wwPDB X-ray Structure Validation Summary Report (i)

Oct 8, 2026 – 11:26 AM EDT

PDB ID	:	14CS / pdb_000014cs
Title	:	Structure of liver pyruvate kinase in complex with allosteric activator 8e
Authors	:	Lulla, A.; Rodriguez Rivero, A.; Grotli, M.; Hyvonen, M.
Deposited on	:	2026-04-28
Resolution	:	2.13 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

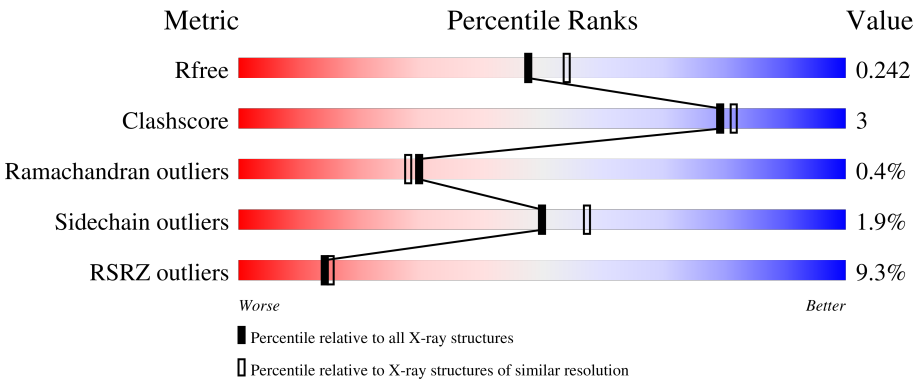
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.13 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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 <=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	9%; 88%; 9% •
1	C	447	6%; 86%; 9% 5%
1	D	447	3%; 87%; 7% • 5%
1	E	447	13%; 85%; 8% • 6%

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Mol	Chain	Length	Quality of chain
1	F	447	7% 88% 8%
1	G	447	6% 85% 10%
1	H	447	3% 89% 6% 5%

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	502	-	X	-	-
3	OXL	B	502	-	X	-	-
3	OXL	C	502	-	X	-	-
3	OXL	D	502	-	X	-	-
3	OXL	E	502	-	X	-	-
3	OXL	G	502	-	X	-	-
3	OXL	H	502	-	X	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 27999 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 Isoform L-type of Pyruvate kinase PKLR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	422	3237	2036	585	596	20	0	6	0
1	B	436	3329	2090	604	615	20	0	4	0
1	C	426	3251	2042	586	604	19	0	4	0
1	D	425	3252	2042	590	601	19	0	6	0
1	E	419	3210	2018	579	593	20	0	5	0
1	F	432	3321	2090	597	614	20	0	7	0
1	G	427	3275	2057	588	611	19	0	6	0
1	H	425	3251	2040	594	598	19	0	4	0

There are 48 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	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	12	ASP	SER	conflict	UNP P30613
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

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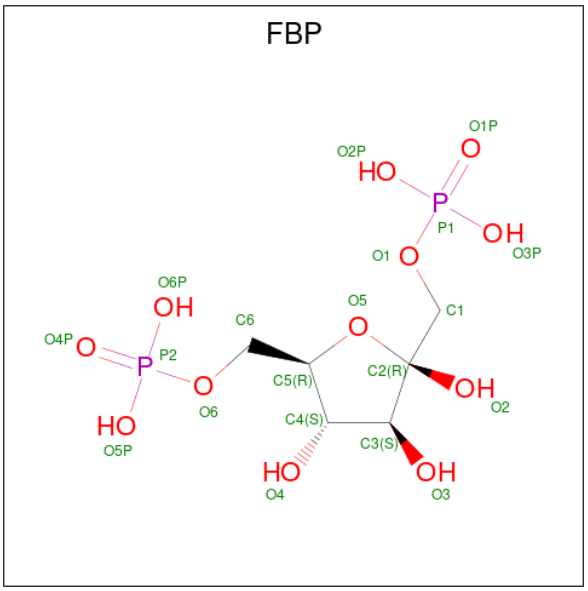
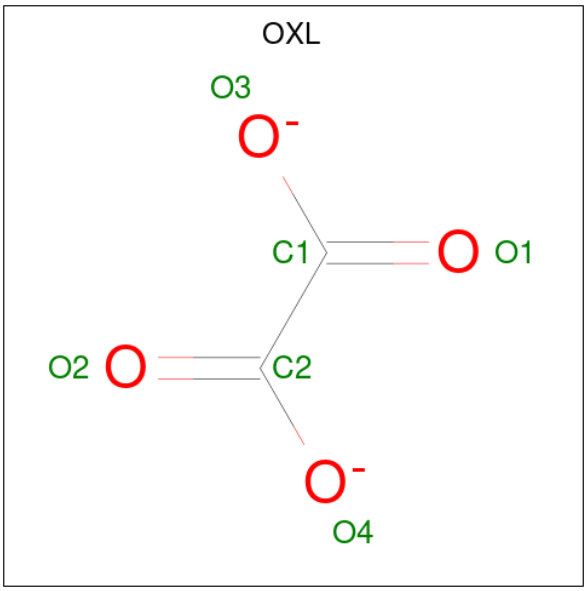
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP P30613
C	12	ASP	SER	conflict	UNP P30613
C	130	GLY	-	linker	UNP P30613
C	131	SER	-	linker	UNP P30613
C	132	GLY	-	linker	UNP P30613
D	-1	GLY	-	expression tag	UNP P30613
D	0	SER	-	expression tag	UNP P30613
D	12	ASP	SER	conflict	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	12	ASP	SER	conflict	UNP P30613
E	130	GLY	-	linker	UNP P30613
E	131	SER	-	linker	UNP P30613
E	132	GLY	-	linker	UNP P30613
F	-1	GLY	-	expression tag	UNP P30613
F	0	SER	-	expression tag	UNP P30613
F	12	ASP	SER	conflict	UNP P30613
F	130	GLY	-	linker	UNP P30613
F	131	SER	-	linker	UNP P30613
F	132	GLY	-	linker	UNP P30613
G	-1	GLY	-	expression tag	UNP P30613
G	0	SER	-	expression tag	UNP P30613
G	12	ASP	SER	conflict	UNP P30613
G	130	GLY	-	linker	UNP P30613
G	131	SER	-	linker	UNP P30613
G	132	GLY	-	linker	UNP P30613
H	-1	GLY	-	expression tag	UNP P30613
H	0	SER	-	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: $C_6H_{14}O_{12}P_2$).



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

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



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

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

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

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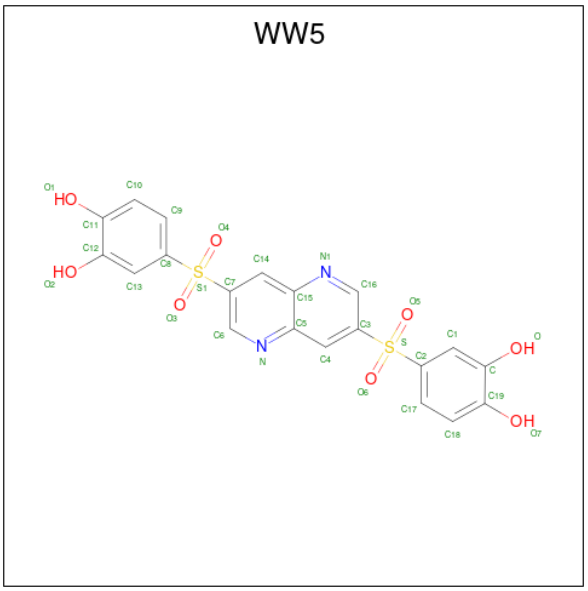
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0
4	G	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0

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

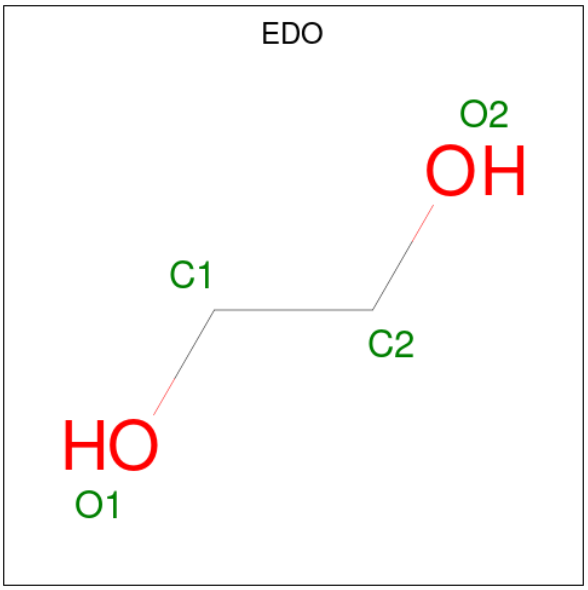
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0
5	B	1	Total K 1 1	0	0
5	C	1	Total K 1 1	0	0
5	D	1	Total K 1 1	0	0
5	E	1	Total K 1 1	0	0
5	F	1	Total K 1 1	0	0
5	G	1	Total K 1 1	0	0
5	H	1	Total K 1 1	0	0

- Molecule 6 is 4,4'-(1,5-naphthyridine-3,7-diyldisulfonyl)di(benzene-1,2-diol) (CCD ID: WW5) (formula: $C_{20}H_{14}N_2O_8S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
6	B	1	46	20	14	2	8	2	14	0
			Total	C	H	N	O	S		
6	C	1	46	20	14	2	8	2	14	0
			Total	C	H	N	O	S		
6	F	1	46	20	14	2	8	2	14	0
			Total	C	H	N	O	S		
6	G	1	46	20	14	2	8	2	14	0

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
7	B	1	10	2	6	2	6	0
			Total	C	H	O		
7	E	1	10	2	6	2	6	0

- Molecule 8 is water.

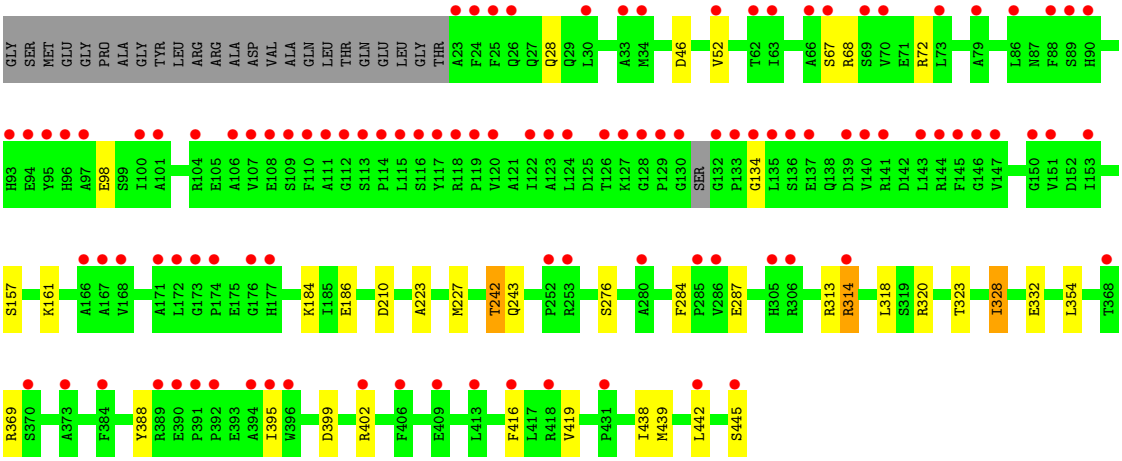
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	110	110	110	0	0
			Total	O		
8	B	173	173	173	0	0
			Total	O		
8	C	192	192	192	0	0
			Total	O		
8	D	244	244	244	0	0
			Total	O		
8	E	135	135	135	0	0
			Total	O		
8	F	169	169	169	0	0
			Total	O		
8	G	201	201	201	0	0
			Total	O		
8	H	221	221	221	0	0

3 Residue-property plots (i)

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

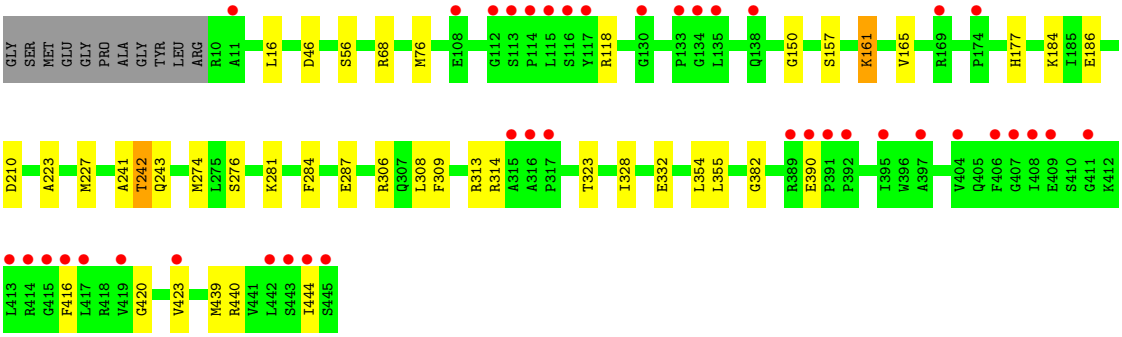
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain A:



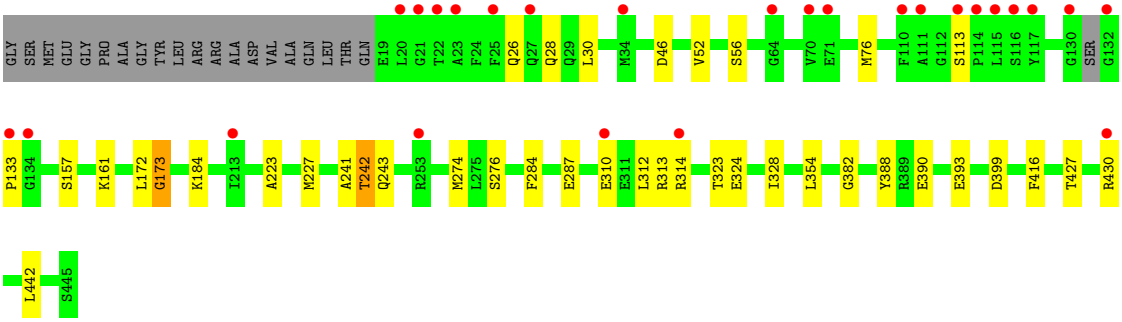
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain B:



