-N	3.40	115.94	110.66
6	A	605	O8X	C1-C2-C3	3.39	122.73	119.44
6	A	605	O8X	C17-C16-C9	3.38	122.73	119.44
6	D	605	O8X	O5-S-C3	3.25	112.08	107.98
6	G	605	O8X	C9-S1-C10	-3.22	98.47	104.37
3	H	602	OXL	O4-C2-C1	3.22	119.07	112.83
6	D	605	O8X	C1-C2-C3	3.18	122.54	119.44
3	G	602	OXL	O4-C2-C1	3.05	118.75	112.83
2	D	601	FBP	O5P-P2-O6	3.02	114.55	106.67
6	H	605	O8X	C1-C2-C3	3.02	122.38	119.44
6	H	605	O8X	C8-C9-C16	-3.01	116.54	120.47
6	G	605	O8X	C5-C4-N	-2.98	106.03	110.66
6	H	605	O8X	C12-C11-C10	2.98	122.00	118.95
6	H	605	O8X	O5-S-C3	2.97	111.73	107.98
6	D	605	O8X	C8-C9-C16	-2.95	116.62	120.47
6	G	605	O8X	C17-C16-C9	2.94	122.30	119.44
3	E	602	OXL	O3-C1-C2	2.92	118.50	112.83
6	D	605	O8X	O-C-C19	2.88	126.12	118.42
6	A	605	O8X	C9-S1-C10	-2.87	99.11	104.37
6	A	605	O8X	O5-S-C3	2.86	111.58	107.98
6	A	605	O8X	C8-C9-C16	-2.82	116.78	120.47
6	D	605	O8X	C2-C3-S	2.82	122.86	119.76
6	G	605	O8X	O1-S-C3	2.80	111.51	107.98
6	D	605	O8X	C17-C16-C9	2.79	122.15	119.44
3	G	602	OXL	O3-C1-C2	2.78	118.22	112.83
6	D	605	O8X	C16-C9-S1	2.77	123.10	119.49
6	G	605	O8X	C13-C14-C15	2.75	123.21	120.19
6	G	605	O8X	C11-C10-S1	2.71	123.03	119.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	OXL	O2-C2-C1	-2.70	115.00	120.63
6	A	605	O8X	C18-C3-S	2.67	121.79	119.06
2	G	601	FBP	O3P-P1-O2P	2.65	117.74	107.80
6	A	605	O8X	O5-S-O1	2.65	122.73	119.52
6	A	605	O8X	O1-S-N	-2.65	102.91	107.03
6	H	605	O8X	C13-C14-C15	2.58	123.02	120.19
3	F	602	OXL	O2-C2-C1	-2.53	115.35	120.63
6	A	605	O8X	C12-C11-C10	2.53	121.54	118.95
6	G	605	O8X	C8-C9-C16	-2.48	117.23	120.47
6	D	605	O8X	C9-S1-C10	-2.45	99.87	104.37
3	C	602	OXL	O3-C1-C2	2.45	117.58	112.83
6	G	605	O8X	C12-C11-C10	2.45	121.45	118.95
3	B	602	OXL	O4-C2-C1	2.41	117.50	112.83
6	A	605	O8X	C2-C1-C	-2.40	118.09	120.50
6	H	605	O8X	C5-C4-N	-2.33	107.05	110.66
3	D	602	OXL	O1-C1-C2	-2.32	115.79	120.63
6	A	605	O8X	C11-C10-C15	-2.32	117.81	120.68
6	D	605	O8X	C12-C11-C10	2.31	121.31	118.95
6	H	605	O8X	O2-C14-C13	-2.30	113.60	120.00
2	E	601	FBP	O3P-P1-O2P	2.27	116.32	107.80
6	G	605	O8X	O-C-C19	2.26	124.47	118.42
6	H	605	O8X	C7-C8-C9	2.22	121.60	119.44
6	D	605	O8X	O2-C14-C13	-2.17	113.94	120.00
6	A	605	O8X	O2-C14-C13	-2.15	114.01	120.00
6	D	605	O8X	C11-C10-S1	2.15	122.29	119.49
2	B	601	FBP	O3P-P1-O2P	2.15	115.84	107.80
2	B	601	FBP	O5P-P2-O6	2.14	112.25	106.67
6	H	605	O8X	C9-S1-C10	-2.13	100.46	104.37
6	H	605	O8X	O-C-C19	2.13	124.11	118.42
3	B	602	OXL	O3-C1-C2	2.12	116.93	112.83
6	D	605	O8X	C7-C8-C9	2.11	121.49	119.44
6	D	605	O8X	C5-C6-C7	-2.09	115.86	121.18
6	G	605	O8X	O3-S1-C10	2.08	110.52	107.96
6	G	605	O8X	O2-C14-C13	-2.06	114.26	120.00
6	H	605	O8X	O4-S1-C10	-2.06	105.42	107.96
6	G	605	O8X	C1-C2-C3	2.05	121.44	119.44
6	D	605	O8X	C11-C10-C15	-2.05	118.14	120.68
6	H	605	O8X	C16-C9-S1	2.04	122.15	119.49
6	D	605	O8X	C2-C1-C	-2.02	118.48	120.50
3	E	602	OXL	O4-C2-C1	2.01	116.73	112.83

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	605	O8X	N-C4-C5-C6
2	A	601	FBP	C4-C5-C6-O6
2	B	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6
2	D	601	FBP	C4-C5-C6-O6
2	E	601	FBP	C4-C5-C6-O6
2	F	601	FBP	C4-C5-C6-O6
2	H	601	FBP	C4-C5-C6-O6
6	D	605	O8X	C4-N-S-O5
6	D	605	O8X	C4-N-S-O1
6	D	605	O8X	C4-N-S-C3
2	G	601	FBP	C4-C5-C6-O6
2	A	601	FBP	O5-C5-C6-O6
2	B	601	FBP	O5-C5-C6-O6
2	C	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
6	A	605	O8X	C4-C5-C6-C17
6	G	605	O8X	C4-C5-C6-C17
6	H	605	O8X	C4-C5-C6-C17
3	D	602	OXL	O3-C1-C2-O4
6	A	605	O8X	C4-C5-C6-C7
6	G	605	O8X	C4-C5-C6-C7
6	H	605	O8X	C4-C5-C6-C7
6	D	605	O8X	C4-C5-C6-C17
3	A	602	OXL	O3-C1-C2-O4
3	C	602	OXL	O3-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O4
3	H	602	OXL	O3-C1-C2-O4
6	D	605	O8X	C4-C5-C6-C7
3	B	602	OXL	O3-C1-C2-O4
3	F	602	OXL	O3-C1-C2-O4
3	G	602	OXL	O3-C1-C2-O4
3	A	602	OXL	O1-C1-C2-O2
3	B	602	OXL	O1-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O2
3	C	602	OXL	O1-C1-C2-O2
3	E	602	OXL	O1-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O2
3	F	602	OXL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

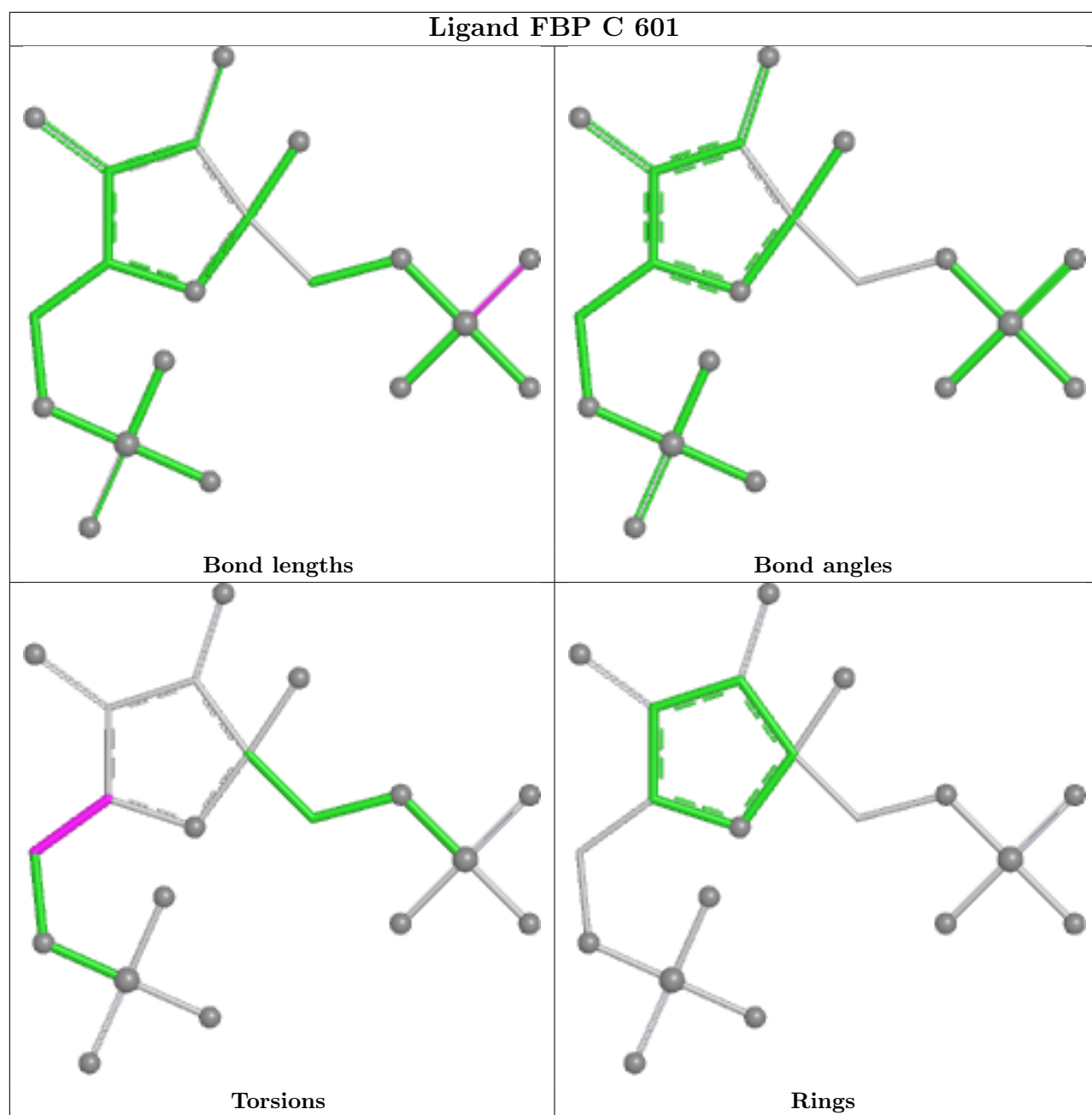
Mol	Chain	Res	Type	Atoms
3	G	602	OXL	O1-C1-C2-O2
3	C	602	OXL	O1-C1-C2-O4
3	A	602	OXL	O1-C1-C2-O4
3	A	602	OXL	O3-C1-C2-O2
3	B	602	OXL	O1-C1-C2-O4
3	C	602	OXL	O3-C1-C2-O2
3	E	602	OXL	O1-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O2
3	F	602	OXL	O3-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O4
3	H	602	OXL	O3-C1-C2-O2
3	B	602	OXL	O3-C1-C2-O2
3	D	602	OXL	O3-C1-C2-O2
3	F	602	OXL	O1-C1-C2-O4
3	G	602	OXL	O1-C1-C2-O4
3	G	602	OXL	O3-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O4
2	G	601	FBP	O5-C5-C6-O6
6	H	605	O8X	C4-N-S-O1

