Full wwPDB X-ray Structure Validation Report (i)

Apr 3, 2023 – 05:48 PM EDT

PDB ID	:	7FS6
Title	:	Structure of liver pyruvate kinase in complex with allosteric modulator 18
Authors	:	Lulla, A.; Nilsson, O.; Brear, P.; Nain-Perez, A.; Grotli, M.; Hyvonen, M.
Deposited on	:	2022-12-18
Resolution	:	2.24 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 (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:

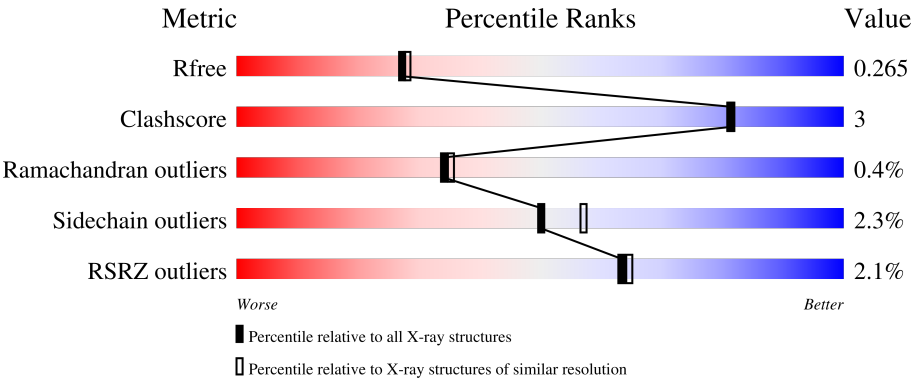
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 2.24 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}	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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	3% 84% 10% 6%
1	B	447	2% 90% 7%
1	C	447	3% 86% 9% 5%
1	D	447	% 88% 6% 5%
1	E	447	2% 86% 8% 6%

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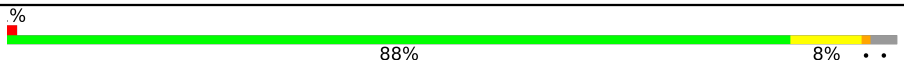
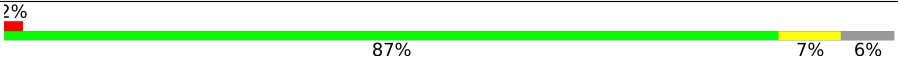
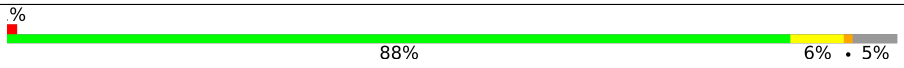
Mol	Chain	Length	Quality of chain
1	F	447	
1	G	447	
1	H	447	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXL	D	603	-	X	-	-
3	OXL	F	602	-	X	-	-
5	K	A	604	-	-	-	X
5	K	B	604	-	-	-	X
5	K	E	604	-	-	-	X
5	K	F	604	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 28136 atoms, of which 273 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pyruvate kinase PKLR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	6	0
			3236	2034	585	597	20			
1	B	436	Total	C	N	O	S	0	4	0
			3329	2090	604	615	20			
1	C	425	Total	C	N	O	S	0	4	0
			3247	2040	585	603	19			
1	D	425	Total	C	N	O	S	0	6	0
			3252	2042	590	601	19			
1	E	419	Total	C	N	O	S	0	5	0
			3210	2018	579	593	20			
1	F	432	Total	C	N	O	S	0	7	0
			3321	2090	597	614	20			
1	G	421	Total	C	N	O	S	0	6	0
			3231	2031	581	600	19			
1	H	425	Total	C	N	O	S	0	4	0
			3251	2040	594	598	19			

There are 64 discrepancies between the modelled and reference sequences:

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

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

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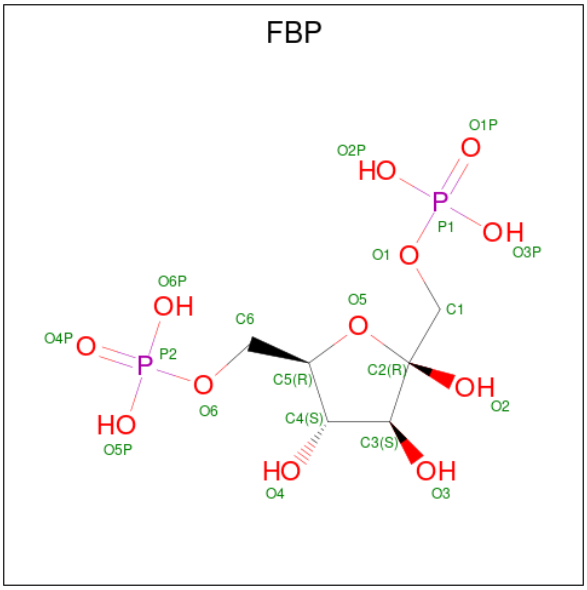
Chain	Residue	Modelled	Actual	Comment	Reference
G	132	GLY	-	linker	UNP P30613
H	-1	GLY	-	expression tag	UNP P30613
H	0	SER	-	expression tag	UNP P30613
H	1	MET	-	expression tag	UNP P30613
H	2	GLU	-	expression tag	UNP P30613
H	12	ASP	SER	conflict	UNP P30613
H	130	GLY	-	linker	UNP P30613
H	131	SER	-	linker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

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



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

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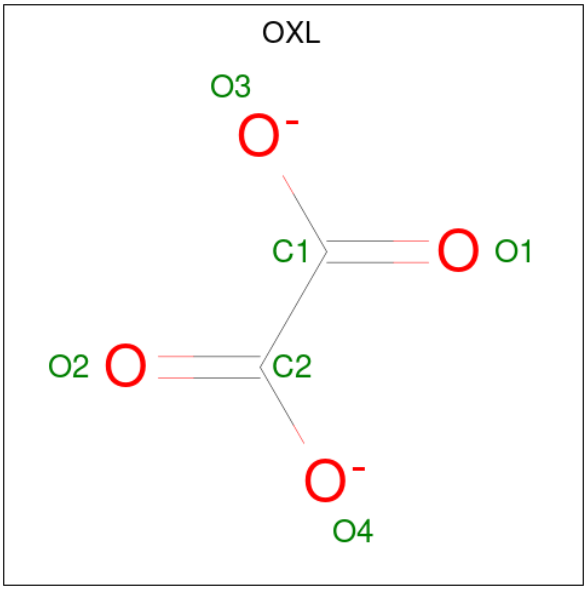
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C O P 20 6 12 2	0	0
2	H	1	Total C O P 20 6 12 2	0	0

- Molecule 3 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).



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

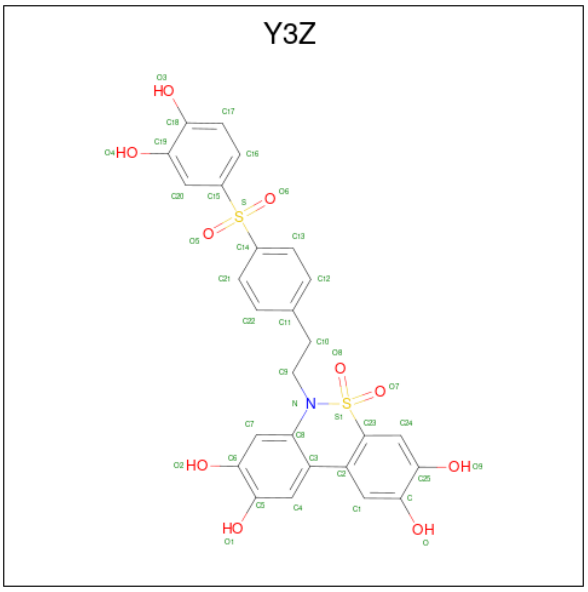
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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 (three-letter code: 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 (10aM)-6-{2-[4-(3,4-dihydroxybenzene-1-sulfonyl)phenyl]ethyl}-2,3,8,9-tetrahydroxy-5lambda 6 -dibenzo[c,e][1,2]thiazine-5,5(6H)-dione (three-letter code: Y3Z) (formula: $C_{26}H_{21}NO_{10}S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	S	42	1
			120	52	42	2	20	4		
6	B	1	Total	C	H	N	O	S	21	0
			60	26	21	1	10	2		
6	B	1	Total	C	H	N	O	S	21	0
			60	26	21	1	10	2		
6	D	1	Total	C	H	N	O	S	21	0
			60	26	21	1	10	2		
6	D	1	Total	C	H	N	O	S	21	0
			60	26	21	1	10	2		
6	D	1	Total	C	H	N	O	S	21	0
			60	26	21	1	10	2		
6	E	1	Total	C	H	N	O	S	21	0
			60	26	21	1	10	2		
6	F	1	Total	C	H	N	O	S	21	0
			60	26	21	1	10	2		
6	F	1	Total	C	H	N	O	S	21	0
			60	26	21	1	10	2		
6	H	1	Total	C	H	N	O	S	21	0
			60	26	21	1	10	2		
6	H	1	Total	C	H	N	O	S	21	0
			60	26	21	1	10	2		
6	H	1	Total	C	H	N	O	S	21	0
			60	26	21	1	10	2		

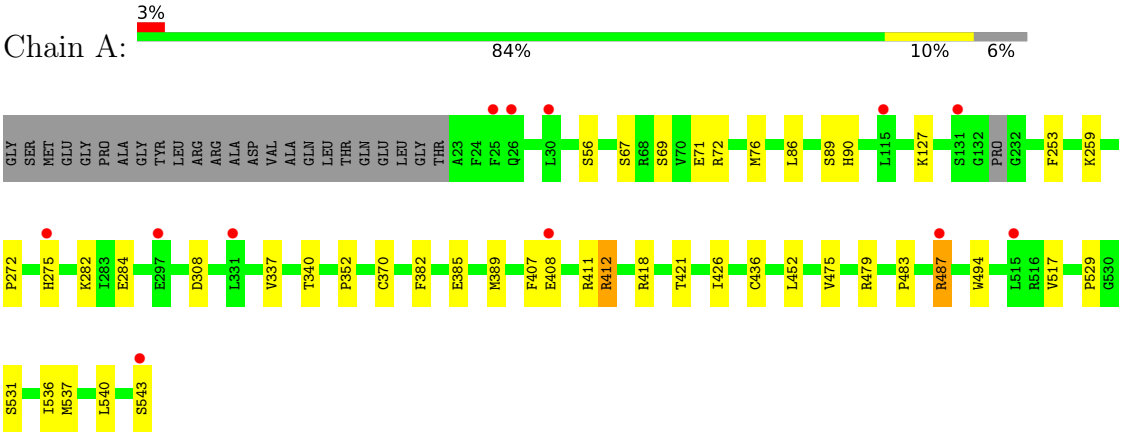
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	78	Total O 78 78	0	0
7	B	123	Total O 123 123	0	0
7	C	170	Total O 170 170	0	0
7	D	158	Total O 158 158	0	0
7	E	72	Total O 72 72	0	0
7	F	123	Total O 123 123	0	0
7	G	182	Total O 182 182	0	0
7	H	149	Total O 149 149	0	0

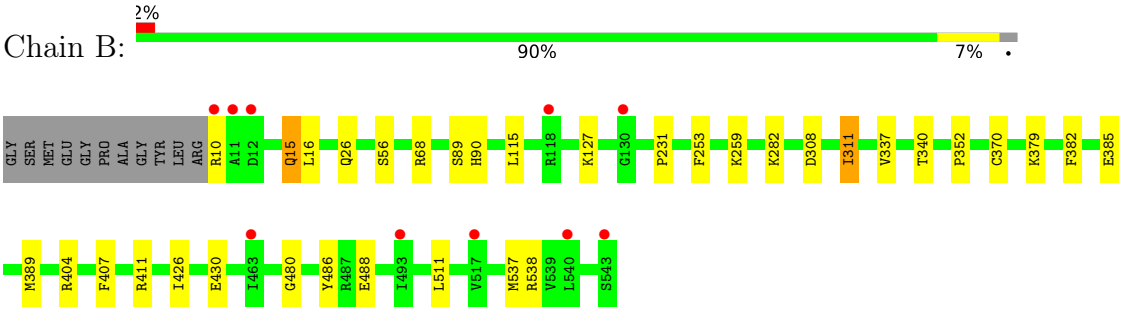
3 Residue-property plots (i)

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

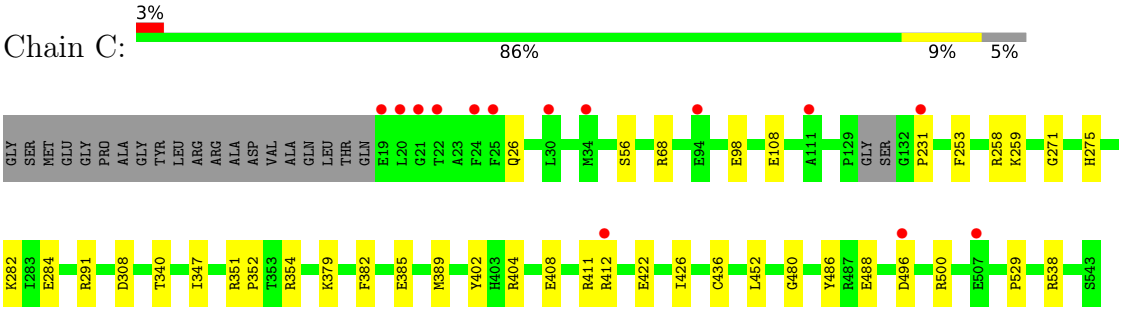
• Molecule 1: Pyruvate kinase PKLR



• Molecule 1: Pyruvate kinase PKLR

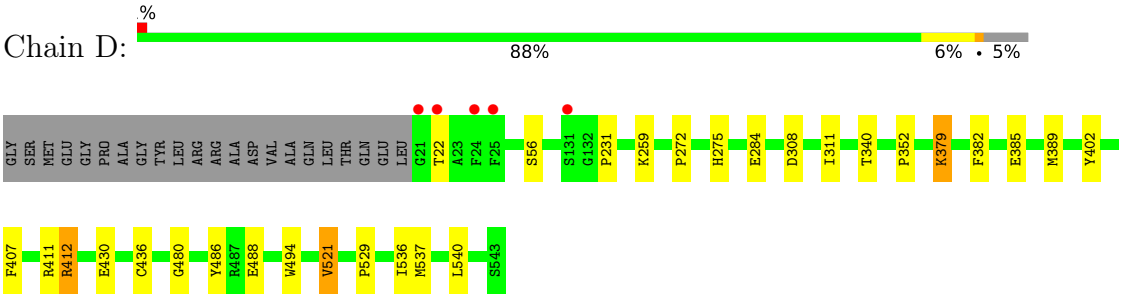


• Molecule 1: Pyruvate kinase PKLR



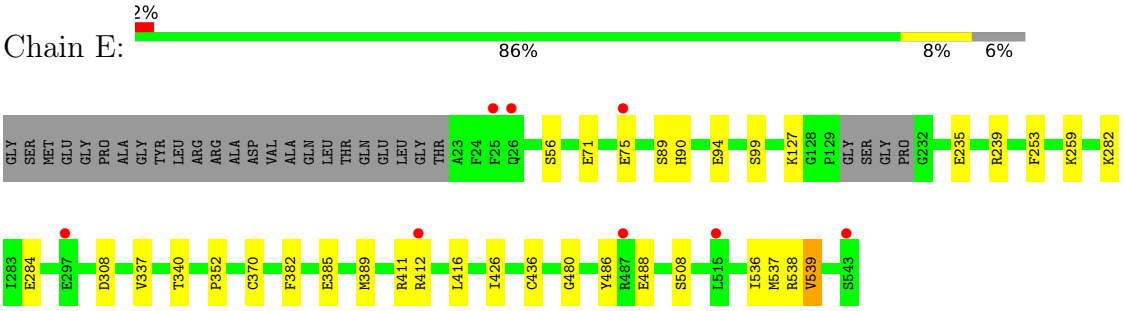
• Molecule 1: Pyruvate kinase PKLR

Chain D:



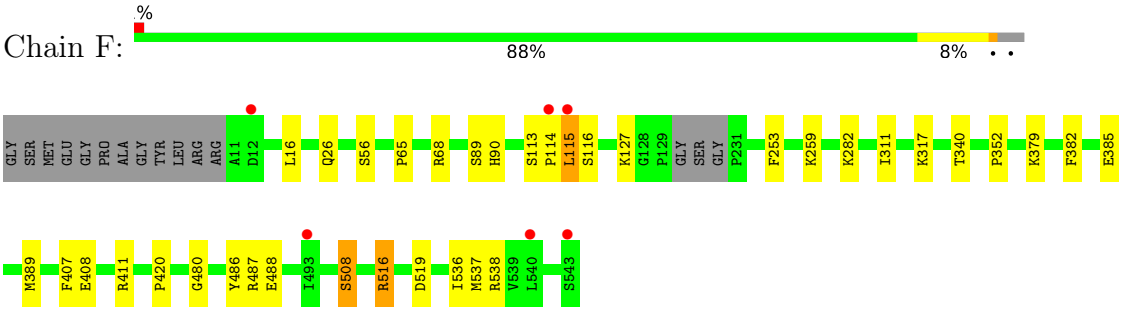
• Molecule 1: Pyruvate kinase PKLR

Chain E:



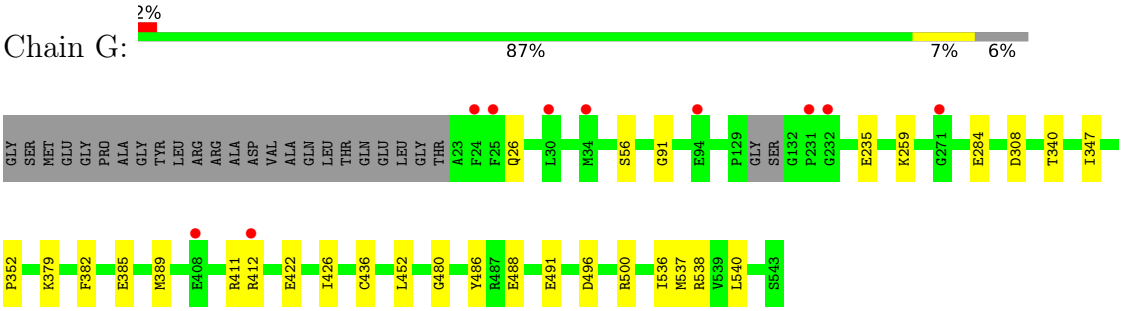
• Molecule 1: Pyruvate kinase PKLR

Chain F:



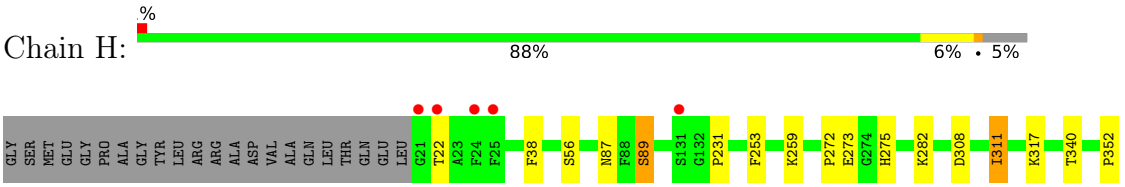
• Molecule 1: Pyruvate kinase PKLR

Chain G:



• Molecule 1: Pyruvate kinase PKLR

Chain H:




K379
F382
E385
M389
R404
F407
R411
C436
G480
Y486
R487
E488
W494
R516
P529
I536
M537
R538
S543

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	210.69Å 117.24Å 188.53Å 90.00° 89.58° 90.00°	Depositor
Resolution (Å)	105.34 – 2.24 105.34 – 2.24	Depositor EDS
% Data completeness (in resolution range)	62.8 (105.34-2.24) 62.8 (105.34-2.24)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.77 (at 2.25Å)	Xtriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, R_{free}	0.250 , 0.275 0.242 , 0.265	Depositor DCC
R_{free} test set	7022 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	39.5	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 62.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.000 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.000 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.005 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	28136	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 98.91 % 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 7.2334e-12. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, OXL, MG, FBP, Y3Z

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	0.38	0/3307	0.54	0/4469
1	B	0.42	0/3396	0.55	0/4592
1	C	0.46	0/3313	0.57	0/4479
1	D	0.45	0/3326	0.56	0/4497
1	E	0.38	0/3278	0.53	0/4430
1	F	0.43	0/3396	0.55	0/4591
1	G	0.47	0/3303	0.58	0/4465
1	H	0.44	0/3316	0.56	0/4483
All	All	0.43	0/26635	0.55	0/36006

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3236	0	3299	24	0
1	B	3329	0	3395	18	0
1	C	3247	0	3299	23	0
1	D	3252	0	3310	17	0
1	E	3210	0	3270	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3321	0	3394	21	0
1	G	3231	0	3284	18	1
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
2	D	20	0	10	0	0
2	E	20	0	10	0	0
2	F	20	0	10	0	0
2	G	20	0	10	0	0
2	H	20	0	10	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0
3	G	6	0	0	0	0
3	H	6	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	78	42	0	1	0
6	B	78	42	0	2	0
6	D	117	63	0	4	0
6	E	39	21	0	0	0
6	F	78	42	0	3	0
6	H	117	63	0	2	0
7	A	78	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	123	0	0	0	0
7	C	170	0	0	2	0
7	D	158	0	0	0	0
7	E	72	0	0	1	0
7	F	123	0	0	1	0
7	G	182	0	0	0	0
7	H	149	0	0	3	1
All	All	27863	273	26637	140	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 (140) 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:H:308:ASP:O	1:H:311:ILE:HG13	1.72	0.88
1:G:538:ARG:HG2	1:H:536:ILE:HG12	1.67	0.77
1:C:529:PRO:HG2	1:G:235:GLU:HG2	1.67	0.75
1:E:235:GLU:O	1:E:239:ARG:HD3	1.91	0.70
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.75	0.69
1:C:538:ARG:HG2	1:D:536:ILE:HG12	1.75	0.69
1:E:536:ILE:HG12	1:F:538:ARG:HG2	1.75	0.69
1:E:538:ARG:HG2	1:F:536:ILE:HG12	1.75	0.68
1:C:411:ARG:HG3	1:C:426:ILE:HD11	1.76	0.66
1:C:500:ARG:HD3	7:C:749:HOH:O	1.94	0.66
1:G:411:ARG:HG3	1:G:426:ILE:HD11	1.80	0.64
6:A:605[A]:Y3Z:O5	1:C:402:TYR:HB3	1.98	0.63
1:B:407:PHE:CD2	1:B:411:ARG:NH1	2.67	0.63
1:D:379:LYS:HE2	6:D:607:Y3Z:O7	2.00	0.61
1:A:418[A]:ARG:HG3	1:B:16:LEU:HD11	1.84	0.59
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.84	0.59
1:A:67:SER:HA	1:A:72:ARG:HG2	1.83	0.59
1:E:411:ARG:HG2	1:E:426:ILE:HD11	1.83	0.59
6:B:606:Y3Z:C21	6:B:606:Y3Z:C20	2.78	0.59
1:A:517:VAL:HG13	1:A:543:SER:HB2	1.85	0.58
1:F:114:PRO:HB3	1:F:487:ARG:HE	1.68	0.57
1:C:422[A]:GLU:HG3	1:C:452:LEU:HD13	1.86	0.56
1:H:379:LYS:HD3	6:H:607:Y3Z:O7	2.06	0.56
1:F:407:PHE:CE2	1:F:411:ARG:NH1	2.74	0.56
1:G:537:MET:HE1	1:H:537:MET:HG2	1.88	0.55
1:F:65:PRO:HG2	1:F:379:LYS:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:412:ARG:CZ	1:H:404:ARG:HD3	2.37	0.55
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.88	0.55
1:G:491:GLU:HG3	1:G:500:ARG:HD2	1.89	0.55
1:H:538[A]:ARG:HD2	7:H:724:HOH:O	2.06	0.55
1:G:537:MET:CE	1:H:537:MET:HG2	2.37	0.54
1:F:311:ILE:HD11	6:F:605:Y3Z:C25	2.37	0.54
1:B:115:LEU:HD13	1:B:511:LEU:HB3	1.91	0.53
1:E:539:VAL:HG22	1:F:420:PRO:HB3	1.91	0.53
1:G:56:SER:HB2	1:G:480:GLY:HA2	1.90	0.53
1:C:351:ARG:HH22	1:C:354:ARG:HH22	1.56	0.52
1:B:308:ASP:O	1:B:311:ILE:HD13	2.10	0.52
1:H:272:PRO:HA	1:H:275[A]:HIS:CE1	2.44	0.52
1:H:56:SER:HB2	1:H:480:GLY:HA2	1.92	0.51
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.93	0.51
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.93	0.51
1:A:272:PRO:HA	1:A:275:HIS:NE2	2.26	0.51
1:D:311:ILE:HD13	6:D:606:Y3Z:O9	2.10	0.51
1:E:89:SER:HA	1:E:127:LYS:HG3	1.92	0.50
1:C:496:ASP:HB3	7:C:797:HOH:O	2.11	0.50
1:D:311:ILE:CD1	6:D:606:Y3Z:O9	2.59	0.50
1:D:402:TYR:HB3	6:D:601:Y3Z:O7	2.11	0.50
1:F:56:SER:HB2	1:F:480:GLY:HA2	1.94	0.50
1:D:272:PRO:HA	1:D:275[A]:HIS:CE1	2.46	0.50
1:G:347:ILE:HD13	1:G:379:LYS:HE3	1.93	0.50
1:G:412:ARG:NH2	1:H:404:ARG:HD3	2.27	0.50
1:B:15:GLN:HE21	1:B:15:GLN:HA	1.76	0.49
1:F:407:PHE:CD2	1:F:411:ARG:NH1	2.75	0.49
1:G:486:TYR:CZ	1:G:488:GLU:HB2	2.47	0.49
1:H:407:PHE:O	1:H:411:ARG:HG3	2.12	0.49
1:C:271:GLY:O	1:C:275:HIS:CE1	2.65	0.49
1:D:521:VAL:HG12	1:D:540:LEU:HB3	1.95	0.49
6:F:606:Y3Z:C20	6:F:606:Y3Z:C13	2.87	0.49
1:C:382:PHE:HB3	1:C:385:GLU:HB2	1.95	0.48
1:C:258:ARG:O	1:C:291:ARG:HD2	2.13	0.48
1:B:411:ARG:HG2	1:B:426:ILE:HD11	1.95	0.48
1:F:89:SER:HA	1:F:127:LYS:HG3	1.94	0.48
1:A:382:PHE:HB3	1:A:385:GLU:HB2	1.95	0.48
1:B:407:PHE:CE2	1:B:411:ARG:NH1	2.81	0.48
1:B:89:SER:HA	1:B:127:LYS:HG3	1.94	0.48
1:C:347:ILE:HD13	1:C:379:LYS:HE3	1.95	0.48
1:G:382:PHE:HB3	1:G:385:GLU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:382:PHE:HB3	1:E:385:GLU:HB2	1.96	0.47
1:A:89:SER:HA	1:A:127:LYS:HG3	1.95	0.47
1:E:486:TYR:CZ	1:E:488:GLU:HB2	2.49	0.47
1:H:494:TRP:CD1	1:H:529:PRO:HG3	2.50	0.47
1:D:494:TRP:CD1	1:D:529:PRO:HG3	2.49	0.47
1:H:317:LYS:NZ	7:H:705:HOH:O	2.46	0.47
1:B:382:PHE:HB3	1:B:385:GLU:HB2	1.96	0.46
1:C:486:TYR:CZ	1:C:488:GLU:HB2	2.50	0.46
1:F:516:ARG:O	1:F:519:ASP:HB2	2.16	0.46
1:D:486:TYR:CZ	1:D:488:GLU:HB2	2.50	0.46
1:F:382:PHE:HB3	1:F:385:GLU:HB2	1.96	0.46
1:C:352:PRO:HG3	1:C:389:MET:HG2	1.96	0.46
1:H:486:TYR:CZ	1:H:488:GLU:HB2	2.50	0.46
1:E:56:SER:HB2	1:E:480:GLY:HA2	1.97	0.46
1:H:382:PHE:HB3	1:H:385:GLU:HB2	1.96	0.46
1:F:352:PRO:HG3	1:F:389:MET:HG2	1.98	0.46
1:H:38:PHE:CE1	6:H:601:Y3Z:C9	2.99	0.46
1:E:416:LEU:HB3	1:F:16:LEU:HD22	1.98	0.45
1:A:408:GLU:OE2	1:B:411:ARG:NH2	2.47	0.45
1:F:311:ILE:CD1	6:F:605:Y3Z:C25	2.94	0.45
1:A:67:SER:HB2	1:A:76[A]:MET:SD	2.57	0.45
1:G:352:PRO:HG3	1:G:389:MET:HG2	1.97	0.45
1:D:382:PHE:HB3	1:D:385:GLU:HB2	1.98	0.45
1:C:538:ARG:CG	1:D:536:ILE:HG12	2.45	0.45
1:E:352:PRO:HG3	1:E:389:MET:HG2	1.98	0.45
1:F:486:TYR:CZ	1:F:488:GLU:HB2	2.52	0.45
1:G:538:ARG:CG	1:H:536:ILE:HG12	2.43	0.45
1:B:486:TYR:CZ	1:B:488:GLU:HB2	2.52	0.45
1:C:68:ARG:NH2	1:C:98:GLU:HB3	2.32	0.44
6:B:605:Y3Z:O9	6:B:606:Y3Z:O	2.36	0.44
1:B:352:PRO:HG3	1:B:389:MET:HG2	1.99	0.44
1:D:352:PRO:HG3	1:D:389:MET:HG2	2.00	0.44
1:H:537:MET:O	1:H:537:MET:HG3	2.17	0.44
1:A:352:PRO:HG3	1:A:389:MET:HG2	1.99	0.44
1:F:317:LYS:NZ	7:H:703:HOH:O	2.51	0.44
1:A:275:HIS:HB2	7:A:764:HOH:O	2.18	0.43
1:A:411:ARG:HG3	1:A:426:ILE:HD11	2.01	0.43
1:C:411:ARG:HD2	1:D:430[B]:GLU:OE1	2.17	0.43
1:C:56:SER:HB2	1:C:480:GLY:CA	2.48	0.43
1:E:75:GLU:HG2	7:E:726:HOH:O	2.19	0.43
1:H:352:PRO:HG3	1:H:389:MET:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:PHE:HB3	1:A:282:LYS:HD2	2.01	0.42
1:A:337:VAL:HG22	1:A:370:CYS:HB2	2.01	0.42
1:E:337:VAL:HG22	1:E:370:CYS:HB2	2.01	0.42
1:A:411:ARG:HD2	1:B:430:GLU:OE1	2.19	0.42
1:B:337:VAL:HG22	1:B:370:CYS:HB2	2.02	0.42
1:D:284:GLU:HB3	1:D:308:ASP:HB2	2.02	0.42
1:A:487:ARG:HH11	1:A:487:ARG:HA	1.85	0.42
1:F:115:LEU:HD23	1:F:508:SER:OG	2.20	0.42
1:C:404:ARG:HD3	1:D:412:ARG:NH2	2.35	0.42
1:G:284:GLU:HB3	1:G:308:ASP:HB2	2.02	0.41
1:B:253:PHE:HB3	1:B:282:LYS:HD2	2.02	0.41
1:C:351:ARG:HH22	1:C:354:ARG:NH2	2.18	0.41
1:G:536:ILE:HG12	1:H:538[A]:ARG:HG2	2.01	0.41
1:A:421:THR:HG22	1:A:452:LEU:HD12	2.01	0.41
1:A:494:TRP:CD1	1:A:529:PRO:HG3	2.55	0.41
1:C:284:GLU:HB3	1:C:308:ASP:HB2	2.01	0.41
1:E:284:GLU:HB3	1:E:308:ASP:HB2	2.02	0.41
1:F:253:PHE:HB3	1:F:282:LYS:HD2	2.03	0.41
1:E:253:PHE:HB3	1:E:282:LYS:HD2	2.02	0.41
1:A:475:VAL:CG2	1:A:483:PRO:HB3	2.51	0.41
1:G:56:SER:HB2	1:G:480:GLY:CA	2.49	0.41
1:A:407:PHE:O	1:A:411:ARG:HB2	2.21	0.41
1:F:408:GLU:HG3	7:F:764:HOH:O	2.20	0.41
1:H:253:PHE:HB3	1:H:282:LYS:HD2	2.03	0.41
1:F:113:SER:C	1:F:115:LEU:H	2.24	0.41
1:A:69:SER:OG	1:A:72:ARG:HB2	2.21	0.40
1:H:87:ASN:OD1	1:H:89:SER:HB2	2.21	0.40
1:A:412:ARG:NH1	1:B:404:ARG:HH11	2.19	0.40
1:A:56:SER:HB3	1:A:479:ARG:HG2	2.03	0.40
1:C:253:PHE:HB3	1:C:282:LYS:HD2	2.03	0.40
1:A:284:GLU:HB3	1:A:308:ASP:HB2	2.03	0.40
1:D:407:PHE:O	1:D:411:ARG:HG3	2.21	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:G:496:ASP:CB	7:H:762:HOH:O[4_546]	2.10	0.10