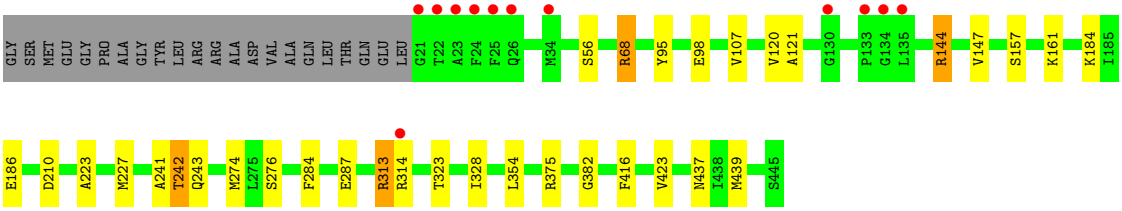
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain C:



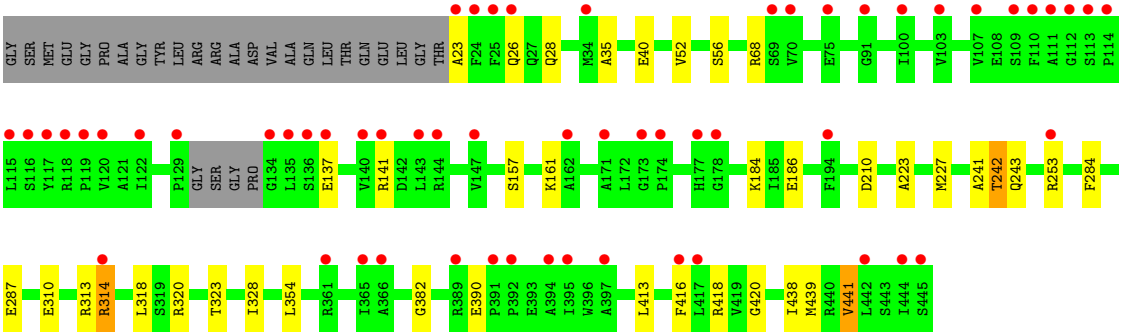
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain D:



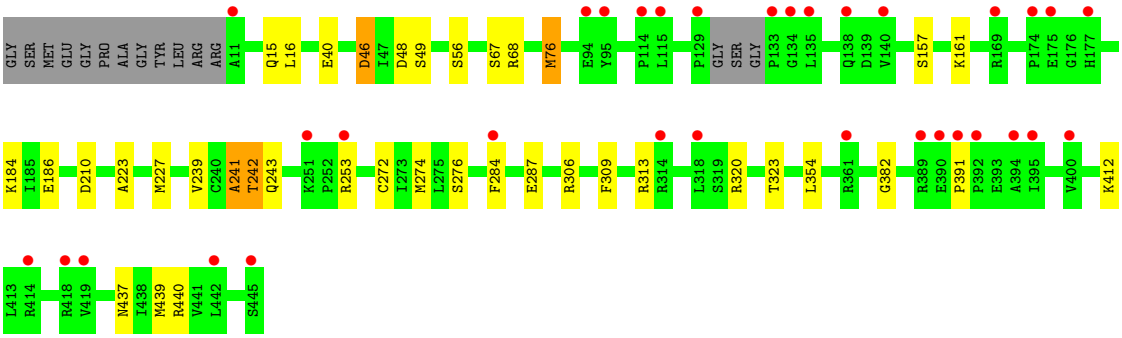
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain E:



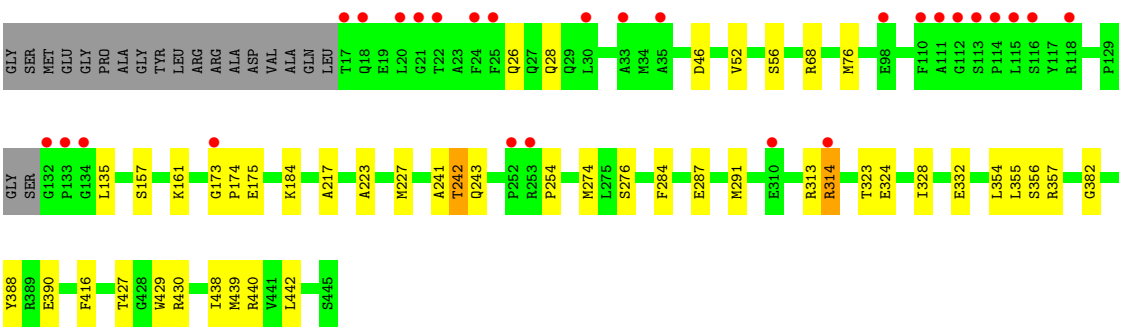
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain F:



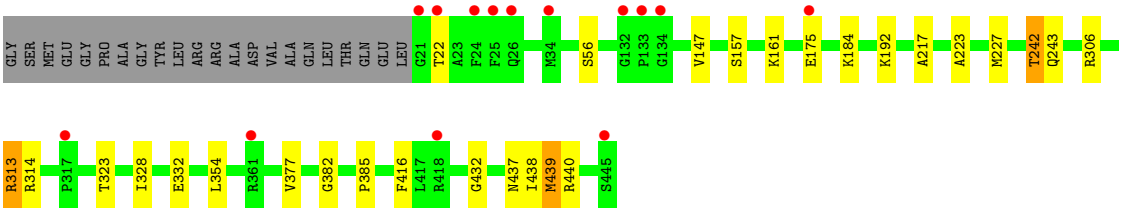
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain G:



• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	206.78Å 112.73Å 187.78Å 90.00° 92.70° 90.00°	Depositor
Resolution (Å)	98.95 – 2.13 98.95 – 2.13	Depositor EDS
% Data completeness (in resolution range)	57.0 (98.95-2.13) 57.0 (98.95-2.13)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.12Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.212 , 0.252 0.203 , 0.242	Depositor DCC
R_{free} test set	6809 reflections (2.83%)	wwPDB-VP
Wilson B-factor (Å^2)	27.2	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	27999	wwPDB-VP
Average B, all atoms (Å^2)	32.0	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 62.37 % 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 1.1388e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: K, WW5, EDO, OXL, MG, FBP

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	0.71	1/3309 (0.0%)	1.05	4/4473 (0.1%)
1	B	0.77	1/3396 (0.0%)	1.04	5/4592 (0.1%)
1	C	0.77	2/3317 (0.1%)	1.05	4/4484 (0.1%)
1	D	0.83	2/3326 (0.1%)	1.06	3/4497 (0.1%)
1	E	0.71	0/3278	1.04	4/4430 (0.1%)
1	F	0.74	1/3396 (0.0%)	1.02	3/4591 (0.1%)
1	G	0.79	3/3347 (0.1%)	1.07	6/4525 (0.1%)
1	H	0.81	0/3316	1.06	1/4483 (0.0%)
All	All	0.77	10/26685 (0.0%)	1.05	30/36075 (0.1%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	276	SER	CA-C	8.27	1.56	1.52
1	B	276	SER	CA-C	8.16	1.56	1.52
1	D	276	SER	CA-C	8.04	1.56	1.52
1	A	276	SER	CA-C	7.94	1.56	1.52
1	C	276	SER	CA-C	7.26	1.56	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	356	SER	CA-C-N	7.21	130.25	120.38
1	G	356	SER	C-N-CA	7.21	130.25	120.38
1	G	416	PHE	CA-CB-CG	7.20	121.00	113.80
1	B	46	ASP	CA-CB-CG	5.98	118.58	112.60
1	H	416	PHE	CA-CB-CG	5.82	119.62	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3237	0	3301	20	0
1	B	3329	0	3394	24	0
1	C	3251	0	3302	19	0
1	D	3252	0	3310	15	0
1	E	3210	0	3270	21	0
1	F	3321	0	3393	25	0
1	G	3275	0	3326	28	0
1	H	3251	0	3306	21	0
2	A	20	0	10	0	0
2	B	20	0	10	0	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
2	E	20	0	10	0	0
2	F	20	0	10	0	0
2	G	20	0	10	0	0
2	H	20	0	10	1	0
3	A	6	0	0	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	B	32	14	0	0	0
6	C	32	14	0	0	0
6	F	32	14	0	0	0
6	G	32	14	0	0	0
7	B	4	6	6	1	0
7	E	4	6	6	0	0
8	A	110	0	0	0	0
8	B	173	0	0	3	0
8	C	192	0	0	1	0
8	D	244	0	0	0	0
8	E	135	0	0	0	0
8	F	169	0	0	2	0
8	G	201	0	0	0	0
8	H	221	0	0	0	0
All	All	27931	68	26694	144	0

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

The worst 5 of 144 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:440:ARG:HG2	1:H:438:ILE:HG12	1.53	0.91
1:G:439:MET:HE3	1:H:439:MET:HG2	1.60	0.84
1:C:324[A]:GLU:HG3	1:C:354:LEU:HD13	1.67	0.77
1:G:324[A]:GLU:HG3	1:G:354:LEU:HD13	1.67	0.77
1:C:313:ARG:HG3	1:C:328:ILE:HD11	1.66	0.77

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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%)	416 (98%)	6 (1%)	2 (0%)	24	22
1	B	438/447 (98%)	431 (98%)	6 (1%)	1 (0%)	43	44
1	C	426/447 (95%)	417 (98%)	6 (1%)	3 (1%)	18	15
1	D	429/447 (96%)	423 (99%)	4 (1%)	2 (0%)	24	22
1	E	420/447 (94%)	414 (99%)	5 (1%)	1 (0%)	43	44
1	F	435/447 (97%)	428 (98%)	6 (1%)	1 (0%)	43	44
1	G	429/447 (96%)	420 (98%)	7 (2%)	2 (0%)	24	22
1	H	427/447 (96%)	419 (98%)	6 (1%)	2 (0%)	24	22
All	All	3428/3576 (96%)	3368 (98%)	46 (1%)	14 (0%)	30	28

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	173	GLY
1	A	134	GLY
1	G	173	GLY
1	D	437	ASN
1	A	242	THR

5.3.2 Protein sidechains (i)

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%)	332 (98%)	8 (2%)	43	48
1	B	349/352 (99%)	339 (97%)	10 (3%)	37	41
1	C	341/352 (97%)	334 (98%)	7 (2%)	47	54
1	D	342/352 (97%)	334 (98%)	8 (2%)	44	50
1	E	338/352 (96%)	330 (98%)	8 (2%)	43	48
1	F	350/352 (99%)	342 (98%)	8 (2%)	44	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	345/352 (98%)	338 (98%)	7 (2%)	48	55
1	H	340/352 (97%)	335 (98%)	5 (2%)	57	65
All	All	2745/2816 (98%)	2684 (98%)	61 (2%)	50	52

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	161	LYS
1	G	442	LEU
1	E	314	ARG
1	G	314	ARG
1	H	314	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	307	GLN
1	F	405	GLN
1	H	376	GLN
1	G	187	ASN
1	D	90	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 16 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FBP	B	501	-	18,20,20	0.46	0	21,32,32	0.59	0
3	OXL	F	502	4	5,5,5	2.21	3 (60%)	6,6,6	2.04	2 (33%)
2	FBP	E	501	-	18,20,20	0.56	0	21,32,32	0.67	0
2	FBP	D	501	-	18,20,20	0.88	1 (5%)	21,32,32	0.94	2 (9%)
3	OXL	A	502	4	5,5,5	1.93	2 (40%)	6,6,6	2.21	3 (50%)
6	WW5	F	505	-	35,35,35	2.65	12 (34%)	50,54,54	1.72	14 (28%)
3	OXL	D	502	4	5,5,5	2.11	2 (40%)	6,6,6	1.89	2 (33%)
7	EDO	E	505	-	3,3,3	0.08	0	2,2,2	0.15	0
2	FBP	G	501	-	18,20,20	0.43	0	21,32,32	0.87	1 (4%)
3	OXL	B	502	4	5,5,5	2.23	1 (20%)	6,6,6	2.03	3 (50%)
2	FBP	C	501	-	18,20,20	0.50	0	21,32,32	0.71	0
2	FBP	H	501	-	18,20,20	0.75	0	21,32,32	0.77	0
3	OXL	H	502	4	5,5,5	2.14	2 (40%)	6,6,6	0.99	0
6	WW5	C	505	-	35,35,35	2.92	10 (28%)	50,54,54	1.60	11 (22%)
2	FBP	F	501	-	18,20,20	0.43	0	21,32,32	0.56	0
3	OXL	E	502	4	5,5,5	2.19	2 (40%)	6,6,6	1.92	2 (33%)
3	OXL	C	502	4	5,5,5	2.09	2 (40%)	6,6,6	1.44	1 (16%)
7	EDO	B	506	-	3,3,3	0.20	0	2,2,2	0.16	0
3	OXL	G	502	4	5,5,5	2.20	2 (40%)	6,6,6	1.16	1 (16%)
6	WW5	G	505	-	35,35,35	2.76	13 (37%)	50,54,54	1.69	15 (30%)
6	WW5	B	505	-	35,35,35	2.32	14 (40%)	50,54,54	1.71	10 (20%)
2	FBP	A	501	-	18,20,20	0.44	0	21,32,32	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	B	501	-	-	4/13/32/32	0/1/1/1
3	OXL	F	502	4	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	E	501	-	-	4/13/32/32	0/1/1/1
2	FBP	D	501	-	-	2/13/32/32	0/1/1/1
3	OXL	A	502	4	-	4/4/4/4	-
6	WW5	F	505	-	-	0/24/24/24	0/4/4/4
3	OXL	D	502	4	-	4/4/4/4	-
7	EDO	E	505	-	-	1/1/1/1	-
2	FBP	G	501	-	-	2/13/32/32	0/1/1/1
3	OXL	B	502	4	-	4/4/4/4	-
2	FBP	C	501	-	-	2/13/32/32	0/1/1/1
2	FBP	H	501	-	-	7/13/32/32	0/1/1/1
3	OXL	H	502	4	-	4/4/4/4	-
6	WW5	C	505	-	-	0/24/24/24	0/4/4/4
2	FBP	F	501	-	-	2/13/32/32	0/1/1/1
3	OXL	E	502	4	-	4/4/4/4	-
3	OXL	C	502	4	-	4/4/4/4	-
7	EDO	B	506	-	-	1/1/1/1	-
3	OXL	G	502	4	-	4/4/4/4	-
6	WW5	G	505	-	-	1/24/24/24	0/4/4/4
6	WW5	B	505	-	-	0/24/24/24	0/4/4/4
2	FBP	A	501	-	-	2/13/32/32	0/1/1/1