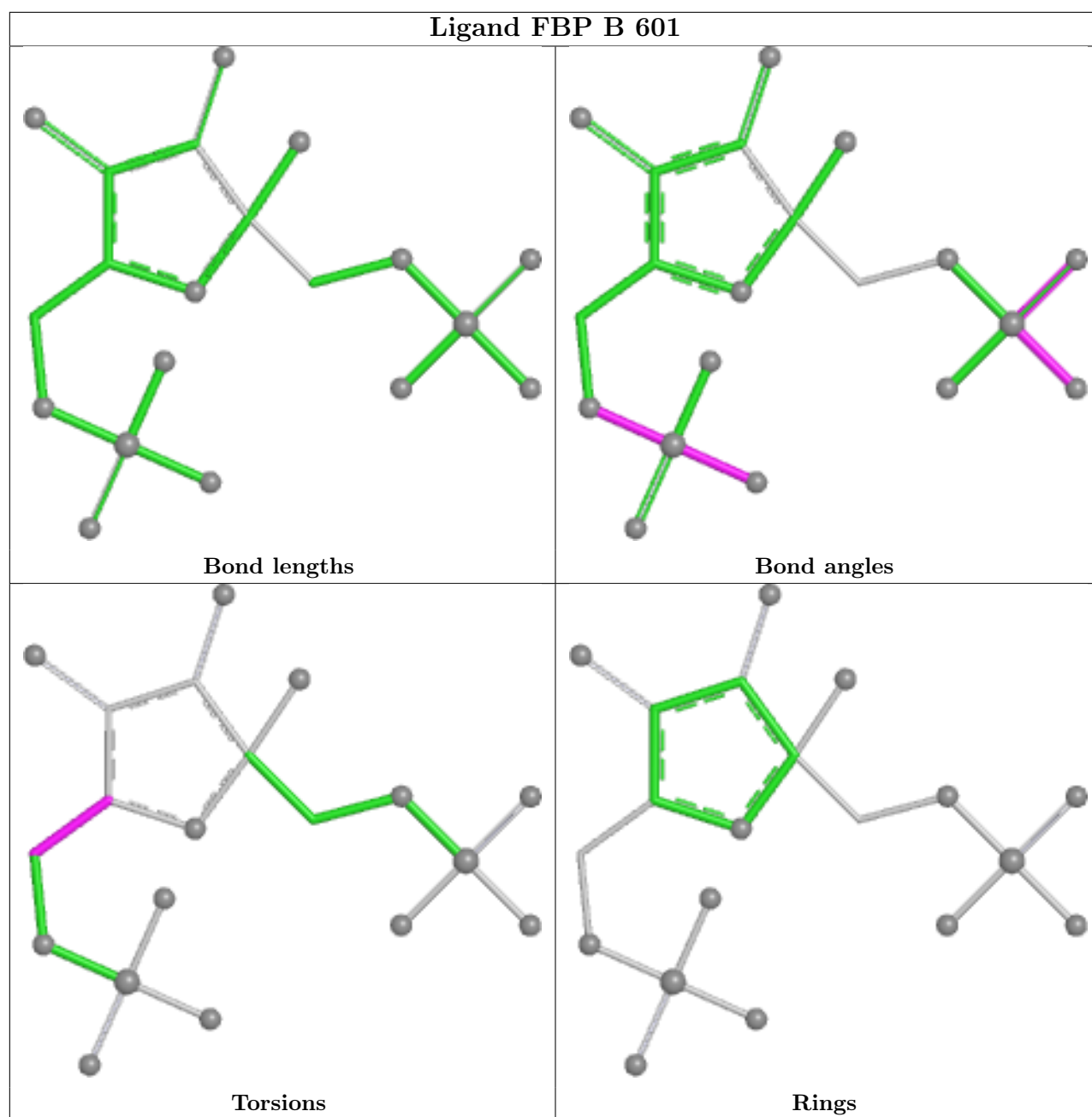
There are no ring outliers.

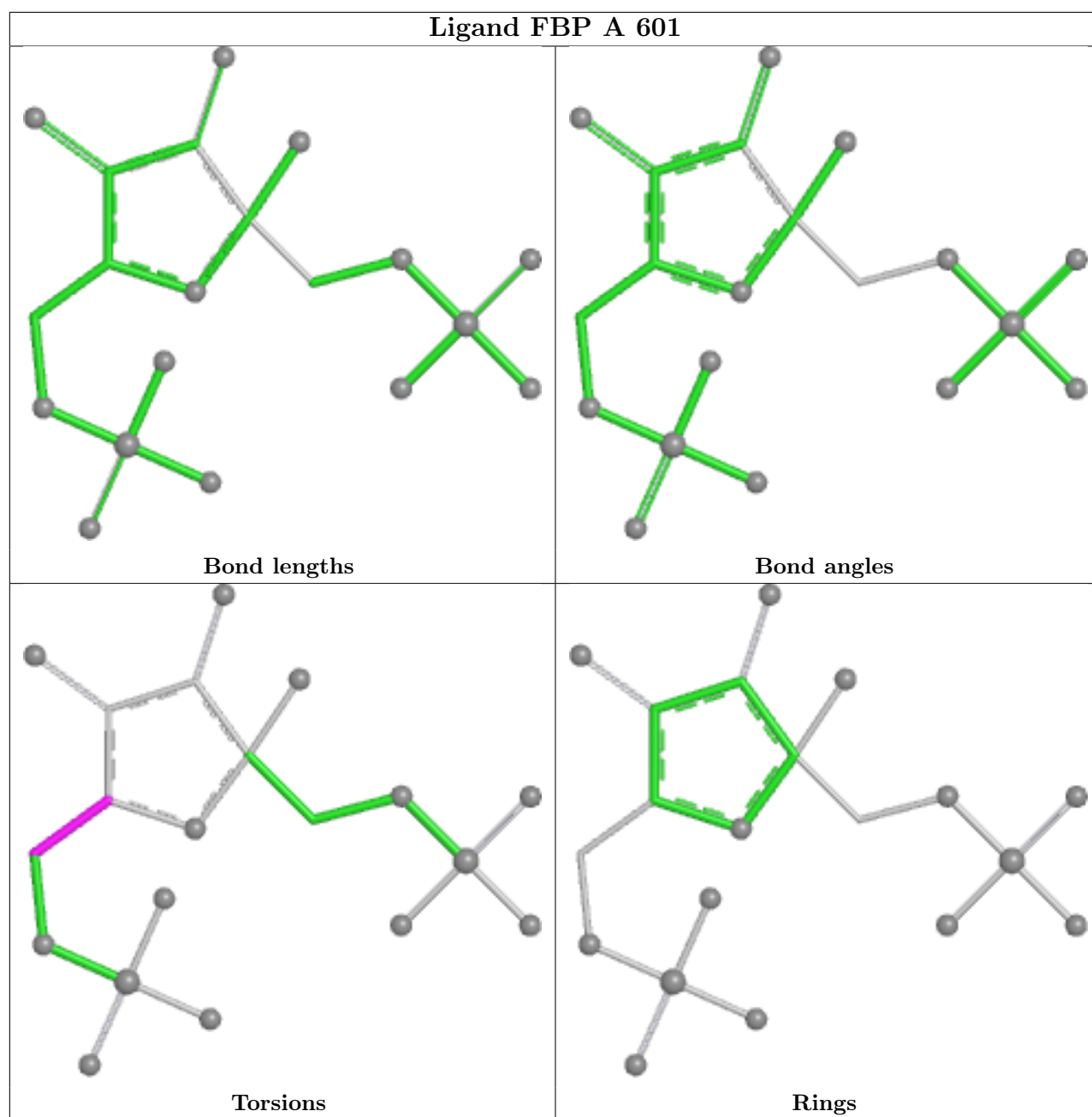
1 monomer is involved in 1 short contact:

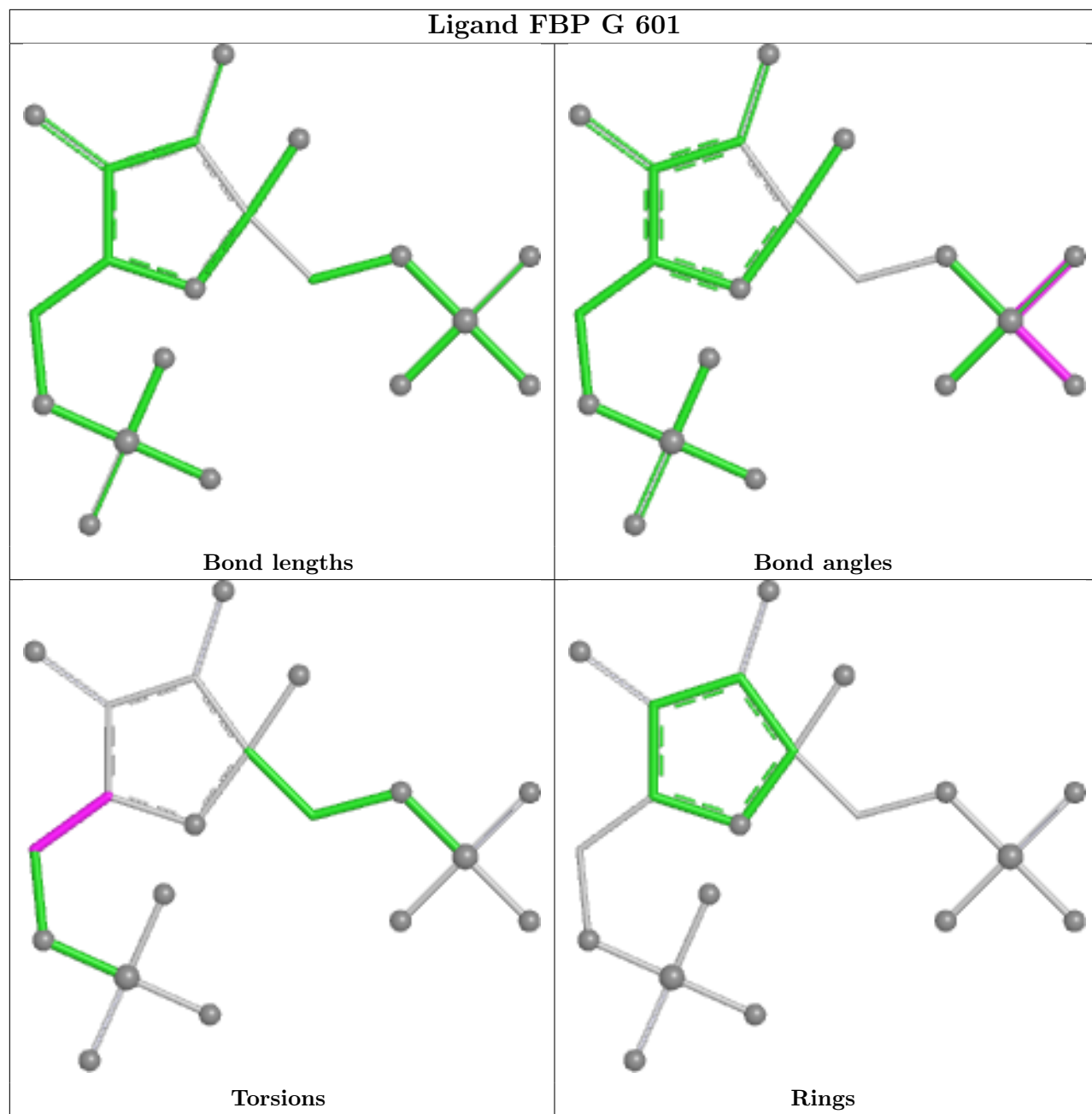
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	601	FBP	1	0

