Full wwPDB X-ray Structure Validation Report (i)

Oct 24, 2026 – 12:09 PM EDT

PDB ID	:	14CT / pdb_000014ct
Title	:	Structure of liver pyruvate kinase in complex with allosteric activator 8f
Authors	:	Lulla, A.; Rodriguez Rivero, A.; Grotli, M.; Hyvonen, M.
Deposited on	:	2026-04-28
Resolution	:	2.48 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:

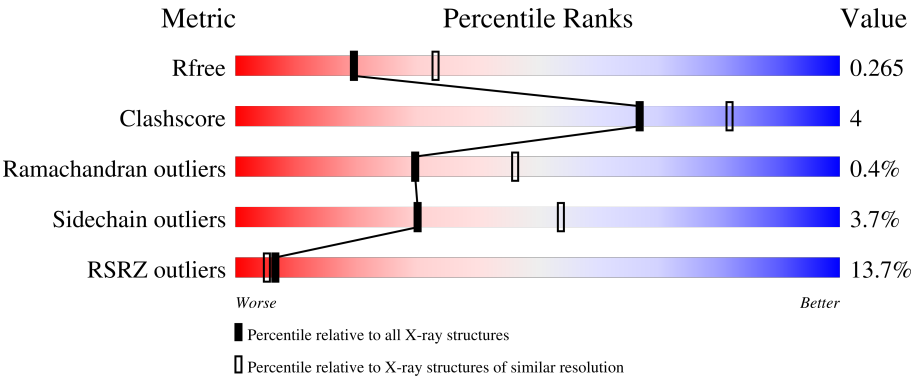
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	26% 83% 10% • 6%
1	B	447	4% 84% 12% ••
1	C	447	13% 83% 11% • 5%
1	D	447	2% 85% 9% • 5%
1	E	447	33% 83% 10% • 6%

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Mol	Chain	Length	Quality of chain
1	F	447	10% 85% 10%
1	G	447	14% 80% 14% 6%
1	H	447	2% 84% 10% 5%

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

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

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 27210 atoms, of which 56 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Isoform L-type of Pyruvate kinase PKLR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	12	0
			3232	2029	581	602	20			
1	B	436	Total	C	N	O	S	3	8	0
			3350	2104	604	622	20			
1	C	424	Total	C	N	O	S	0	9	0
			3268	2058	584	607	19			
1	D	424	Total	C	N	O	S	0	8	0
			3254	2043	589	603	19			
1	E	420	Total	C	N	O	S	0	12	0
			3255	2047	585	603	20			
1	F	432	Total	C	N	O	S	0	8	0
			3324	2092	597	615	20			
1	G	422	Total	C	N	O	S	0	10	0
			3256	2049	584	604	19			
1	H	425	Total	C	N	O	S	0	9	0
			3269	2053	593	604	19			

There are 48 discrepancies between the modelled and reference sequences:

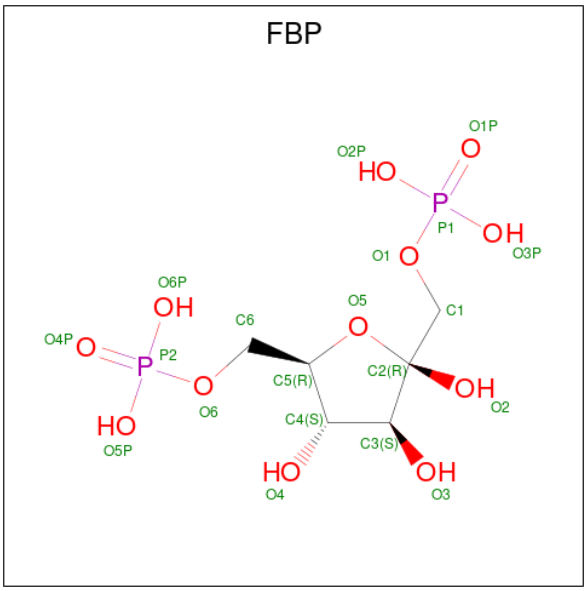
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P30613
A	0	SER	-	expression tag	UNP P30613
A	12	ASP	SER	conflict	UNP P30613
A	130	GLY	-	linker	UNP P30613
A	131	SER	-	linker	UNP P30613
A	132	GLY	-	linker	UNP P30613
B	-1	GLY	-	expression tag	UNP P30613
B	0	SER	-	expression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