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	505	WW5	C2-S	-8.72	1.63	1.77
6	G	505	WW5	C2-S	-8.00	1.64	1.77
6	G	505	WW5	C8-S1	-7.67	1.65	1.77
6	C	505	WW5	C8-S1	-7.63	1.65	1.77
6	F	505	WW5	C2-S	-7.63	1.65	1.77

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	505	WW5	C14-C7-S1	5.50	126.45	119.14
6	B	505	WW5	C14-C7-S1	4.69	125.38	119.14
6	G	505	WW5	C4-C3-S	4.58	125.23	119.14
6	C	505	WW5	C4-C3-S	4.12	124.62	119.14
3	A	502	OXL	O4-C2-C1	4.06	120.70	112.83

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	501	FBP	C1-O1-P1-O2P
2	H	501	FBP	C1-O1-P1-O3P
2	H	501	FBP	O1-C1-C2-O2
2	H	501	FBP	O1-C1-C2-C3
2	H	501	FBP	O1-C1-C2-O5

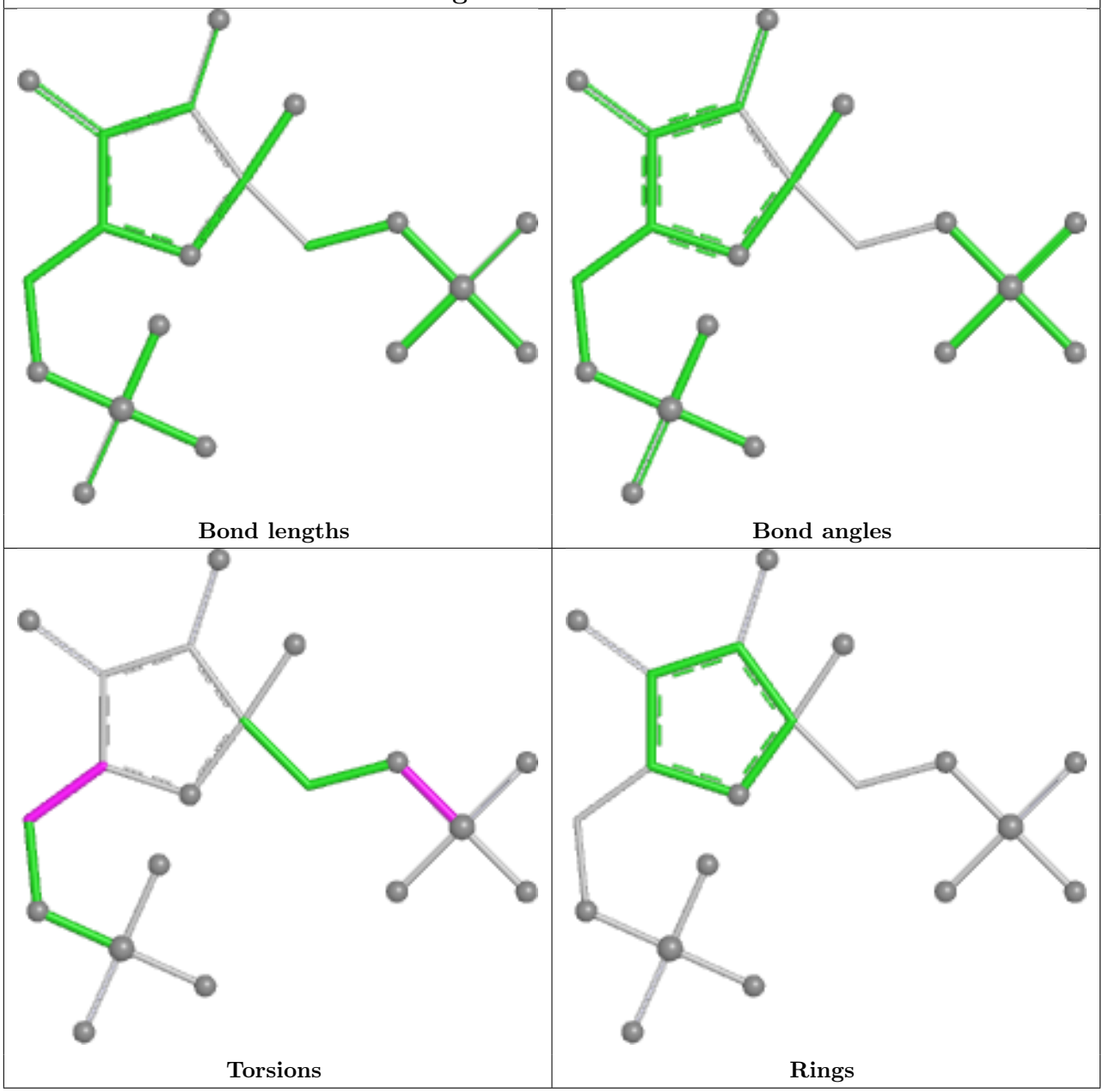
There are no ring outliers.

3 monomers are involved in 3 short contacts:

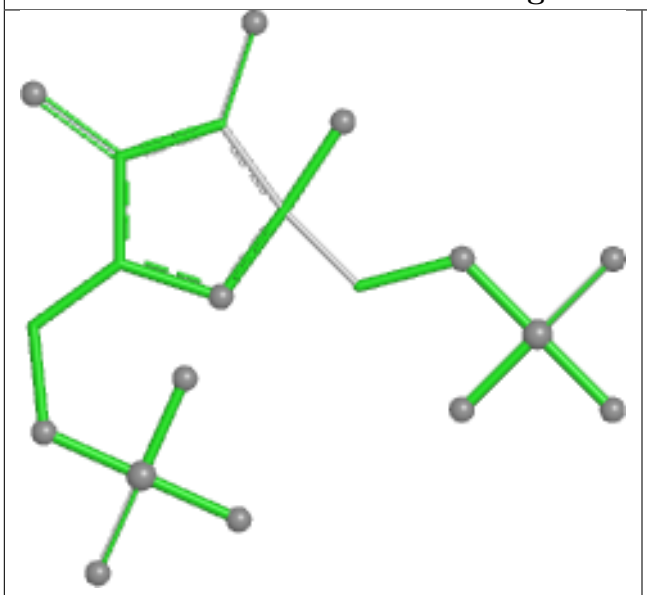
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	OXL	1	0
2	H	501	FBP	1	0
7	B	506	EDO	1	0

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 then 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.

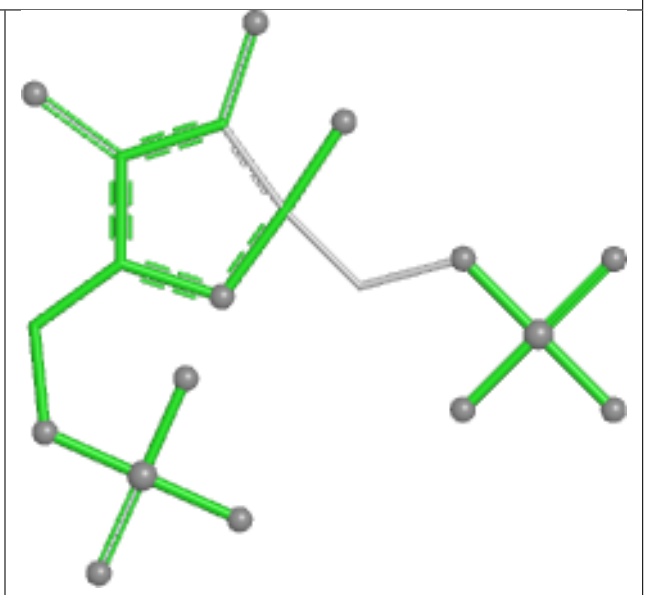
Ligand FBP B 501



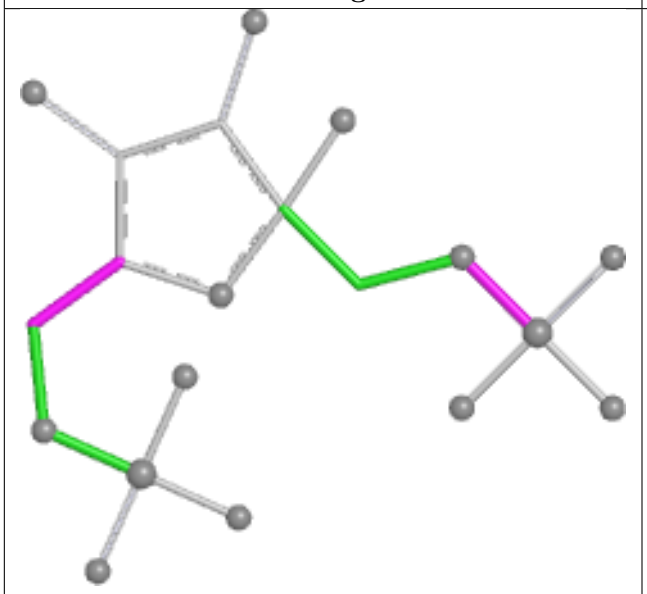
Ligand FBP E 501



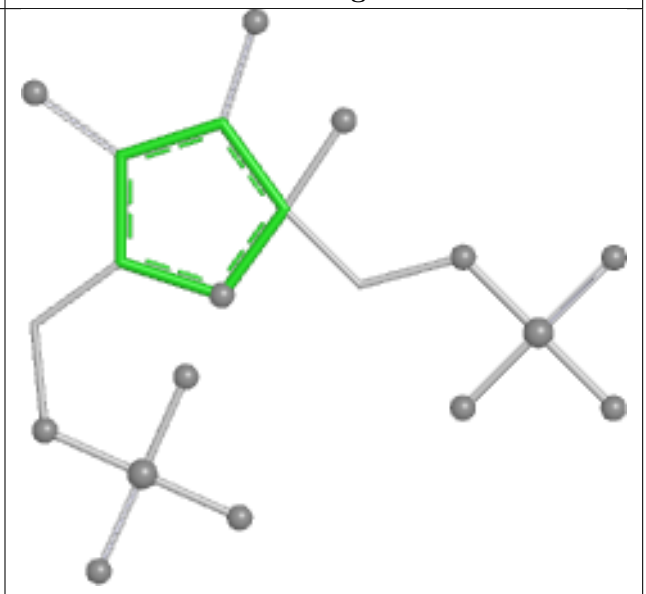
Bond lengths



Bond angles

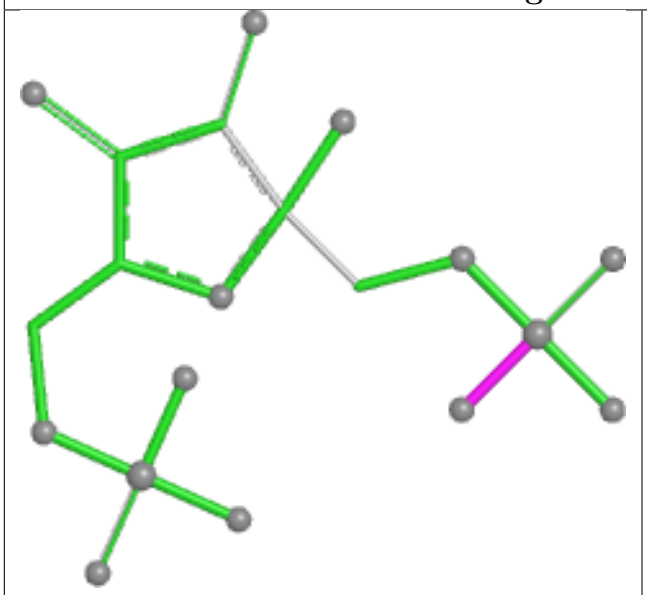


Torsions



Rings

Ligand FBP D 501



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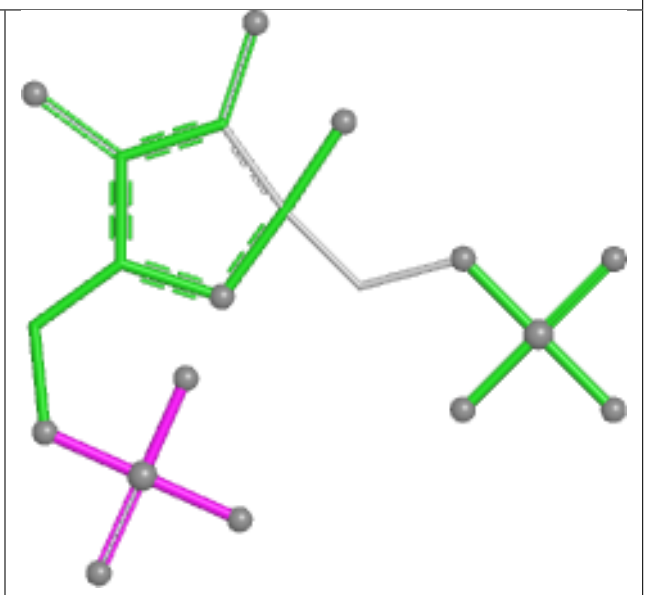

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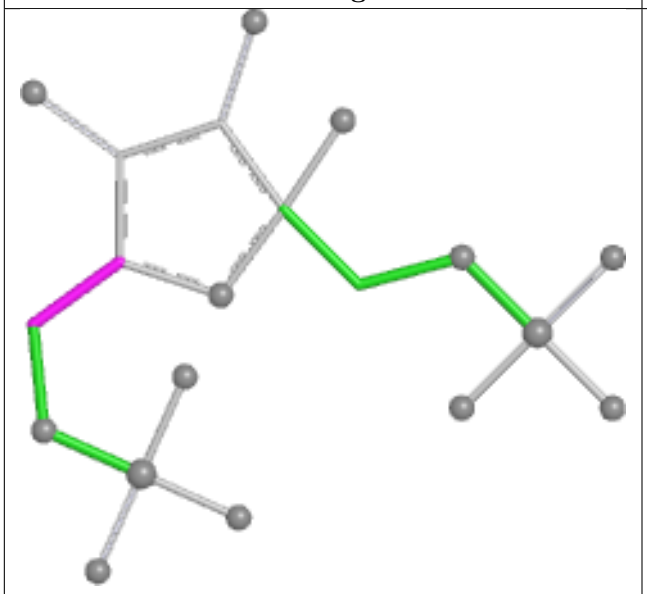