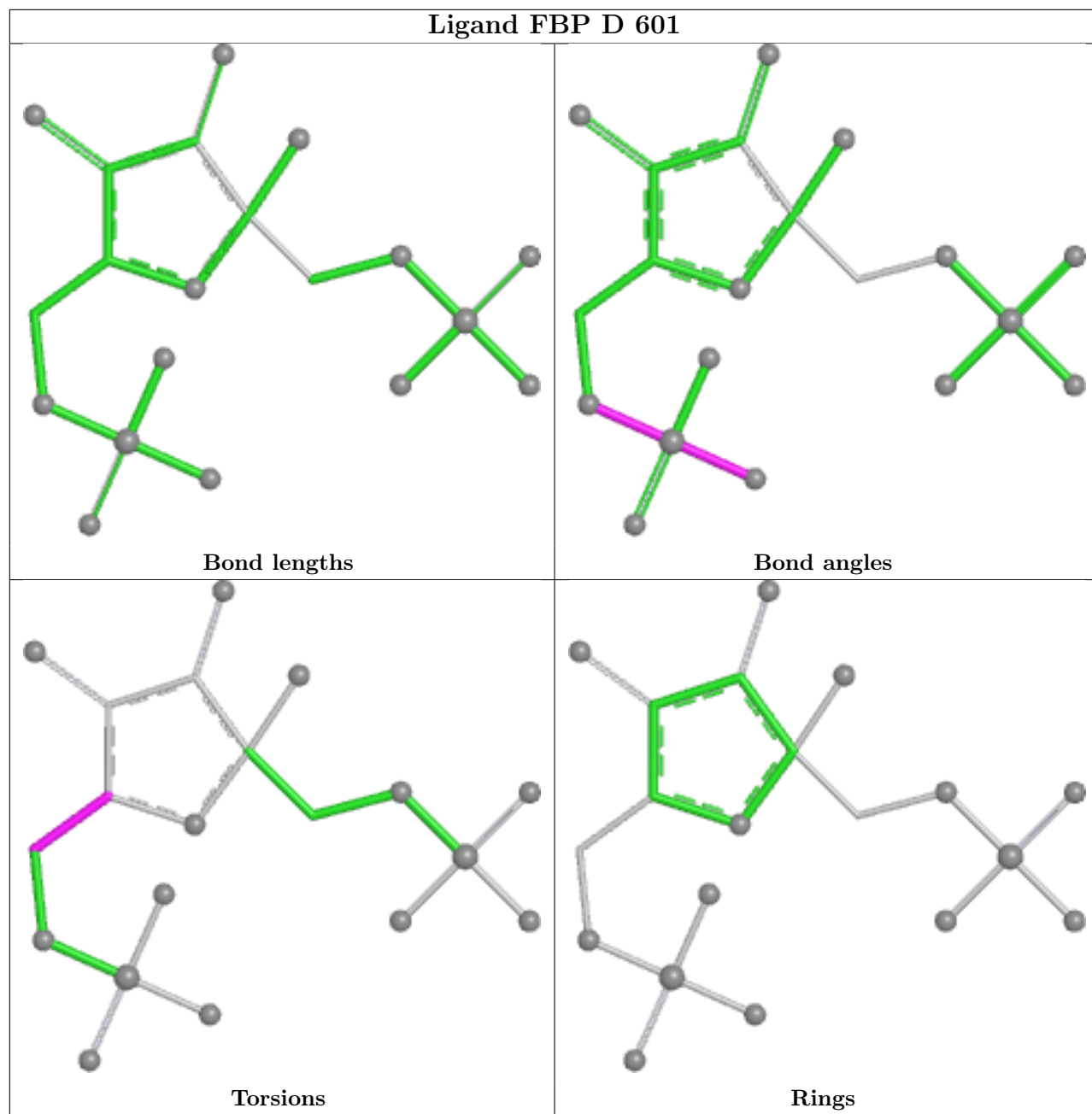
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