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%)	418 (99%)	5 (1%)	1 (0%)	47	53
1	B	438/447 (98%)	429 (98%)	7 (2%)	2 (0%)	29	28
1	C	425/447 (95%)	417 (98%)	6 (1%)	2 (0%)	29	28
1	D	429/447 (96%)	421 (98%)	6 (1%)	2 (0%)	29	28
1	E	420/447 (94%)	414 (99%)	5 (1%)	1 (0%)	47	53
1	F	435/447 (97%)	426 (98%)	7 (2%)	2 (0%)	29	28
1	G	423/447 (95%)	412 (97%)	9 (2%)	2 (0%)	29	28
1	H	427/447 (96%)	421 (99%)	4 (1%)	2 (0%)	29	28
All	All	3421/3576 (96%)	3358 (98%)	49 (1%)	14 (0%)	34	35

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	116	SER
1	C	231	PRO
1	C	340	THR
1	E	340	THR
1	G	340	THR
1	A	340	THR
1	B	340	THR
1	D	340	THR
1	F	340	THR
1	H	340	THR
1	B	231	PRO
1	D	231	PRO
1	G	91	GLY
1	H	231	PRO

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%)	329 (97%)	11 (3%)	39	44
1	B	349/352 (99%)	339 (97%)	10 (3%)	42	48
1	C	341/352 (97%)	335 (98%)	6 (2%)	59	66
1	D	342/352 (97%)	335 (98%)	7 (2%)	55	62
1	E	338/352 (96%)	327 (97%)	11 (3%)	38	43
1	F	350/352 (99%)	341 (97%)	9 (3%)	46	52
1	G	340/352 (97%)	336 (99%)	4 (1%)	71	78
1	H	340/352 (97%)	332 (98%)	8 (2%)	49	55
All	All	2740/2816 (97%)	2674 (98%)	66 (2%)	50	55

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	86	LEU
1	A	90	HIS
1	A	259	LYS
1	A	412	ARG
1	A	436	CYS
1	A	487	ARG
1	A	531	SER
1	A	537[A]	MET
1	A	537[B]	MET
1	A	540	LEU
1	B	10	ARG
1	B	15	GLN
1	B	26	GLN
1	B	68	ARG
1	B	90	HIS
1	B	259	LYS
1	B	311	ILE
1	B	379	LYS

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Mol	Chain	Res	Type
1	B	537[A]	MET
1	B	537[B]	MET
1	C	26	GLN
1	C	108	GLU
1	C	259	LYS
1	C	408	GLU
1	C	412	ARG
1	C	436	CYS
1	D	22	THR
1	D	259	LYS
1	D	379	LYS
1	D	412	ARG
1	D	436	CYS
1	D	521	VAL
1	D	537	MET
1	E	71	GLU
1	E	90	HIS
1	E	94	GLU
1	E	99	SER
1	E	259	LYS
1	E	412	ARG
1	E	436	CYS
1	E	508	SER
1	E	537[A]	MET
1	E	537[B]	MET
1	E	539	VAL
1	F	26	GLN
1	F	68	ARG
1	F	90	HIS
1	F	115	LEU
1	F	259	LYS
1	F	508	SER
1	F	516	ARG
1	F	537[A]	MET
1	F	537[B]	MET
1	G	26	GLN
1	G	259	LYS
1	G	436	CYS
1	G	540	LEU
1	H	22	THR
1	H	89	SER
1	H	259	LYS

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Mol	Chain	Res	Type
1	H	273	GLU
1	H	311	ILE
1	H	411	ARG
1	H	436	CYS
1	H	537	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	15	GLN
1	D	90	HIS
1	F	90	HIS
1	G	503	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 45 ligands modelled in this entry, 16 are monoatomic - leaving 29 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	$\#\|Z\|>2$
6	Y3Z	D	601	-	43,43,43	2.84	14 (32%)	60,67,67	2.42	21 (35%)
3	OXL	D	603	4	5,5,5	1.78	2 (40%)	6,6,6	2.58	4 (66%)
6	Y3Z	H	606	-	43,43,43	2.38	10 (23%)	60,67,67	2.23	17 (28%)
6	Y3Z	D	606	-	43,43,43	2.43	11 (25%)	60,67,67	2.23	19 (31%)
6	Y3Z	B	606	-	43,43,43	2.30	10 (23%)	60,67,67	2.22	20 (33%)
2	FBP	G	601	-	18,20,20	0.73	0	23,32,32	0.86	0
2	FBP	C	601	-	18,20,20	0.43	0	23,32,32	0.64	0
2	FBP	D	602	-	18,20,20	0.83	1 (5%)	23,32,32	0.75	0
6	Y3Z	A	605[B]	-	43,43,43	2.23	8 (18%)	60,67,67	2.37	17 (28%)
6	Y3Z	F	605	-	43,43,43	2.22	6 (13%)	60,67,67	2.02	15 (25%)
3	OXL	H	603	4	5,5,5	2.02	2 (40%)	6,6,6	1.10	1 (16%)
3	OXL	G	602	4	5,5,5	1.71	2 (40%)	6,6,6	1.69	2 (33%)
2	FBP	F	601	-	18,20,20	0.44	0	23,32,32	0.70	0
6	Y3Z	D	607	-	43,43,43	2.29	12 (27%)	60,67,67	1.82	16 (26%)
3	OXL	E	602	4	5,5,5	2.00	2 (40%)	6,6,6	1.04	0
6	Y3Z	E	605	-	43,43,43	2.72	18 (41%)	60,67,67	2.08	19 (31%)
3	OXL	A	602	4	5,5,5	1.90	2 (40%)	6,6,6	1.14	1 (16%)
6	Y3Z	B	605	-	43,43,43	2.34	16 (37%)	60,67,67	2.56	23 (38%)
2	FBP	E	601	-	18,20,20	0.63	0	23,32,32	0.83	2 (8%)
6	Y3Z	H	607	-	43,43,43	2.24	13 (30%)	60,67,67	1.73	14 (23%)
6	Y3Z	A	605[A]	-	43,43,43	2.09	6 (13%)	60,67,67	2.07	20 (33%)
2	FBP	H	602	-	18,20,20	0.79	0	23,32,32	1.25	3 (13%)
3	OXL	B	602	4	5,5,5	2.19	2 (40%)	6,6,6	0.65	0
3	OXL	C	602	4	5,5,5	2.11	2 (40%)	6,6,6	0.58	0
2	FBP	A	601	-	18,20,20	0.57	0	23,32,32	0.76	0
6	Y3Z	H	601	-	43,43,43	2.31	9 (20%)	60,67,67	2.91	19 (31%)
2	FBP	B	601	-	18,20,20	0.76	0	23,32,32	0.97	1 (4%)
6	Y3Z	F	606	-	43,43,43	2.03	11 (25%)	60,67,67	2.24	15 (25%)
3	OXL	F	602	4	5,5,5	2.76	4 (80%)	6,6,6	1.87	2 (33%)

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
6	Y3Z	D	601	-	-	4/17/37/37	0/4/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OXL	D	603	4	-	0/4/4/4	-
6	Y3Z	H	606	-	-	0/17/37/37	0/4/5/5
6	Y3Z	D	606	-	-	0/17/37/37	0/4/5/5
6	Y3Z	B	606	-	-	13/17/37/37	0/4/5/5
2	FBP	G	601	-	-	3/13/32/32	0/1/1/1
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
2	FBP	D	602	-	-	2/13/32/32	0/1/1/1
6	Y3Z	A	605[B]	-	-	4/17/37/37	0/4/5/5
6	Y3Z	F	605	-	-	0/17/37/37	0/4/5/5
3	OXL	H	603	4	-	1/4/4/4	-
3	OXL	G	602	4	-	1/4/4/4	-
2	FBP	F	601	-	-	2/13/32/32	0/1/1/1
6	Y3Z	D	607	-	-	2/17/37/37	0/4/5/5
3	OXL	E	602	4	-	1/4/4/4	-
6	Y3Z	E	605	-	-	4/17/37/37	0/4/5/5
3	OXL	A	602	4	-	0/4/4/4	-
6	Y3Z	B	605	-	-	4/17/37/37	0/4/5/5
2	FBP	E	601	-	-	3/13/32/32	0/1/1/1
6	Y3Z	H	607	-	-	3/17/37/37	0/4/5/5
6	Y3Z	A	605[A]	-	-	3/17/37/37	0/4/5/5
2	FBP	H	602	-	-	2/13/32/32	0/1/1/1
3	OXL	B	602	4	-	0/4/4/4	-
3	OXL	C	602	4	-	0/4/4/4	-
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
6	Y3Z	H	601	-	-	2/17/37/37	0/4/5/5
2	FBP	B	601	-	-	3/13/32/32	0/1/1/1
6	Y3Z	F	606	-	-	9/17/37/37	0/4/5/5
3	OXL	F	602	4	-	0/4/4/4	-

All (163) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	605	Y3Z	C23-S1	-10.78	1.60	1.75
6	A	605[A]	Y3Z	C23-S1	-10.29	1.61	1.75
6	D	606	Y3Z	C23-S1	-9.74	1.61	1.75
6	A	605[B]	Y3Z	C23-S1	-9.26	1.62	1.75
6	B	606	Y3Z	C23-S1	-9.15	1.62	1.75
6	H	606	Y3Z	C23-S1	-8.40	1.63	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	601	Y3Z	C23-S1	-8.32	1.63	1.75
6	F	606	Y3Z	C23-S1	-8.26	1.63	1.75
6	H	607	Y3Z	C23-S1	-8.15	1.64	1.75
6	D	601	Y3Z	C23-S1	-8.13	1.64	1.75
6	D	601	Y3Z	C15-S	-8.09	1.64	1.77
6	E	605	Y3Z	C23-S1	-7.46	1.65	1.75
6	D	607	Y3Z	C23-S1	-7.32	1.65	1.75
6	H	606	Y3Z	C15-S	-7.26	1.65	1.77
6	H	601	Y3Z	C15-S	-7.08	1.66	1.77
6	D	606	Y3Z	C15-S	-6.96	1.66	1.77
6	D	601	Y3Z	C3-C8	6.82	1.49	1.41
6	B	605	Y3Z	C8-N	-6.80	1.35	1.43
6	D	601	Y3Z	C8-N	-6.57	1.35	1.43
6	E	605	Y3Z	C3-C8	6.42	1.49	1.41
6	A	605[B]	Y3Z	C14-S	-6.00	1.67	1.77
6	E	605	Y3Z	C15-S	-5.58	1.68	1.77
6	H	607	Y3Z	C15-S	-5.46	1.68	1.77
6	B	605	Y3Z	C15-S	-5.11	1.69	1.77
6	D	607	Y3Z	C15-S	-4.93	1.69	1.77
6	E	605	Y3Z	C8-N	-4.83	1.37	1.43
6	D	607	Y3Z	C8-N	-4.80	1.37	1.43
6	F	605	Y3Z	C15-S	-4.76	1.69	1.77
6	B	605	Y3Z	S1-N	-4.76	1.56	1.64
6	F	605	Y3Z	C14-S	-4.69	1.69	1.77
6	E	605	Y3Z	C24-C23	4.65	1.46	1.39
6	B	605	Y3Z	C24-C23	4.46	1.46	1.39
6	A	605[B]	Y3Z	C15-S	-4.44	1.70	1.77
6	E	605	Y3Z	C1-C	4.42	1.45	1.38
6	E	605	Y3Z	C-C25	4.33	1.47	1.40
6	D	607	Y3Z	O8-S1	-4.21	1.38	1.43
6	D	607	Y3Z	C14-S	-4.11	1.70	1.77
6	D	606	Y3Z	C24-C25	-4.11	1.33	1.38
6	D	607	Y3Z	C24-C23	4.05	1.45	1.39
6	E	605	Y3Z	S1-N	4.05	1.71	1.64
6	B	606	Y3Z	C21-C14	4.04	1.45	1.38
6	H	601	Y3Z	C9-N	-4.02	1.45	1.48
6	B	605	Y3Z	C9-C10	3.97	1.63	1.52
6	D	601	Y3Z	C24-C23	3.92	1.45	1.39
3	B	602	OXL	O2-C2	3.90	1.33	1.22
6	B	606	Y3Z	C9-N	3.90	1.51	1.48
6	A	605[A]	Y3Z	C14-S	-3.90	1.70	1.77
6	H	607	Y3Z	C18-C19	3.86	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	606	Y3Z	S1-N	3.83	1.70	1.64
6	B	606	Y3Z	O8-S1	-3.82	1.39	1.43
6	B	606	Y3Z	C15-S	-3.74	1.71	1.77
6	B	606	Y3Z	C24-C23	3.71	1.44	1.39
3	E	602	OXL	O1-C1	3.68	1.32	1.22
3	F	602	OXL	O2-C2	3.67	1.32	1.22
6	H	607	Y3Z	C14-S	-3.64	1.71	1.77
6	H	601	Y3Z	C3-C8	3.54	1.45	1.41
6	F	606	Y3Z	C15-S	-3.52	1.71	1.77
6	H	601	Y3Z	O7-S1	3.51	1.47	1.43
6	F	606	Y3Z	O8-S1	-3.49	1.39	1.43
3	A	602	OXL	O2-C2	3.48	1.31	1.22
6	H	606	Y3Z	C13-C14	3.46	1.44	1.38
6	H	607	Y3Z	C8-N	-3.45	1.39	1.43
6	A	605[A]	Y3Z	C15-S	-3.44	1.71	1.77
6	H	606	Y3Z	C8-N	-3.41	1.39	1.43
6	H	606	Y3Z	C24-C25	-3.41	1.34	1.38
6	H	606	Y3Z	C18-C19	3.38	1.45	1.40
6	D	606	Y3Z	C4-C5	-3.38	1.34	1.38
3	C	602	OXL	O1-C1	3.36	1.31	1.22
6	B	605	Y3Z	C23-S1	-3.32	1.71	1.75
6	D	606	Y3Z	C14-S	-3.29	1.71	1.77
6	F	606	Y3Z	C21-C14	3.27	1.44	1.38
6	H	601	Y3Z	C14-S	-3.24	1.71	1.77
6	D	601	Y3Z	C13-C14	3.20	1.43	1.38
6	B	606	Y3Z	C13-C14	3.18	1.43	1.38
6	H	607	Y3Z	O8-S1	-3.17	1.40	1.43
6	D	601	Y3Z	C-C25	3.14	1.45	1.40
3	C	602	OXL	O3-C1	-3.12	1.21	1.30
3	H	603	OXL	O2-C2	3.07	1.30	1.22
6	D	601	Y3Z	C7-C8	-3.07	1.34	1.39
6	H	606	Y3Z	S1-N	3.07	1.69	1.64
3	D	603	OXL	O2-C2	3.04	1.30	1.22
6	D	607	Y3Z	O7-S1	-3.02	1.40	1.43
3	F	602	OXL	O1-C1	3.00	1.30	1.22
6	D	601	Y3Z	C1-C	2.98	1.43	1.38
6	B	605	Y3Z	C5-C6	2.96	1.44	1.40
6	H	606	Y3Z	C16-C15	2.94	1.43	1.38
6	D	606	Y3Z	S1-N	2.94	1.69	1.64
6	E	605	Y3Z	C1-C2	2.93	1.44	1.39
6	E	605	Y3Z	C24-C25	2.89	1.43	1.38
3	F	602	OXL	O3-C1	-2.88	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	606	Y3Z	C14-S	-2.87	1.72	1.77
6	H	607	Y3Z	C24-C23	2.87	1.43	1.39
6	H	601	Y3Z	C24-C23	2.79	1.43	1.39
3	G	602	OXL	O3-C1	-2.79	1.22	1.30
6	B	606	Y3Z	C4-C3	2.77	1.44	1.39
6	A	605[B]	Y3Z	C24-C23	2.76	1.43	1.39
6	D	607	Y3Z	C18-C19	2.72	1.44	1.40
6	D	601	Y3Z	C9-C10	2.72	1.59	1.52
3	H	603	OXL	O4-C2	-2.69	1.22	1.30
6	E	605	Y3Z	O9-C25	2.68	1.41	1.36
6	B	605	Y3Z	C24-C25	2.66	1.42	1.38
6	D	601	Y3Z	O7-S1	-2.65	1.40	1.43
6	D	607	Y3Z	C16-C15	2.64	1.43	1.38
6	F	606	Y3Z	C8-N	-2.63	1.40	1.43
6	F	606	Y3Z	C24-C23	2.63	1.43	1.39
6	E	605	Y3Z	C21-C14	2.61	1.42	1.38
6	A	605[B]	Y3Z	C9-N	-2.60	1.46	1.48
6	D	606	Y3Z	C1-C	-2.59	1.35	1.38
6	B	605	Y3Z	O7-S1	-2.59	1.40	1.43
6	H	606	Y3Z	O8-S1	2.59	1.46	1.43
6	F	606	Y3Z	C22-C21	2.57	1.43	1.38
6	D	606	Y3Z	C18-C19	2.55	1.44	1.40
6	A	605[B]	Y3Z	C16-C15	2.54	1.42	1.38
6	H	607	Y3Z	C2-C23	2.53	1.44	1.40
6	B	605	Y3Z	C14-S	-2.52	1.73	1.77
3	E	602	OXL	O3-C1	-2.50	1.23	1.30
3	G	602	OXL	O1-C1	2.50	1.29	1.22
6	F	605	Y3Z	C18-C19	2.49	1.44	1.40
6	D	601	Y3Z	C13-C12	2.48	1.43	1.38
6	B	605	Y3Z	C13-C12	2.47	1.43	1.38
6	B	606	Y3Z	C13-C12	2.47	1.43	1.38
2	D	602	FBP	P2-O5P	-2.46	1.45	1.54
6	F	606	Y3Z	C20-C15	2.46	1.43	1.39
3	A	602	OXL	O4-C2	-2.46	1.23	1.30
6	E	605	Y3Z	C16-C15	2.44	1.42	1.38
6	D	606	Y3Z	C21-C14	2.42	1.42	1.38
3	B	602	OXL	O4-C2	-2.39	1.23	1.30
6	A	605[B]	Y3Z	C24-C25	-2.38	1.35	1.38
6	D	607	Y3Z	C7-C6	-2.37	1.35	1.38
6	D	601	Y3Z	C4-C5	-2.37	1.35	1.38
6	E	605	Y3Z	C9-C10	2.36	1.58	1.52
6	A	605[A]	Y3Z	C13-C14	2.35	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	605	Y3Z	C5-C6	2.32	1.43	1.40
6	D	601	Y3Z	C1-C2	2.31	1.43	1.39
6	A	605[B]	Y3Z	C7-C6	-2.31	1.35	1.38
6	D	607	Y3Z	O2-C6	-2.31	1.31	1.36
6	D	606	Y3Z	O8-S1	2.27	1.46	1.43
6	A	605[A]	Y3Z	C24-C25	-2.27	1.35	1.38
6	E	605	Y3Z	C17-C18	2.25	1.43	1.39
6	H	607	Y3Z	C3-C8	2.25	1.43	1.41
6	H	607	Y3Z	O5-S	2.24	1.48	1.44
6	E	605	Y3Z	C2-C23	2.24	1.43	1.40
6	H	601	Y3Z	C5-C6	2.23	1.43	1.40
6	B	605	Y3Z	C3-C8	2.22	1.43	1.41
6	B	605	Y3Z	C13-C14	2.20	1.42	1.38
6	F	605	Y3Z	C4-C3	2.19	1.43	1.39
6	E	605	Y3Z	C14-S	-2.19	1.73	1.77
6	A	605[A]	Y3Z	C24-C23	2.18	1.42	1.39
6	H	607	Y3Z	C9-N	-2.17	1.46	1.48
6	H	607	Y3Z	S1-N	2.16	1.68	1.64
6	H	607	Y3Z	C24-C25	-2.13	1.35	1.38
6	B	605	Y3Z	O9-C25	2.12	1.40	1.36
3	F	602	OXL	O4-C2	-2.11	1.24	1.30
6	D	606	Y3Z	C9-N	-2.10	1.46	1.48
6	F	606	Y3Z	C5-C6	2.09	1.43	1.40
6	F	606	Y3Z	C24-C25	-2.09	1.36	1.38
3	D	603	OXL	O4-C2	-2.07	1.24	1.30
6	F	606	Y3Z	S1-N	2.06	1.68	1.64
6	B	605	Y3Z	C1-C2	2.05	1.43	1.39
6	F	605	Y3Z	C-C25	2.04	1.43	1.40
6	D	607	Y3Z	C20-C15	2.03	1.42	1.39
6	B	605	Y3Z	C7-C8	-2.03	1.36	1.39
6	H	601	Y3Z	C7-C6	2.01	1.41	1.38