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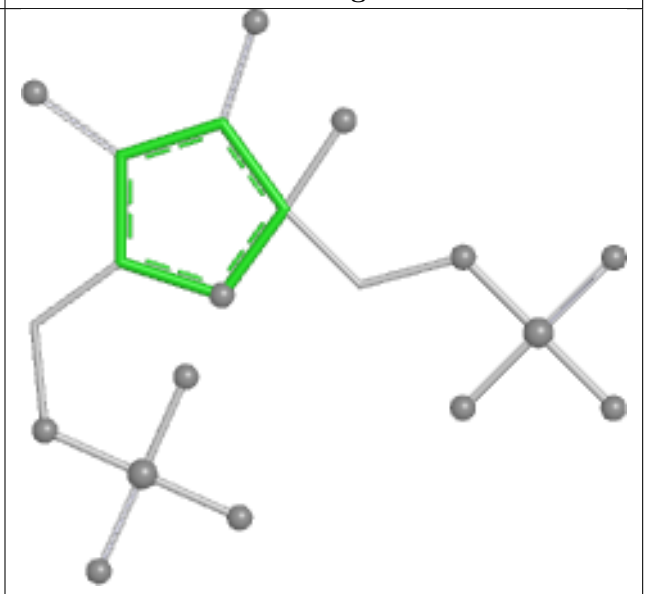
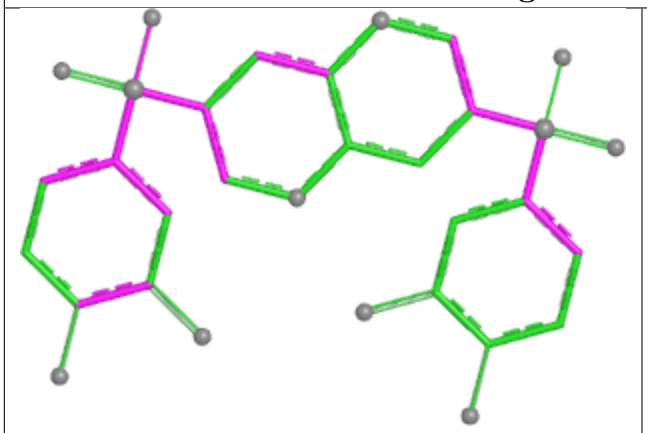


Rings

Ligand WW5 F 505



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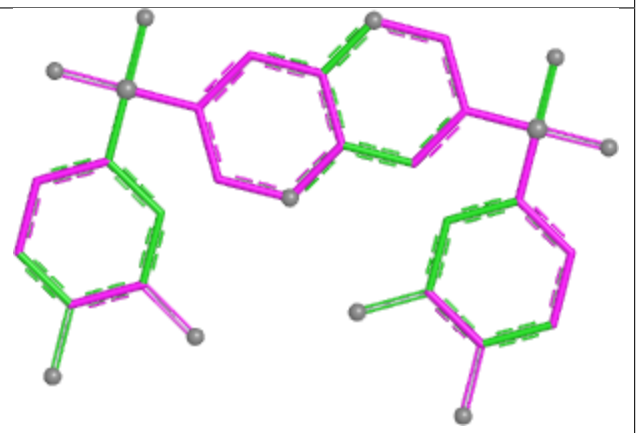
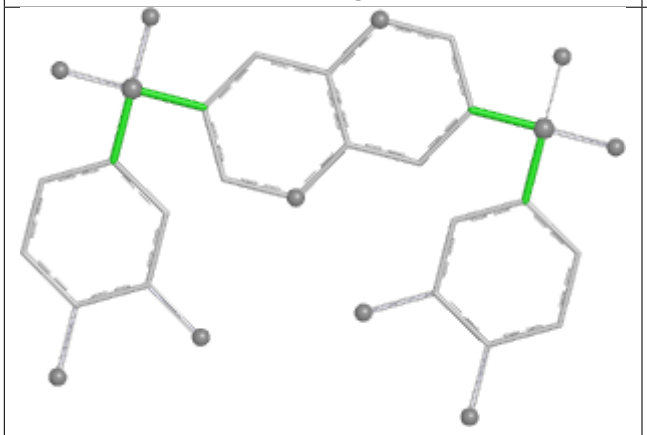


Bond angles



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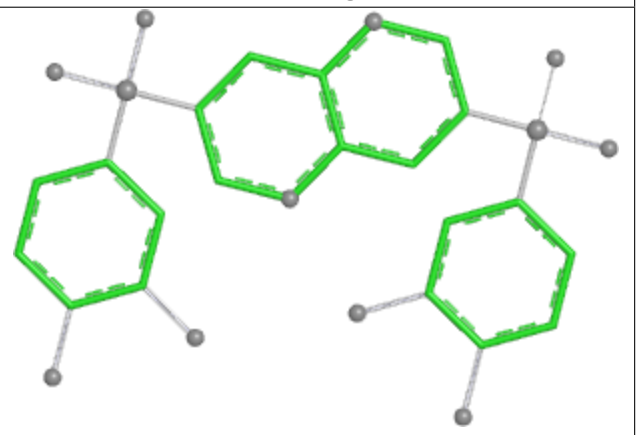
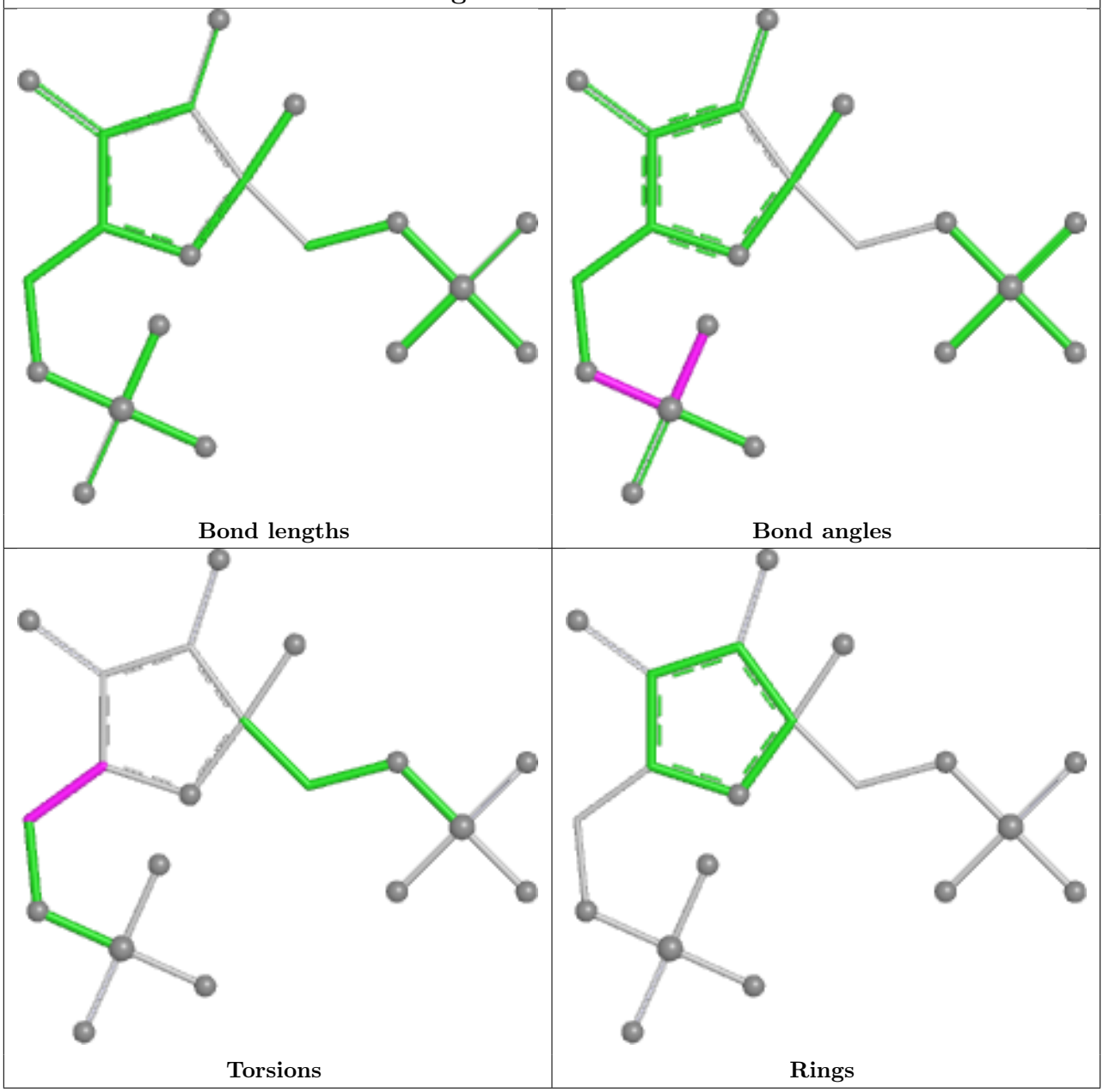
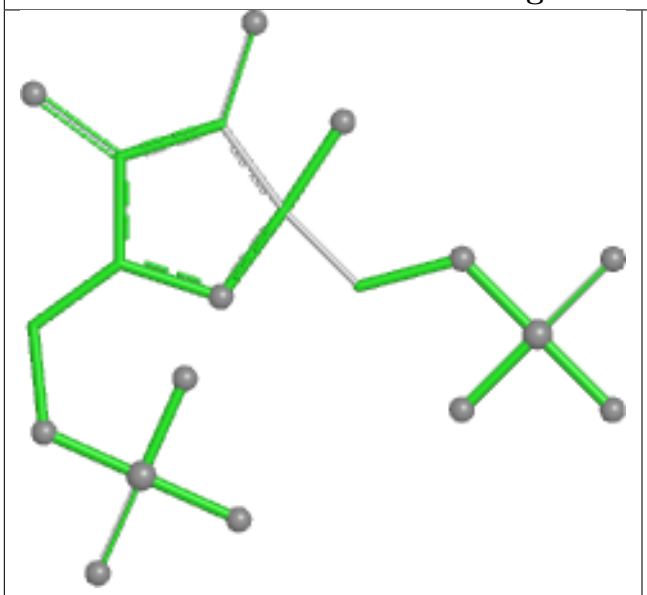


Rings

Ligand FBP G 501



Ligand FBP C 501



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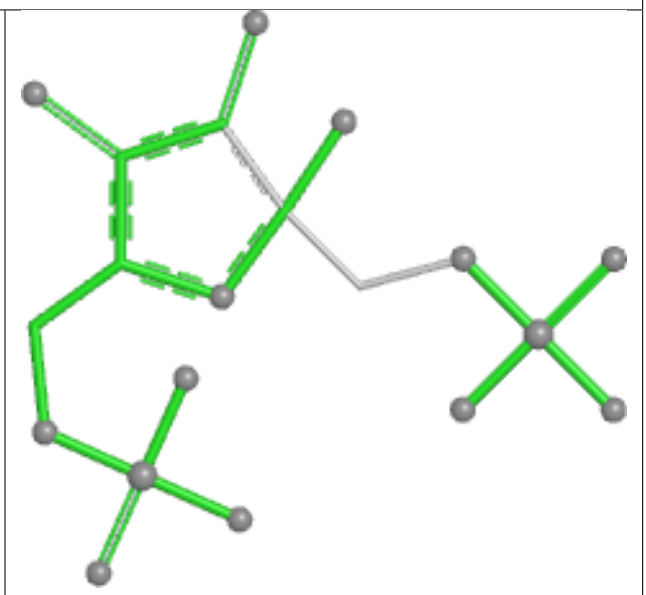
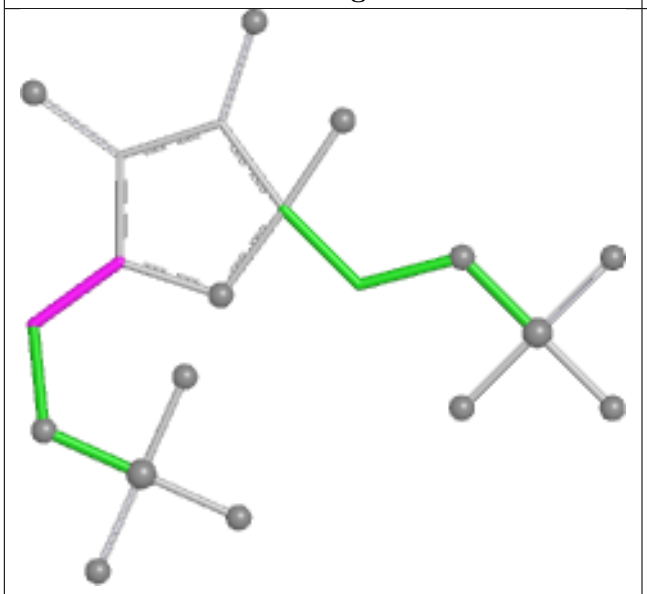