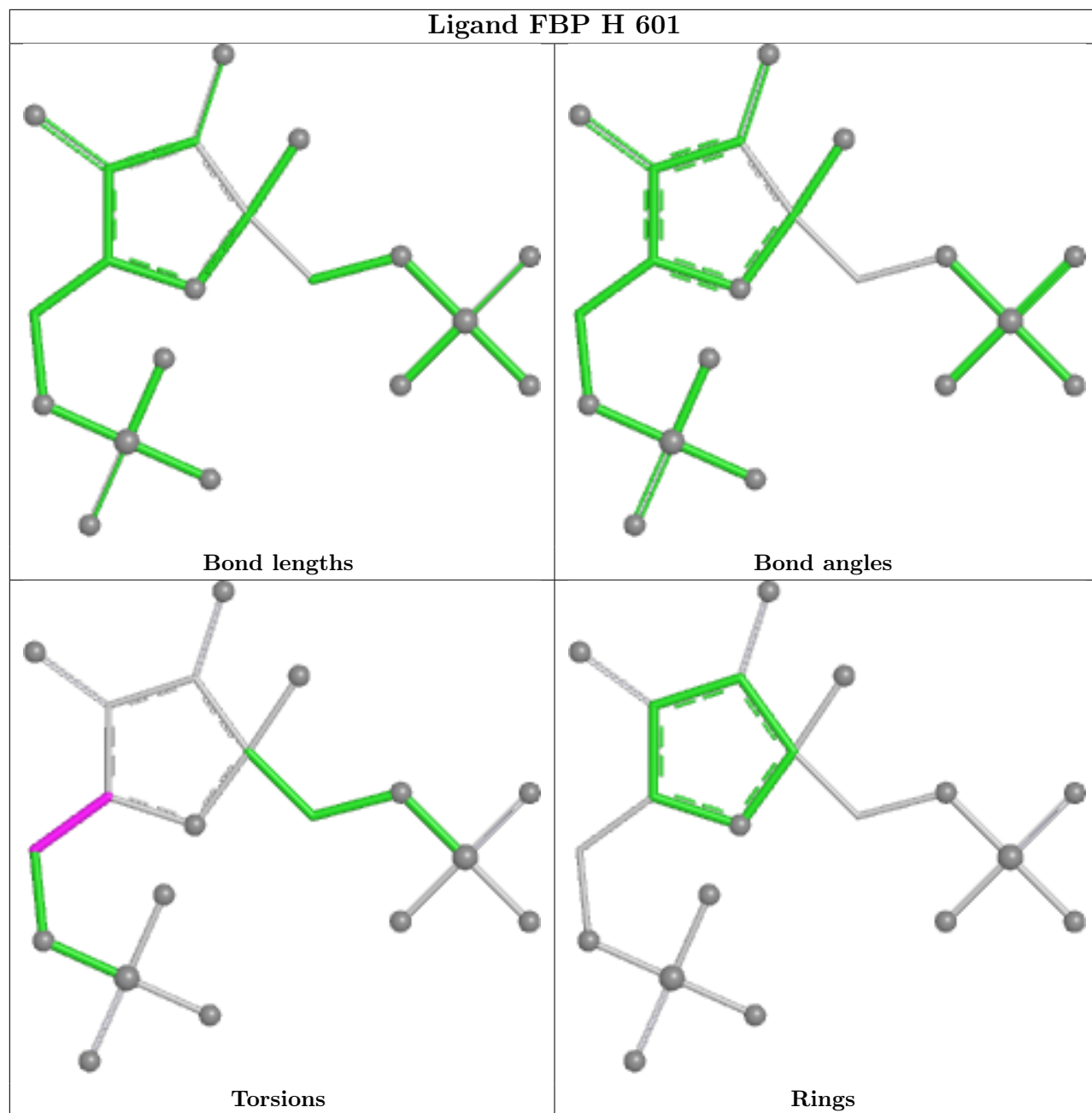




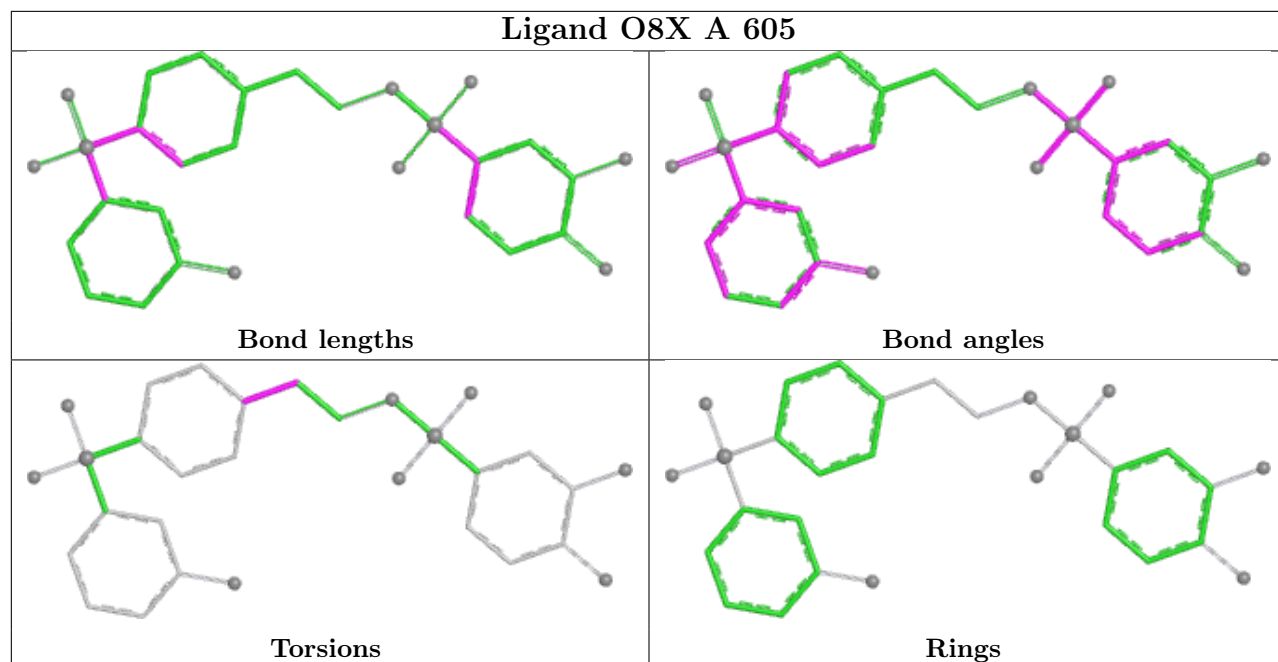




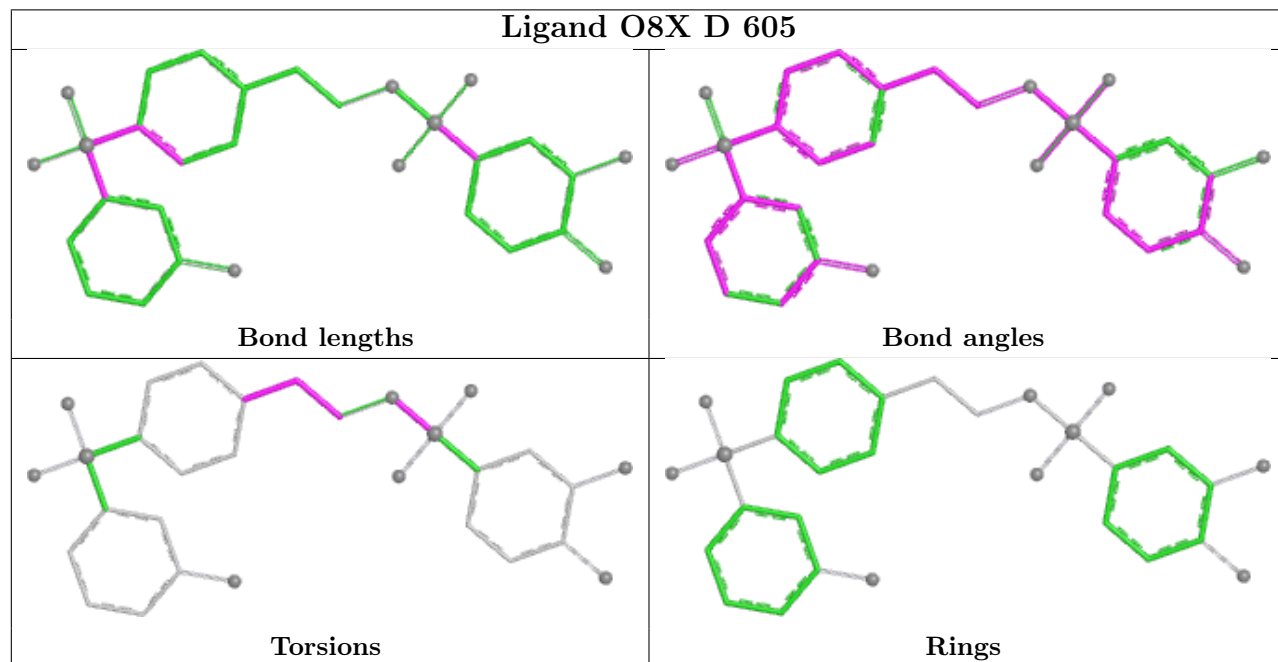
Ligand FBP H 601

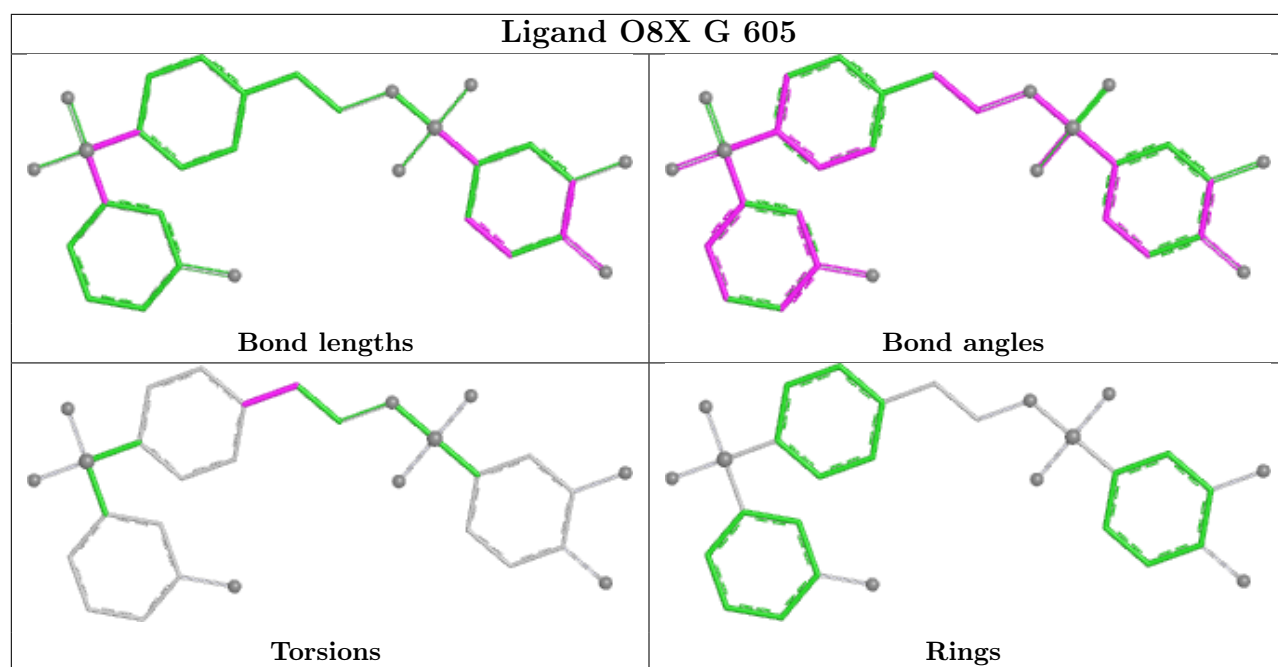


Ligand O8X A 605

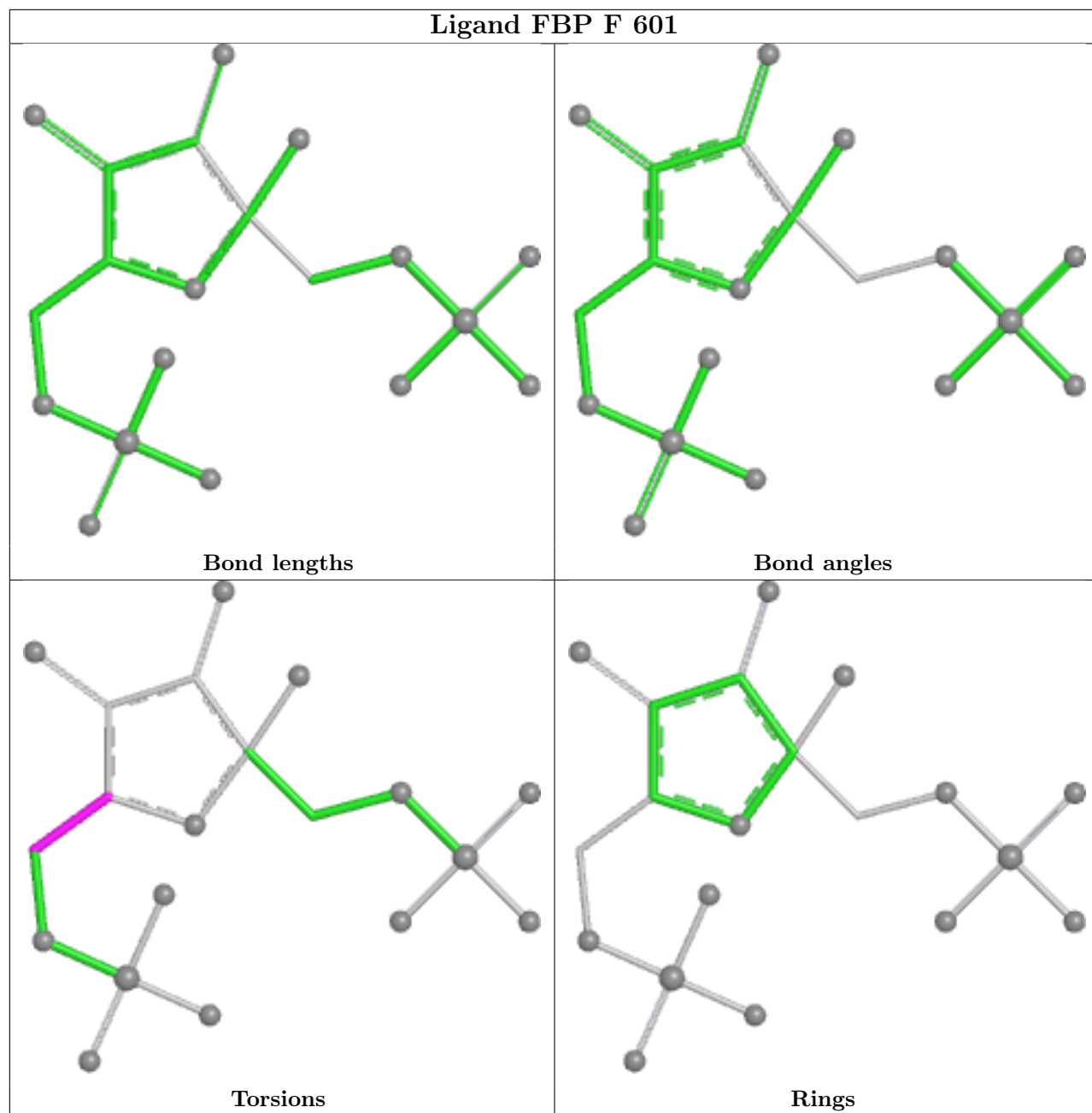


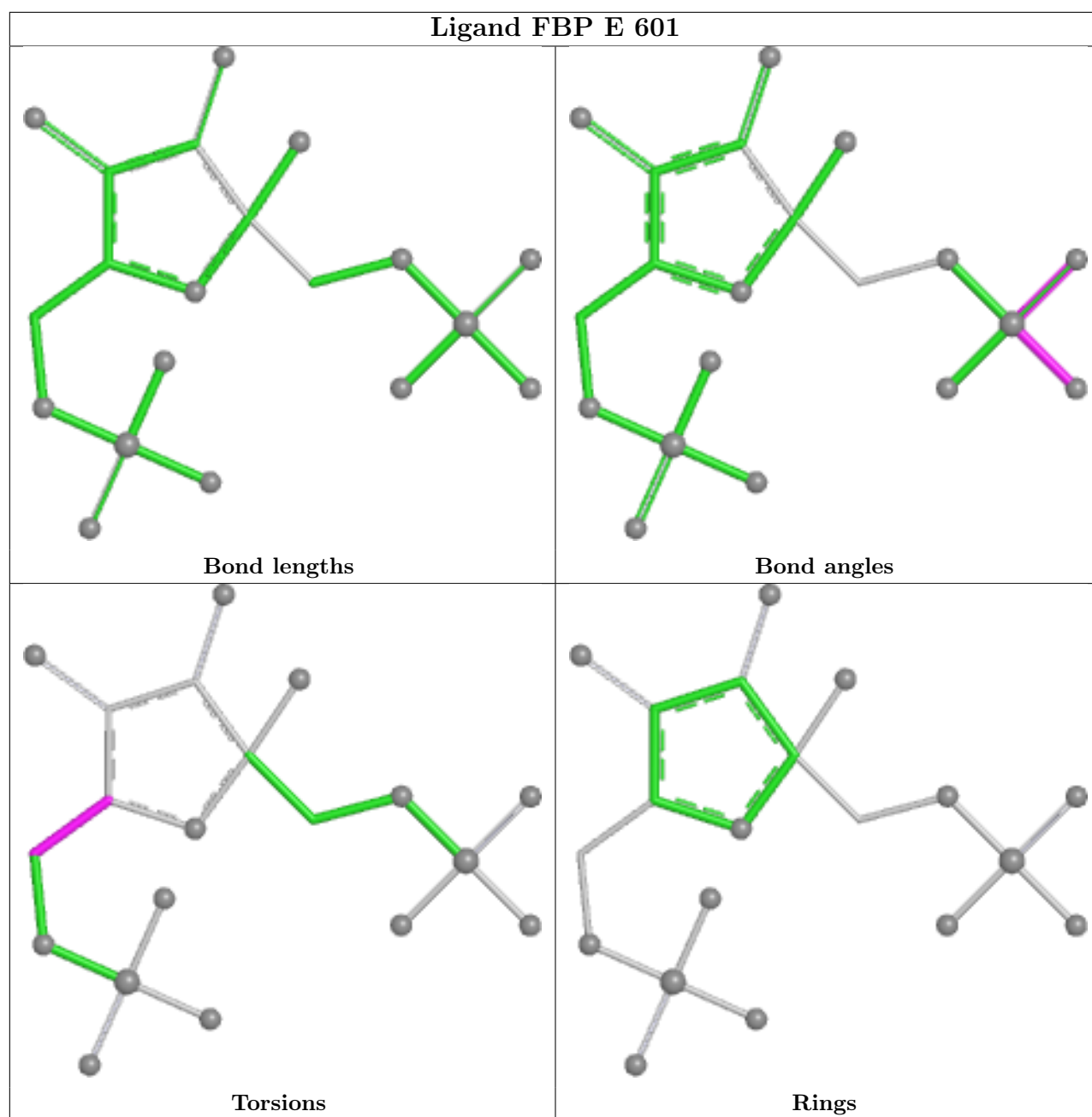
Ligand O8X D 605

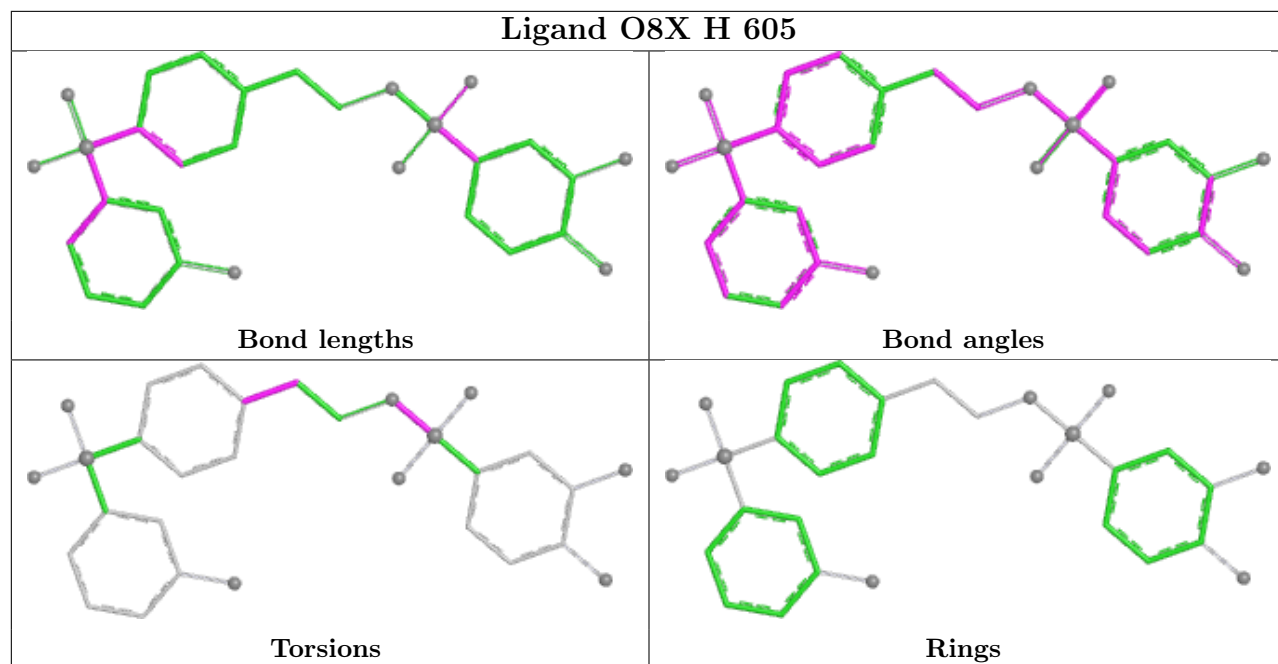




Ligand FBP F 601







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%)	1.50	104 (24%) 2 1	43, 82, 112, 131	6 (1%)
1	B	436/447 (97%)	1.32	95 (21%) 2 2	43, 74, 108, 125	4 (0%)
1	C	425/447 (95%)	0.88	79 (18%) 3 2	28, 61, 95, 140	4 (0%)
1	D	425/447 (95%)	-0.01	10 (2%) 59 56	22, 44, 69, 121	6 (1%)
1	E	419/447 (93%)	1.04	64 (15%) 5 4	32, 70, 102, 123	5 (1%)
1	F	432/447 (96%)	0.50	33 (7%) 20 16	34, 54, 86, 105	7 (1%)
1	G	421/447 (94%)	0.07	11 (2%) 57 54	27, 48, 68, 100	7 (1%)
1	H	425/447 (95%)	-0.17	9 (2%) 63 60	20, 39, 63, 103	4 (0%)
All	All	3405/3576 (95%)	0.64	405 (11%) 9 6	20, 58, 100, 140	43 (1%)