All (251) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	601	Y3Z	O7-S1-N	-13.14	93.63	108.13
6	B	605	Y3Z	O7-S1-C23	8.41	119.90	109.13
6	A	605[B]	Y3Z	O7-S1-N	-8.28	99.00	108.13
6	B	605	Y3Z	C23-S1-N	-7.91	89.73	101.82
6	H	601	Y3Z	O7-S1-C23	7.56	118.81	109.13
6	D	606	Y3Z	C2-C23-S1	6.98	125.77	117.27
6	F	605	Y3Z	C2-C23-S1	6.90	125.67	117.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	606	Y3Z	C2-C23-S1	6.67	125.39	117.27
6	H	606	Y3Z	C2-C23-S1	6.63	125.35	117.27
6	H	606	Y3Z	C13-C14-S	6.46	127.75	119.52
6	H	601	Y3Z	O5-S-C14	6.31	115.08	107.97
6	F	606	Y3Z	C12-C13-C14	6.29	125.96	119.45
6	F	606	Y3Z	C21-C14-S	6.28	127.52	119.52
6	D	601	Y3Z	O7-S1-N	6.09	114.85	108.13
6	B	606	Y3Z	C13-C14-C21	-6.01	112.05	120.44
6	H	607	Y3Z	C2-C23-S1	6.00	124.58	117.27
6	A	605[B]	Y3Z	C15-S-C14	-5.98	93.81	104.35
6	D	601	Y3Z	O5-S-C14	5.89	114.61	107.97
6	B	606	Y3Z	C22-C21-C14	5.88	125.54	119.45
6	D	606	Y3Z	C23-S1-N	-5.78	92.98	101.82
6	F	605	Y3Z	C23-S1-N	-5.78	92.99	101.82
6	A	605[B]	Y3Z	C2-C23-S1	5.57	124.05	117.27
6	H	601	Y3Z	C2-C23-S1	5.45	123.90	117.27
6	D	606	Y3Z	C21-C14-S	5.42	126.42	119.52
6	A	605[A]	Y3Z	C15-S-C14	-5.41	94.81	104.35
6	B	605	Y3Z	C9-N-C8	5.37	128.13	121.72
6	A	605[A]	Y3Z	C2-C23-S1	5.35	123.78	117.27
6	F	606	Y3Z	C13-C14-C21	-5.32	113.02	120.44
6	B	606	Y3Z	O5-S-C14	5.15	113.78	107.97
6	H	601	Y3Z	O5-S-C15	5.12	113.75	107.97
6	B	605	Y3Z	O8-S1-C23	5.10	115.67	109.13
6	A	605[A]	Y3Z	O6-S-C14	5.05	113.66	107.97
6	E	605	Y3Z	C22-C21-C14	5.05	124.67	119.45
6	A	605[B]	Y3Z	O6-S-C14	5.05	113.66	107.97
6	A	605[B]	Y3Z	O7-S1-C23	4.92	115.44	109.13
6	H	606	Y3Z	C23-S1-N	-4.87	94.36	101.82
6	D	607	Y3Z	O8-S1-C23	4.72	115.18	109.13
6	D	606	Y3Z	O6-S-C14	4.69	113.25	107.97
6	B	606	Y3Z	C2-C23-S1	4.68	122.97	117.27
6	H	601	Y3Z	C15-S-C14	-4.67	96.11	104.35
6	D	601	Y3Z	C13-C14-C21	-4.64	113.97	120.44
6	D	601	Y3Z	C9-N-C8	4.61	127.22	121.72
6	E	605	Y3Z	O5-S-C14	4.61	113.16	107.97
6	H	606	Y3Z	O7-S1-C23	4.56	114.98	109.13
6	H	601	Y3Z	O7-S1-O8	4.56	124.17	118.59
6	D	607	Y3Z	C2-C23-S1	4.54	122.80	117.27
6	D	601	Y3Z	C13-C14-S	4.48	125.23	119.52
6	D	601	Y3Z	O6-S-C15	-4.42	102.99	107.97
6	D	601	Y3Z	C12-C13-C14	4.40	124.00	119.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	605	Y3Z	C9-N-C8	4.24	126.78	121.72
6	A	605[B]	Y3Z	O8-S1-N	4.21	112.77	108.13
6	D	607	Y3Z	C23-S1-N	-4.19	95.41	101.82
6	E	605	Y3Z	C13-C14-C21	-4.16	114.64	120.44
6	D	601	Y3Z	C9-C10-C11	4.15	124.02	112.16
6	D	606	Y3Z	C12-C13-C14	4.14	123.74	119.45
6	H	606	Y3Z	O7-S1-O8	-4.08	113.58	118.59
6	E	605	Y3Z	C23-S1-N	-4.04	95.64	101.82
6	F	606	Y3Z	O7-S1-C23	4.04	114.31	109.13
6	D	601	Y3Z	O5-S-C15	4.02	112.51	107.97
6	H	606	Y3Z	O5-S-C14	3.99	112.47	107.97
6	D	607	Y3Z	O7-S1-O8	-3.93	113.76	118.59
6	D	601	Y3Z	O8-S1-N	-3.92	103.80	108.13
6	F	605	Y3Z	O8-S1-C23	3.92	114.15	109.13
6	B	606	Y3Z	O8-S1-N	3.90	112.44	108.13
6	B	605	Y3Z	C13-C14-C21	-3.88	115.02	120.44
3	D	603	OXL	O4-C2-C1	3.87	124.65	113.16
6	B	606	Y3Z	C13-C14-S	3.79	124.35	119.52
6	H	607	Y3Z	C23-S1-N	-3.79	96.02	101.82
6	H	601	Y3Z	C13-C14-C21	-3.78	115.16	120.44
6	D	606	Y3Z	C13-C14-C21	-3.77	115.18	120.44
6	B	606	Y3Z	C23-S1-N	-3.76	96.06	101.82
6	H	606	Y3Z	C22-C21-C14	3.74	123.32	119.45
6	A	605[B]	Y3Z	C23-S1-N	-3.73	96.11	101.82
6	D	606	Y3Z	O8-S1-C23	3.71	113.88	109.13
6	H	601	Y3Z	O8-S1-N	3.68	112.19	108.13
6	B	605	Y3Z	C13-C14-S	3.68	124.20	119.52
6	B	605	Y3Z	O8-S1-N	-3.65	104.10	108.13
2	H	602	FBP	O6P-P2-O6	-3.65	97.03	106.73
6	H	607	Y3Z	O7-S1-N	3.62	112.13	108.13
6	D	601	Y3Z	C23-S1-N	-3.61	96.30	101.82
6	D	601	Y3Z	C2-C23-S1	3.60	121.65	117.27
6	E	605	Y3Z	C9-C10-C11	3.59	122.41	112.16
6	A	605[B]	Y3Z	C12-C13-C14	3.58	123.16	119.45
6	B	605	Y3Z	C16-C15-S	3.50	123.97	119.52
6	A	605[A]	Y3Z	C13-C14-C21	-3.49	115.57	120.44
6	F	605	Y3Z	C17-C16-C15	3.46	123.03	119.45
6	A	605[A]	Y3Z	C13-C14-S	3.45	123.92	119.52
6	H	606	Y3Z	C17-C16-C15	3.45	123.02	119.45
6	E	605	Y3Z	C15-S-C14	-3.44	98.29	104.35
6	H	601	Y3Z	C12-C13-C14	3.43	123.00	119.45
6	H	606	Y3Z	O8-S1-C23	3.40	113.49	109.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	606	Y3Z	O7-S1-C23	3.36	113.43	109.13
6	A	605[A]	Y3Z	C16-C15-C20	-3.35	116.50	120.62
6	B	605	Y3Z	C22-C21-C14	3.35	122.92	119.45
6	H	606	Y3Z	C13-C14-C21	-3.35	115.77	120.44
6	F	606	Y3Z	C20-C15-S	3.35	123.26	119.21
6	H	601	Y3Z	C23-S1-N	-3.32	96.75	101.82
6	B	605	Y3Z	C12-C13-C14	3.29	122.85	119.45
6	F	606	Y3Z	O6-S-C15	3.29	111.68	107.97
3	D	603	OXL	O2-C2-C1	-3.27	110.27	120.78
6	F	606	Y3Z	C17-C16-C15	3.27	122.83	119.45
6	A	605[B]	Y3Z	C17-C16-C15	3.26	122.83	119.45
6	A	605[A]	Y3Z	O8-S1-C23	3.26	113.31	109.13
6	F	605	Y3Z	C15-S-C14	-3.25	98.62	104.35
6	F	605	Y3Z	O6-S-C14	3.24	111.62	107.97
6	B	606	Y3Z	C21-C14-S	3.20	123.59	119.52
6	B	605	Y3Z	C2-C23-S1	3.19	121.15	117.27
6	A	605[A]	Y3Z	C17-C16-C15	3.19	122.75	119.45
6	B	605	Y3Z	C24-C23-C2	-3.18	116.64	120.18
6	F	606	Y3Z	C15-S-C14	-3.16	98.78	104.35
6	E	605	Y3Z	O8-S1-C23	3.16	113.18	109.13
6	A	605[A]	Y3Z	O7-S1-N	-3.16	104.65	108.13
6	E	605	Y3Z	O8-S1-N	3.15	111.61	108.13
6	B	606	Y3Z	C15-S-C14	-3.14	98.80	104.35
6	A	605[A]	Y3Z	C23-S1-N	-3.13	97.04	101.82
6	B	605	Y3Z	O6-S-C14	3.12	111.49	107.97
6	A	605[B]	Y3Z	O6-S-C15	3.11	111.48	107.97
6	E	605	Y3Z	C10-C11-C12	-3.11	113.36	121.23
6	H	607	Y3Z	C17-C16-C15	3.10	122.66	119.45
6	D	607	Y3Z	C17-C16-C15	3.07	122.63	119.45
6	A	605[A]	Y3Z	O6-S-C15	3.07	111.43	107.97
6	F	605	Y3Z	O3-C18-C19	3.04	126.54	118.45
6	E	605	Y3Z	O7-S1-N	-3.04	104.78	108.13
6	B	606	Y3Z	O7-S1-C23	3.03	113.01	109.13
6	H	607	Y3Z	O3-C18-C19	2.99	126.43	118.45
6	F	605	Y3Z	C16-C15-C20	-2.99	116.94	120.62
6	D	606	Y3Z	O7-S1-O8	-2.97	114.94	118.59
6	D	601	Y3Z	C16-C15-S	2.96	123.28	119.52
6	E	605	Y3Z	C2-C23-S1	2.95	120.86	117.27
3	F	602	OXL	O4-C2-C1	2.94	121.91	113.16
6	A	605[A]	Y3Z	C16-C15-S	2.92	123.24	119.52
6	B	606	Y3Z	C16-C15-C20	-2.90	117.06	120.62
6	F	606	Y3Z	O3-C18-C19	2.90	126.17	118.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	606	Y3Z	C16-C15-C20	-2.89	117.07	120.62
6	B	605	Y3Z	C1-C2-C23	2.88	120.63	117.61
6	D	606	Y3Z	C17-C16-C15	2.87	122.42	119.45
6	D	601	Y3Z	C22-C21-C14	2.86	122.41	119.45
6	D	607	Y3Z	C4-C5-C6	-2.84	117.35	119.86
6	D	601	Y3Z	C15-S-C14	-2.84	99.35	104.35
6	B	605	Y3Z	O7-S1-N	-2.84	105.00	108.13
3	D	603	OXL	O3-C1-C2	2.83	121.58	113.16
3	G	602	OXL	O3-C1-C2	2.83	121.58	113.16
6	H	607	Y3Z	C13-C14-C21	-2.81	116.52	120.44
6	F	605	Y3Z	C13-C14-C21	-2.81	116.52	120.44
6	F	605	Y3Z	O7-S1-C23	2.81	112.73	109.13
6	A	605[A]	Y3Z	C22-C21-C14	2.80	122.35	119.45
6	F	605	Y3Z	C22-C21-C14	2.79	122.33	119.45
6	B	605	Y3Z	O1-C5-C6	2.78	125.86	118.45
6	H	607	Y3Z	C13-C14-S	2.76	123.04	119.52
6	H	606	Y3Z	O3-C18-C19	2.76	125.79	118.45
6	D	601	Y3Z	C10-C11-C22	-2.74	114.29	121.23
6	B	606	Y3Z	O3-C18-C19	2.72	125.70	118.45
6	D	607	Y3Z	C7-C6-C5	2.71	122.26	119.86
6	H	601	Y3Z	C9-N-C8	2.70	124.94	121.72
6	B	605	Y3Z	C17-C16-C15	2.69	122.23	119.45
6	A	605[A]	Y3Z	C12-C13-C14	2.68	122.22	119.45
6	B	606	Y3Z	C12-C13-C14	2.67	122.21	119.45
6	A	605[B]	Y3Z	O5-S-C14	-2.67	104.97	107.97
6	D	607	Y3Z	C13-C14-S	2.66	122.91	119.52
6	A	605[A]	Y3Z	C19-C20-C15	2.66	121.94	119.63
3	F	602	OXL	O3-C1-C2	2.64	121.01	113.16
6	D	607	Y3Z	O3-C18-C19	2.64	125.48	118.45
6	H	601	Y3Z	C21-C14-S	2.61	122.84	119.52
6	H	606	Y3Z	C21-C14-S	-2.61	116.19	119.52
6	H	601	Y3Z	O6-S-C15	-2.60	105.04	107.97
6	H	606	Y3Z	C16-C17-C18	-2.59	117.84	120.50
6	H	607	Y3Z	O7-S1-C23	2.57	112.43	109.13
6	D	607	Y3Z	O7-S1-C23	2.57	112.42	109.13
6	H	607	Y3Z	O8-S1-N	-2.54	105.33	108.13
6	A	605[B]	Y3Z	C16-C15-C20	-2.53	117.51	120.62
6	D	607	Y3Z	O9-C25-C24	2.53	126.25	119.46
6	A	605[B]	Y3Z	O5-S-C15	2.53	110.83	107.97
6	B	606	Y3Z	C17-C16-C15	2.53	122.07	119.45
6	D	601	Y3Z	C10-C11-C12	2.52	127.61	121.23
6	B	606	Y3Z	C4-C5-C6	-2.52	117.63	119.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	605	Y3Z	C13-C14-S	2.51	122.72	119.52
6	D	606	Y3Z	C7-C8-C3	-2.51	118.03	120.98
6	H	601	Y3Z	C16-C15-S	2.48	122.68	119.52
6	E	605	Y3Z	C10-C11-C22	2.48	127.50	121.23
6	E	605	Y3Z	C21-C22-C11	-2.46	117.65	121.03
6	E	605	Y3Z	O1-C5-C6	2.45	124.98	118.45
6	F	605	Y3Z	C12-C13-C14	2.45	121.98	119.45
6	B	605	Y3Z	C9-C10-C11	2.44	119.14	112.16
6	E	605	Y3Z	C21-C14-S	2.44	122.63	119.52
6	A	605[B]	Y3Z	C16-C15-S	2.44	122.63	119.52
6	D	607	Y3Z	O1-C5-C6	2.44	124.95	118.45
6	D	606	Y3Z	O1-C5-C6	2.44	124.95	118.45
6	F	606	Y3Z	O6-S-C14	2.43	110.71	107.97
6	D	606	Y3Z	O-C-C25	2.43	124.92	118.45
6	H	601	Y3Z	C22-C21-C14	2.42	121.95	119.45
6	A	605[B]	Y3Z	C13-C14-C21	-2.42	117.07	120.44
6	B	605	Y3Z	C16-C15-C20	-2.41	117.66	120.62
6	E	605	Y3Z	C16-C15-S	2.40	122.57	119.52
6	D	607	Y3Z	O7-S1-N	2.38	110.76	108.13
6	D	607	Y3Z	C16-C15-C20	-2.37	117.70	120.62
6	F	606	Y3Z	O1-C5-C6	2.37	124.77	118.45
3	H	603	OXL	O4-C2-C1	2.36	120.17	113.16
6	F	606	Y3Z	C23-S1-N	-2.35	98.22	101.82
3	D	603	OXL	O1-C1-C2	-2.35	113.23	120.78
6	H	607	Y3Z	C22-C21-C14	2.33	121.86	119.45
6	H	601	Y3Z	O3-C18-C19	2.33	124.66	118.45
6	D	607	Y3Z	C12-C13-C14	2.33	121.86	119.45
6	A	605[A]	Y3Z	O5-S-C15	2.32	110.59	107.97
6	H	606	Y3Z	O-C-C25	2.32	124.63	118.45
6	D	607	Y3Z	C13-C14-C21	-2.31	117.22	120.44
6	D	601	Y3Z	O8-S1-C23	2.30	112.08	109.13
6	D	601	Y3Z	O1-C5-C6	2.30	124.57	118.45
2	B	601	FBP	P1-O1-C1	2.29	124.61	118.30
2	H	602	FBP	O5P-P2-O6	2.29	112.82	106.73
6	H	606	Y3Z	C9-N-C8	2.29	124.45	121.72
6	F	605	Y3Z	C8-C7-C6	2.28	122.98	118.68
6	F	605	Y3Z	O-C-C25	2.27	124.50	118.45
6	B	605	Y3Z	O3-C18-C19	2.27	124.50	118.45
6	A	605[A]	Y3Z	O7-S1-C23	2.26	112.02	109.13
6	B	605	Y3Z	C19-C20-C15	2.24	121.58	119.63
6	D	606	Y3Z	O7-S1-N	2.23	110.59	108.13
6	A	605[A]	Y3Z	O-C-C25	2.22	124.37	118.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	606	Y3Z	O7-S1-O8	-2.22	115.86	118.59
6	H	606	Y3Z	C1-C2-C23	2.22	119.94	117.61
6	B	606	Y3Z	O7-S1-O8	-2.22	115.87	118.59
6	A	605[B]	Y3Z	O-C-C25	2.22	124.36	118.45
6	D	606	Y3Z	C1-C2-C23	2.21	119.93	117.61
6	D	601	Y3Z	C4-C3-C8	2.20	120.11	117.96
6	H	607	Y3Z	O6-S-C15	-2.20	105.50	107.97
6	B	606	Y3Z	O9-C25-C24	2.19	125.33	119.46
6	B	605	Y3Z	O9-C25-C24	2.19	125.33	119.46
6	D	606	Y3Z	O3-C18-C19	2.19	124.28	118.45
6	A	605[B]	Y3Z	C9-N-C8	2.18	124.32	121.72
6	B	605	Y3Z	O6-S-O5	-2.18	115.08	119.23
6	B	606	Y3Z	C19-C20-C15	2.17	121.52	119.63
6	H	607	Y3Z	C12-C13-C14	2.17	121.69	119.45
6	B	606	Y3Z	C8-C7-C6	2.16	122.74	118.68
6	B	606	Y3Z	O6-S-O5	-2.15	115.11	119.23
6	H	606	Y3Z	O7-S1-N	2.14	110.49	108.13
6	A	605[A]	Y3Z	O3-C18-C19	2.14	124.15	118.45
6	D	606	Y3Z	C22-C21-C14	2.10	121.63	119.45
6	H	601	Y3Z	C2-C3-C8	2.10	122.41	119.79
6	H	607	Y3Z	C16-C15-C20	-2.10	118.04	120.62
6	D	606	Y3Z	C9-N-C8	2.10	124.22	121.72
3	G	602	OXL	O4-C2-C1	2.09	119.36	113.16
3	A	602	OXL	O4-C2-C1	2.08	119.34	113.16
2	E	601	FBP	O3P-P1-O2P	2.08	115.58	107.64
6	H	607	Y3Z	C19-C20-C15	2.07	121.43	119.63
6	F	605	Y3Z	C7-C8-C3	-2.06	118.56	120.98
6	D	601	Y3Z	C7-C6-C5	2.04	121.67	119.86
6	H	601	Y3Z	O2-C6-C7	2.04	124.92	119.46
2	H	602	FBP	O2P-P1-O1	2.03	112.12	106.73
6	E	605	Y3Z	C7-C6-C5	2.01	121.64	119.86
6	A	605[A]	Y3Z	O8-S1-N	2.01	110.35	108.13
2	E	601	FBP	P1-O1-C1	2.01	123.83	118.30
6	D	606	Y3Z	O6-S-C15	2.00	110.23	107.97

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FBP	C4-C5-C6-O6
2	B	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	D	602	FBP	C4-C5-C6-O6
2	E	601	FBP	C1-O1-P1-O2P
2	E	601	FBP	C4-C5-C6-O6
2	F	601	FBP	C4-C5-C6-O6
2	G	601	FBP	C6-O6-P2-O5P
2	H	602	FBP	C4-C5-C6-O6
6	A	605[A]	Y3Z	C11-C10-C9-N
6	B	605	Y3Z	C10-C9-N-C8
6	B	606	Y3Z	C11-C10-C9-N
6	B	606	Y3Z	C10-C9-N-S1
6	F	606	Y3Z	C11-C10-C9-N
6	F	606	Y3Z	C20-C15-S-C14
6	B	606	Y3Z	C21-C14-S-O5
6	F	606	Y3Z	C20-C15-S-O6
6	B	606	Y3Z	C13-C14-S-O5
6	B	606	Y3Z	C21-C14-S-C15
2	A	601	FBP	O5-C5-C6-O6
2	E	601	FBP	O5-C5-C6-O6
6	B	606	Y3Z	C20-C15-S-O6
6	B	606	Y3Z	C13-C14-S-C15
6	F	606	Y3Z	C16-C15-S-O6
6	B	606	Y3Z	C20-C15-S-C14
6	A	605[B]	Y3Z	C10-C9-N-C8
6	B	606	Y3Z	C10-C9-N-C8
6	D	601	Y3Z	C10-C9-N-C8
6	E	605	Y3Z	C10-C9-N-C8
2	C	601	FBP	O5-C5-C6-O6
2	D	602	FBP	O5-C5-C6-O6
2	H	602	FBP	O5-C5-C6-O6
2	B	601	FBP	O5-C5-C6-O6
2	F	601	FBP	O5-C5-C6-O6
6	B	605	Y3Z	C9-C10-C11-C12
6	D	601	Y3Z	C9-C10-C11-C12
6	E	605	Y3Z	C9-C10-C11-C22
6	F	606	Y3Z	C16-C15-S-C14
6	F	606	Y3Z	C13-C14-S-O5
6	D	601	Y3Z	C9-C10-C11-C22
6	E	605	Y3Z	C9-C10-C11-C12
6	B	605	Y3Z	C9-C10-C11-C22
6	F	606	Y3Z	C21-C14-S-O5
2	B	601	FBP	C1-O1-P1-O2P
2	G	601	FBP	C4-C5-C6-O6

Continued on next page...

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Mol	Chain	Res	Type	Atoms
6	A	605[A]	Y3Z	C9-C10-C11-C12
6	F	606	Y3Z	C13-C14-S-C15
6	A	605[B]	Y3Z	C11-C10-C9-N
6	D	601	Y3Z	C11-C10-C9-N
6	E	605	Y3Z	C11-C10-C9-N
6	H	601	Y3Z	C11-C10-C9-N
6	H	607	Y3Z	C11-C10-C9-N
6	H	601	Y3Z	C10-C9-N-C8
6	B	606	Y3Z	C16-C15-S-O6
6	B	605	Y3Z	C10-C9-N-S1
6	D	607	Y3Z	C21-C14-S-O6
6	F	606	Y3Z	C21-C14-S-C15
6	B	606	Y3Z	C9-C10-C11-C12
6	H	607	Y3Z	C13-C14-S-O5
6	B	606	Y3Z	C9-C10-C11-C22
6	H	607	Y3Z	C21-C14-S-O5
6	A	605[A]	Y3Z	C9-C10-C11-C22
6	D	607	Y3Z	C13-C14-S-O6
6	A	605[B]	Y3Z	C9-C10-C11-C12
2	G	601	FBP	C6-O6-P2-O6P
6	B	606	Y3Z	C16-C15-S-C14
3	E	602	OXL	O3-C1-C2-O4
3	G	602	OXL	O3-C1-C2-O4
3	H	603	OXL	O3-C1-C2-O4
6	A	605[B]	Y3Z	C9-C10-C11-C22

There are no ring outliers.

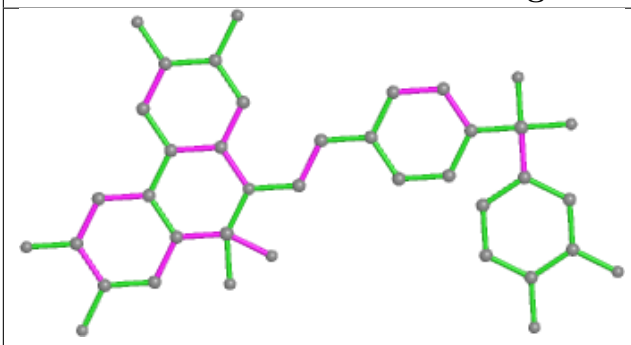
10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	601	Y3Z	1	0
6	D	606	Y3Z	2	0
6	B	606	Y3Z	2	0
6	F	605	Y3Z	2	0
6	D	607	Y3Z	1	0
6	B	605	Y3Z	1	0
6	H	607	Y3Z	1	0
6	A	605[A]	Y3Z	1	0
6	H	601	Y3Z	1	0
6	F	606	Y3Z	1	0

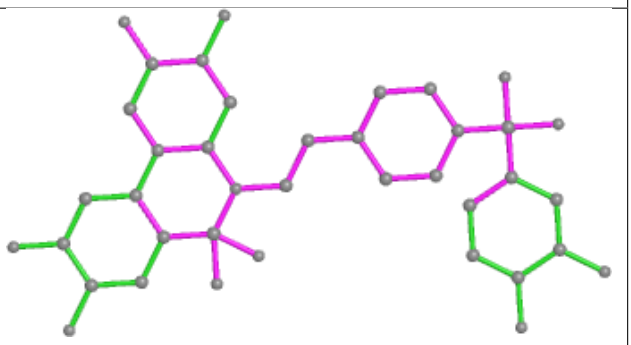
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

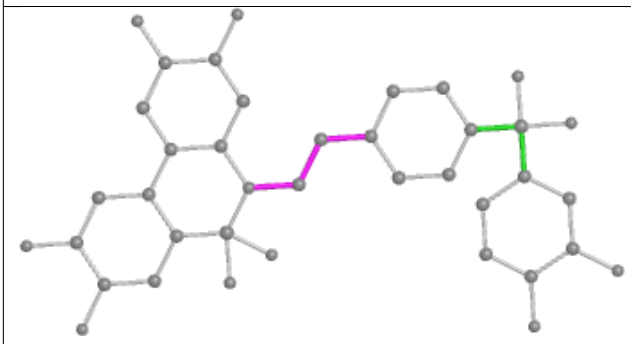
Ligand Y3Z D 601



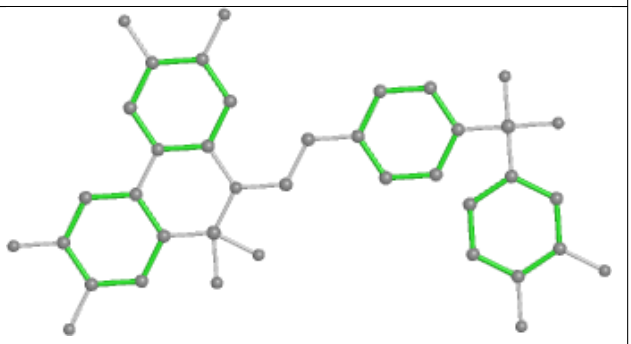
Bond lengths



Bond angles

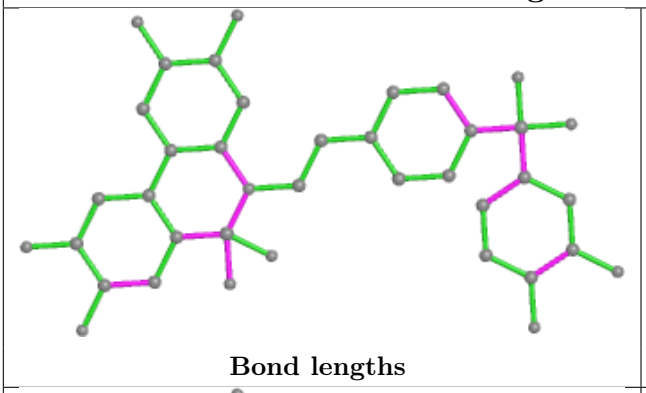


Torsions

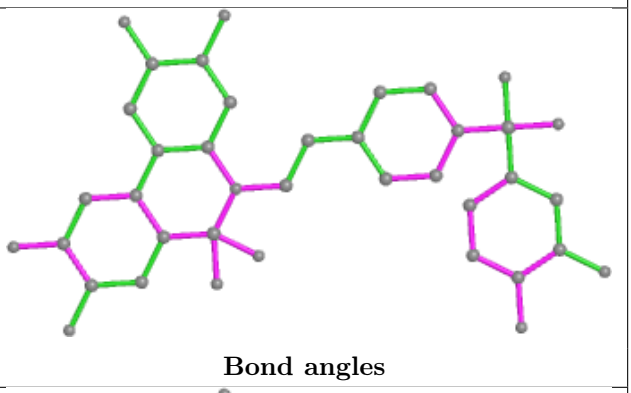


Rings

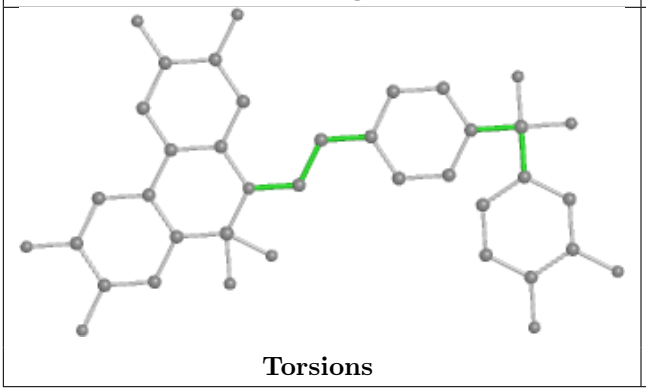
Ligand Y3Z H 606



Bond lengths



Bond angles



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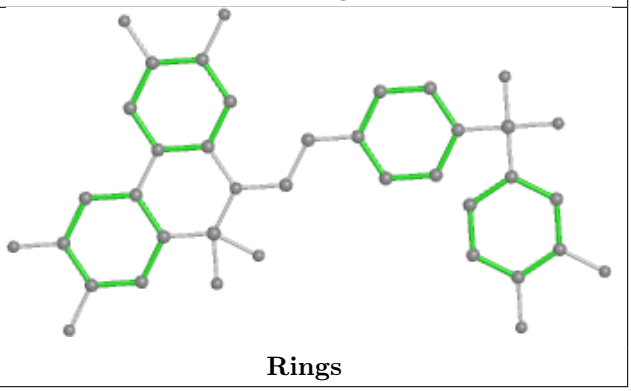
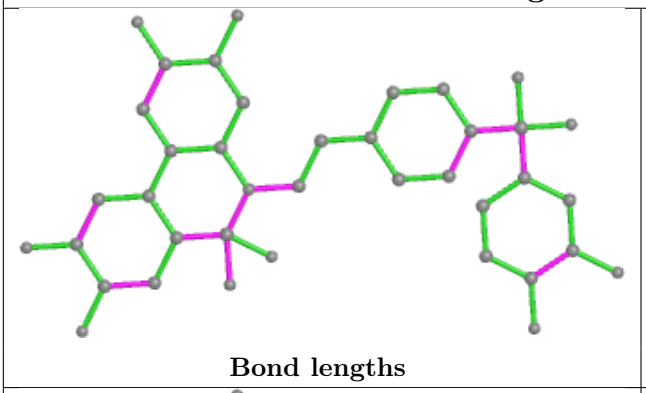