Bond angles



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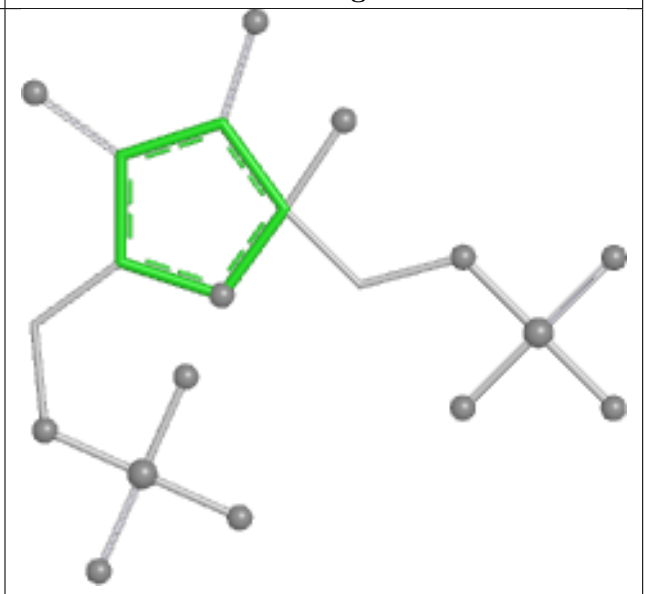
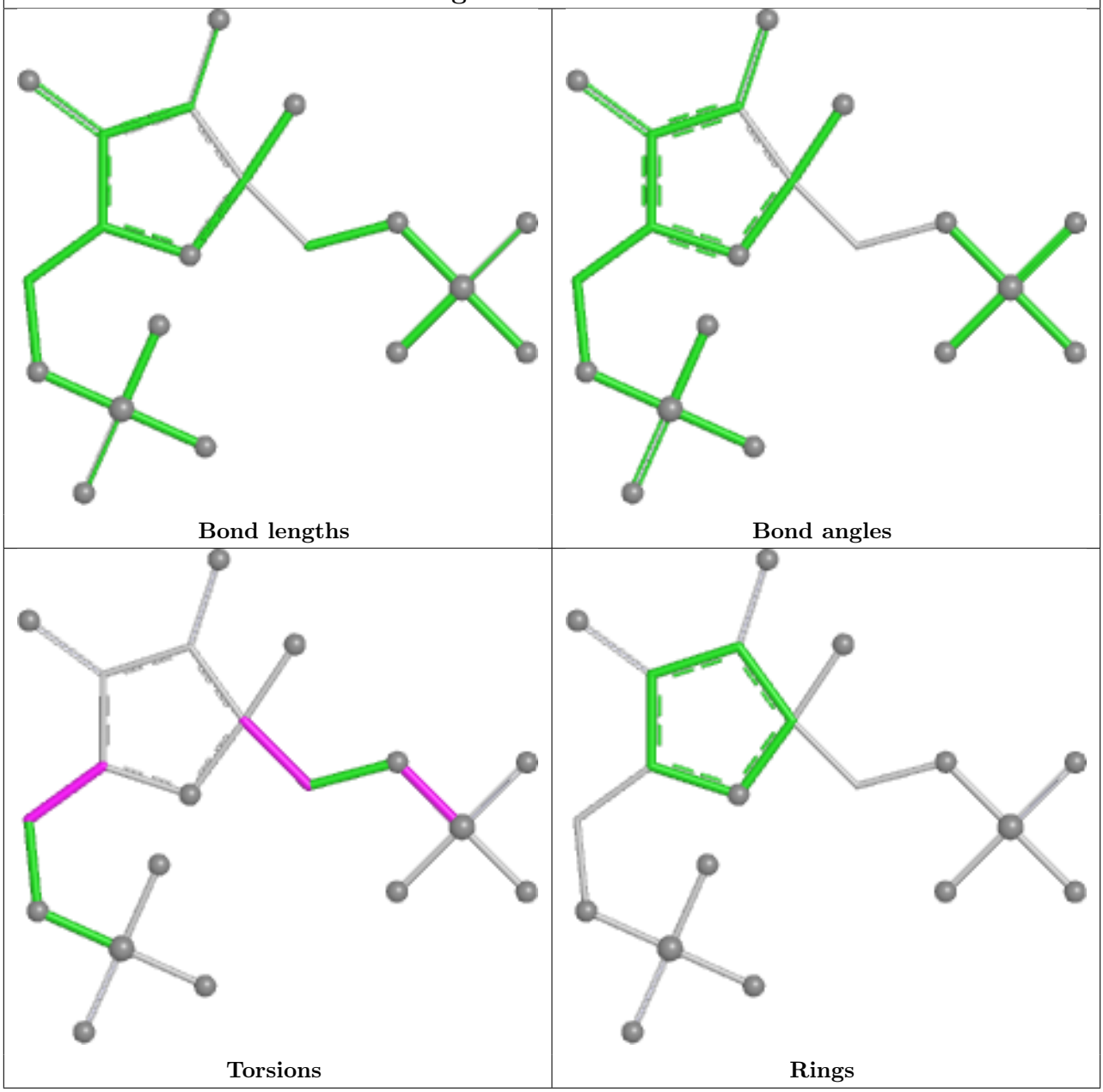
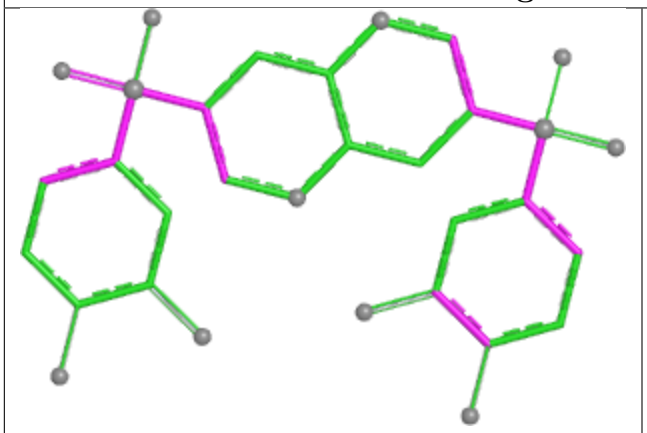


Rings

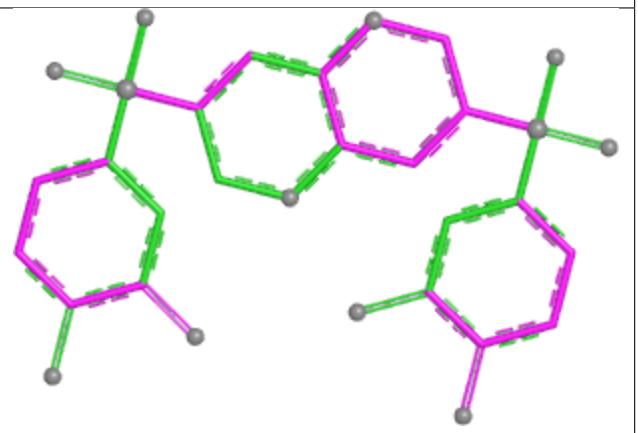
Ligand FBP H 501



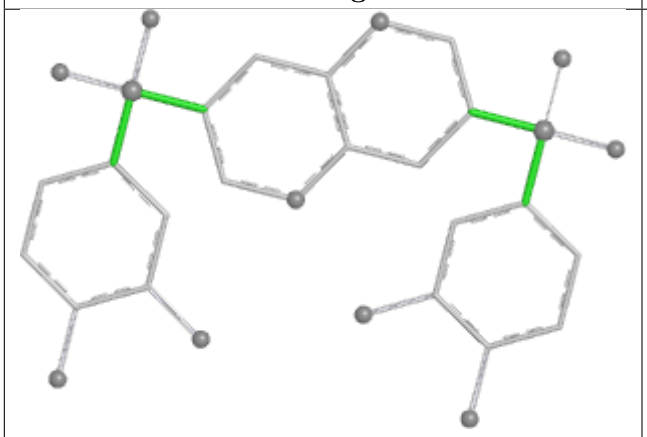
Ligand WW5 C 505



Bond lengths



Bond angles



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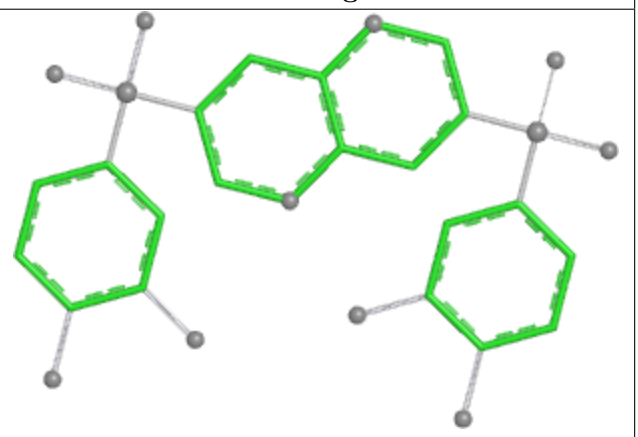
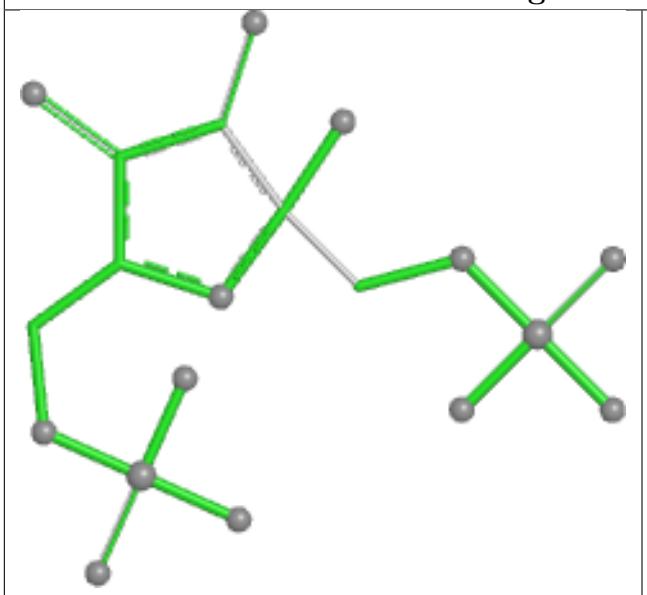
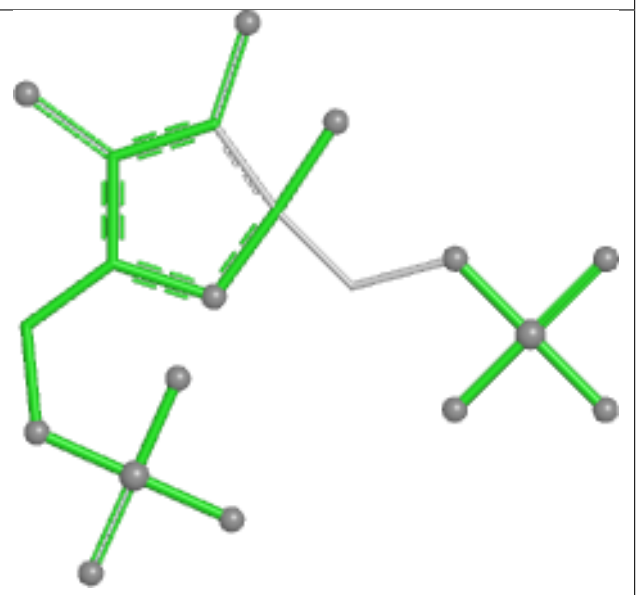