All (405) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	21	GLY	7.4
1	A	63	ILE	6.3
1	A	482	PHE	5.8
1	C	114	PRO	5.7
1	B	115	LEU	5.6
1	A	132	GLY	5.6
1	A	232	GLY	5.3
1	F	231	PRO	5.3
1	A	361	ALA	5.2
1	E	232	GLY	5.1
1	A	377	THR	5.0
1	B	511	LEU	4.9
1	A	238	VAL	4.8
1	B	61	ALA	4.8
1	D	25	PHE	4.8
1	E	244	GLY	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	543	SER	4.6
1	A	357	THR	4.5
1	H	25	PHE	4.5
1	B	116	SER	4.5
1	F	116	SER	4.4
1	E	23	ALA	4.4
1	E	25	PHE	4.4
1	C	132	GLY	4.4
1	E	249	VAL	4.3
1	E	129	PRO	4.3
1	C	36	ASP	4.3
1	C	34	MET	4.2
1	C	116	SER	4.1
1	D	21	GLY	4.1
1	E	238	VAL	4.1
1	C	80	GLY	4.1
1	F	115	LEU	4.1
1	F	232	GLY	4.1
1	C	20	LEU	4.1
1	E	115	LEU	4.1
1	G	132	GLY	4.0
1	B	267[A]	ARG	4.0
1	C	70	VAL	4.0
1	A	25	PHE	4.0
1	F	511	LEU	3.9
1	B	490	PRO	3.9
1	H	24	PHE	3.9
1	A	378	ALA	3.9
1	C	115	LEU	3.9
1	C	103	VAL	3.9
1	A	241	LEU	3.9
1	C	117	TYR	3.9
1	C	79	ALA	3.8
1	C	75	GLU	3.8
1	A	475	VAL	3.8
1	A	464	ALA	3.8
1	C	386	ALA	3.8
1	B	232	GLY	3.7
1	B	379	LYS	3.7
1	C	111	ALA	3.6
1	E	493	ILE	3.6
1	E	490	PRO	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	517	VAL	3.6
1	E	97	ALA	3.6
1	C	366	ASP	3.6
1	B	249	VAL	3.6
1	G	25	PHE	3.6
1	A	543	SER	3.5
1	A	488[A]	GLU	3.4
1	B	114	PRO	3.4
1	B	120	VAL	3.4
1	B	540[A]	LEU	3.4
1	F	36	ASP	3.3
1	B	484	LEU	3.3
1	B	91	GLY	3.3
1	D	24	PHE	3.3
1	A	114	PRO	3.3
1	E	114	PRO	3.3
1	B	256	PHE	3.3
1	E	272	PRO	3.3
1	H	22	THR	3.3
1	A	34	MET	3.3
1	A	84	ALA	3.3
1	B	231	PRO	3.3
1	B	489	PRO	3.3
1	A	24	PHE	3.2
1	C	383	PRO	3.2
1	C	384	VAL	3.2
1	E	101	ALA	3.2
1	F	516	ARG	3.2
1	F	129	PRO	3.2
1	B	498	VAL	3.2
1	C	63	ILE	3.2
1	B	495	ALA	3.2
1	A	374	SER	3.2
1	A	343	LEU	3.2
1	A	254	ALA	3.2
1	E	464	ALA	3.2
1	F	269	ALA	3.2
1	A	253	PHE	3.1
1	C	385	GLU	3.1
1	C	43	CYS	3.1
1	C	382	PHE	3.1
1	A	527	TRP	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	542	ILE	3.1
1	C	402	TYR	3.1
1	C	397	ALA	3.1
1	F	114	PRO	3.1
1	F	487	ARG	3.1
1	F	267[A]	ARG	3.0
1	A	465	VAL	3.0
1	B	445	THR	3.0
1	E	447	GLY	3.0
1	G	23	ALA	3.0
1	E	275	HIS	3.0
1	B	416	LEU	3.0
1	D	242[A]	ARG	3.0
1	A	463	ILE	3.0
1	C	371	ILE	3.0
1	E	491	GLU	3.0
1	A	373	LEU	3.0
1	C	25	PHE	3.0
1	B	509	GLY	3.0
1	A	249	VAL	2.9
1	B	502	VAL	2.9
1	E	111	ALA	2.9
1	C	22	THR	2.9
1	D	22	THR	2.9
1	D	23	ALA	2.9
1	E	511	LEU	2.9
1	A	311	ILE	2.9
1	A	101	ALA	2.9
1	H	30	LEU	2.9
1	G	34	MET	2.9
1	A	273	GLU	2.9
1	C	113	SER	2.9
1	C	408	GLU	2.9
1	B	251	ILE	2.9
1	C	107	VAL	2.9
1	A	471	ALA	2.9
1	C	23	ALA	2.9
1	C	101	ALA	2.9
1	E	257	VAL	2.8
1	E	502	VAL	2.8
1	B	515	LEU	2.8
1	A	333	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	112	GLY	2.8
1	A	100	ILE	2.8
1	A	280	ILE	2.8
1	D	275[A]	HIS	2.8
1	A	268	ALA	2.8
1	A	460	ALA	2.8
1	A	125	ASP	2.8
1	C	110	PHE	2.8
1	C	380	GLY	2.8
1	A	330	ASN	2.8
1	E	120	VAL	2.8
1	C	338	CYS	2.8
1	C	77	ILE	2.8
1	B	508	SER	2.8
1	A	23	ALA	2.8
1	B	79	ALA	2.8
1	C	66	ALA	2.8
1	B	118	ARG	2.8
1	B	88	PHE	2.8
1	A	86	LEU	2.7
1	A	124	LEU	2.7
1	A	495	ALA	2.7
1	E	126	THR	2.7
1	F	490	PRO	2.7
1	A	107	VAL	2.7
1	E	234	SER	2.7
1	C	76[A]	MET	2.7
1	A	118	ARG	2.7
1	C	232	GLY	2.7
1	A	279	ILE	2.7
1	E	233	LEU	2.7
1	F	484	LEU	2.7
1	F	540[A]	LEU	2.7
1	A	62	THR	2.7
1	B	122	ILE	2.7
1	B	493	ILE	2.7
1	E	485	LEU	2.7
1	B	348	THR	2.7
1	E	495	ALA	2.7
1	B	12	ASP	2.6
1	C	65	PRO	2.6
1	A	524	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	465	VAL	2.6
1	A	95	TYR	2.6
1	B	268	ALA	2.6
1	C	95	TYR	2.6
1	C	361	ALA	2.6
1	E	269	ALA	2.6
1	B	276	GLY	2.6
1	B	512	ARG	2.6
1	F	415	PRO	2.6
1	C	59	ILE	2.6
1	B	382	PHE	2.6
1	A	115	LEU	2.6
1	G	30	LEU	2.6
1	B	107	VAL	2.6
1	B	423	VAL	2.6
1	A	305	ALA	2.6
1	C	348	THR	2.6
1	E	100	ILE	2.6
1	C	337	VAL	2.6
1	B	378	ALA	2.6
1	E	116	SER	2.6
1	E	264	ALA	2.6
1	B	308	ASP	2.5
1	C	19	GLU	2.5
1	C	108	GLU	2.5
1	A	492	ALA	2.5
1	B	344	GLU	2.5
1	A	30	LEU	2.5
1	B	514	PHE	2.5
1	E	24	PHE	2.5
1	A	298	VAL	2.5
1	B	349	LYS	2.5
1	A	92	SER	2.5
1	A	478	CYS	2.5
1	C	404	ARG	2.5
1	F	512	ARG	2.5
1	F	489	PRO	2.5
1	B	233	LEU	2.5
1	B	485	LEU	2.5
1	B	520	LEU	2.5
1	C	319	PHE	2.5
1	H	275[A]	HIS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	400	ALA	2.5
1	E	113	SER	2.5
1	E	489	PRO	2.5
1	A	248	GLY	2.5
1	B	100	ILE	2.5
1	D	30	LEU	2.5
1	F	233	LEU	2.5
1	A	88	PHE	2.5
1	C	68	ARG	2.5
1	D	351	ARG	2.5
1	B	272	PRO	2.4
1	C	231	PRO	2.4
1	A	532	GLY	2.4
1	H	408	GLU	2.4
1	A	496	ASP	2.4
1	C	393	ILE	2.4
1	C	343	LEU	2.4
1	F	110	PHE	2.4
1	C	97	ALA	2.4
1	A	531	SER	2.4
1	A	83	ILE	2.4
1	B	443	LEU	2.4
1	F	351	ARG	2.4
1	B	507	GLU	2.4
1	C	345	SER	2.4
1	C	350	PRO	2.4
1	A	130	GLY	2.4
1	B	506	ILE	2.4
1	E	30	LEU	2.4
1	E	86	LEU	2.4
1	G	487	ARG	2.4
1	E	442	VAL	2.4
1	B	305	ALA	2.4
1	E	254	ALA	2.4
1	F	408	GLU	2.4
1	A	58	SER	2.4
1	A	104	ARG	2.4
1	A	365	LEU	2.4
1	E	540	LEU	2.4
1	F	309	LEU	2.4
1	A	70	VAL	2.4
1	B	123	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	505	GLY	2.3
1	E	104	ARG	2.3
1	A	90	HIS	2.3
1	A	233	LEU	2.3
1	A	540	LEU	2.3
1	E	90	HIS	2.3
1	H	34	MET	2.3
1	B	486	TYR	2.3
1	B	238	VAL	2.3
1	B	11	ALA	2.3
1	A	417	SER	2.3
1	E	541[A]	SER	2.3
1	B	124	LEU	2.3
1	E	103	VAL	2.3
1	C	102	ASN	2.3
1	C	357	THR	2.3
1	E	351	ARG	2.3
1	A	494	TRP	2.3
1	A	296	LEU	2.3
1	B	270	LEU	2.3
1	A	240	ASP	2.3
1	A	256	PHE	2.3
1	A	514	PHE	2.3
1	C	24	PHE	2.3
1	A	350	PRO	2.3
1	B	14	ALA	2.3
1	C	72	ARG	2.3
1	B	377	THR	2.3
1	B	132	GLY	2.3
1	B	274	GLY	2.3
1	C	390	GLN	2.3
1	E	28	GLN	2.3
1	G	271	GLY	2.3
1	A	252	VAL	2.3
1	A	404	ARG	2.3
1	B	126	THR	2.2
1	C	37	THR	2.2
1	B	90	HIS	2.2
1	B	86	LEU	2.2
1	B	347	ILE	2.2
1	A	237	ASP	2.2
1	A	407	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	352	PRO	2.2
1	A	469	ALA	2.2
1	C	33	ALA	2.2
1	C	305	ALA	2.2
1	G	33	ALA	2.2
1	A	91	GLY	2.2
1	A	327	GLY	2.2
1	C	21	GLY	2.2
1	A	426	ILE	2.2
1	A	493	ILE	2.2
1	B	77	ILE	2.2
1	B	463	ILE	2.2
1	B	504	PHE	2.2
1	G	24	PHE	2.2
1	E	465	VAL	2.2
1	G	231	PRO	2.2
1	B	121	ALA	2.2
1	A	28	GLN	2.2
1	B	117	TYR	2.2
1	C	90	HIS	2.2
1	E	26	GLN	2.2
1	B	16	LEU	2.2
1	F	485	LEU	2.2
1	G	63	ILE	2.2
1	B	92	SER	2.2
1	E	242	ARG	2.2
1	A	110	PHE	2.2
1	E	514	PHE	2.2
1	C	289	VAL	2.2
1	A	450	ALA	2.2
1	B	84	ALA	2.2
1	E	268	ALA	2.2
1	A	348	THR	2.2
1	C	42	LEU	2.2
1	E	241	LEU	2.2
1	F	118	ARG	2.2
1	B	13	VAL	2.1
1	A	80	GLY	2.1
1	B	518	GLY	2.1
1	B	59	ILE	2.1
1	B	468	SER	2.1
1	F	242	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	379	LYS	2.1
1	E	494	TRP	2.1
1	F	514	PHE	2.1
1	A	537[A]	MET	2.1
1	B	76[A]	MET	2.1
1	C	106	ALA	2.1
1	E	400	ALA	2.1
1	F	11	ALA	2.1
1	C	64	GLY	2.1
1	D	412	ARG	2.1
1	E	488	GLU	2.1
1	A	99	SER	2.1
1	B	131	SER	2.1
1	F	543	SER	2.1
1	C	129	PRO	2.1
1	B	539	VAL	2.1
1	C	405	GLN	2.1
1	E	29	GLN	2.1
1	F	13	VAL	2.1
1	A	375	GLY	2.1
1	E	270	LEU	2.1
1	C	412	ARG	2.1
1	C	109	SER	2.1
1	A	383	PRO	2.1
1	H	231	PRO	2.1
1	E	263	VAL	2.1
1	E	266	VAL	2.1
1	B	33	ALA	2.1
1	B	494	TRP	2.1
1	B	351	ARG	2.1
1	F	416	LEU	2.1
1	E	274	GLY	2.1
1	F	491	GLU	2.1
1	E	63	ILE	2.1
1	A	449	SER	2.1
1	A	342	MET	2.1
1	A	384	VAL	2.0
1	E	245	VAL	2.0
1	A	33	ALA	2.0
1	B	501	ARG	2.0
1	A	484	LEU	2.0
1	B	381	ASN	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	130	GLY	2.0
1	C	74	LYS	2.0
1	B	483	PRO	2.0
1	E	89	SER	2.0
1	F	272	PRO	2.0
1	B	516	ARG	2.0
1	C	35	ALA	2.0
1	C	339	ALA	2.0
1	E	33	ALA	2.0
1	A	347	ILE	2.0
1	A	119	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	K	A	604	1/1	0.71	0.16	149,149,149,149	0
5	K	E	604	1/1	0.73	0.39	127,127,127,127	0
5	K	G	604	1/1	0.83	0.14	88,88,88,88	0
3	OXL	A	602	6/6	0.84	0.17	143,144,144,144	0
5	K	C	604	1/1	0.84	0.19	100,100,100,100	0
5	K	B	604	1/1	0.85	0.11	130,130,130,130	0
3	OXL	C	602	6/6	0.85	0.12	77,78,78,78	0
3	OXL	E	602	6/6	0.88	0.13	89,89,89,90	0
5	K	F	604	1/1	0.88	0.09	118,118,118,118	0
2	FBP	B	601	20/20	0.88	0.12	76,76,77,78	0
2	FBP	A	601	20/20	0.89	0.12	77,79,82,82	0
3	OXL	B	602	6/6	0.90	0.11	77,77,79,80	0

Continued on next page...

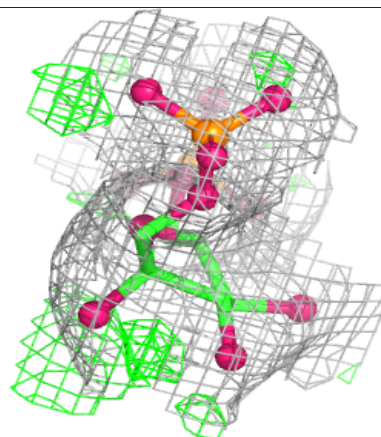
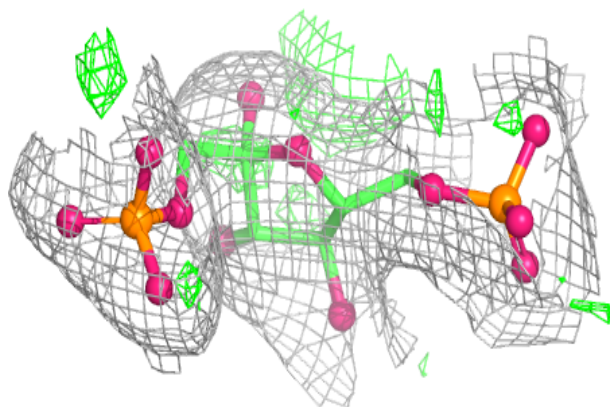
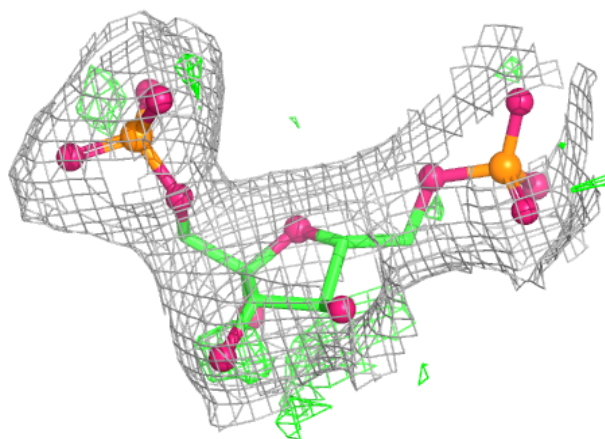
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	OXL	G	602	6/6	0.90	0.11	55,56,58,58	0
6	O8X	A	605	30/30	0.90	0.14	78,80,82,82	19
3	OXL	D	602	6/6	0.91	0.11	62,62,63,64	0
3	OXL	F	602	6/6	0.91	0.14	90,90,90,91	0
6	O8X	G	605	30/30	0.91	0.13	63,66,67,68	19
6	O8X	D	605	30/30	0.92	0.12	51,58,65,66	19
2	FBP	E	601	20/20	0.92	0.10	68,69,72,72	0
6	O8X	H	605	30/30	0.93	0.11	52,55,56,56	19
2	FBP	F	601	20/20	0.94	0.09	56,61,66,66	0
3	OXL	H	602	6/6	0.94	0.14	54,55,56,56	0
4	MG	D	603	1/1	0.95	0.14	36,36,36,36	0
4	MG	F	603	1/1	0.95	0.14	38,38,38,38	0
4	MG	B	603	1/1	0.95	0.12	59,59,59,59	0
4	MG	C	603	1/1	0.96	0.13	56,56,56,56	0
4	MG	H	603	1/1	0.96	0.12	28,28,28,28	0
4	MG	A	603	1/1	0.97	0.04	61,61,61,61	0
5	K	H	604	1/1	0.97	0.10	76,76,76,76	0
4	MG	G	603	1/1	0.97	0.14	31,31,31,31	0
2	FBP	D	601	20/20	0.98	0.05	36,37,38,38	0
5	K	D	604	1/1	0.98	0.17	70,70,70,70	0
2	FBP	G	601	20/20	0.98	0.05	32,34,35,36	0
2	FBP	H	601	20/20	0.98	0.05	28,31,33,33	0
2	FBP	C	601	20/20	0.98	0.05	33,34,38,39	0
4	MG	E	603	1/1	0.99	0.04	46,46,46,46	0