Rings

Ligand Y3Z D 606



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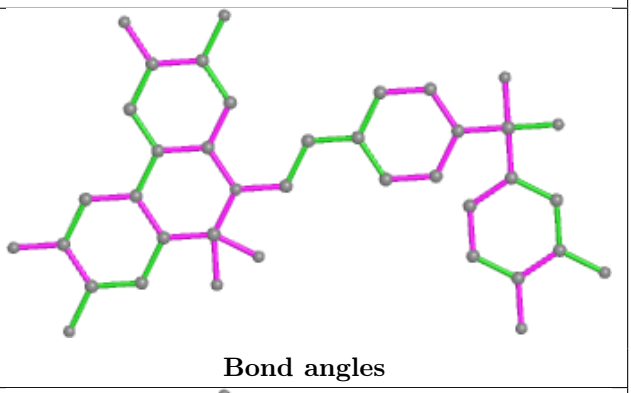
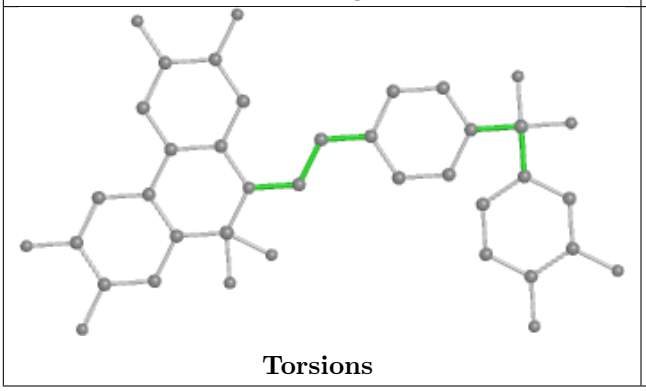


Bond angles



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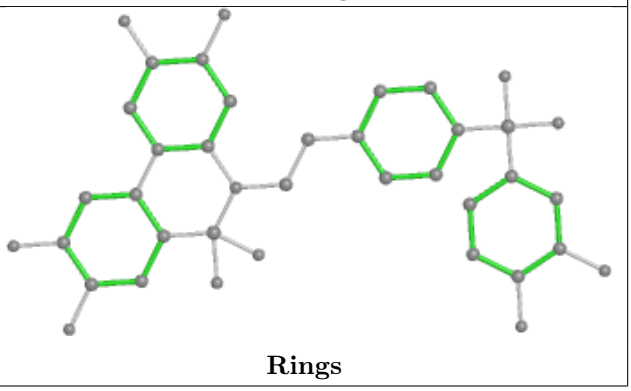
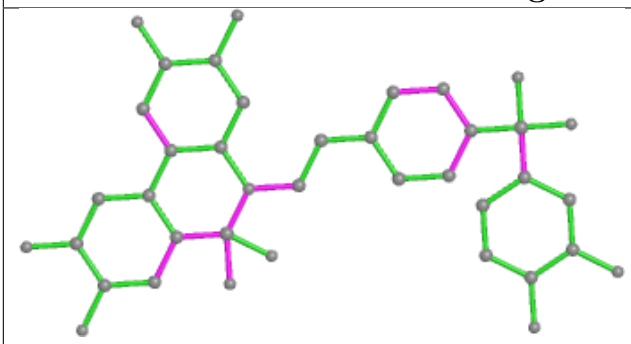


Rings

Ligand Y3Z B 606



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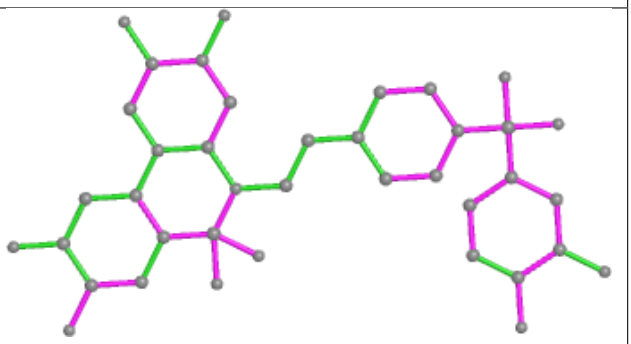
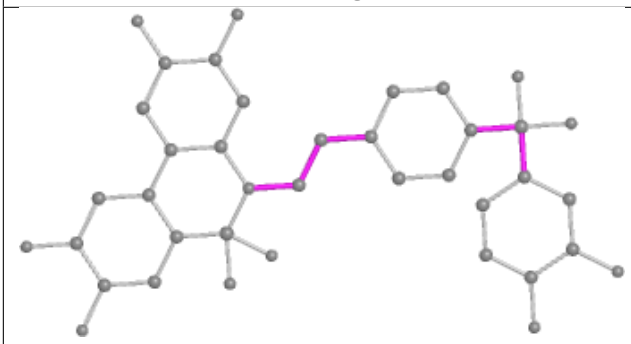


Bond angles



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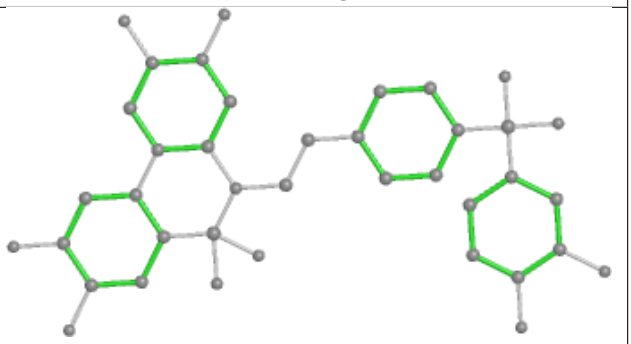
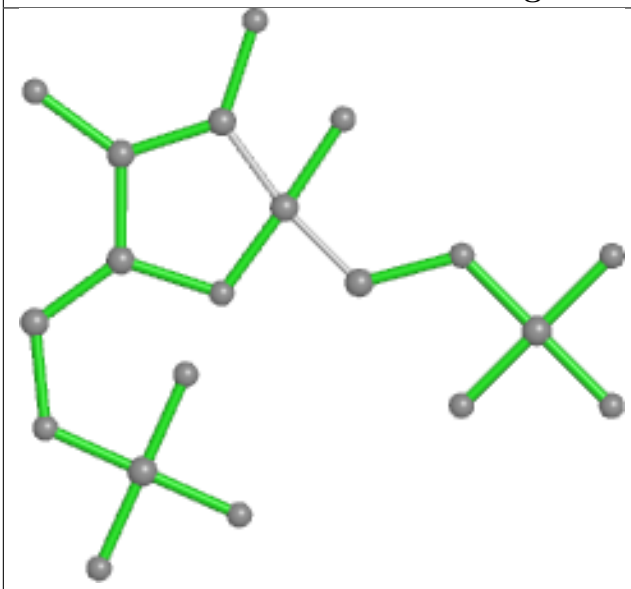


Rings

Ligand FBP G 601



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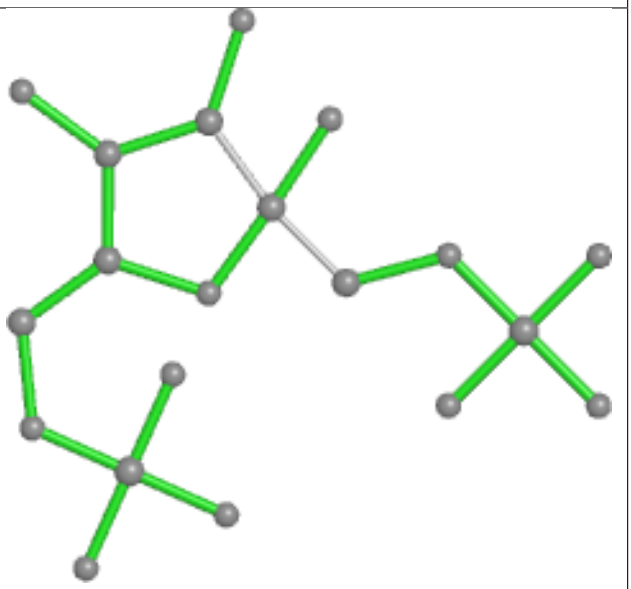
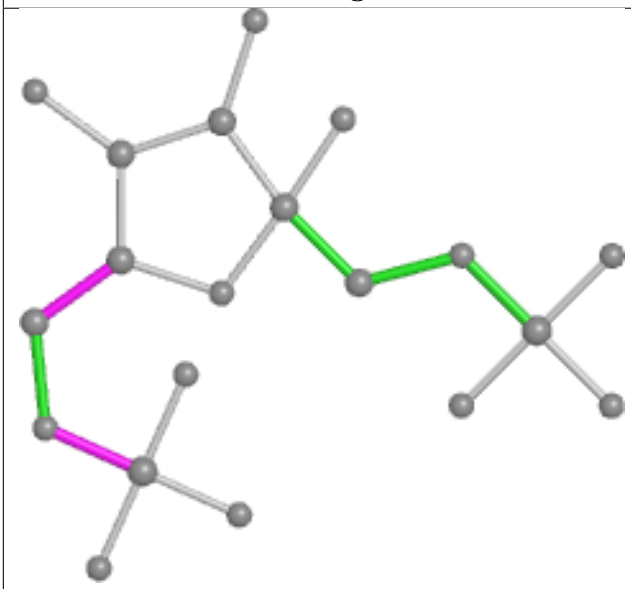


Bond angles



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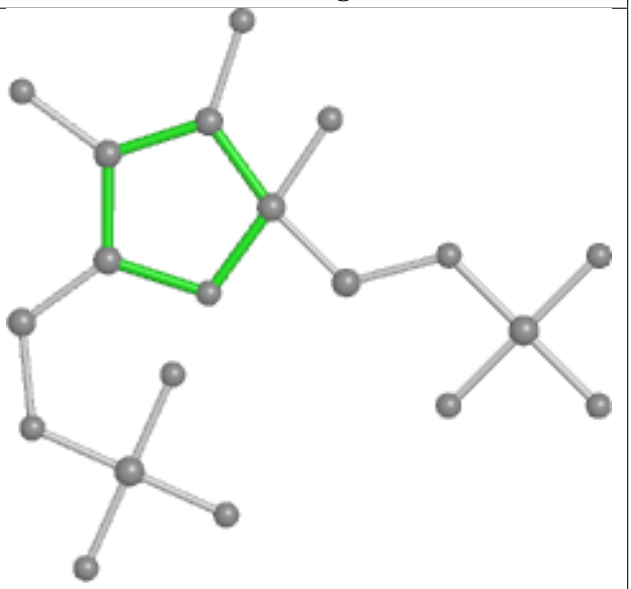
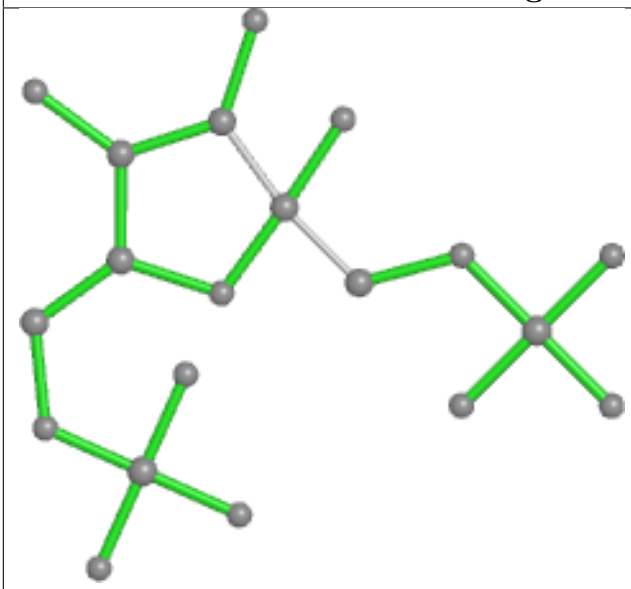


Rings

Ligand FBP C 601



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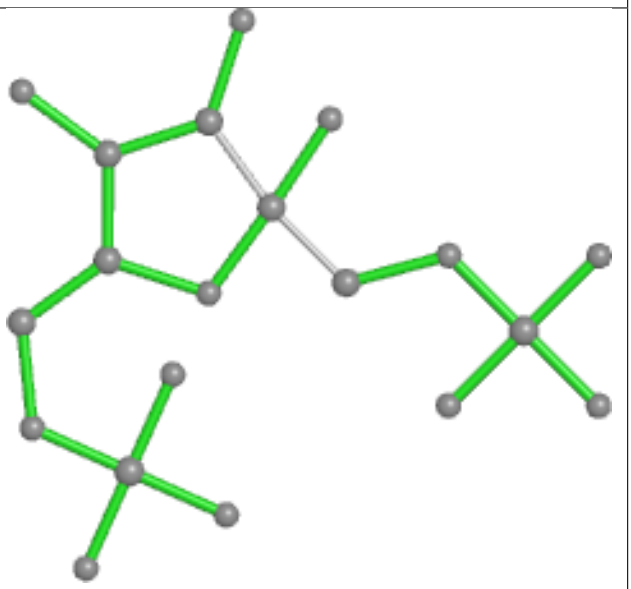

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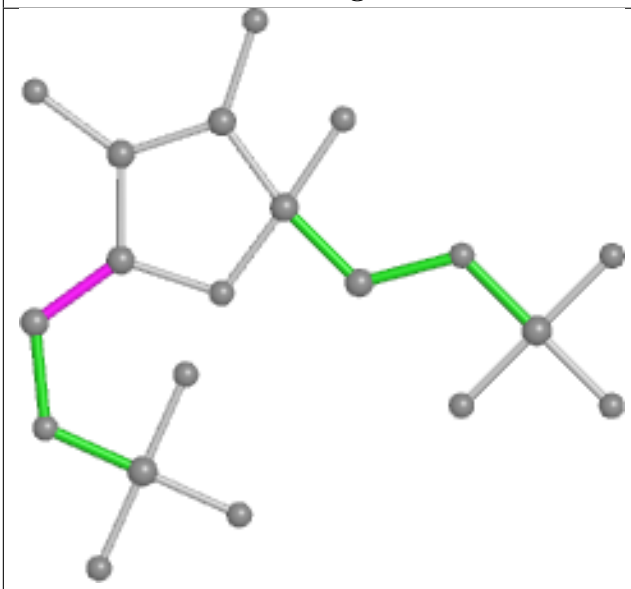

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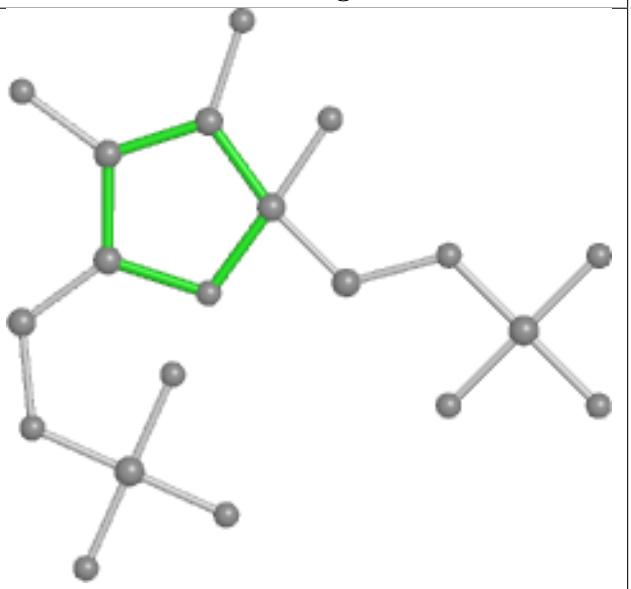

Rings

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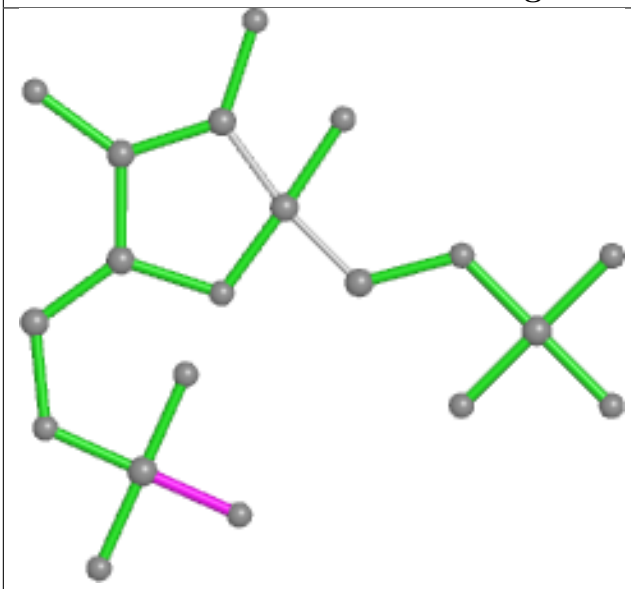

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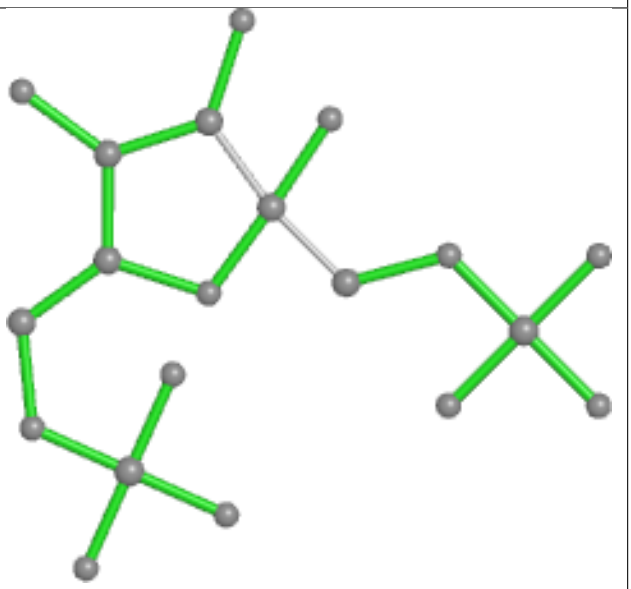

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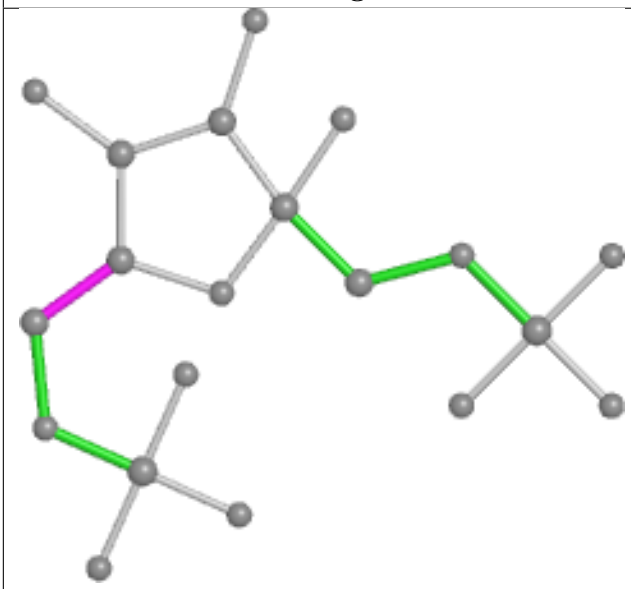

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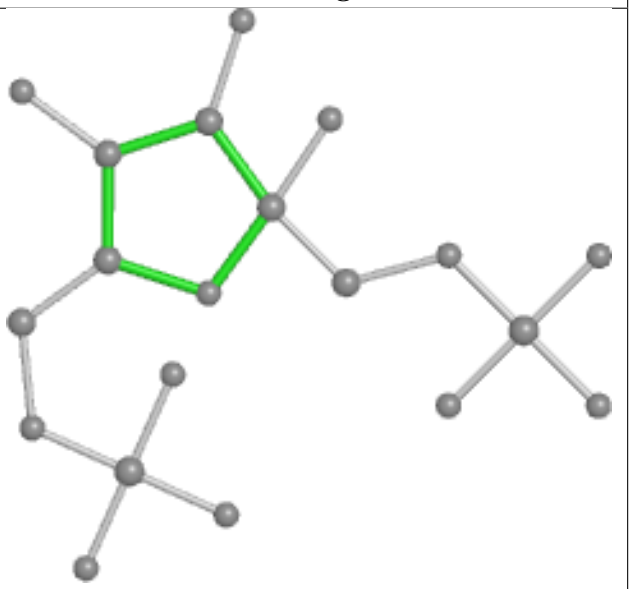
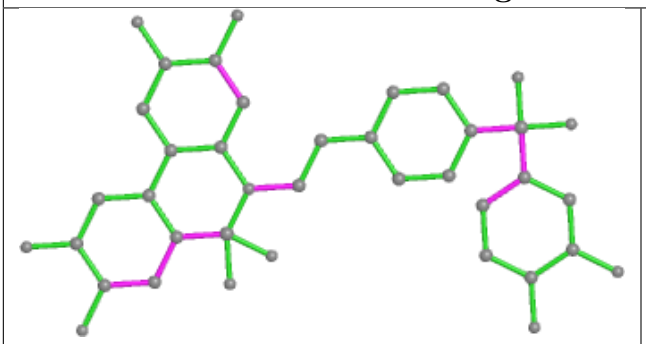


Rings

Ligand Y3Z A 605 (B)



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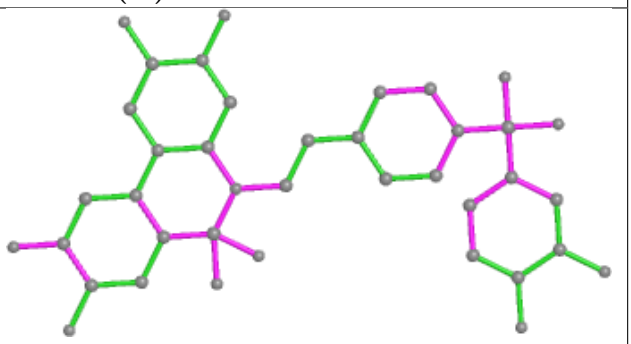
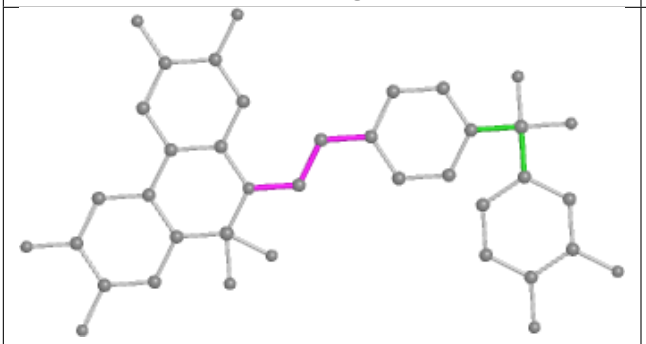


Bond angles



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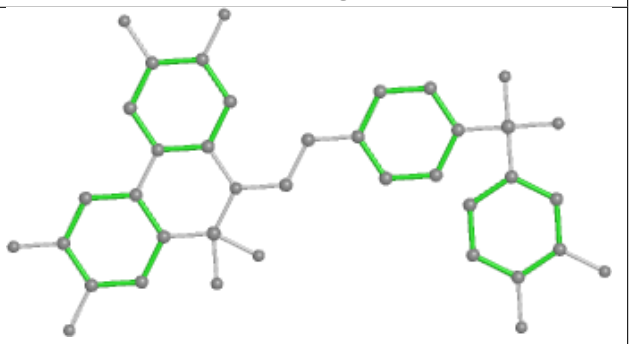
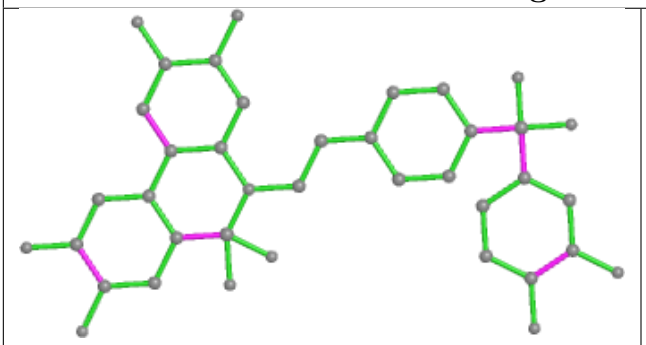


Rings

Ligand Y3Z F 605



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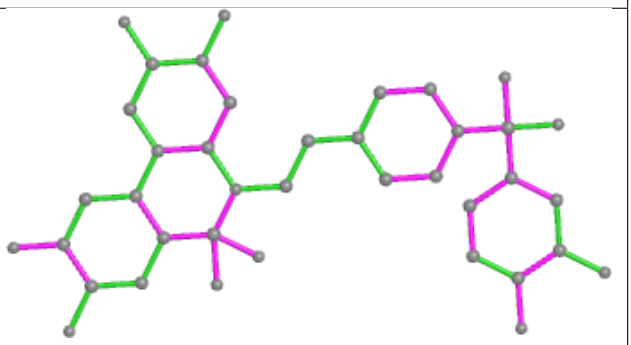

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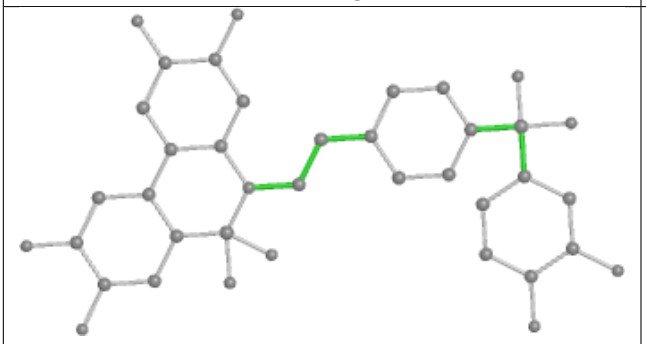