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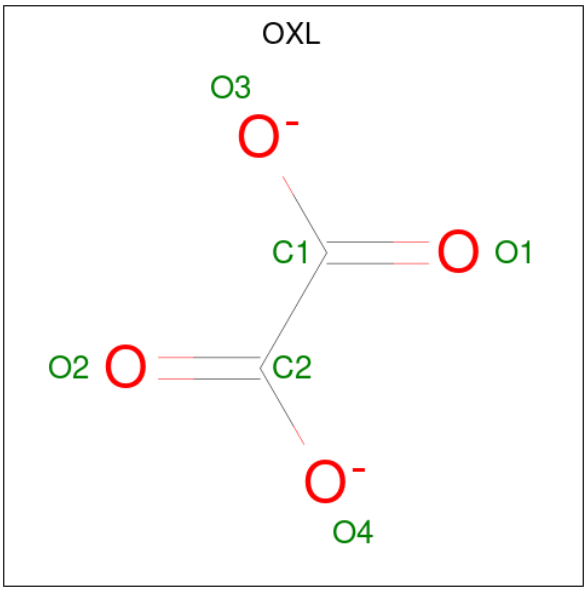
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP P30613
C	12	ASP	SER	conflict	UNP P30613
C	130	GLY	-	linker	UNP P30613
C	131	SER	-	linker	UNP P30613
C	132	GLY	-	linker	UNP P30613
D	-1	GLY	-	expression tag	UNP P30613
D	0	SER	-	expression tag	UNP P30613
D	12	ASP	SER	conflict	UNP P30613
D	130	GLY	-	linker	UNP P30613
D	131	SER	-	linker	UNP P30613
D	132	GLY	-	linker	UNP P30613
E	-1	GLY	-	expression tag	UNP P30613
E	0	SER	-	expression tag	UNP P30613
E	12	ASP	SER	conflict	UNP P30613
E	130	GLY	-	linker	UNP P30613
E	131	SER	-	linker	UNP P30613
E	132	GLY	-	linker	UNP P30613
F	-1	GLY	-	expression tag	UNP P30613
F	0	SER	-	expression tag	UNP P30613
F	12	ASP	SER	conflict	UNP P30613
F	130	GLY	-	linker	UNP P30613
F	131	SER	-	linker	UNP P30613
F	132	GLY	-	linker	UNP P30613
G	-1	GLY	-	expression tag	UNP P30613
G	0	SER	-	expression tag	UNP P30613
G	12	ASP	SER	conflict	UNP P30613
G	130	GLY	-	linker	UNP P30613
G	131	SER	-	linker	UNP P30613
G	132	GLY	-	linker	UNP P30613
H	-1	GLY	-	expression tag	UNP P30613
H	0	SER	-	expression tag	UNP P30613
H	12	ASP	SER	conflict	UNP P30613
H	130	GLY	-	linker	UNP P30613
H	131	SER	-	linker	UNP P30613
H	132	GLY	-	linker	UNP P30613

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



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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 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 (CCD ID: MG) (formula: Mg).

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

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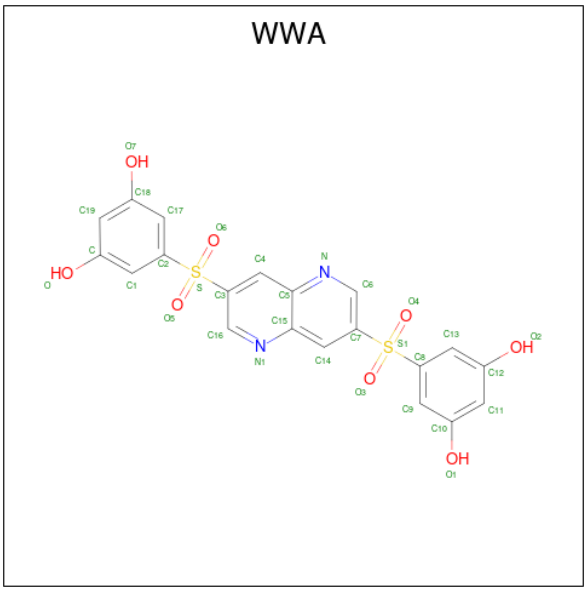
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0
4	G	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0

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

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

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



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

- Molecule 7 is water.