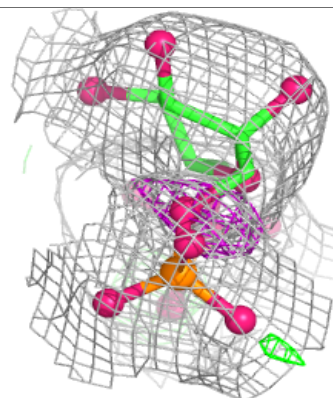
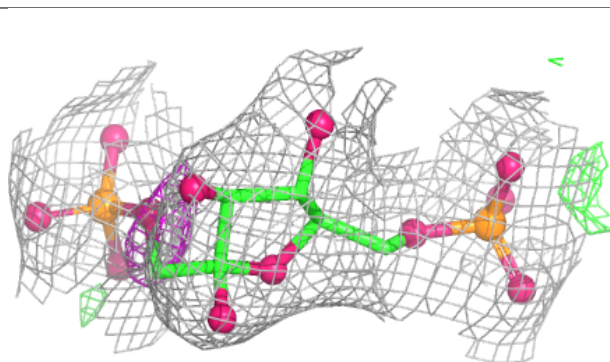
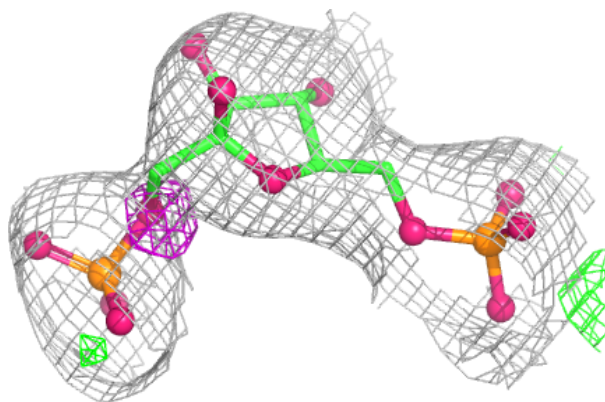
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FBP 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)

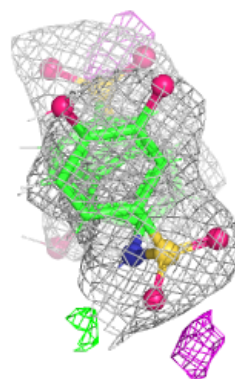
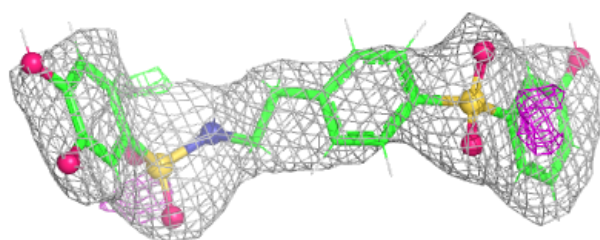
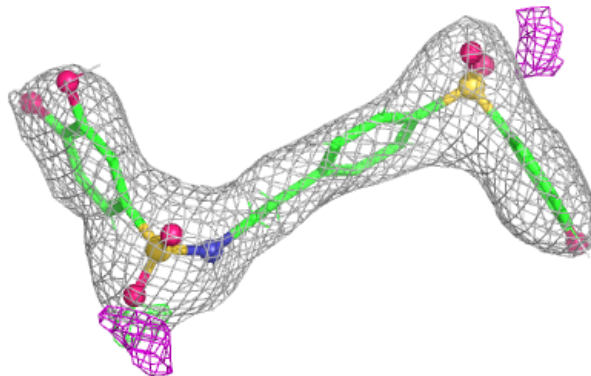
**Electron density around FBP A 601:**

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

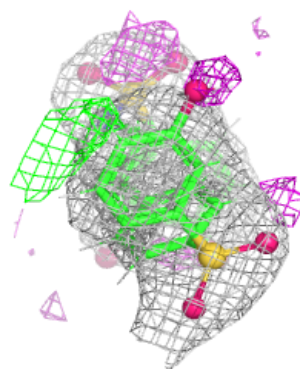
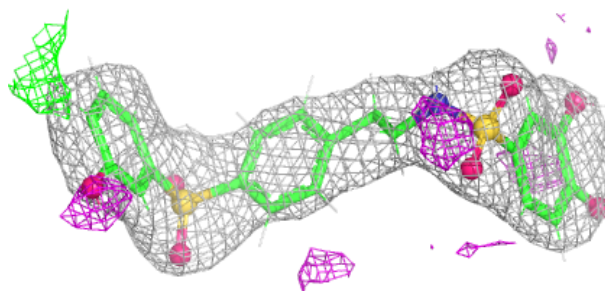
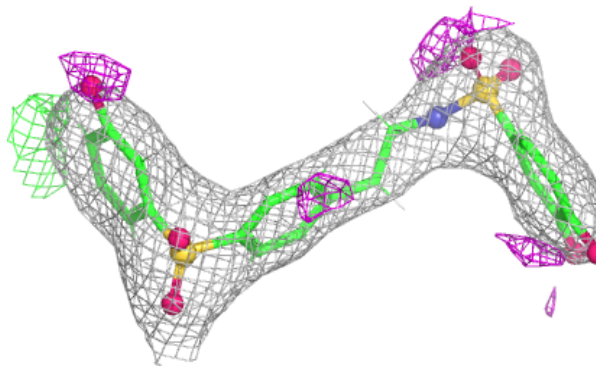


Electron density around O8X A 605:

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

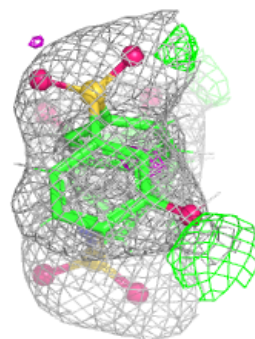
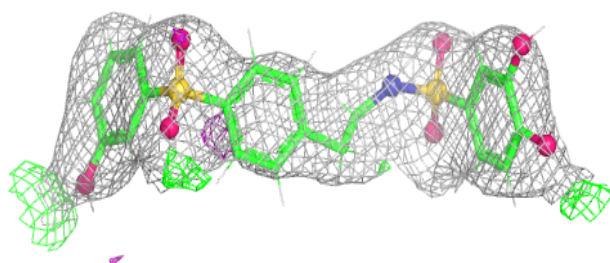
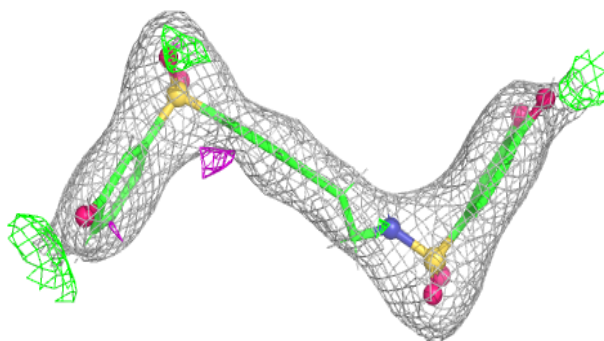
**Electron density around O8X G 605:**

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

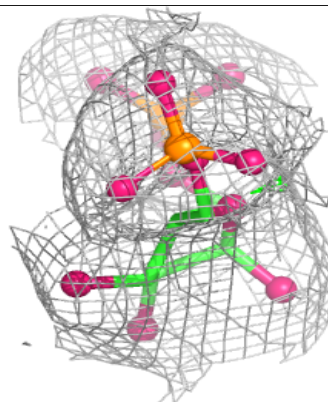
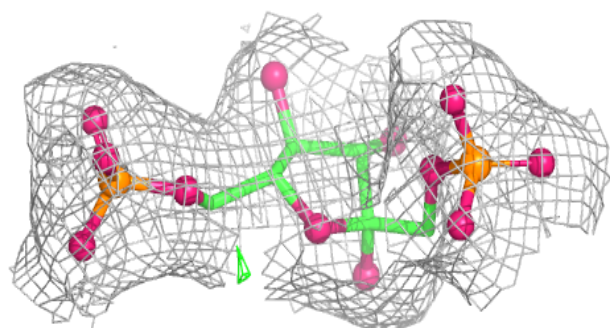
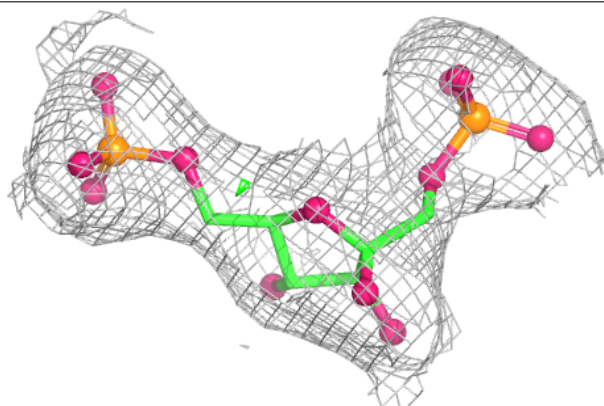


Electron density around O8X D 605:

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

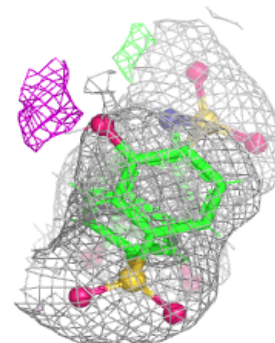
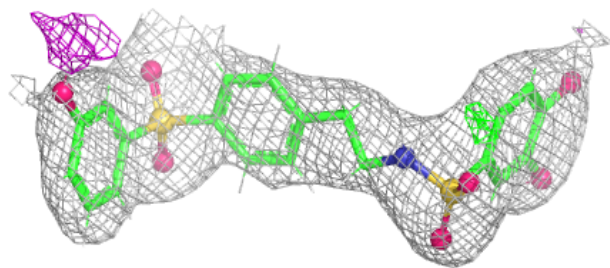
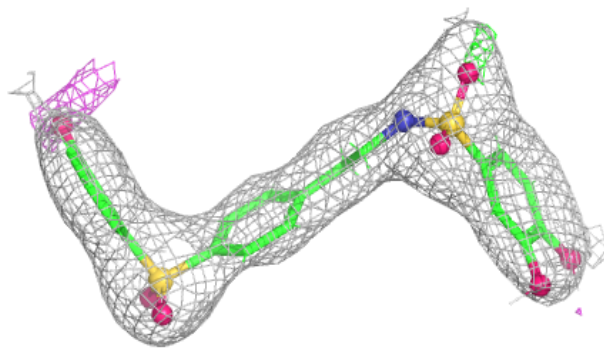
**Electron density around FBP E 601:**