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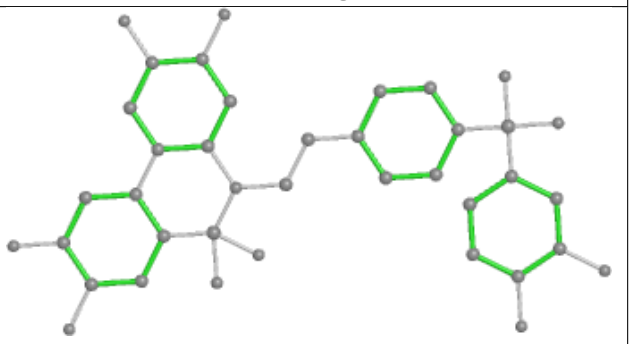
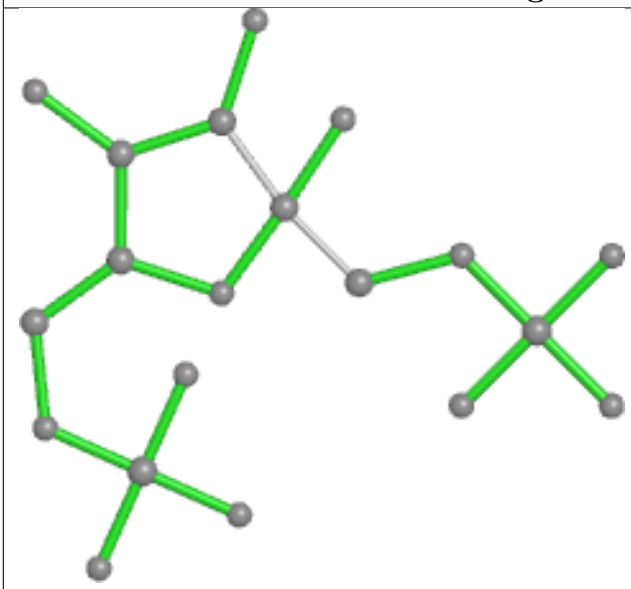


Rings

Ligand FBP F 601



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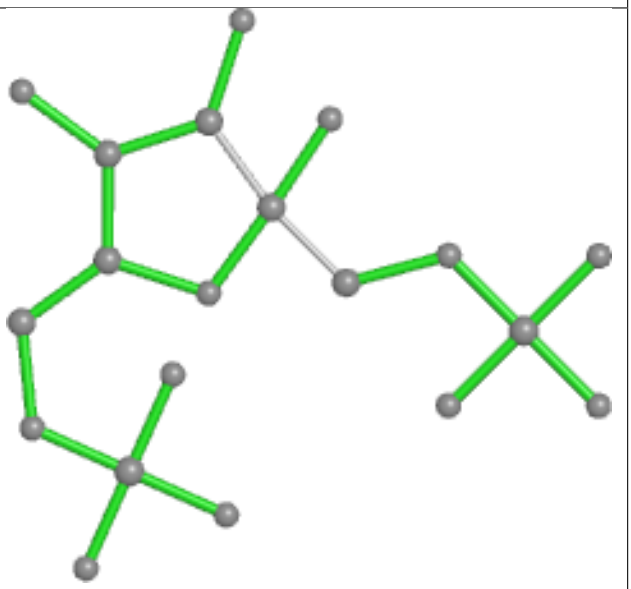
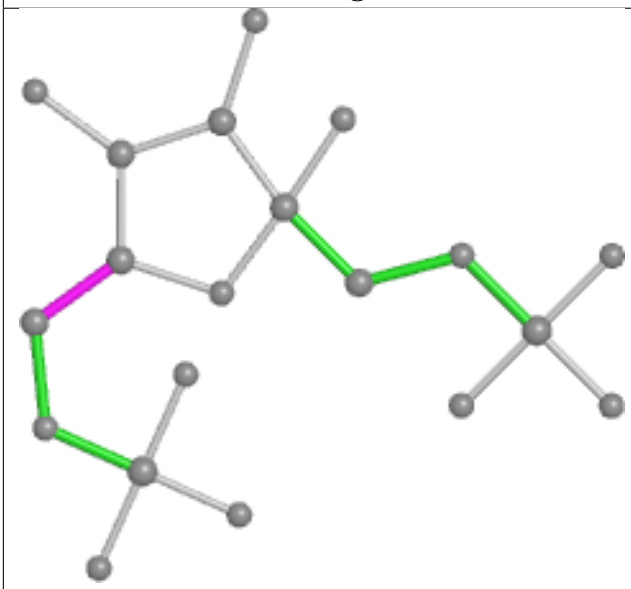


Bond angles



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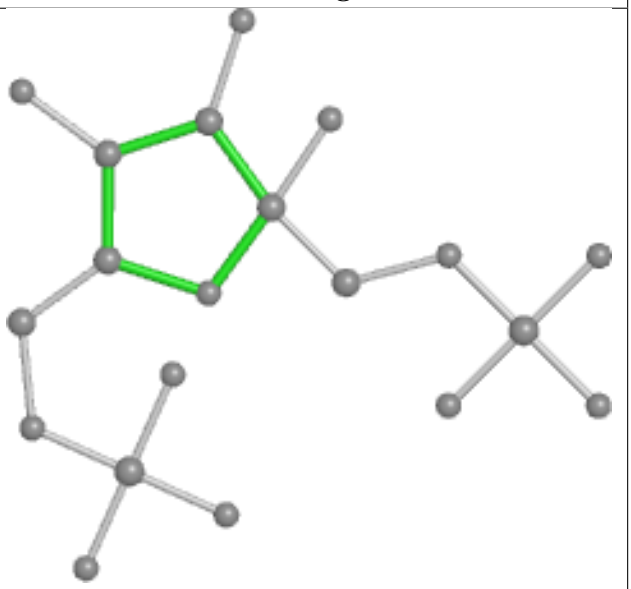
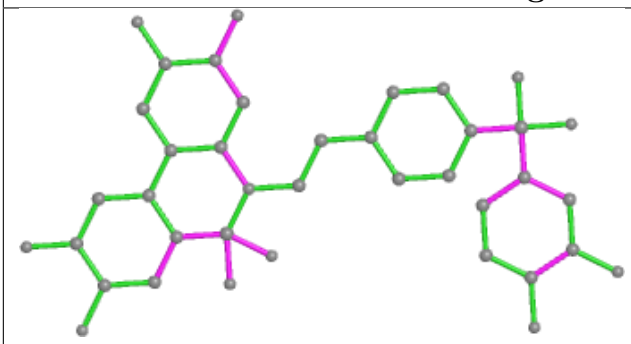


Rings

Ligand Y3Z D 607



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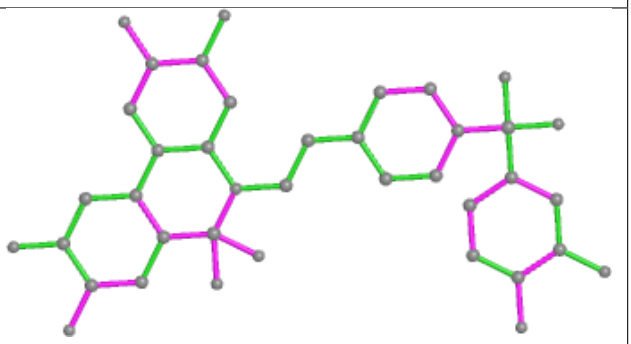
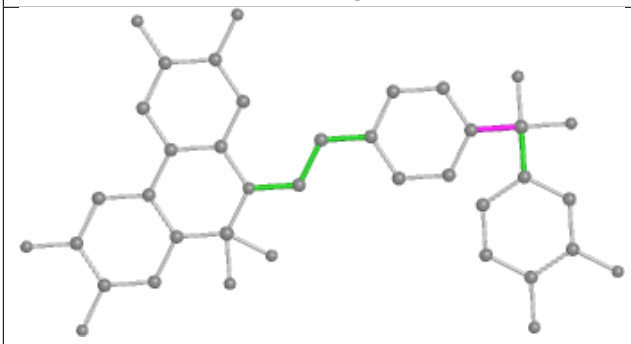


Bond angles



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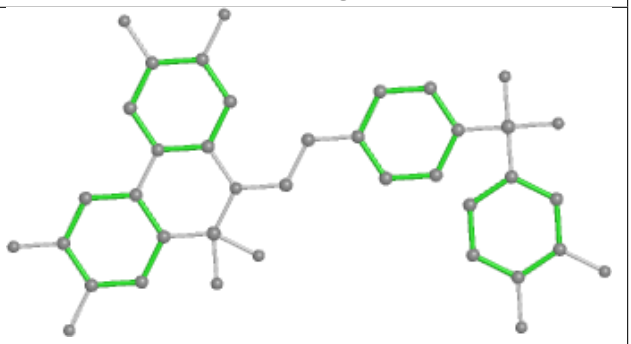
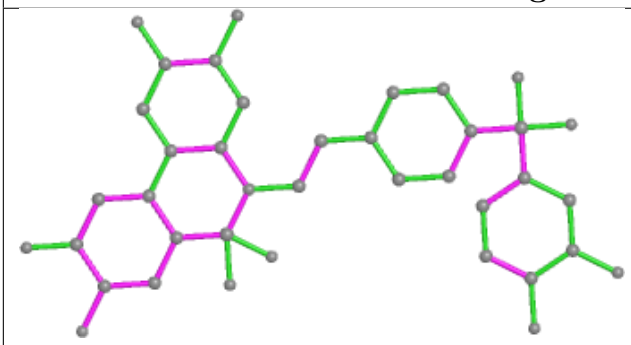
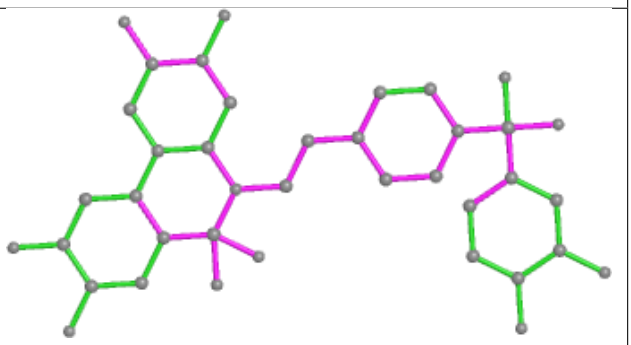


Rings

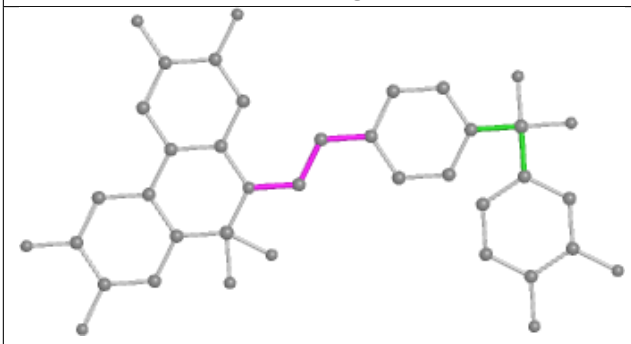
Ligand Y3Z E 605



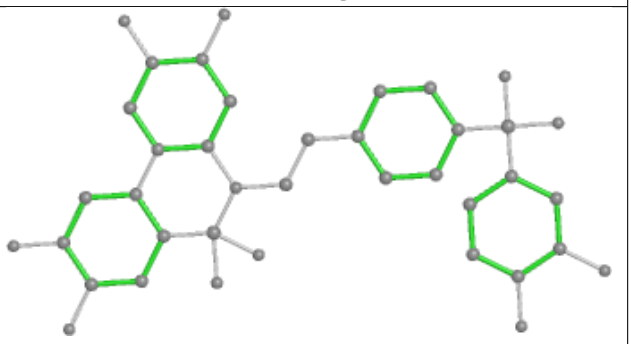
Bond lengths



Bond angles

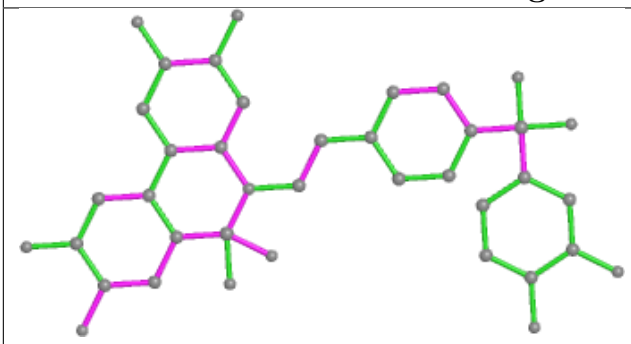


Torsions

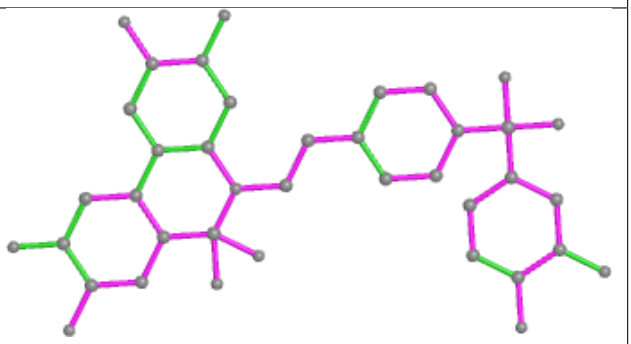


Rings

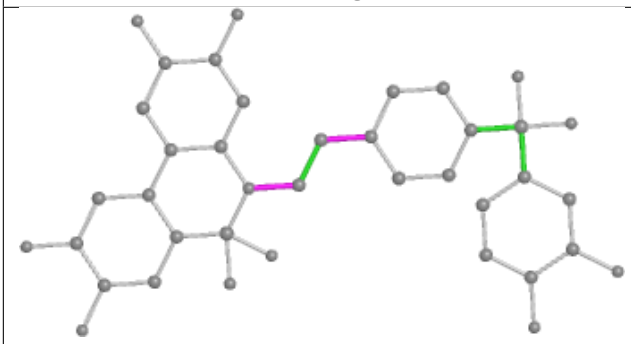
Ligand Y3Z B 605



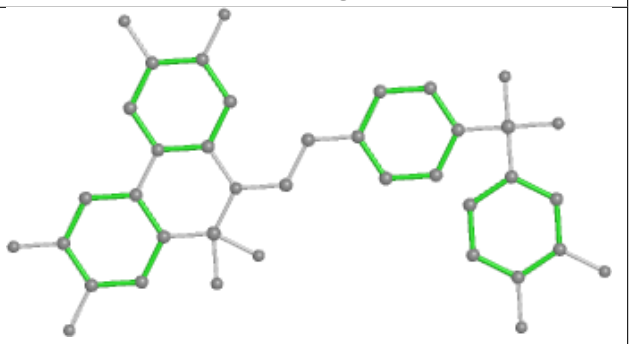
Bond lengths



Bond angles

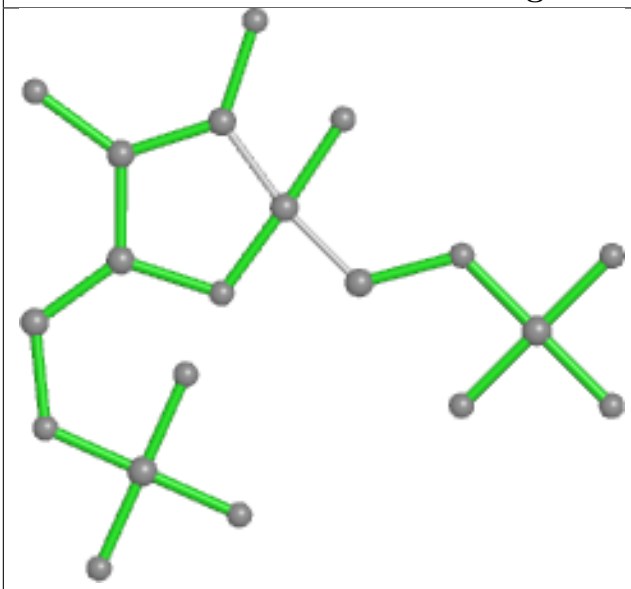


Torsions

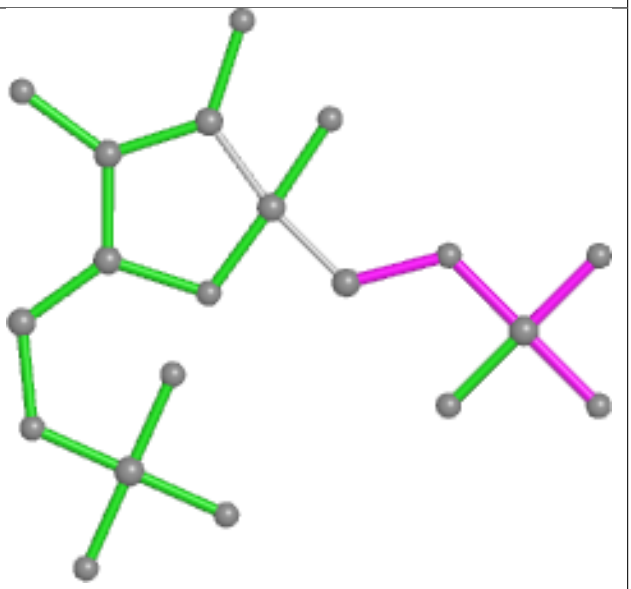


Rings

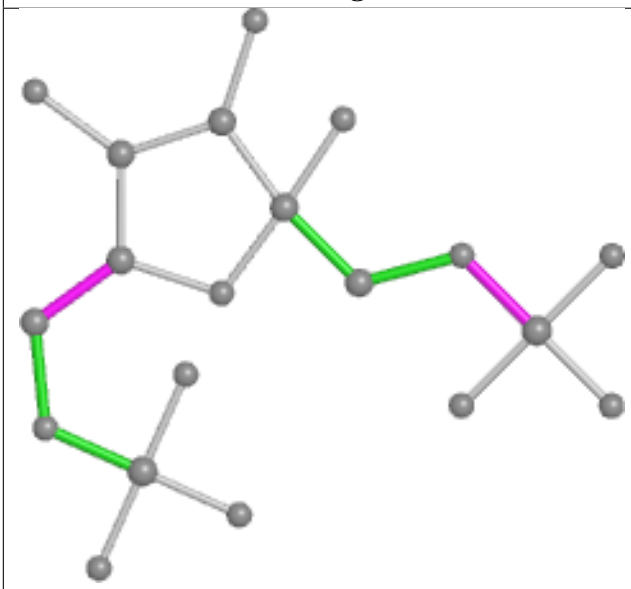
Ligand FBP E 601



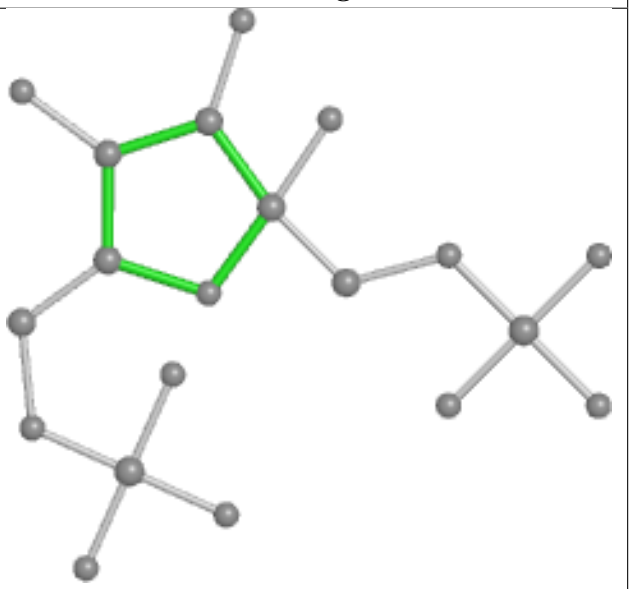
Bond lengths



Bond angles

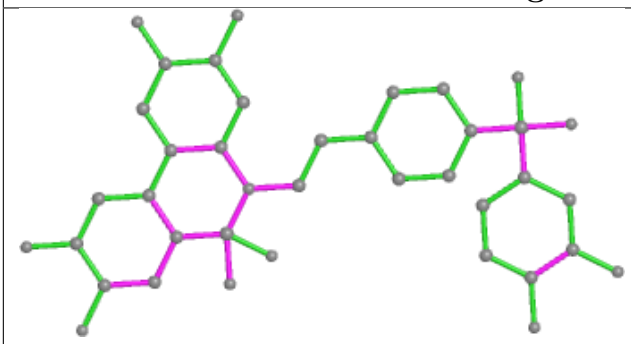


Torsions

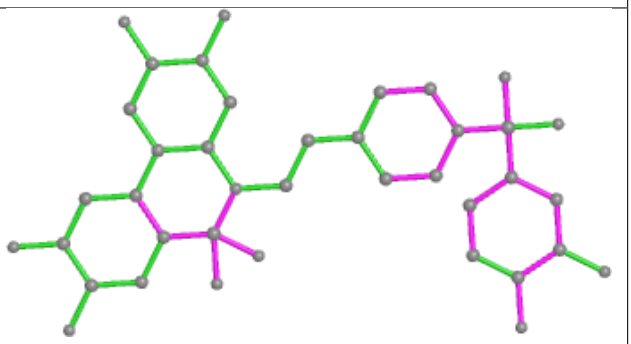


Rings

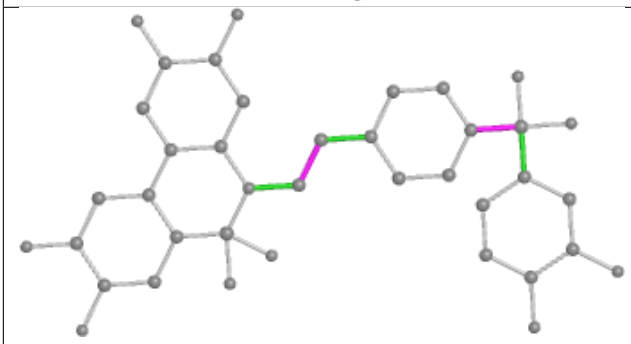
Ligand Y3Z H 607



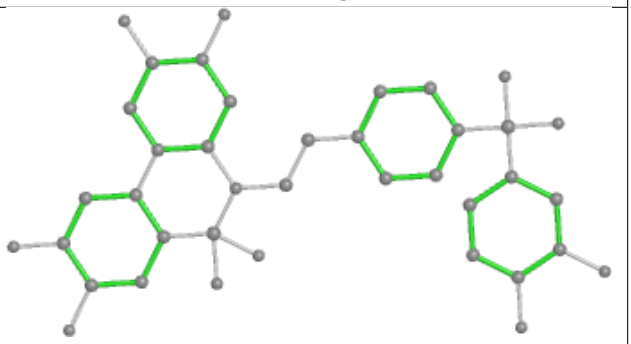
Bond lengths



Bond angles

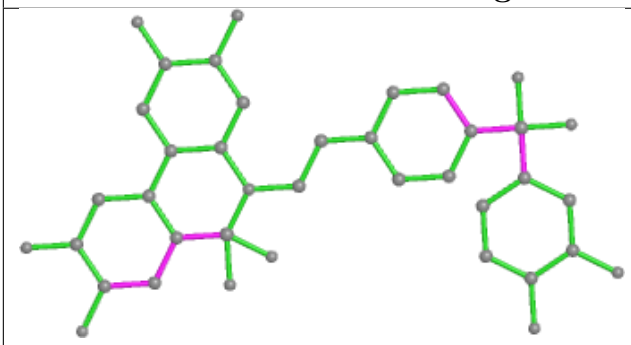


Torsions

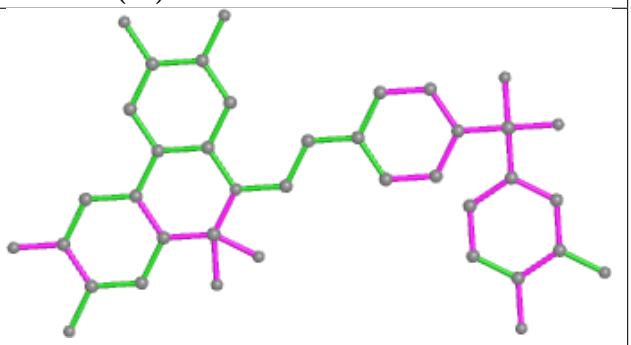


Rings

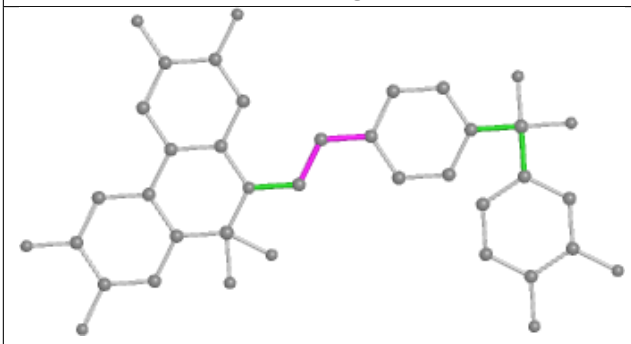
Ligand Y3Z A 605 (A)