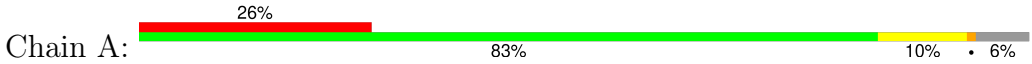
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	39	Total	O	0	0
			39	39		
7	B	86	Total	O	0	0
			86	86		
7	C	61	Total	O	0	0
			61	61		
7	D	97	Total	O	0	0
			97	97		
7	E	34	Total	O	0	0
			34	34		
7	F	77	Total	O	0	0
			77	77		
7	G	70	Total	O	0	0
			70	70		
7	H	130	Total	O	0	0
			130	130		

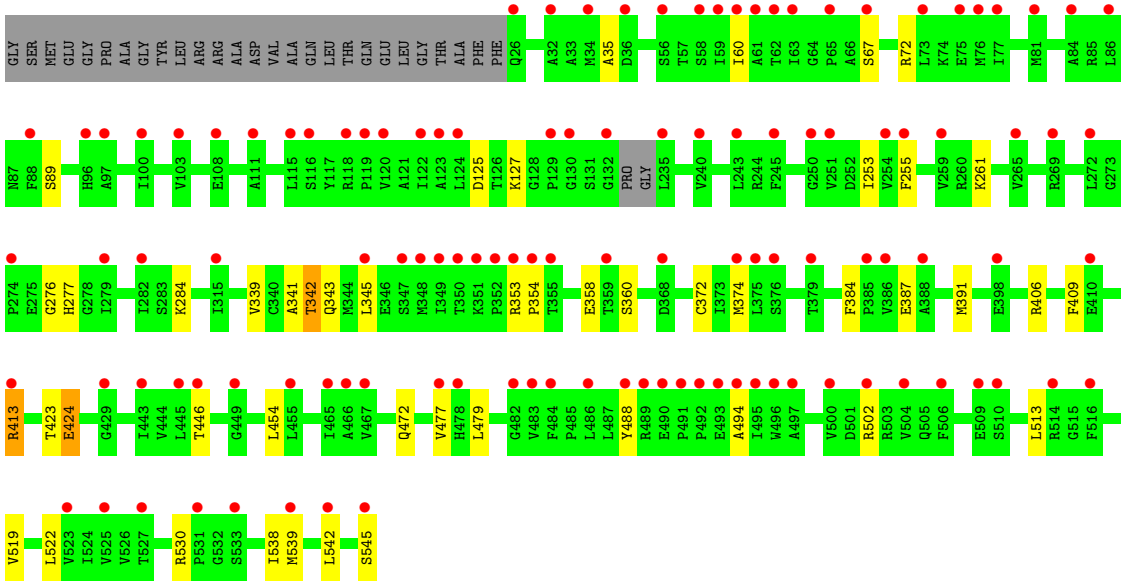
3 Residue-property plots (i)

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

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

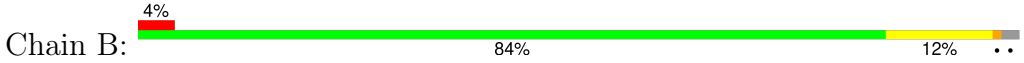
Chain A:

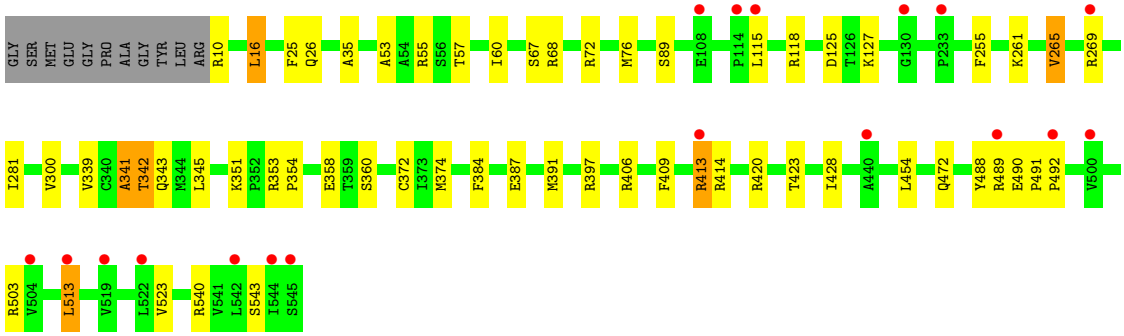




• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

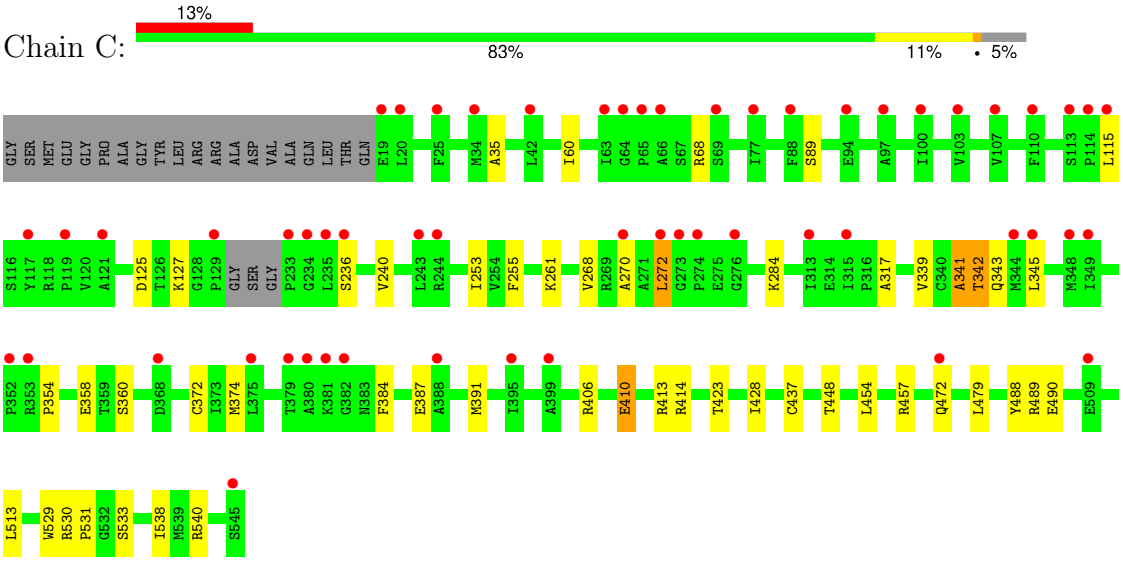
Chain B:





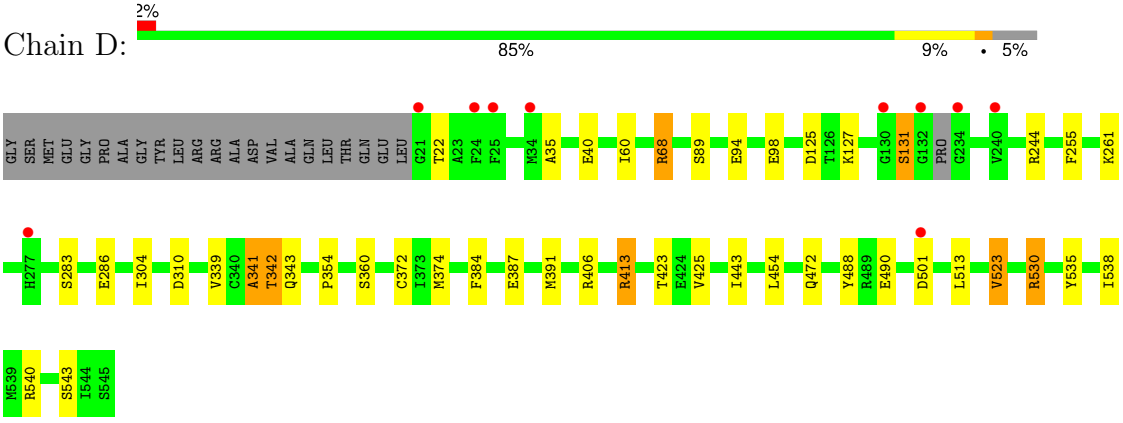
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain C:



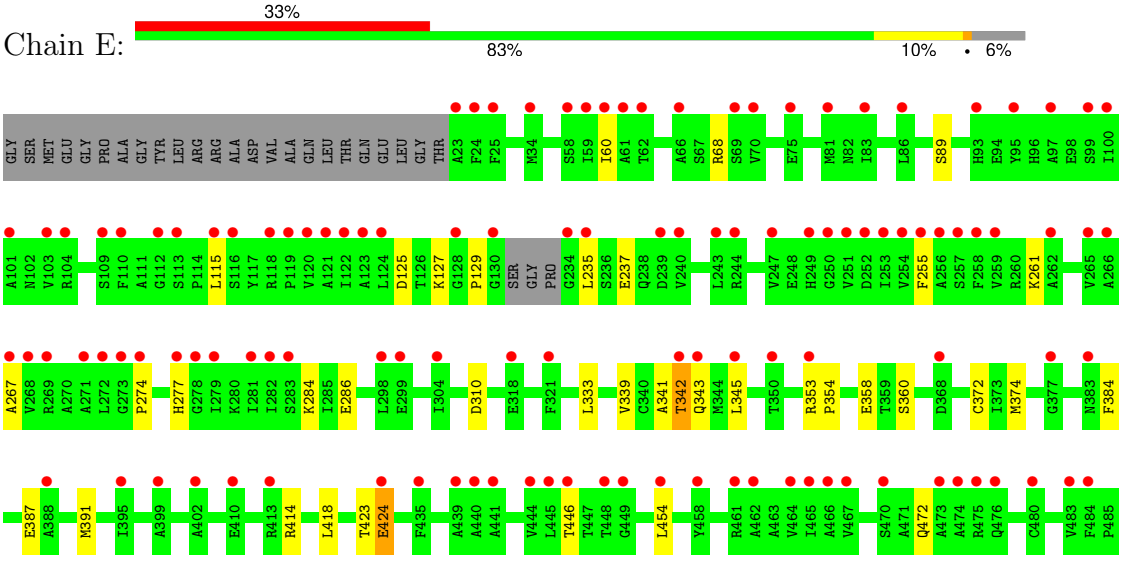
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

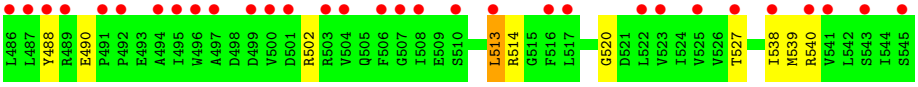
Chain D:



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

Chain E:

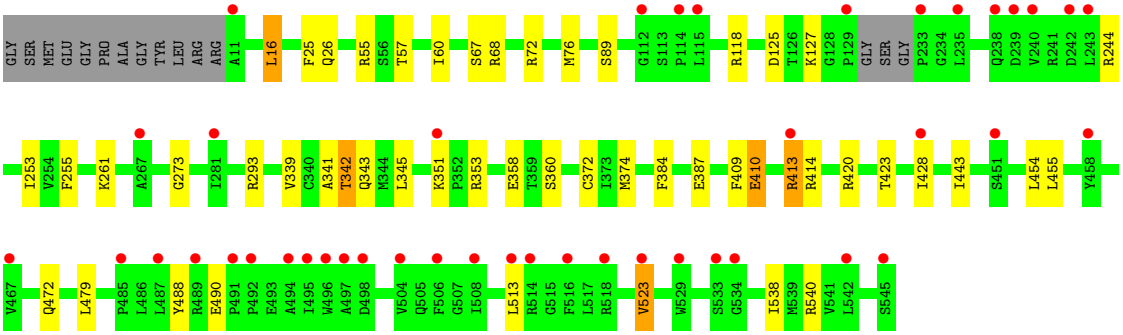




• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain F:

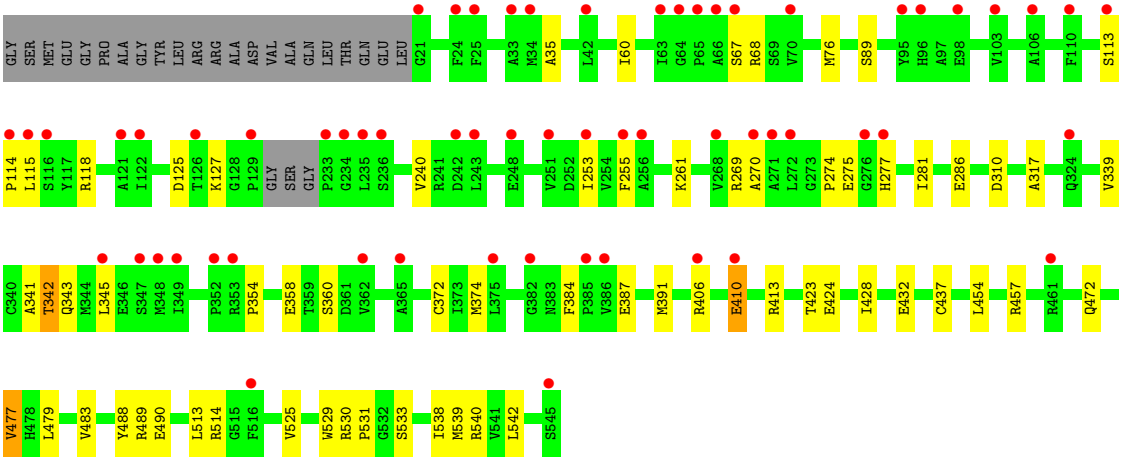




• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain G:

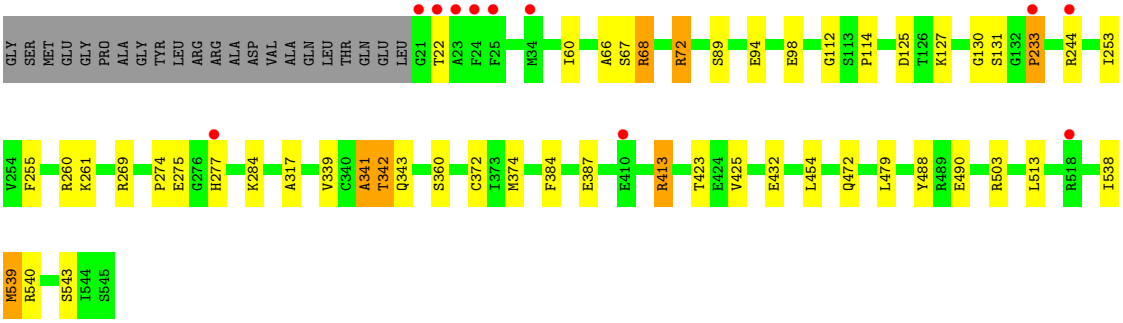




• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	205.76Å 112.90Å 185.80Å 90.00° 93.41° 90.00°	Depositor
Resolution (Å)	102.70 – 2.48 102.70 – 2.48	Depositor EDS
% Data completeness (in resolution range)	69.0 (102.70-2.48) 69.0 (102.70-2.48)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.48Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.255 , 0.281 0.240 , 0.265	Depositor DCC
R_{free} test set	5170 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	49.8	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	27210	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 89.57 % 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 3.2404e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.61	0/3319	1.01	4/4484 (0.1%)
1	B	0.68	0/3429	1.03	4/4636 (0.1%)
1	C	0.63	0/3349	1.01	3/4527 (0.1%)
1	D	0.68	0/3332	1.03	2/4502 (0.0%)
1	E	0.61	0/3345	1.01	2/4519 (0.0%)
1	F	0.66	0/3402	1.02	4/4599 (0.1%)
1	G	0.65	0/3341	1.03	4/4516 (0.1%)
1	H	0.70	0/3352	1.03	3/4531 (0.1%)
All	All	0.65	0/26869	1.02	26/36314 (0.1%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	114	PRO	CA-C-N	7.01	130.25	120.29
1	G	114	PRO	C-N-CA	7.01	130.25	120.29
1	D	341	ALA	CA-C-N	5.53	132.09	121.54
1	D	341	ALA	C-N-CA	5.53	132.09	121.54
1	B	341	ALA	CA-C-N	5.45	131.94	121.54
1	B	341	ALA	C-N-CA	5.45	131.94	121.54
1	H	233	PRO	N-CA-CB	-5.30	97.69	103.25
1	G	341	ALA	CA-C-N	5.28	131.63	121.54
1	G	341	ALA	C-N-CA	5.28	131.63	121.54
1	F	341	ALA	CA-C-N	5.26	131.59	121.54
1	F	341	ALA	C-N-CA	5.26	131.59	121.54
1	F	455	LEU	CA-C-N	5.24	127.30	120.28
1	F	455	LEU	C-N-CA	5.24	127.30	120.28
1	A	341	ALA	CA-C-N	5.19	131.44	121.54
1	A	341	ALA	C-N-CA	5.19	131.44	121.54
1	C	410	GLU	CB-CG-CD	5.18	121.41	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	341	ALA	CA-C-N	5.18	131.44	121.54
1	E	341	ALA	C-N-CA	5.18	131.44	121.54
1	B	115	LEU	CA-C-N	5.16	129.97	122.08
1	B	115	LEU	C-N-CA	5.16	129.97	122.08
1	C	341	ALA	CA-C-N	5.11	131.30	121.54
1	C	341	ALA	C-N-CA	5.11	131.30	121.54
1	A	276	GLY	CA-C-N	5.08	127.08	120.28
1	A	276	GLY	C-N-CA	5.08	127.08	120.28
1	H	341	ALA	CA-C-N	5.06	131.21	121.54
1	H	341	ALA	C-N-CA	5.06	131.21	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3232	0	3307	22	0
1	B	3350	0	3417	27	1
1	C	3268	0	3336	30	0
1	D	3254	0	3313	24	0
1	E	3255	0	3320	25	0
1	F	3324	0	3398	26	0
1	G	3256	0	3320	38	0
1	H	3269	0	3334	29	0
2	A	20	0	10	1	0
2	B	20	0	10	1	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
2	E	20	0	10	1	0
2	F	20	0	10	0	0
2	G	20	0	10	0	0
2	H	20	0	10	1	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	B	32	14	0	0	0
6	C	32	14	0	0	0
6	F	32	14	0	0	0
6	G	32	14	0	0	0
7	A	39	0	0	0	0
7	B	86	0	0	0	0
7	C	61	0	0	0	0
7	D	97	0	0	0	0
7	E	34	0	0	0	0
7	F	77	0	0	0	0
7	G	70	0	0	0	0
7	H	130	0	0	0	0
All	All	27154	56	26825	197	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 4.