Rings

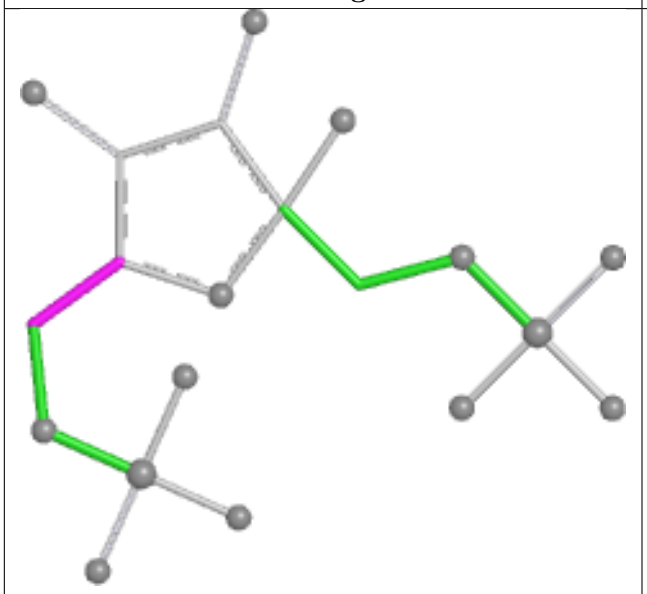
Ligand FBP F 501



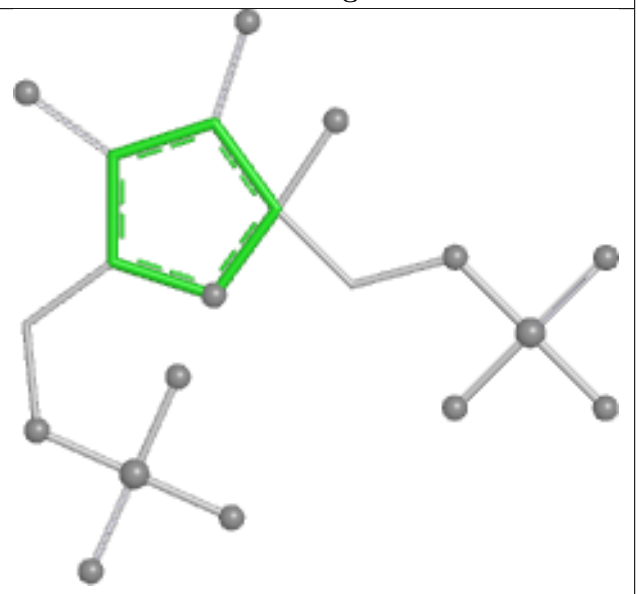
Bond lengths



Bond angles

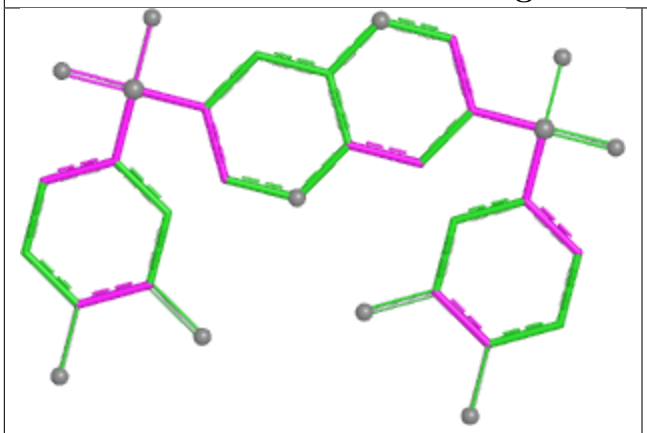


Torsions

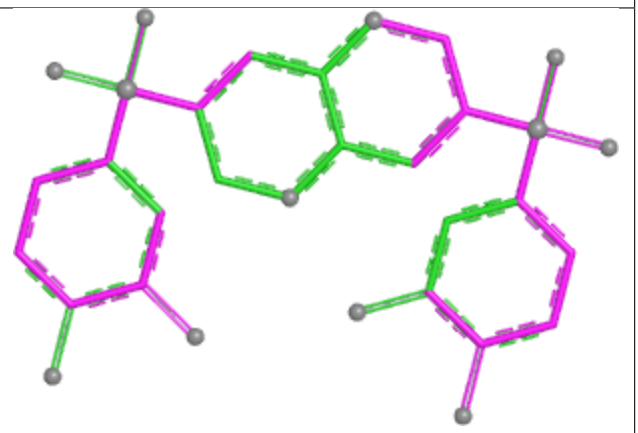


Rings

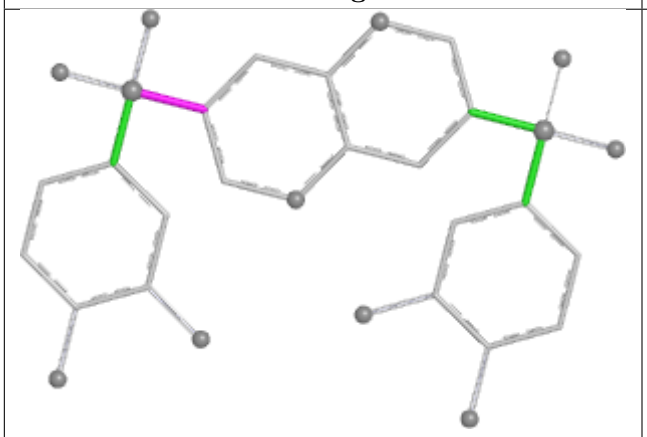
Ligand WW5 G 505



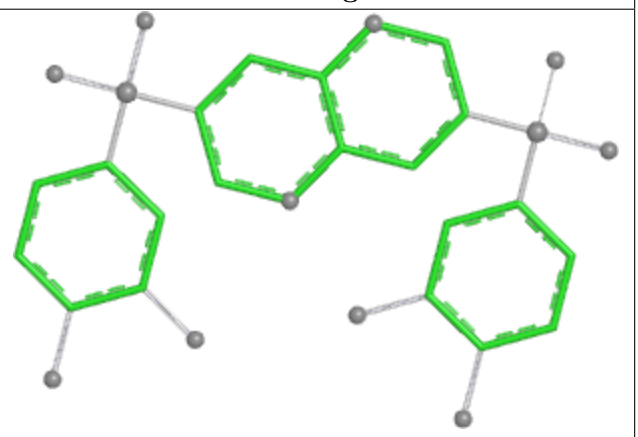
Bond lengths



Bond angles

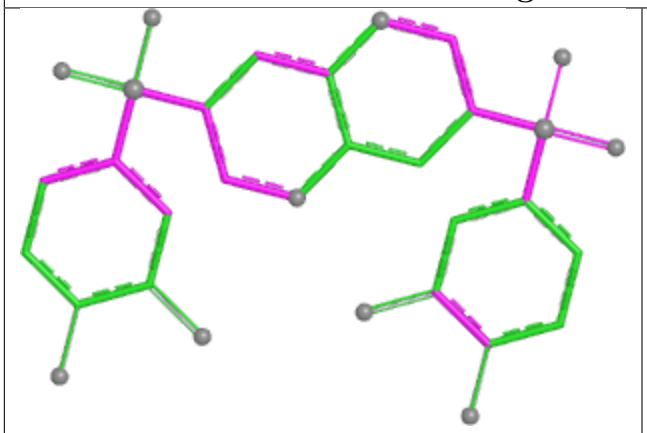


Torsions

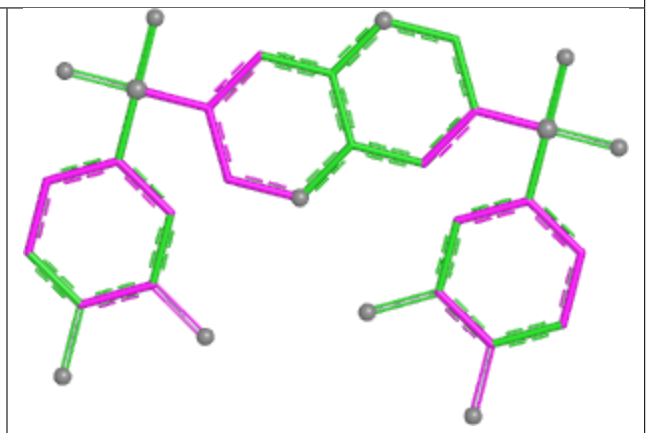


Rings

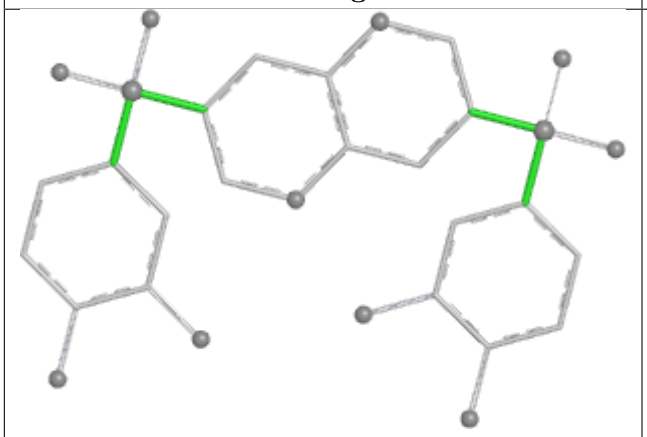
Ligand WW5 B 505



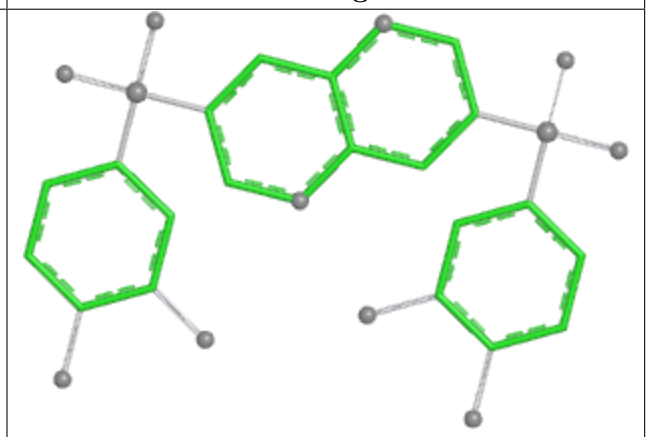
Bond lengths



Bond angles

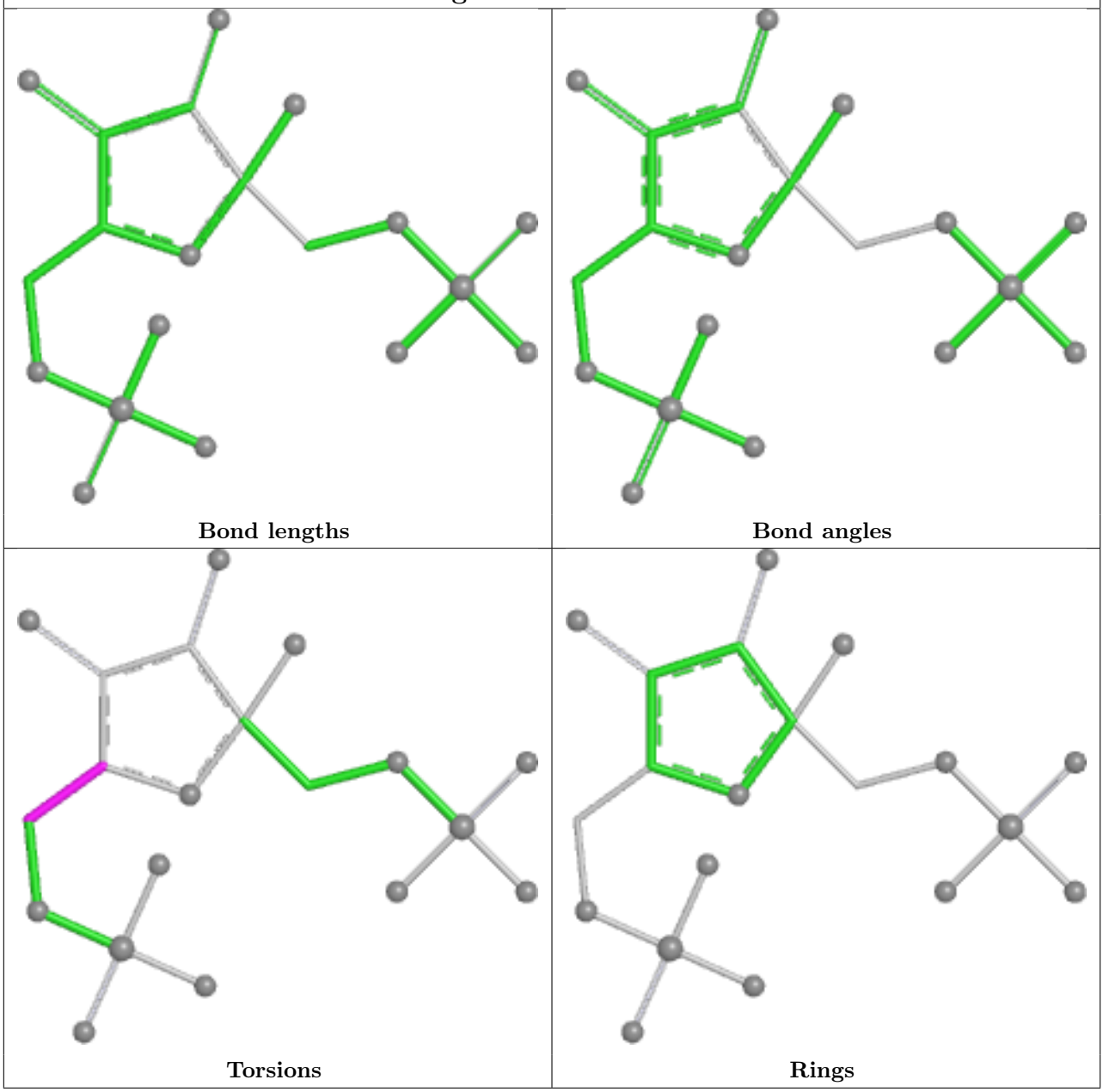


Torsions



Rings

Ligand FBP A 501



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	1.35	105 (24%)	2	2	19, 43, 74, 91	6 (1%)
1	B	436/447 (97%)	0.58	41 (9%)	14	15	11, 30, 61, 76	4 (0%)
1	C	426/447 (95%)	0.31	26 (6%)	27	29	11, 28, 53, 69	4 (0%)
1	D	425/447 (95%)	-0.10	12 (2%)	55	58	7, 20, 40, 79	6 (1%)
1	E	419/447 (93%)	0.87	58 (13%)	6	7	15, 37, 67, 85	5 (1%)
1	F	432/447 (96%)	0.49	33 (7%)	20	21	13, 31, 54, 76	7 (1%)
1	G	427/447 (95%)	0.24	27 (6%)	26	28	9, 26, 51, 87	7 (1%)
1	H	425/447 (95%)	-0.03	14 (3%)	49	52	8, 22, 44, 75	4 (0%)
All	All	3412/3576 (95%)	0.46	316 (9%)	14	15	7, 29, 62, 91	43 (1%)

The worst 5 of 316 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	115	LEU	6.6
1	A	395	ILE	6.5
1	F	133	PRO	6.5
1	E	114	PRO	6.4
1	B	115	LEU	6.4

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	A	503	1/1	0.81	0.17	44,44,44,44	0
4	MG	F	503	1/1	0.86	0.10	38,38,38,38	0
4	MG	B	503	1/1	0.87	0.10	31,31,31,31	0
4	MG	C	503	1/1	0.88	0.14	34,34,34,34	0
3	OXL	C	502	6/6	0.89	0.11	40,41,42,42	0
3	OXL	H	502	6/6	0.89	0.11	30,31,31,31	0
3	OXL	B	502	6/6	0.89	0.09	32,32,33,34	0
7	EDO	E	505	4/4	0.90	0.12	43,43,44,44	6
3	OXL	F	502	6/6	0.91	0.10	41,42,42,43	0
4	MG	E	503	1/1	0.91	0.10	36,36,36,36	0
3	OXL	E	502	6/6	0.92	0.09	35,36,37,37	0
2	FBP	A	501	20/20	0.92	0.11	42,46,47,47	0
4	MG	D	503	1/1	0.92	0.12	31,31,31,31	0
4	MG	H	503	1/1	0.93	0.14	28,28,28,28	0
3	OXL	D	502	6/6	0.94	0.08	32,32,32,33	0
2	FBP	E	501	20/20	0.94	0.09	33,35,39,39	0
5	K	E	504	1/1	0.94	0.07	70,70,70,70	0
5	K	F	504	1/1	0.94	0.07	55,55,55,55	0
6	WW5	F	505	32/32	0.94	0.09	28,30,34,34	14
3	OXL	A	502	6/6	0.94	0.07	49,49,50,50	0
6	WW5	G	505	32/32	0.95	0.08	32,33,36,37	14
5	K	A	504	1/1	0.95	0.07	59,59,59,59	0
2	FBP	F	501	20/20	0.96	0.07	30,33,38,38	0
6	WW5	C	505	32/32	0.96	0.07	28,30,31,31	14
3	OXL	G	502	6/6	0.96	0.06	29,30,32,32	0
5	K	B	504	1/1	0.96	0.10	57,57,57,57	0
7	EDO	B	506	4/4	0.96	0.07	26,26,26,26	6
2	FBP	B	501	20/20	0.96	0.07	28,31,37,37	0
6	WW5	B	505	32/32	0.97	0.07	25,27,28,29	14
4	MG	G	503	1/1	0.97	0.06	23,23,23,23	0
5	K	G	504	1/1	0.97	0.07	39,39,39,39	0
2	FBP	D	501	20/20	0.98	0.05	11,14,15,15	0
5	K	C	504	1/1	0.98	0.05	42,42,42,42	0
2	FBP	G	501	20/20	0.98	0.04	20,21,24,24	0
2	FBP	H	501	20/20	0.98	0.05	13,15,17,17	0
2	FBP	C	501	20/20	0.98	0.06	18,21,25,26	0
5	K	H	504	1/1	0.98	0.05	35,35,35,35	0