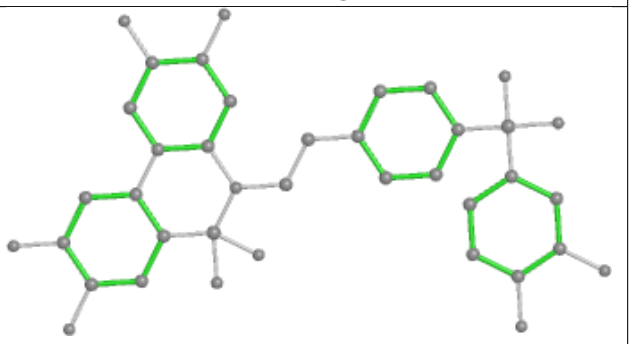
Bond lengths



Bond angles

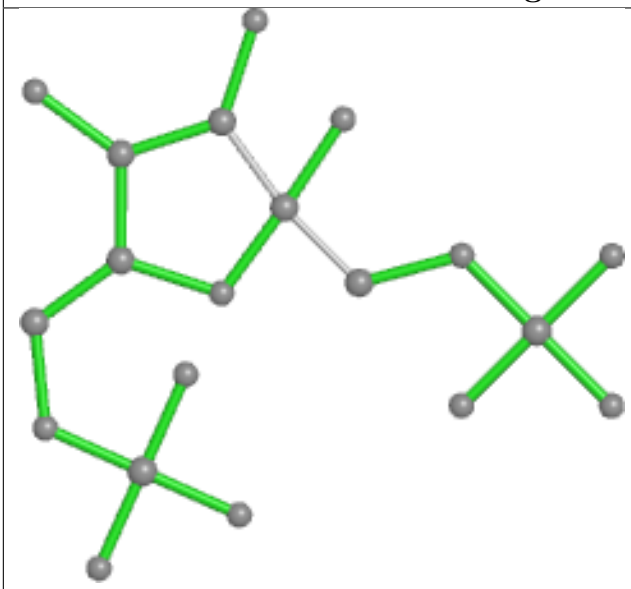


Torsions

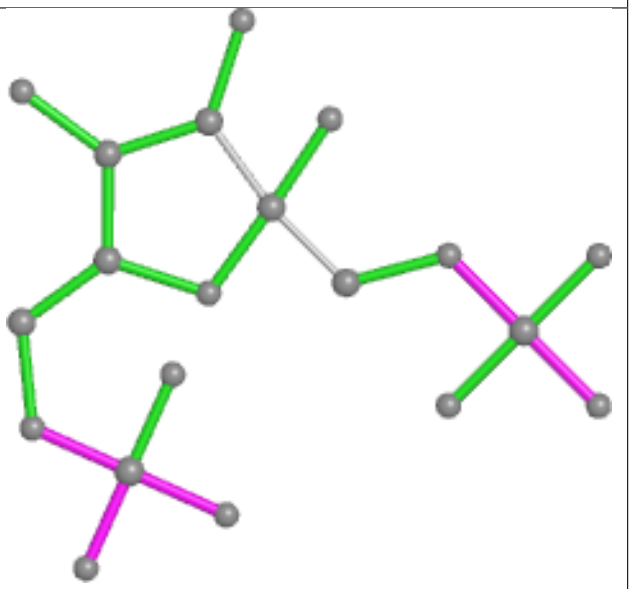


Rings

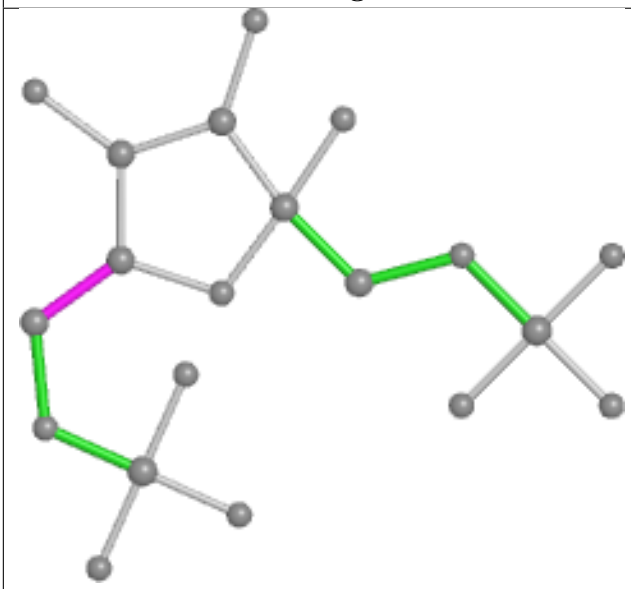
Ligand FBP H 602



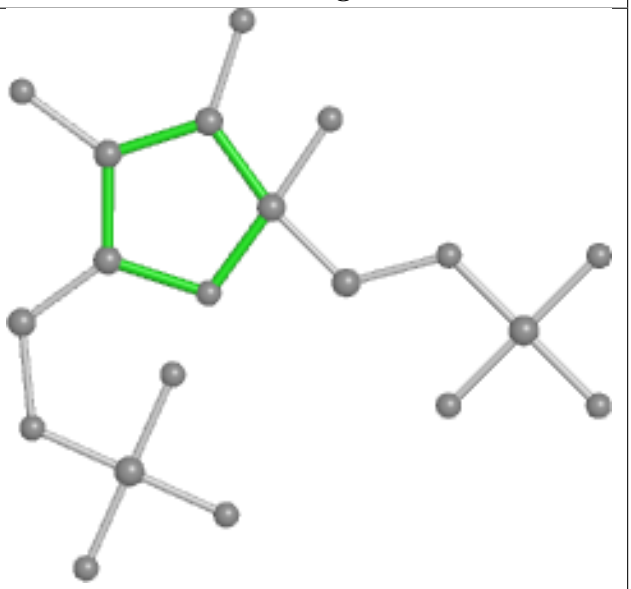
Bond lengths



Bond angles

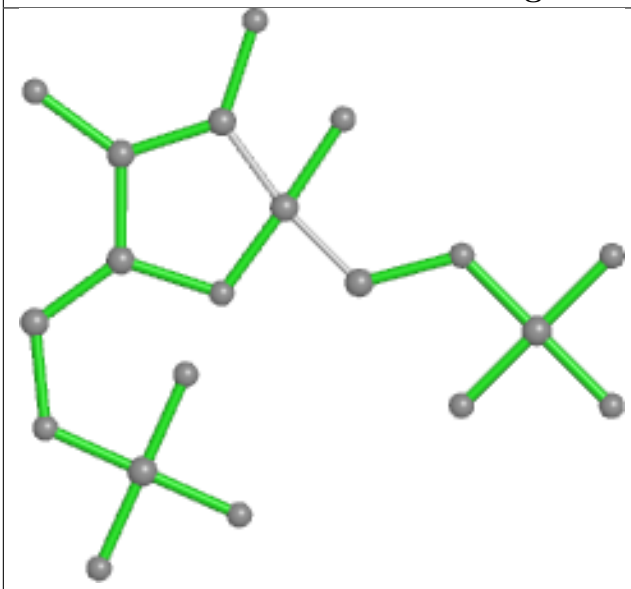


Torsions

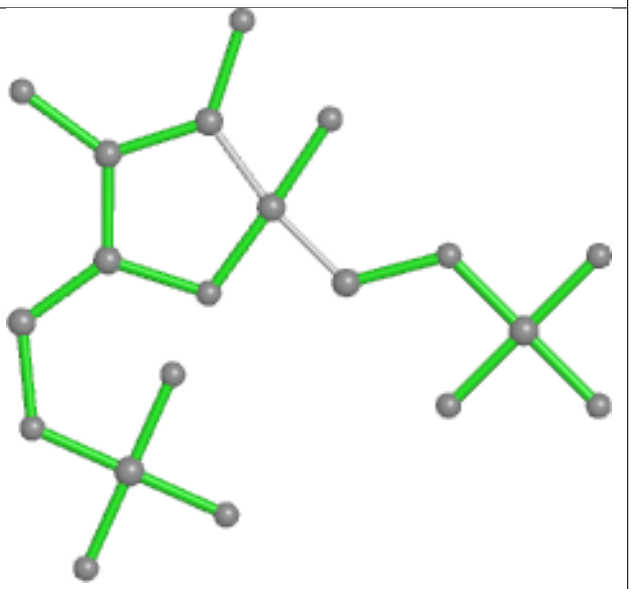


Rings

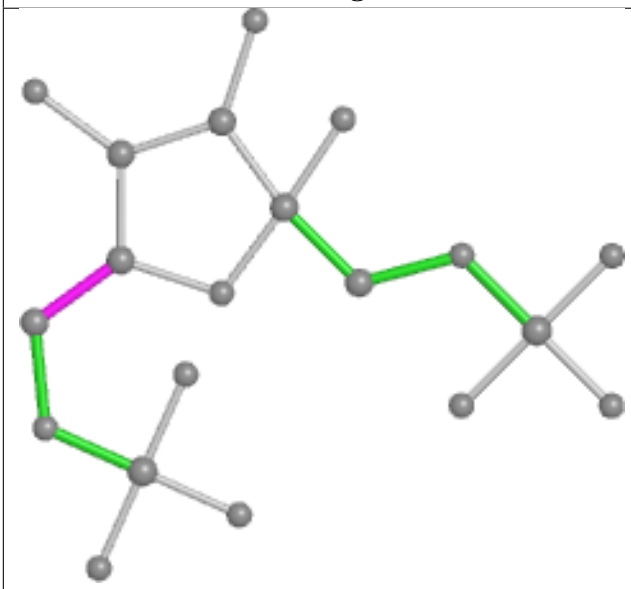
Ligand FBP A 601



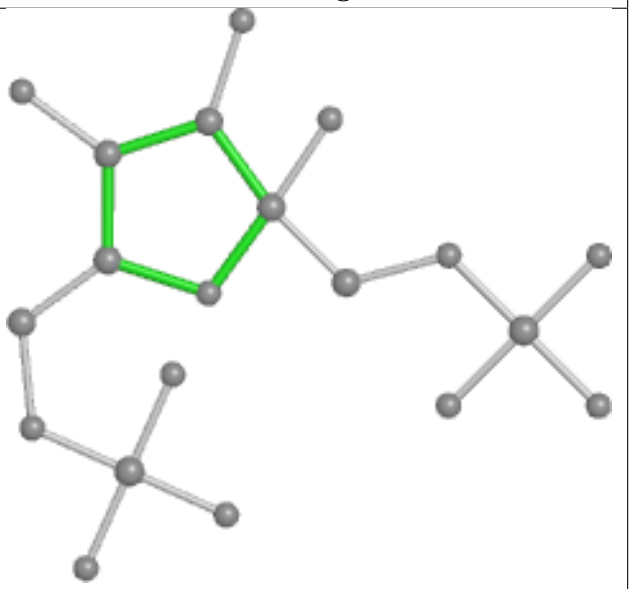
Bond lengths



Bond angles

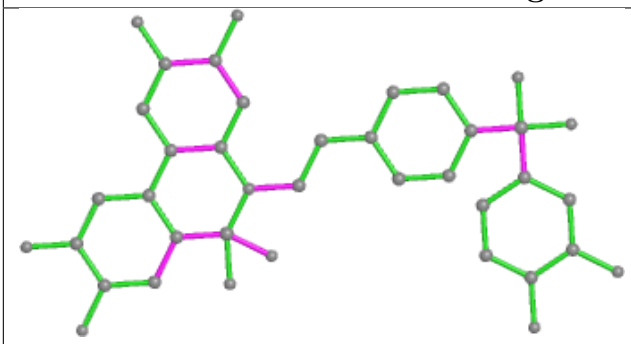


Torsions

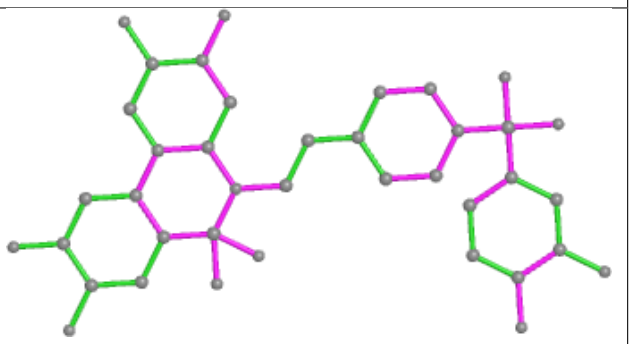


Rings

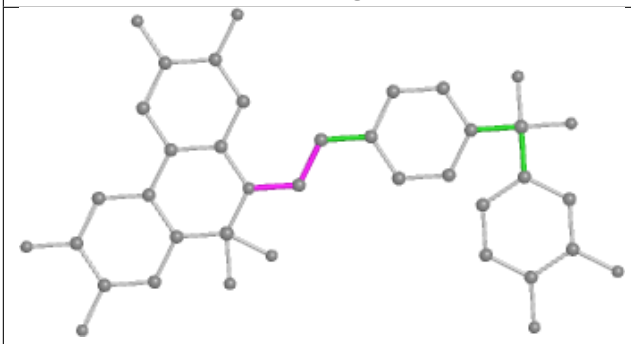
Ligand Y3Z H 601



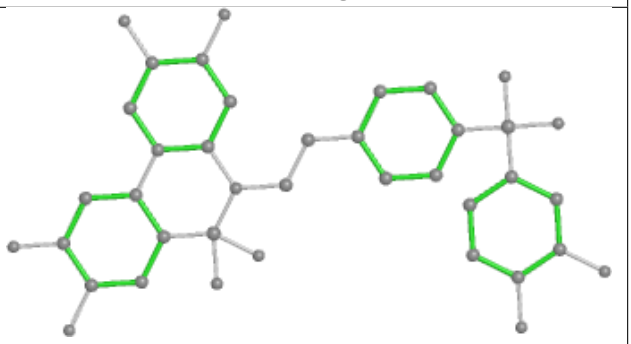
Bond lengths



Bond angles

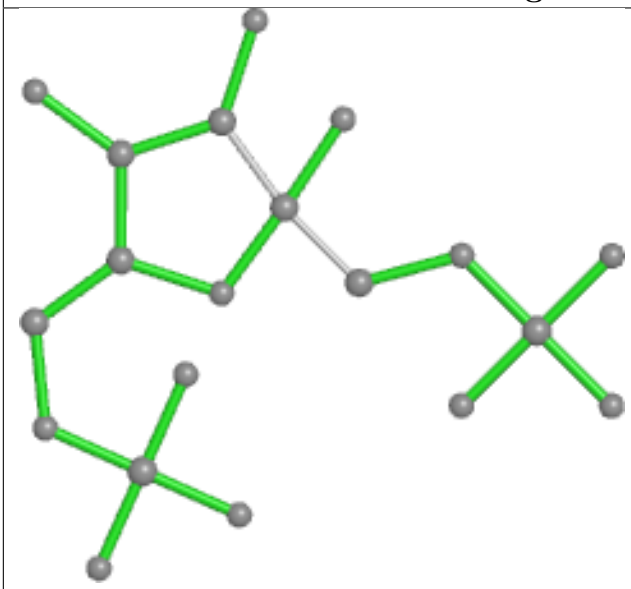


Torsions

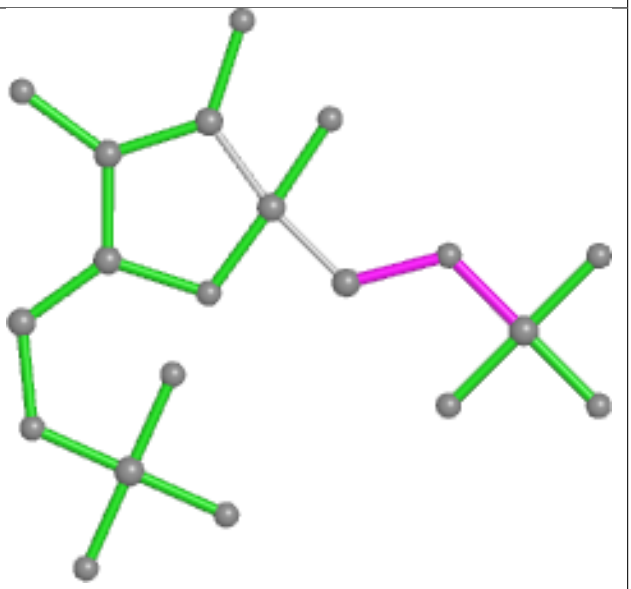


Rings

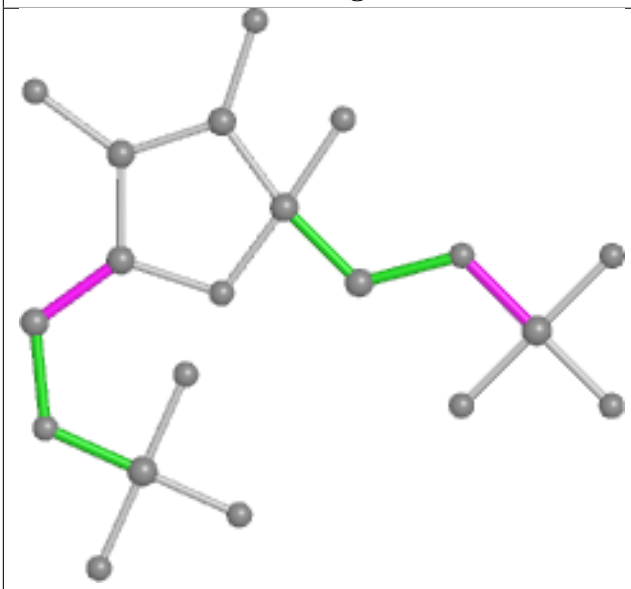
Ligand FBP B 601



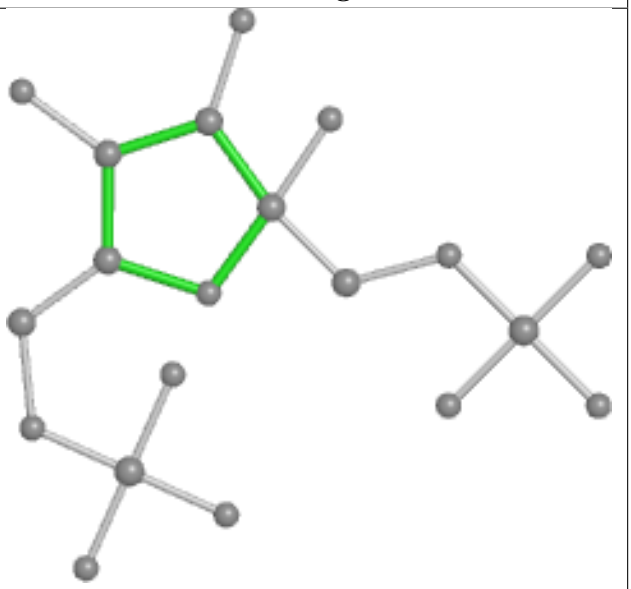
Bond lengths



Bond angles

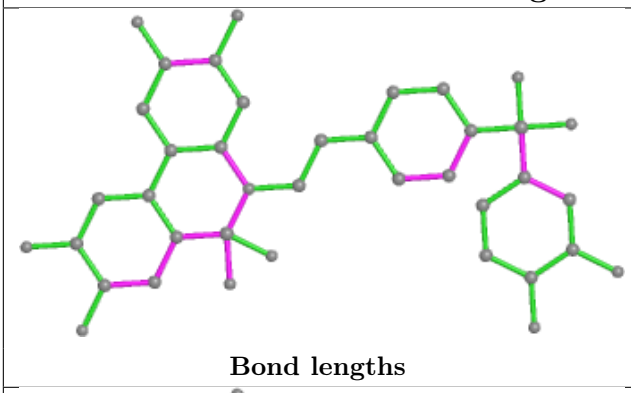


Torsions

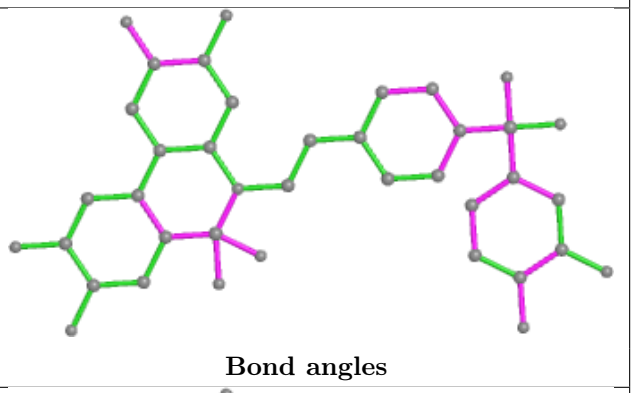


Rings

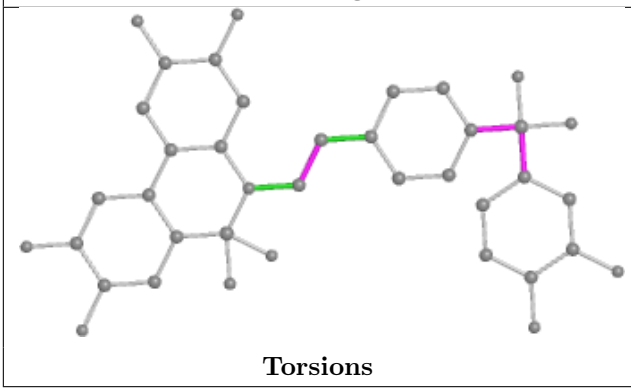
Ligand Y3Z F 606



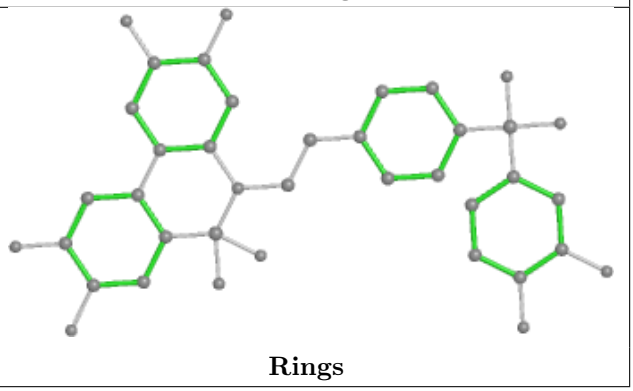
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	0.22	12 (2%)	53	53	37, 63, 99, 125	0
1	B	436/447 (97%)	0.18	10 (2%)	60	61	29, 47, 80, 106	0
1	C	425/447 (95%)	0.12	14 (3%)	46	46	23, 43, 66, 135	0
1	D	425/447 (95%)	0.04	5 (1%)	79	80	26, 39, 66, 106	0
1	E	419/447 (93%)	0.20	8 (1%)	66	68	34, 61, 99, 126	0
1	F	432/447 (96%)	0.15	6 (1%)	75	76	30, 47, 75, 105	0
1	G	421/447 (94%)	0.07	10 (2%)	59	60	23, 44, 63, 96	1 (0%)
1	H	425/447 (95%)	0.02	6 (1%)	75	76	24, 39, 65, 108	0
All	All	3405/3576 (95%)	0.13	71 (2%)	63	65	23, 47, 85, 135	1 (0%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	ARG	12.4
1	E	543	SER	7.8
1	A	543	SER	7.6
1	C	21	GLY	7.3
1	C	22	THR	6.6
1	H	25	PHE	5.9
1	D	25	PHE	5.8
1	B	543	SER	5.6
1	D	21	GLY	5.5
1	F	114	PRO	5.2
1	H	21	GLY	4.9
1	F	543	SER	4.9
1	B	130	GLY	4.8
1	E	25	PHE	4.5
1	D	22	THR	4.5
1	A	25	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	H	22	THR	4.1
1	C	19	GLU	4.0
1	C	20	LEU	3.9
1	E	412	ARG	3.9
1	B	12	ASP	3.7
1	G	232	GLY	3.6
1	F	12	ASP	3.5
1	C	231	PRO	3.5
1	G	34	MET	3.5
1	G	231	PRO	3.4
1	A	275	HIS	3.3
1	A	131	SER	3.3
1	F	540[A]	LEU	3.2
1	C	34	MET	3.1
1	A	487	ARG	3.0
1	A	26	GLN	2.9
1	B	11	ALA	2.8
1	B	540[A]	LEU	2.8
1	G	30	LEU	2.8
1	G	271	GLY	2.8
1	A	30	LEU	2.8
1	G	25	PHE	2.7
1	C	25	PHE	2.7
1	F	493	ILE	2.6
1	D	24	PHE	2.5
1	E	75	GLU	2.5
1	C	30	LEU	2.5
1	E	515	LEU	2.5
1	H	24	PHE	2.5
1	G	408	GLU	2.5
1	A	515	LEU	2.5
1	C	111	ALA	2.4
1	E	487	ARG	2.4
1	F	115	LEU	2.4
1	B	118	ARG	2.4
1	A	297	GLU	2.4
1	E	297	GLU	2.3
1	C	507	GLU	2.3
1	C	412	ARG	2.3
1	A	331[A]	LEU	2.3
1	D	131	SER	2.3
1	H	516	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	94	GLU	2.3
1	B	517	VAL	2.2
1	E	26	GLN	2.2
1	H	131	SER	2.2
1	B	493	ILE	2.2
1	G	24	PHE	2.1
1	G	412	ARG	2.1
1	B	463	ILE	2.1
1	A	115	LEU	2.1
1	C	496	ASP	2.1
1	C	24	PHE	2.1
1	A	408	GLU	2.0
1	G	94	GLU	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 monosaccharides 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, 95^{th} 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	E	604	1/1	-0.18	0.41	156,156,156,156	0
5	K	A	604	1/1	0.14	0.45	166,166,166,166	0
5	K	F	604	1/1	0.14	0.57	168,168,168,168	0
5	K	B	604	1/1	0.29	0.53	147,147,147,147	0
6	Y3Z	F	606	39/39	0.83	0.22	60,73,93,95	21
6	Y3Z	B	606	39/39	0.86	0.20	60,71,91,91	21
6	Y3Z	A	605[A]	39/39	0.87	0.24	77,79,79,80	60
6	Y3Z	A	605[B]	39/39	0.87	0.24	25,32,35,36	60
3	OXL	C	602	6/6	0.89	0.18	69,70,71,71	0
6	Y3Z	D	606	39/39	0.89	0.18	63,66,70,72	21

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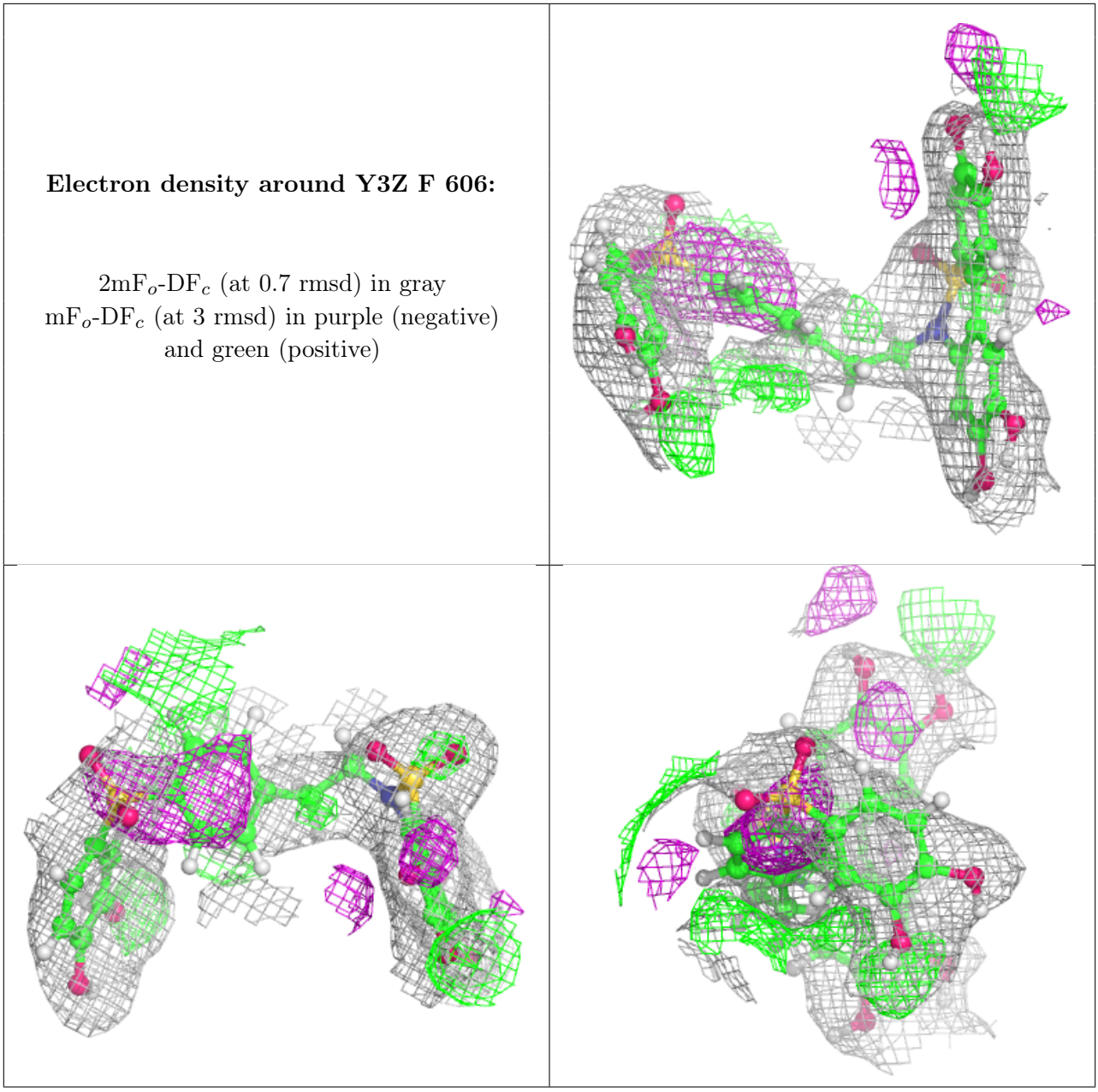
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	Y3Z	E	605	39/39	0.89	0.21	53,58,63,63	21
5	K	H	605	1/1	0.89	0.14	83,83,83,83	0
3	OXL	D	603	6/6	0.90	0.14	50,51,52,52	0
6	Y3Z	H	606	39/39	0.90	0.18	60,63,68,70	21
6	Y3Z	H	607	39/39	0.90	0.23	49,60,90,91	21
5	K	G	604	1/1	0.91	0.09	86,86,86,86	0
6	Y3Z	B	605	39/39	0.91	0.17	59,65,74,75	21
3	OXL	F	602	6/6	0.92	0.12	70,70,71,71	0
6	Y3Z	H	601	39/39	0.92	0.17	46,51,53,53	21
6	Y3Z	D	607	39/39	0.92	0.23	47,59,84,85	21
6	Y3Z	D	601	39/39	0.92	0.20	48,51,55,56	21
5	K	D	605	1/1	0.93	0.13	89,89,89,89	0
3	OXL	E	602	6/6	0.94	0.20	107,107,107,108	0
3	OXL	B	602	6/6	0.94	0.13	67,68,69,70	0
3	OXL	G	602	6/6	0.94	0.14	58,59,60,61	0
6	Y3Z	F	605	39/39	0.94	0.15	59,62,76,76	21
3	OXL	H	603	6/6	0.95	0.13	50,51,51,52	0
4	MG	D	604	1/1	0.95	0.19	24,24,24,24	0
3	OXL	A	602	6/6	0.97	0.16	111,111,111,111	0
2	FBP	A	601	20/20	0.97	0.13	44,48,52,52	0
4	MG	C	603	1/1	0.97	0.21	33,33,33,33	0
2	FBP	F	601	20/20	0.98	0.12	43,48,52,52	0
5	K	C	604	1/1	0.98	0.07	66,66,66,66	0
2	FBP	B	601	20/20	0.98	0.13	41,47,54,54	0
4	MG	E	603	1/1	0.98	0.15	45,45,45,45	0
2	FBP	E	601	20/20	0.98	0.13	46,49,50,50	0
2	FBP	G	601	20/20	0.99	0.12	26,29,30,31	0
4	MG	F	603	1/1	0.99	0.15	30,30,30,30	0
4	MG	G	603	1/1	0.99	0.14	27,27,27,27	0
2	FBP	H	602	20/20	0.99	0.15	30,35,37,37	0
4	MG	A	603	1/1	0.99	0.13	42,42,42,42	0
4	MG	B	603	1/1	0.99	0.18	30,30,30,30	0
2	FBP	C	601	20/20	0.99	0.12	27,28,30,32	0
2	FBP	D	602	20/20	0.99	0.15	33,35,36,36	0
4	MG	H	604	1/1	1.00	0.16	10,10,10,10	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.