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



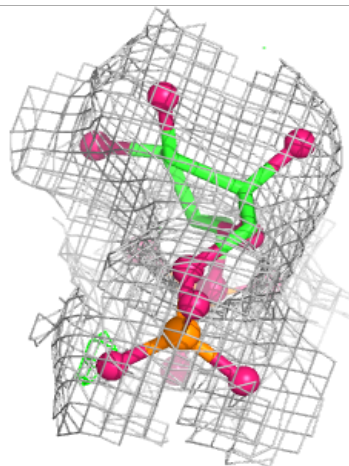
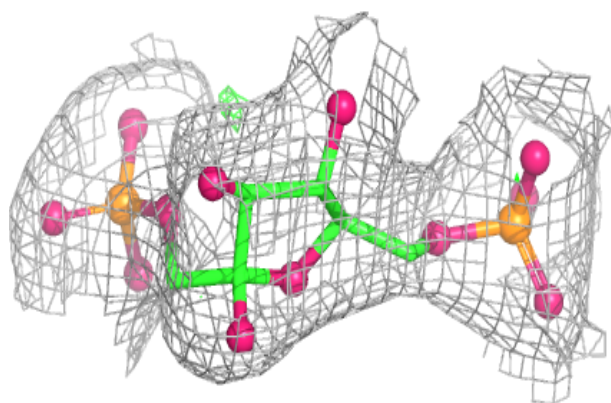
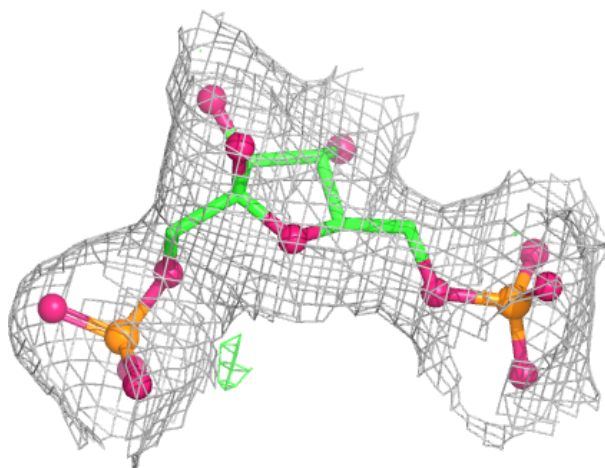
Electron density around O8X H 605:

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



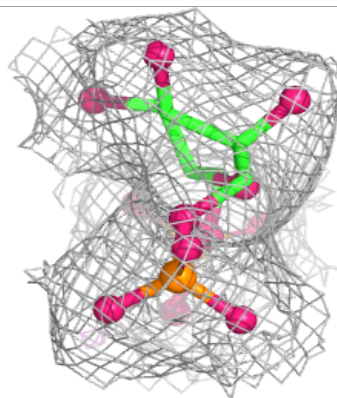
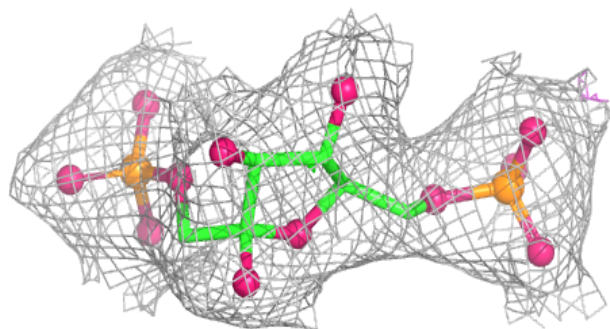
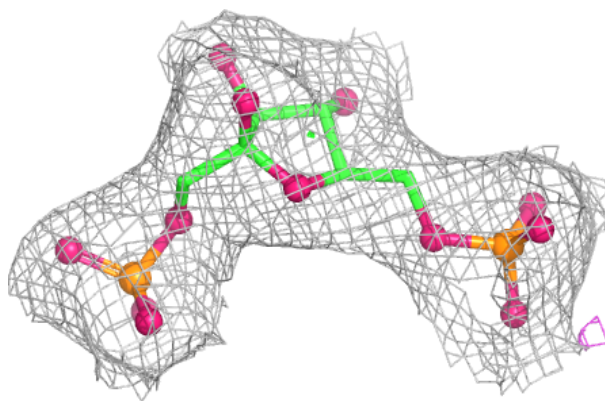
Electron density around FBP F 601:

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

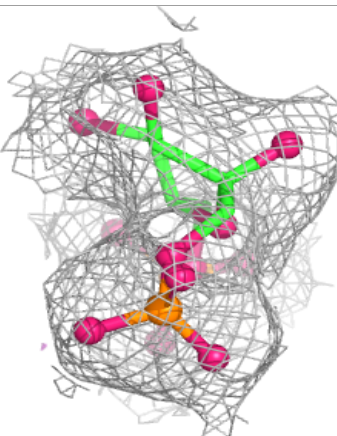
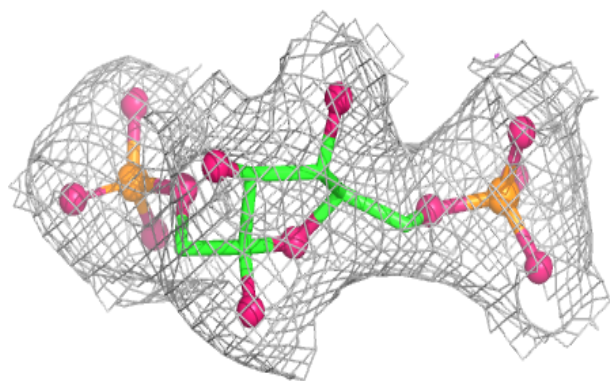
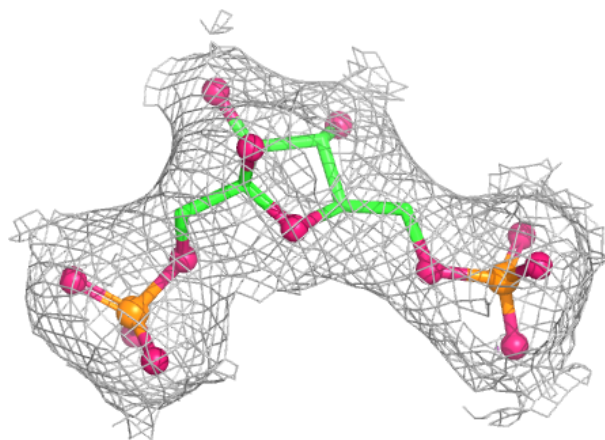


Electron density around FBP D 601:

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

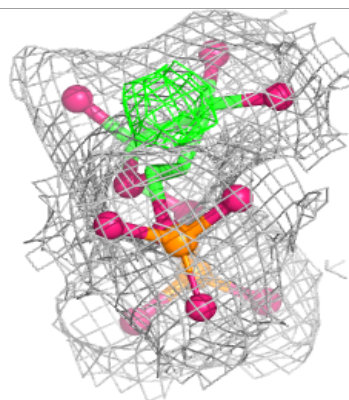
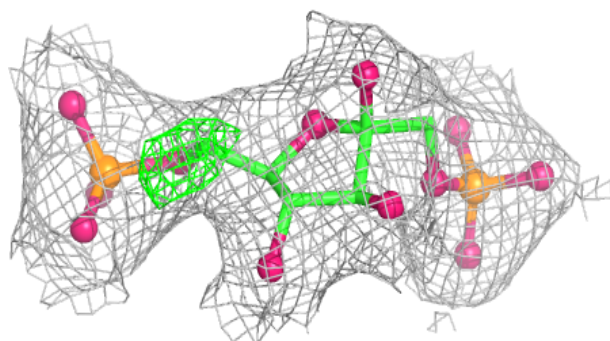
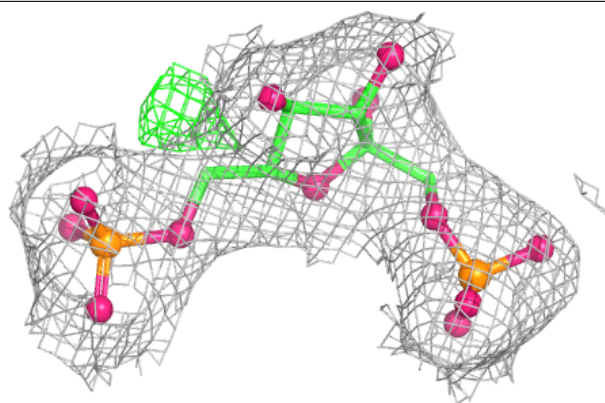
**Electron density around FBP G 601:**

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

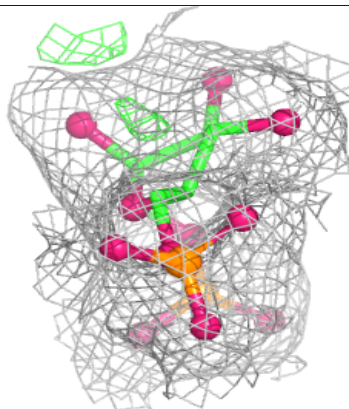
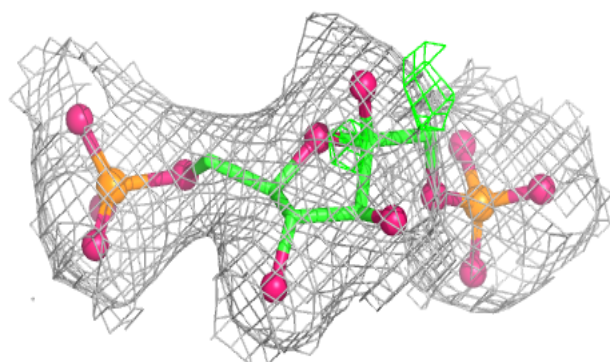
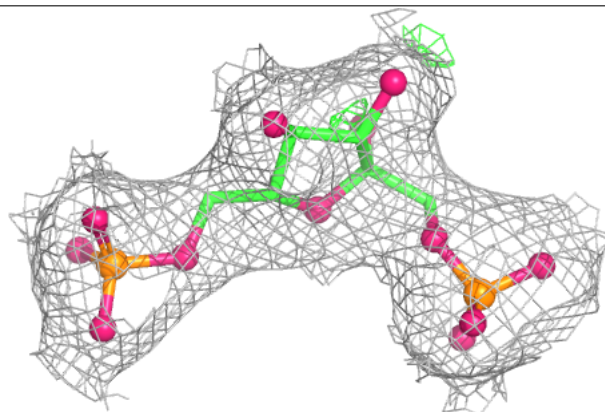


Electron density around FBP H 601:

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

**Electron density around FBP C 601:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.