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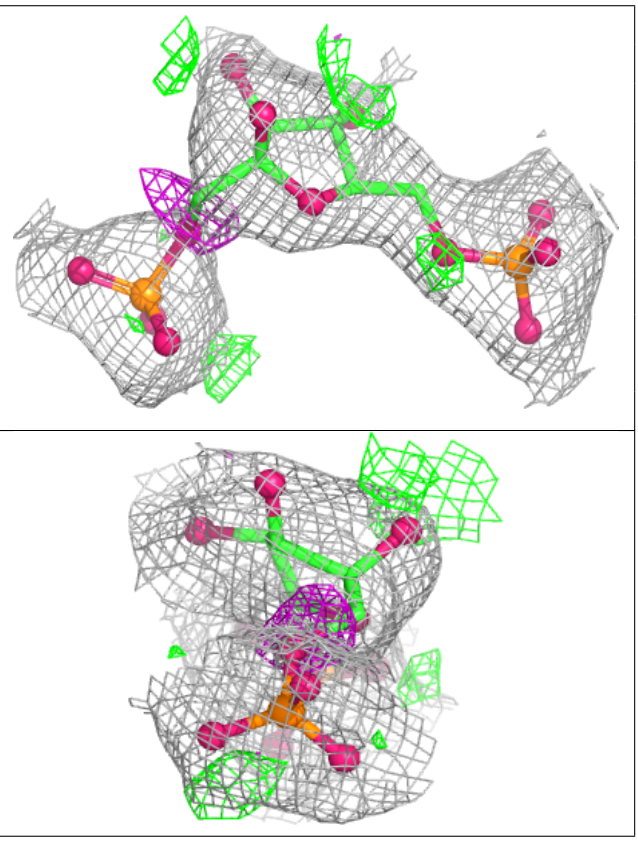
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	K	D	504	1/1	0.99	0.04	29,29,29,29	0

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.

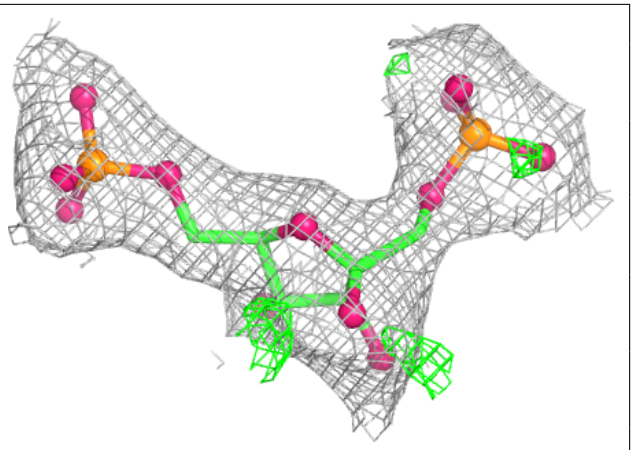
Electron density around FBP A 501:

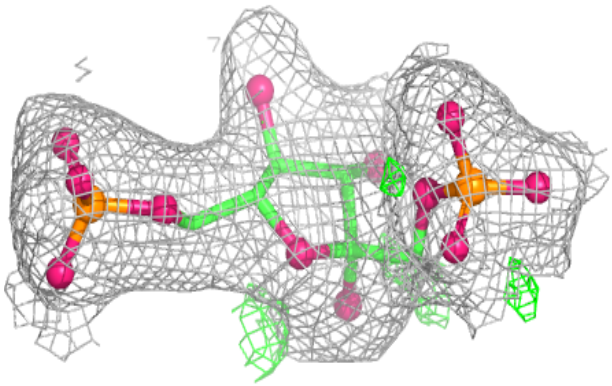
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

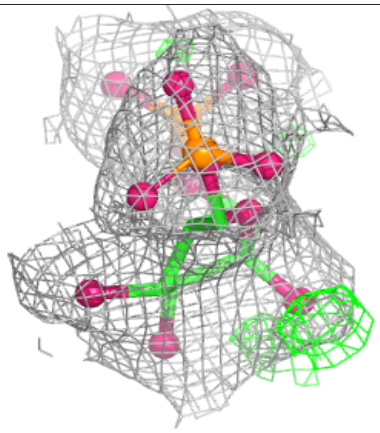


Electron density around FBP E 501:

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

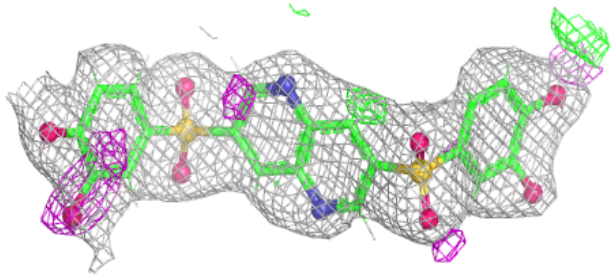


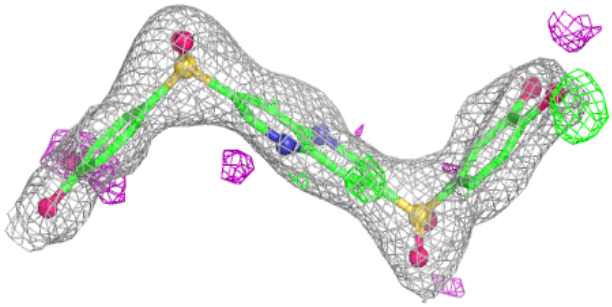


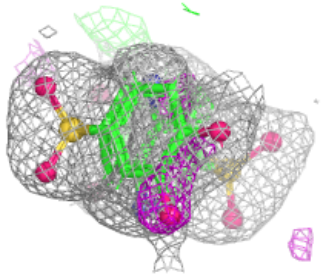


Electron density around WW5 F 505:

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

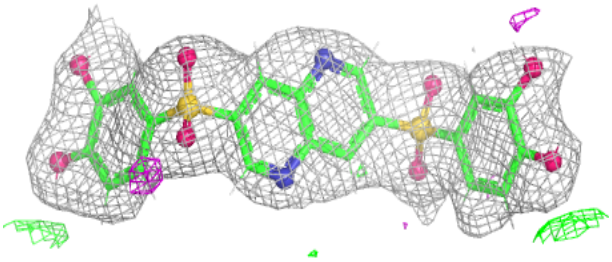


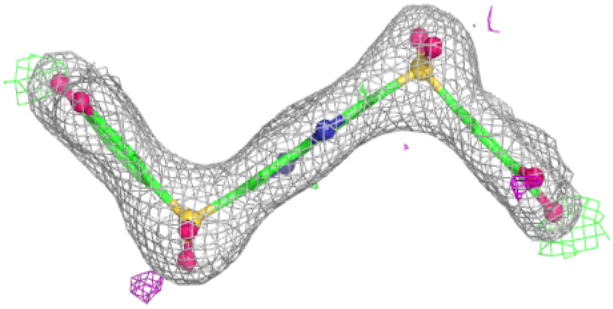


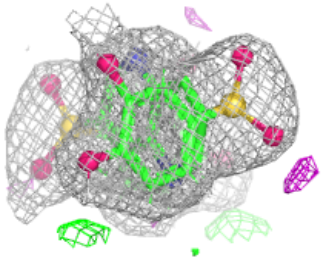


Electron density around WW5 G 505:

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

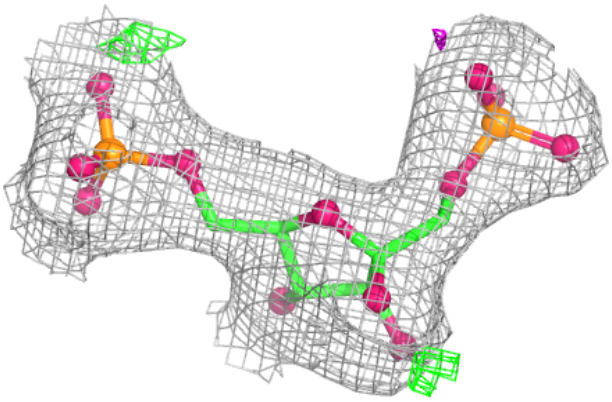


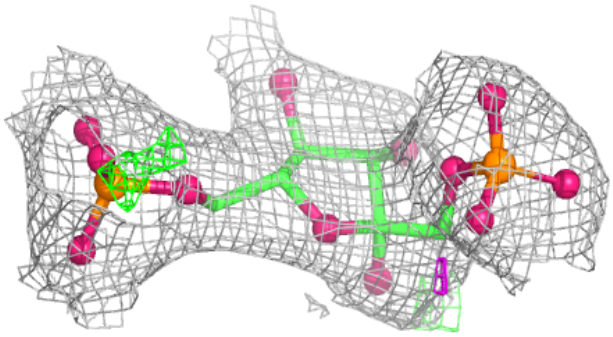


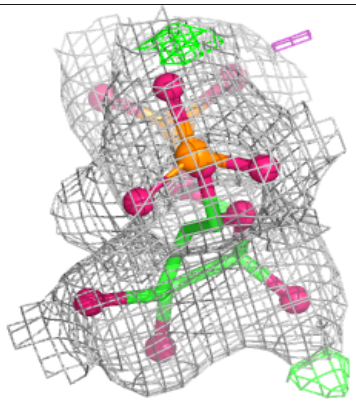


Electron density around FBP F 501:

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

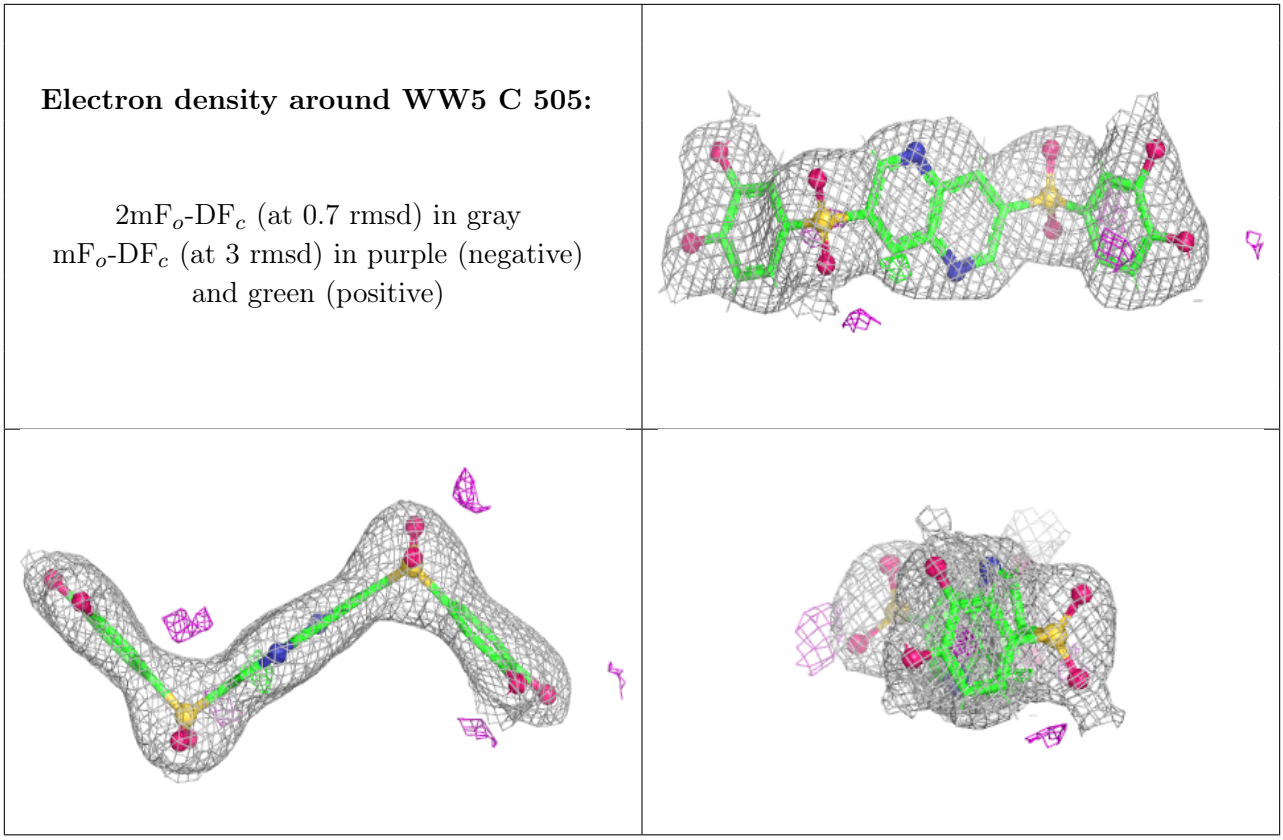






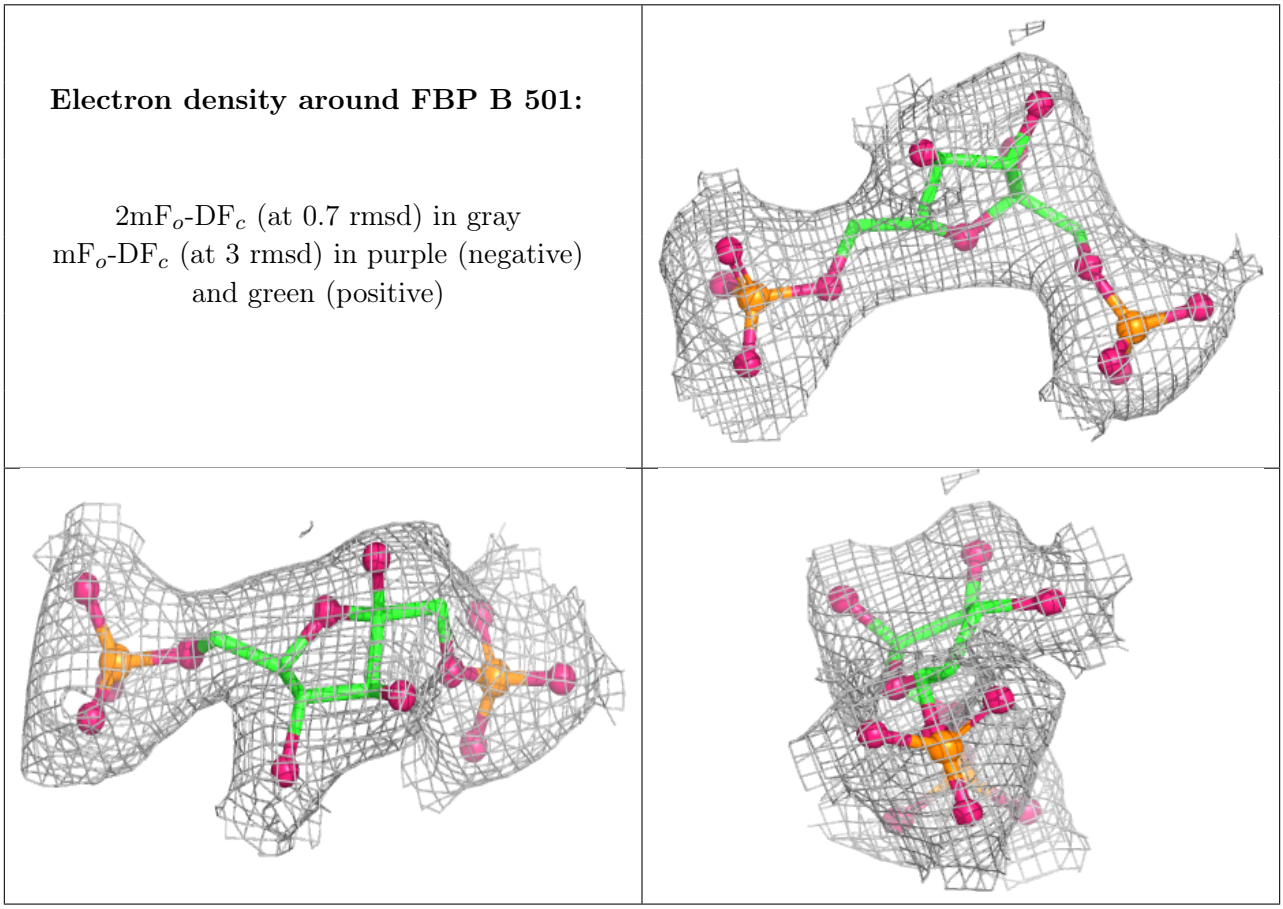
Electron density around WW5 C 505:

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



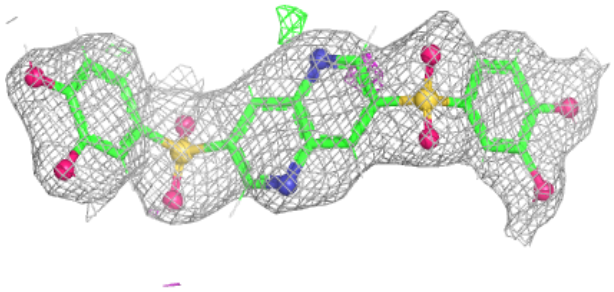
Electron density around FBP B 501:

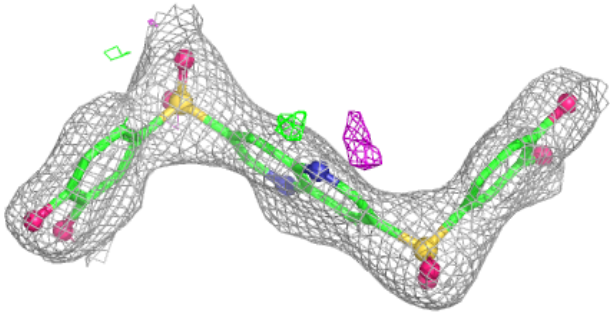
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

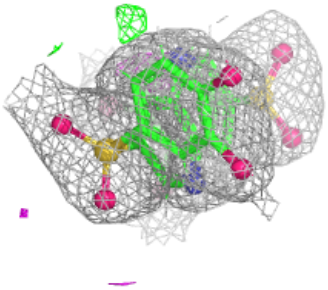


Electron density around WW5 B 505:

$2mF_o$-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 501:

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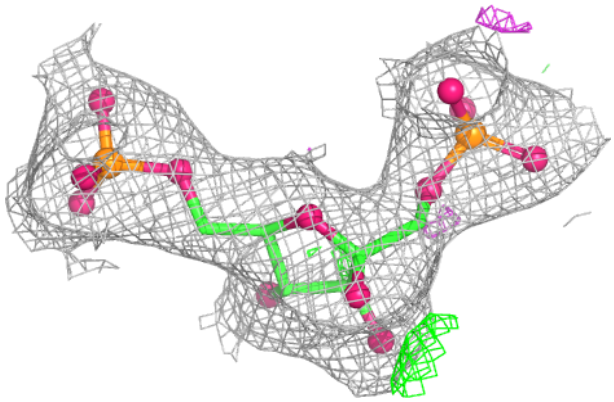
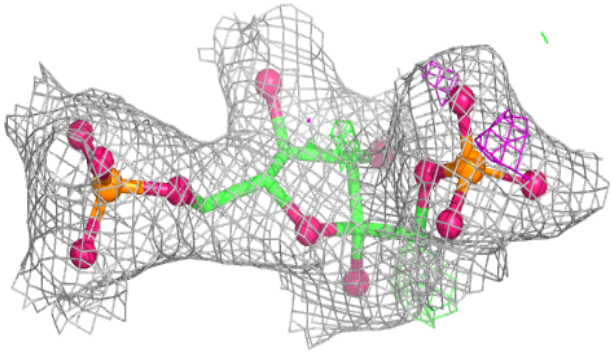
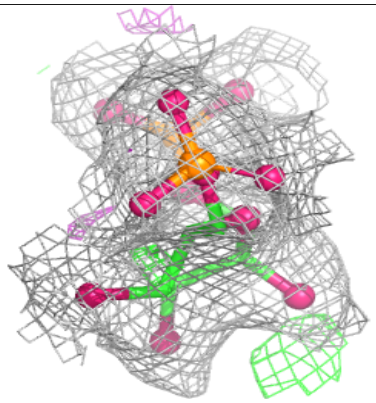
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

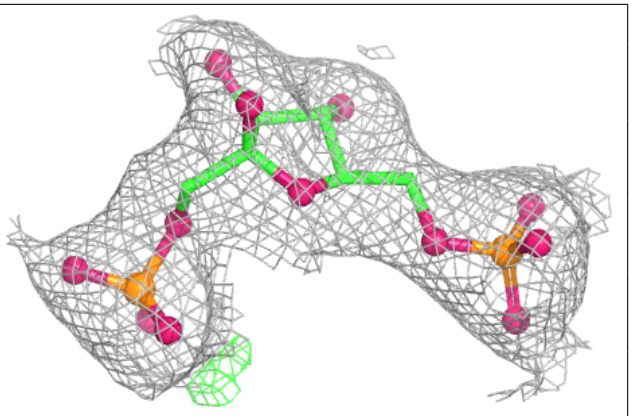


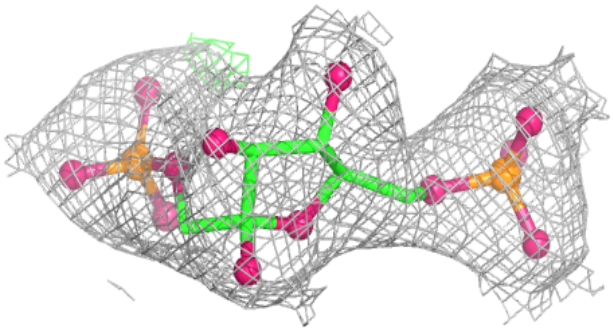


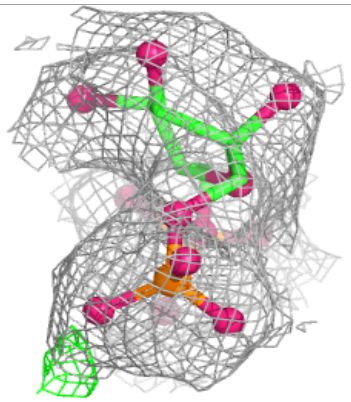


Electron density around FBP G 501:

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

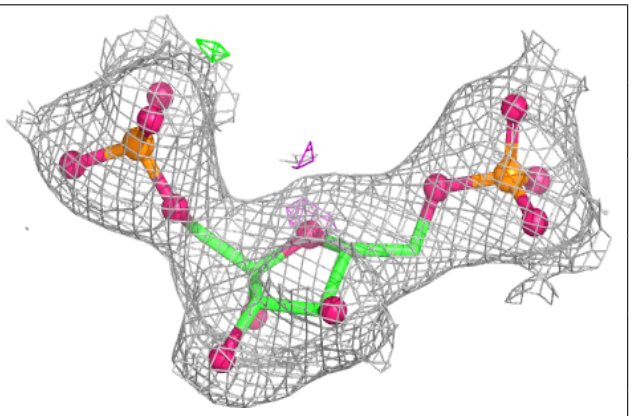


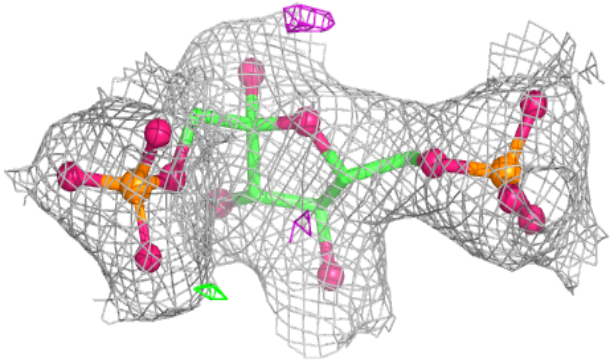


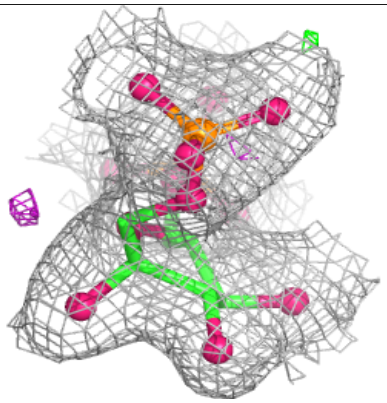


Electron density around FBP H 501:

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

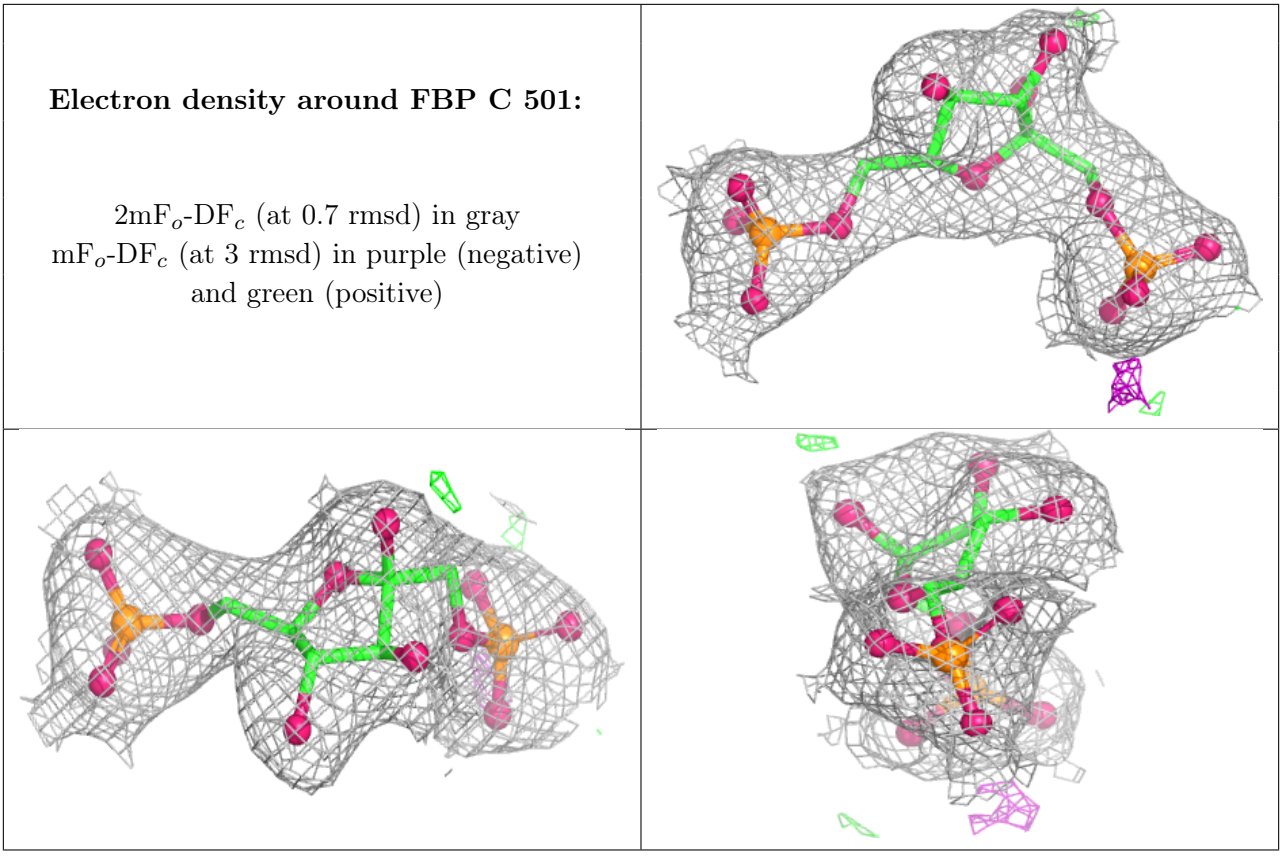






Electron density around FBP C 501:

$2mF_o$-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.