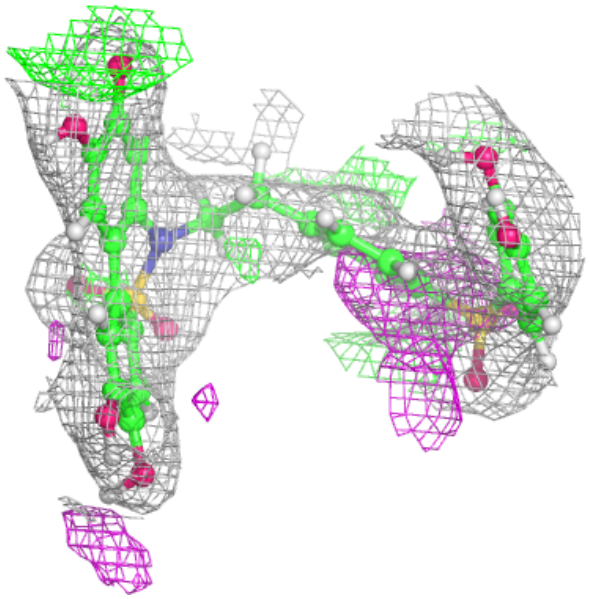
Electron density around Y3Z F 606:

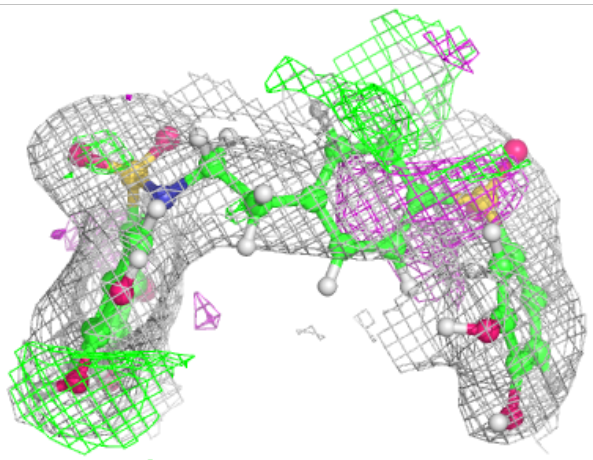
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

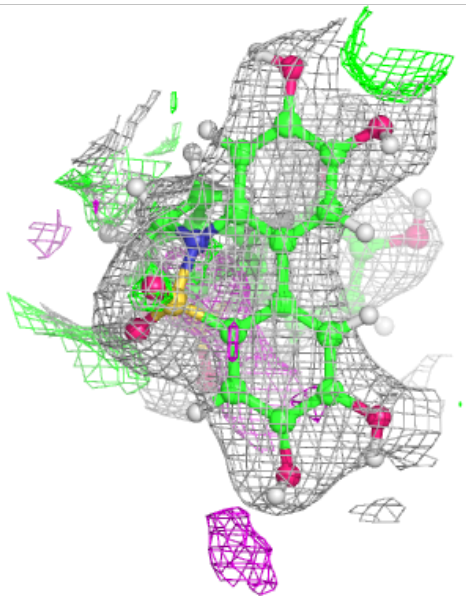


Electron density around Y3Z B 606:

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

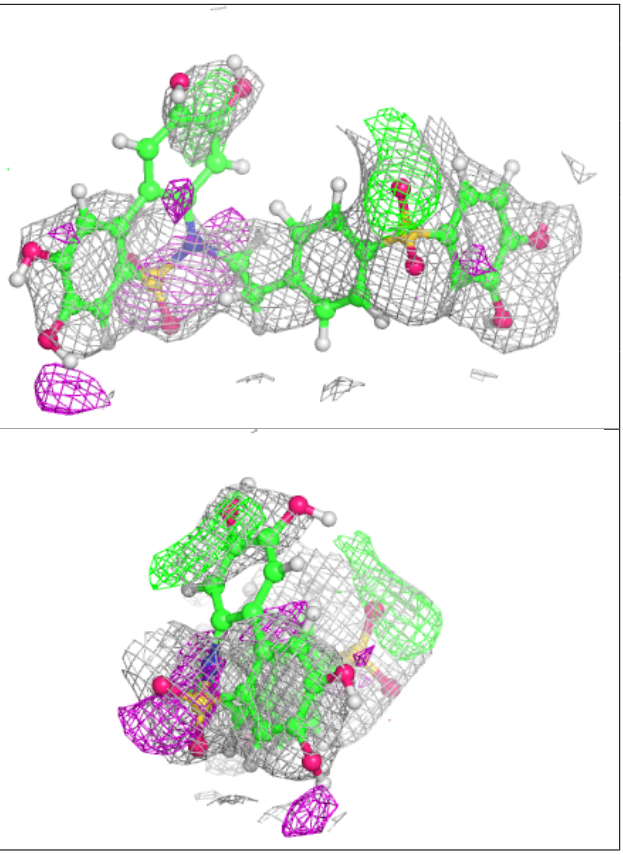






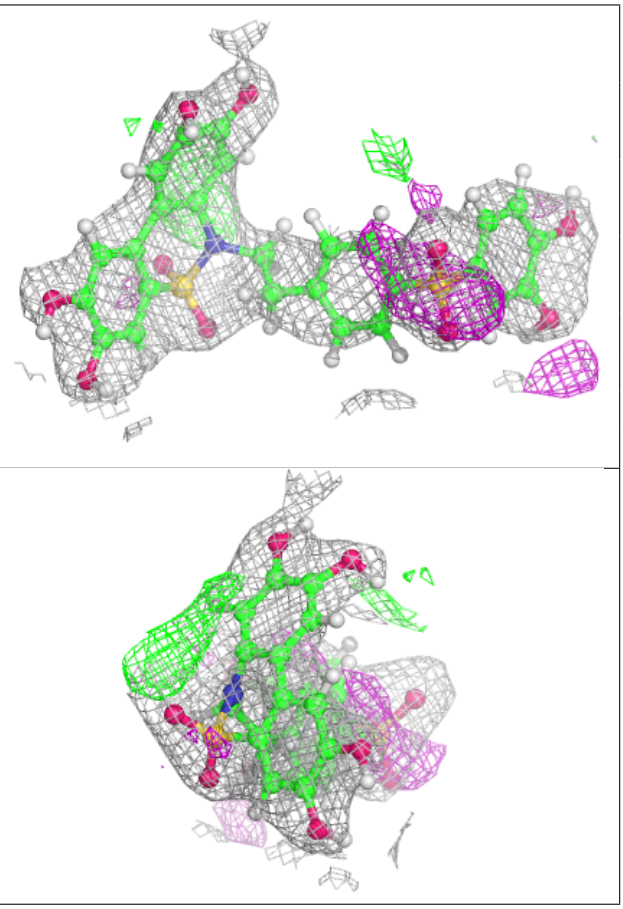
Electron density around Y3Z A 605 (A):

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



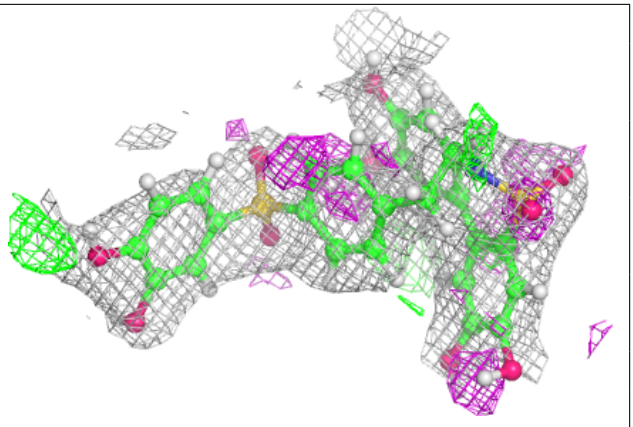
Electron density around Y3Z A 605 (B):

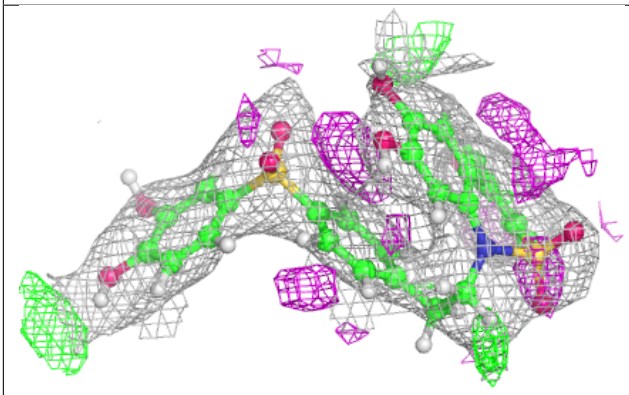
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

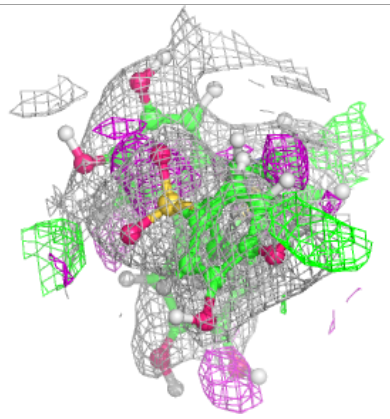


Electron density around Y3Z D 606:

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

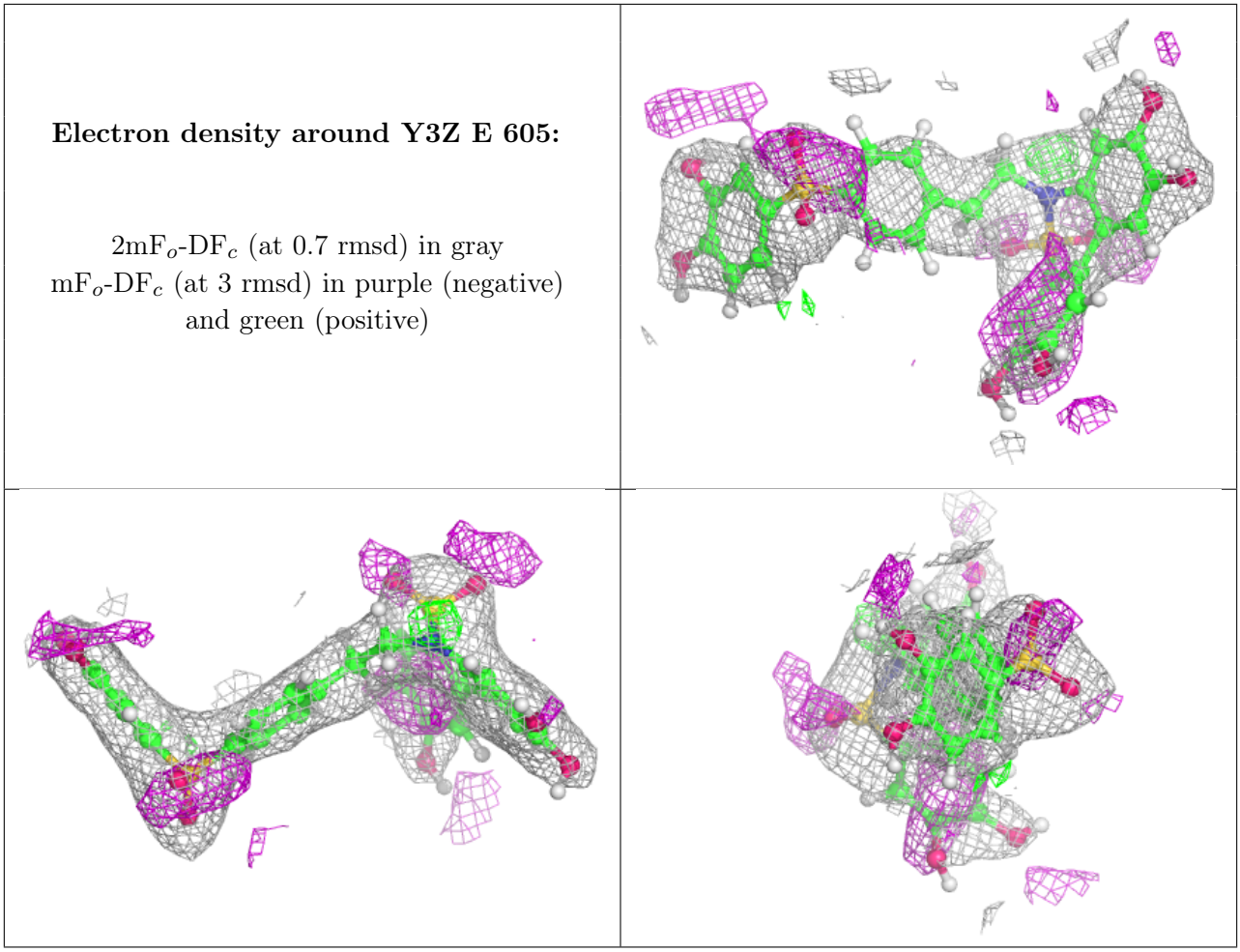






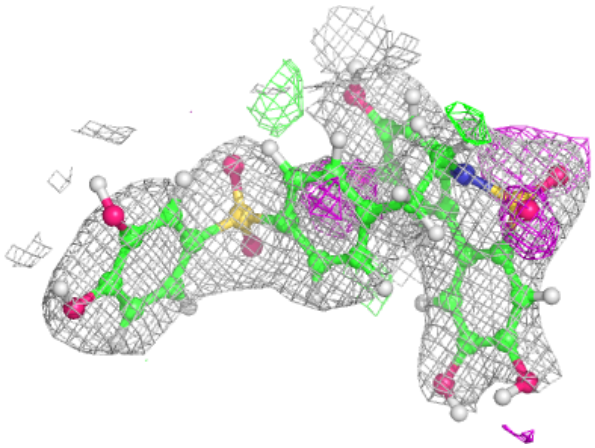
Electron density around Y3Z E 605:

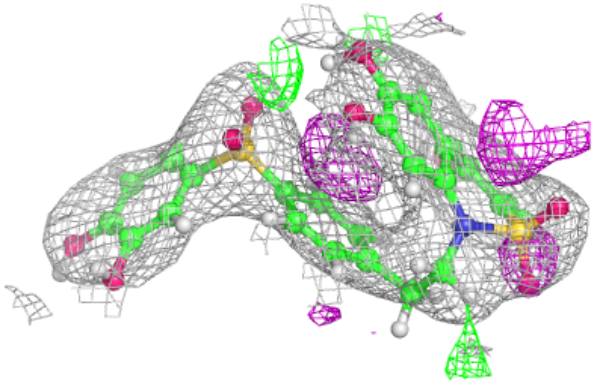
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

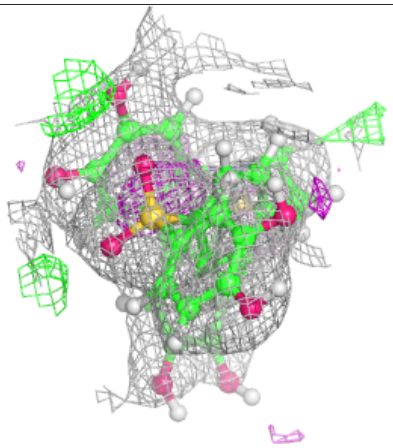


Electron density around Y3Z H 606:

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

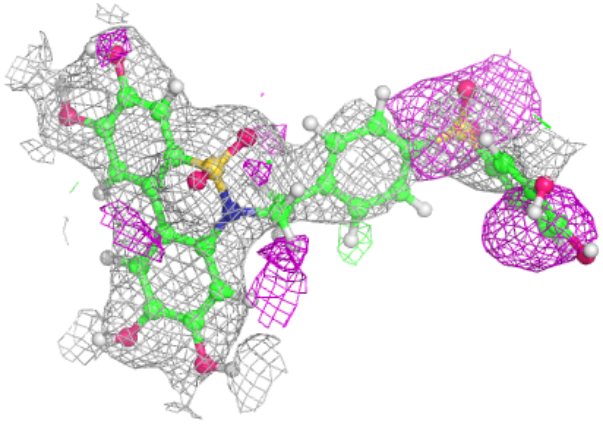


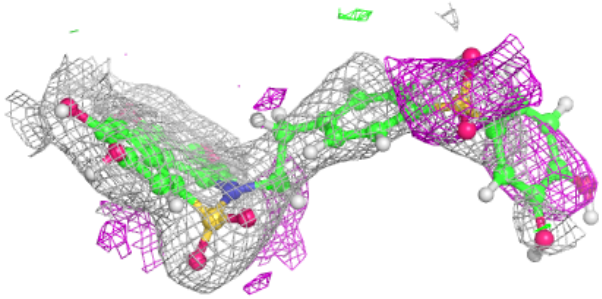


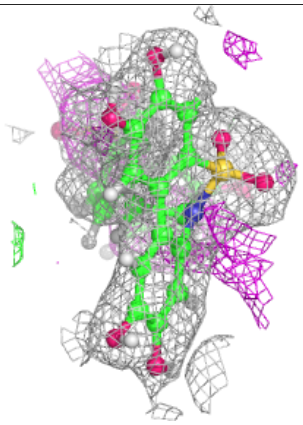


Electron density around Y3Z H 607:

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

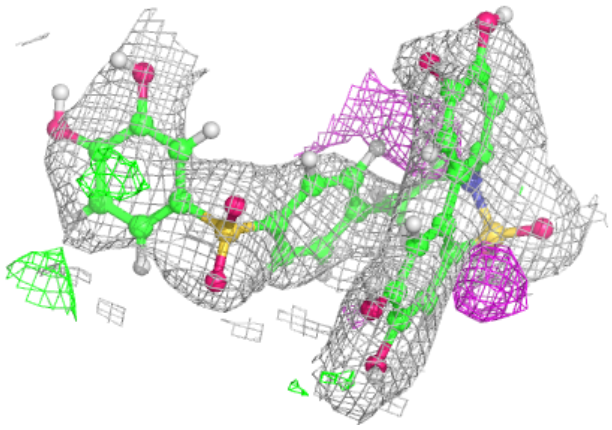


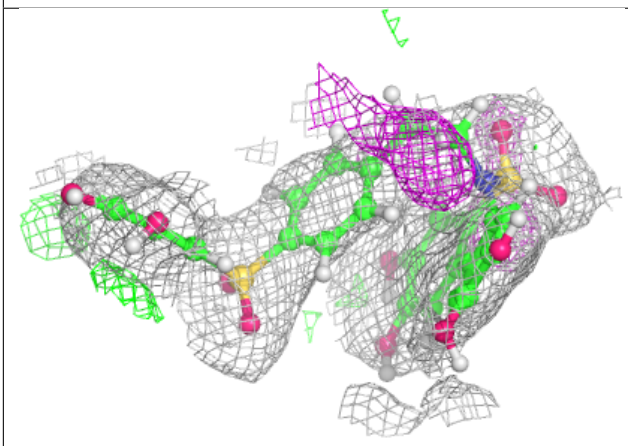


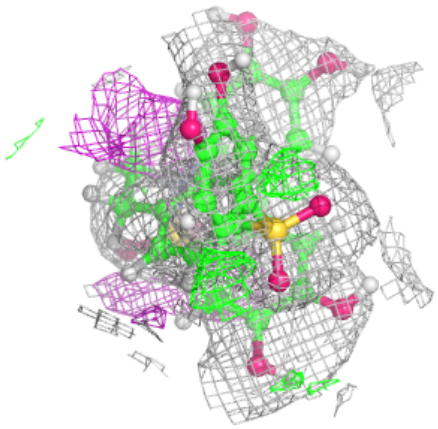


Electron density around Y3Z B 605:

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

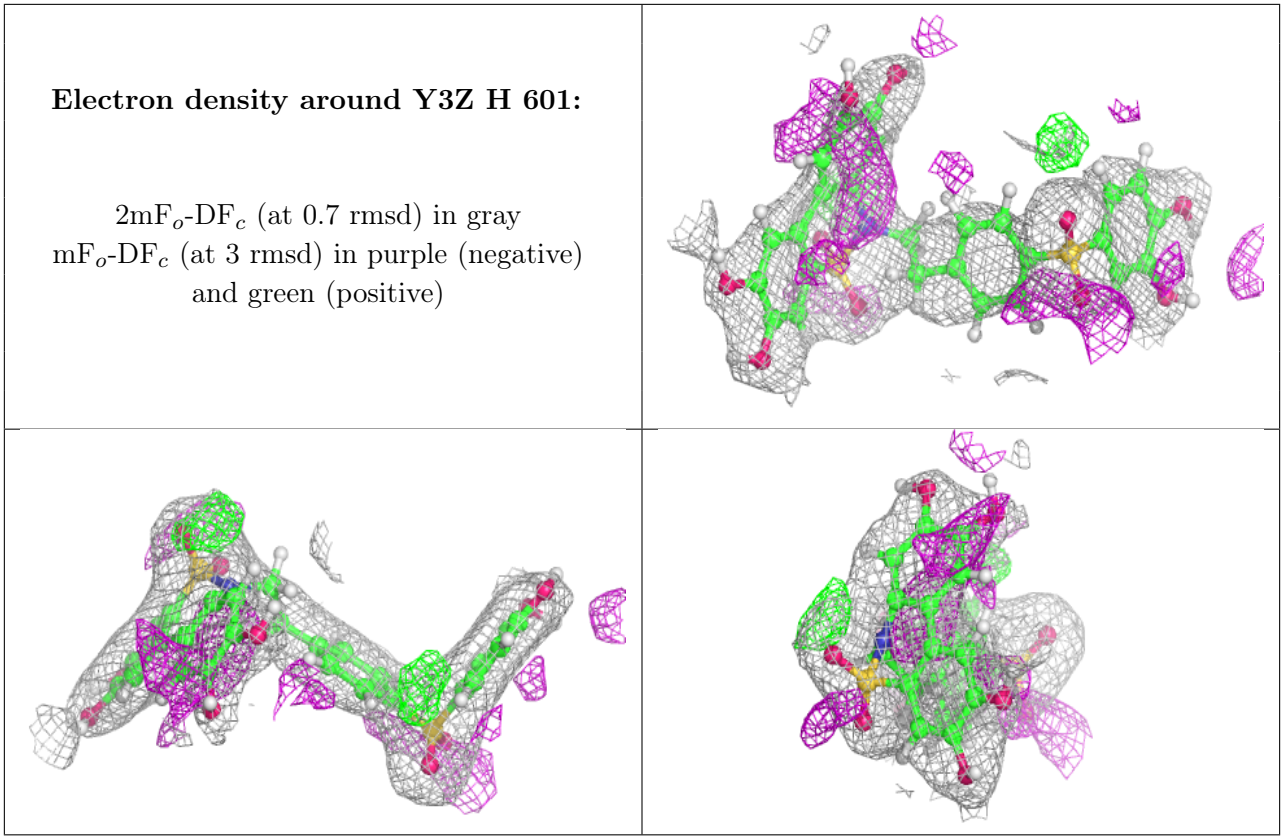






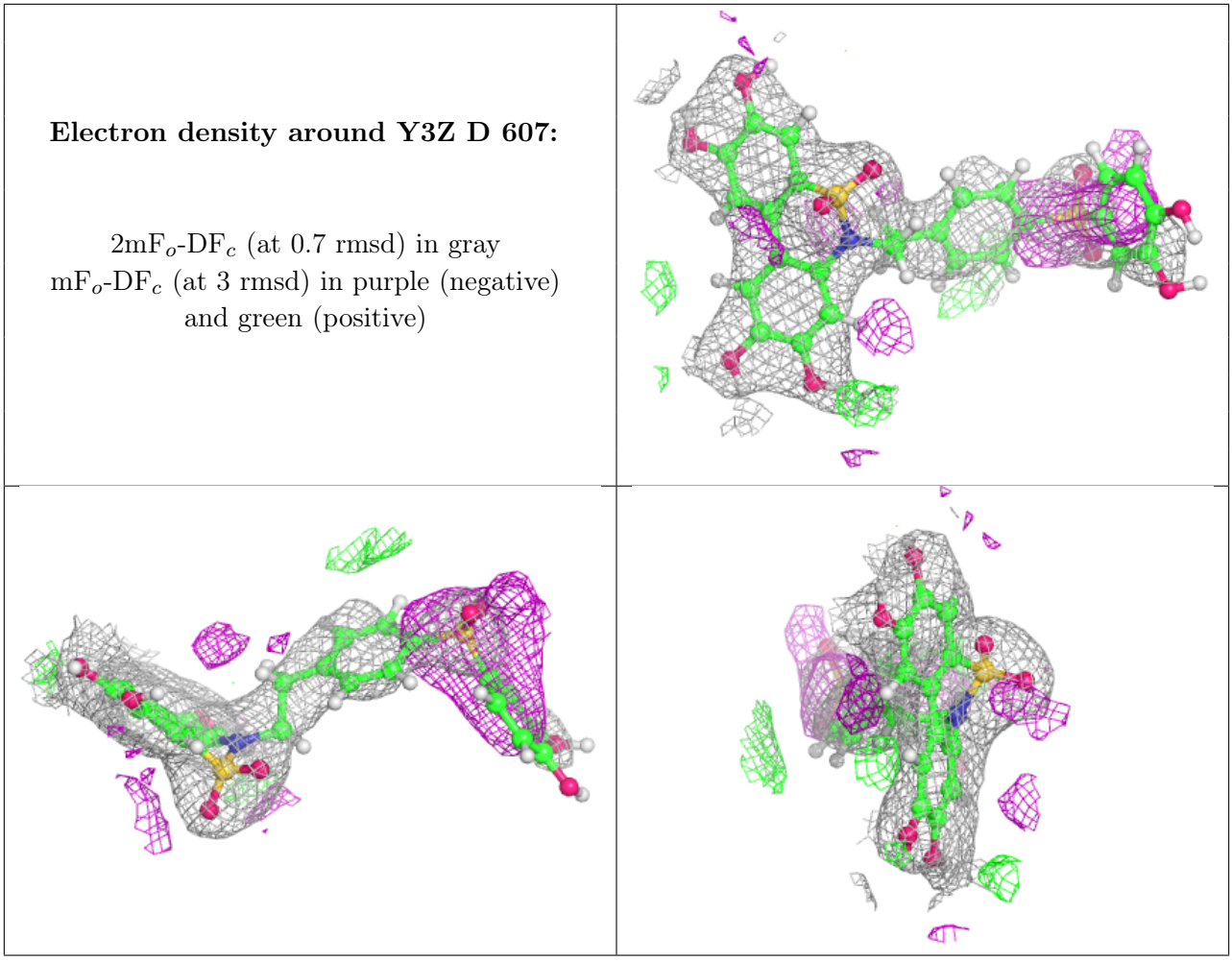
Electron density around Y3Z H 601:

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



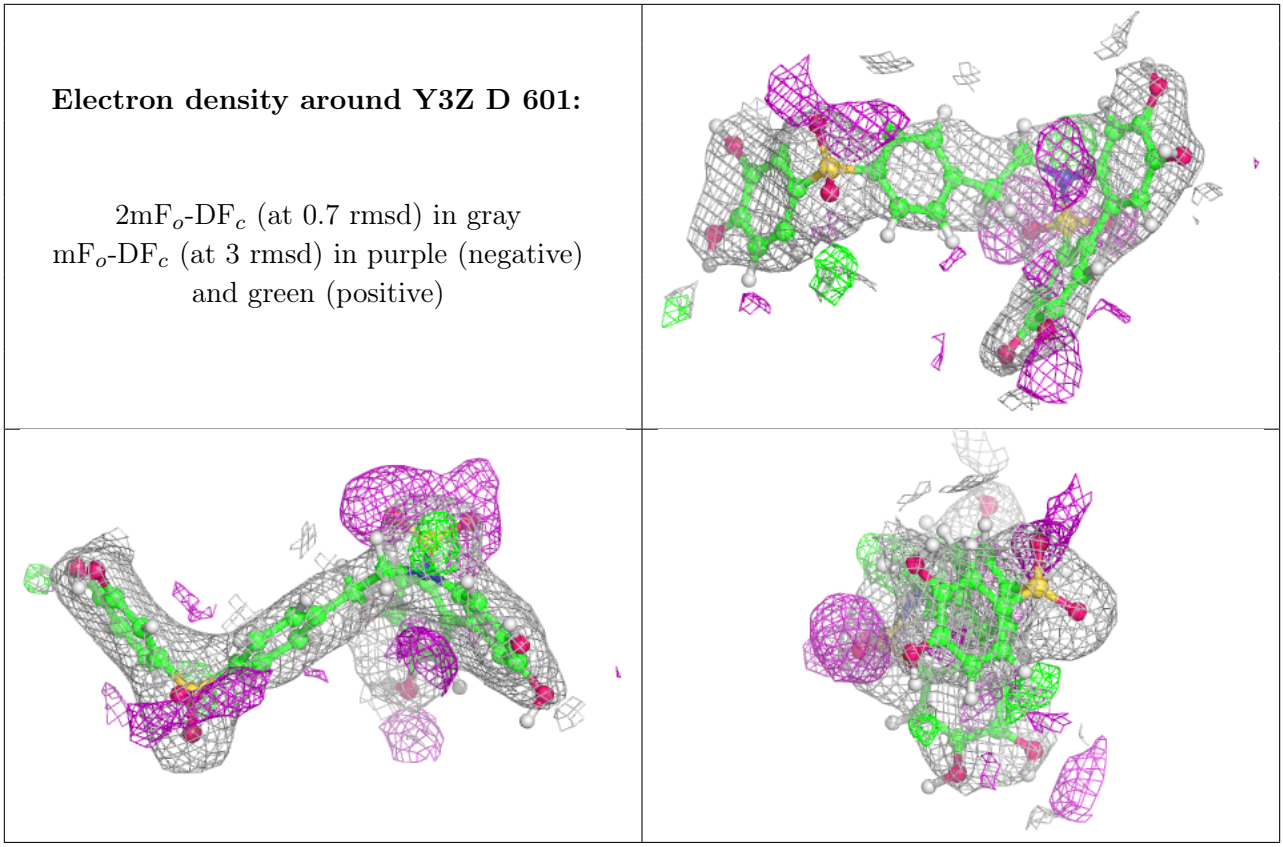
Electron density around Y3Z D 607:

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



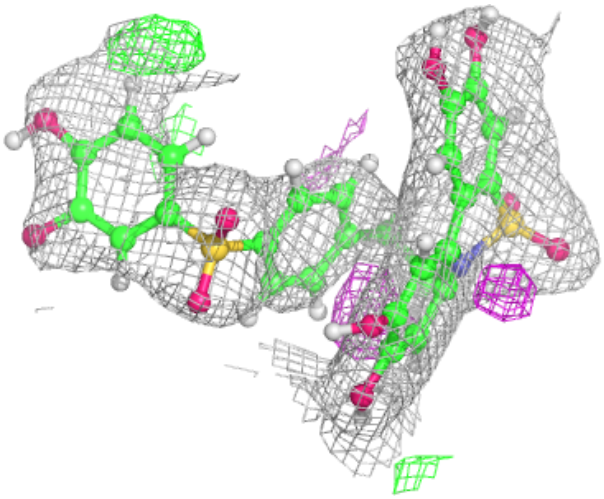
Electron density around Y3Z D 601:

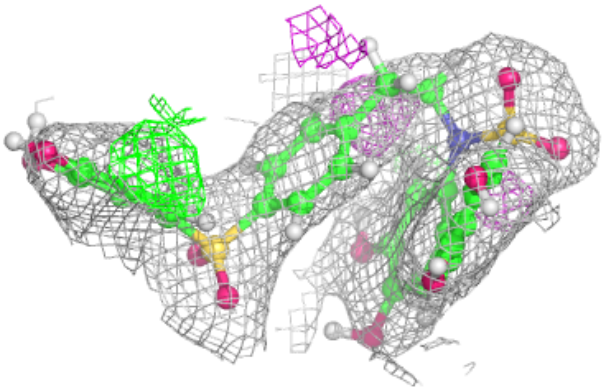
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

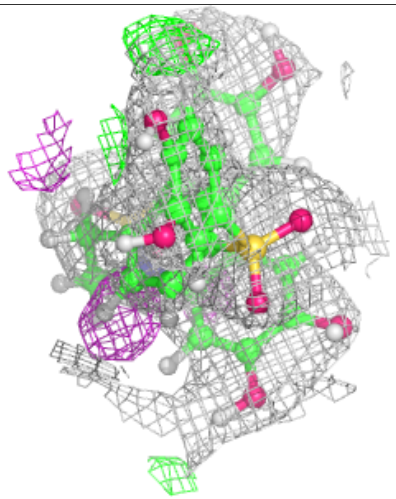


Electron density around Y3Z F 605:

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

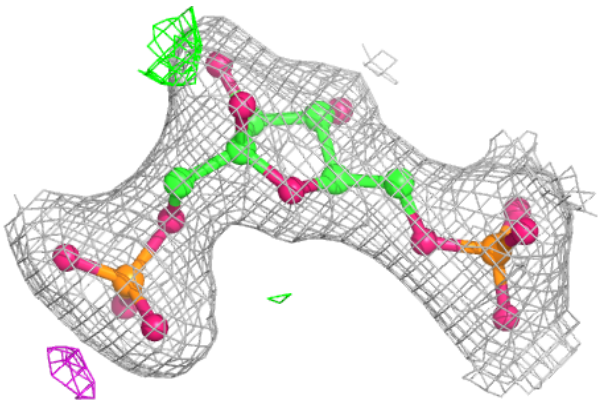


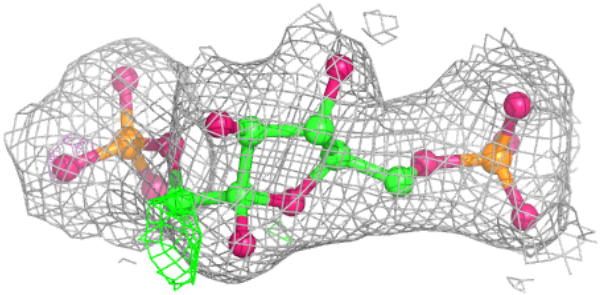


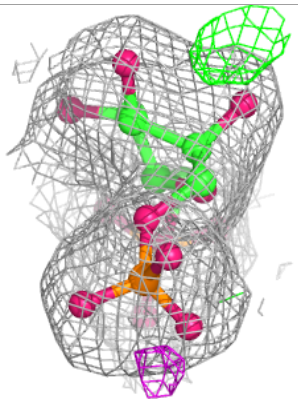


Electron density around FBP A 601:

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

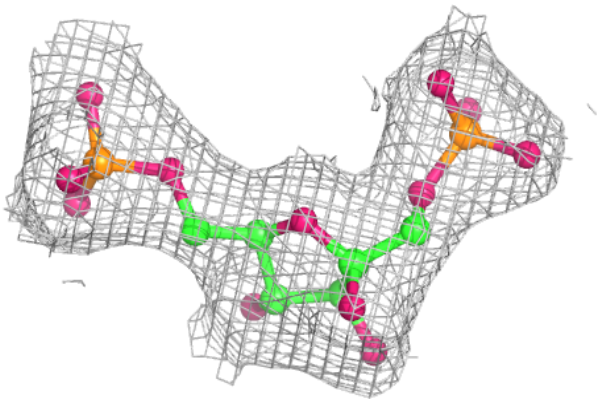


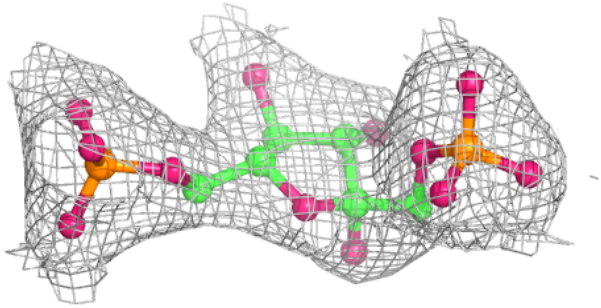


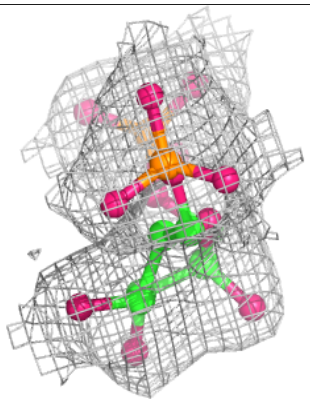


Electron density around FBP F 601:

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

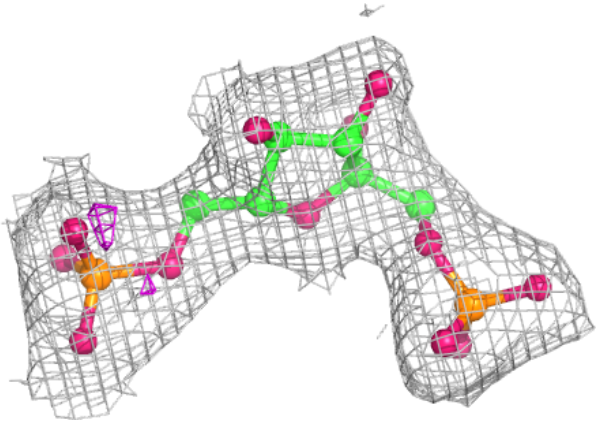


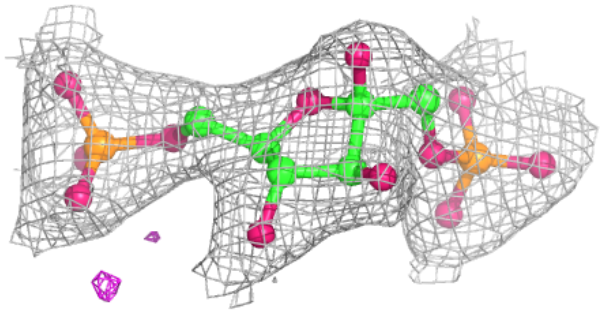


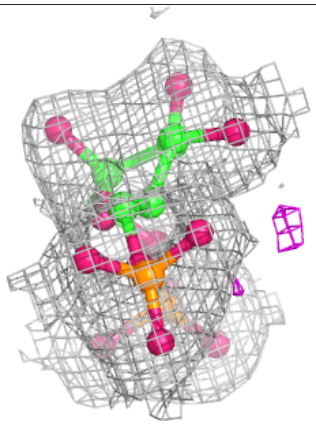


Electron density around FBP B 601:

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

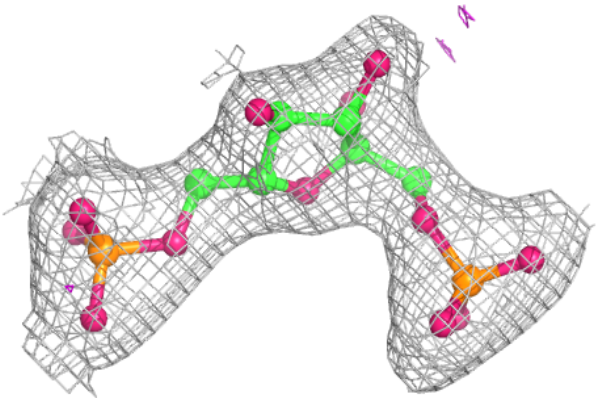


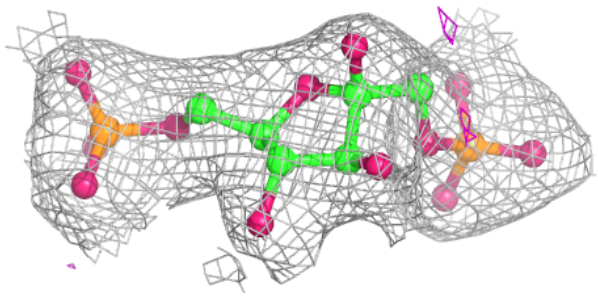


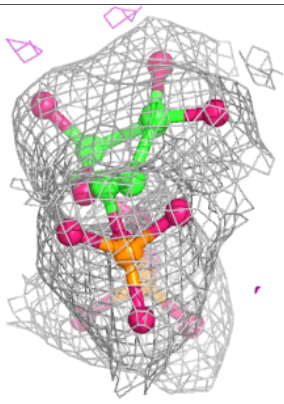


Electron density around FBP E 601:

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

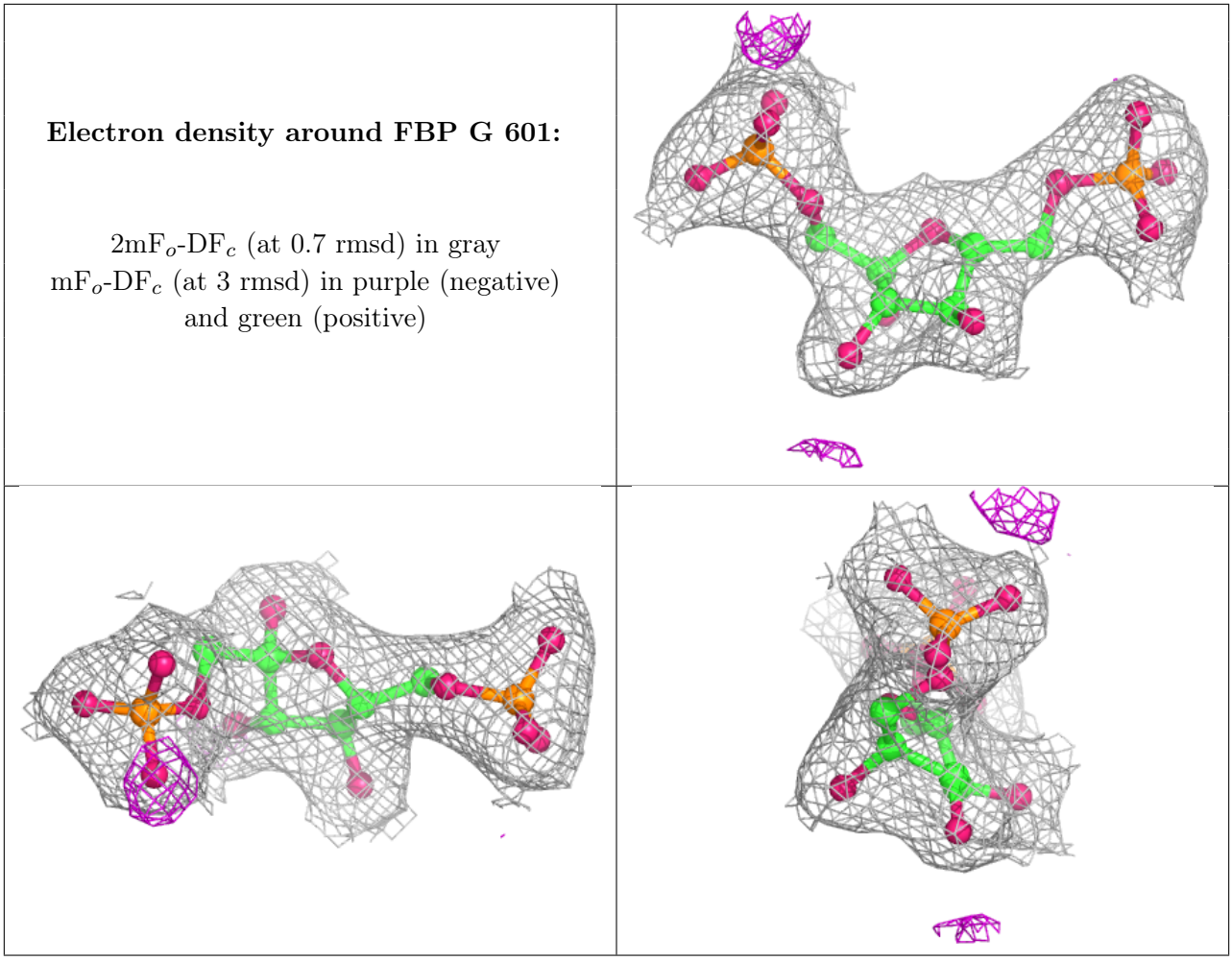






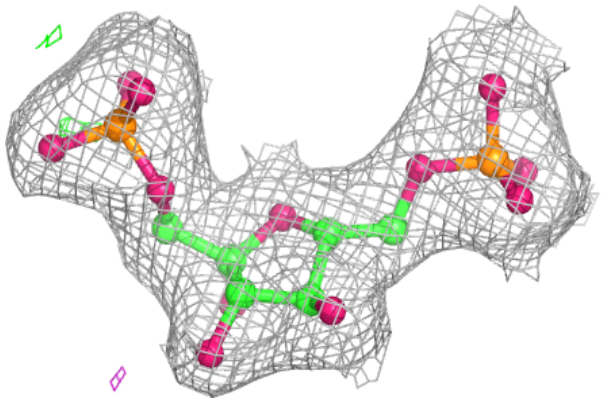
Electron density around FBP G 601:

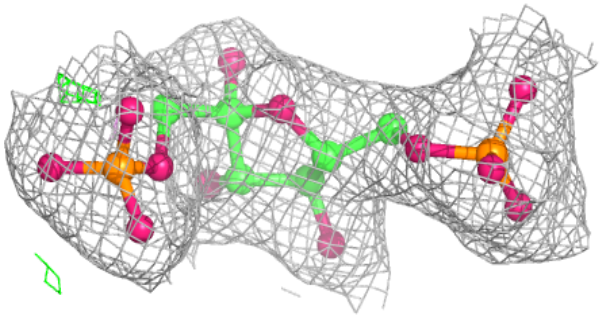
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

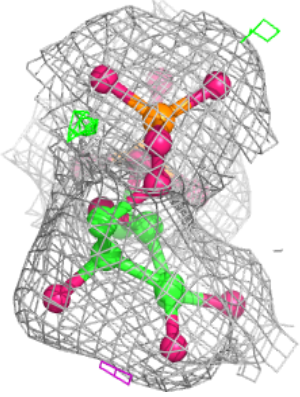


Electron density around FBP H 602:

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

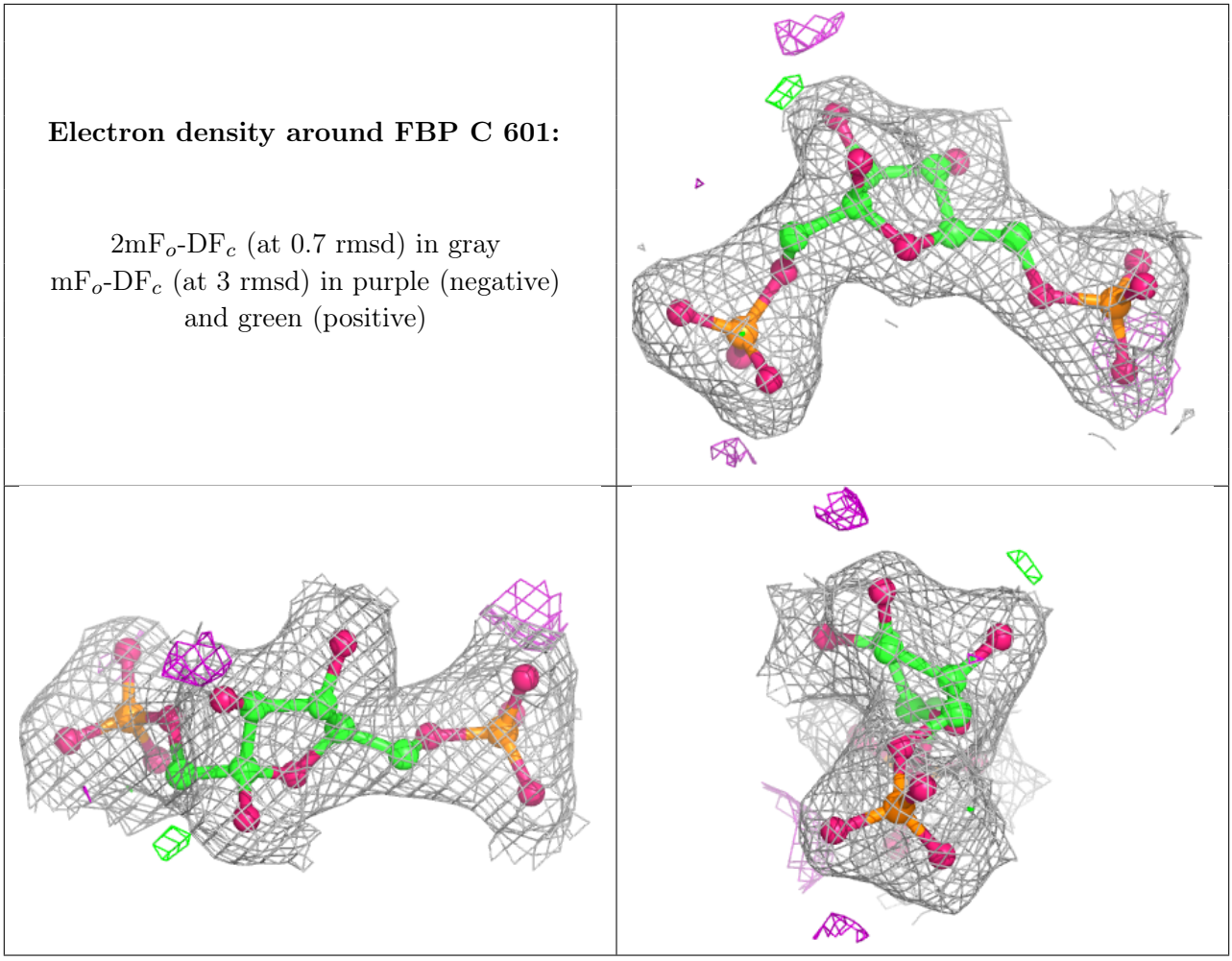






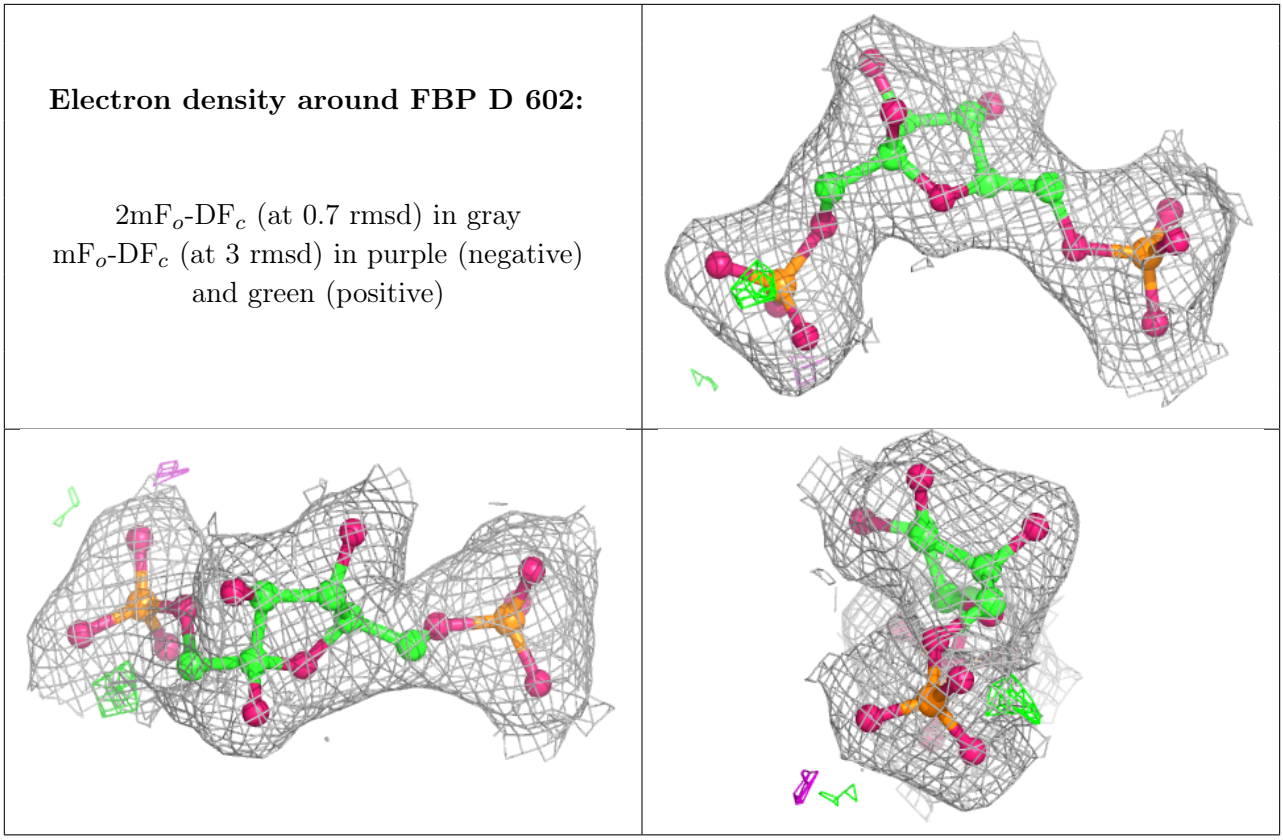
Electron density around FBP C 601:

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



Electron density around FBP D 602:

$2mF_o$-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.