All (197) 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:E:115:LEU:HG	1:E:513:LEU:HB3	1.66	0.77
1:A:519:VAL:HG13	1:A:545:SER:HB3	1.72	0.72
1:G:410:GLU:HG3	1:G:413:ARG:HH22	1.59	0.67
1:G:118:ARG:HH11	1:G:514:ARG:HH12	1.41	0.66
1:G:118:ARG:NH1	1:G:514:ARG:HH12	1.92	0.66
1:B:89:SER:HA	1:B:127:LYS:HG3	1.78	0.66
1:G:539:MET:HE3	1:H:539:MET:HG2	1.76	0.65
1:F:89:SER:HA	1:F:127:LYS:HG3	1.79	0.64
1:G:118:ARG:HH11	1:G:514:ARG:NH1	1.97	0.63
1:C:531:PRO:HB2	1:G:240:VAL:HG11	1.80	0.62
1:H:89:SER:HA	1:H:127:LYS:HG3	1.82	0.62
1:C:413:ARG:HG3	1:C:428:ILE:HD11	1.81	0.61
1:E:115:LEU:HD12	1:E:514:ARG:HE	1.65	0.61
1:D:89:SER:HA	1:D:127:LYS:HG3	1.82	0.61
1:C:538:ILE:HG12	1:D:540:ARG:HG3	1.82	0.61
1:G:413:ARG:NH2	1:H:413:ARG:HE	1.99	0.60
1:E:89:SER:HA	1:E:127:LYS:HG3	1.81	0.60
1:C:89:SER:HA	1:C:127:LYS:HG3	1.82	0.60
1:C:423:THR:HG22	1:C:454:LEU:HD12	1.83	0.60
1:F:339:VAL:HG22	1:F:372:CYS:HB2	1.84	0.59
1:A:89:SER:HA	1:A:127:LYS:HG3	1.85	0.59
1:G:89:SER:HA	1:G:127:LYS:HG3	1.85	0.58
1:G:423:THR:HG22	1:G:454:LEU:HD12	1.86	0.58
1:F:353:ARG:HH21	1:H:317:ALA:HB2	1.69	0.57
1:D:423:THR:HG22	1:D:454:LEU:HD12	1.87	0.57
1:E:115:LEU:HG	1:E:513:LEU:CB	2.35	0.57
1:A:60:ILE:HB	1:A:374:MET:HG3	1.87	0.56
1:B:16:LEU:HD23	1:B:25:PHE:HZ	1.69	0.56
1:F:67:SER:HA	1:F:72:ARG:HG2	1.87	0.56
1:F:413:ARG:HG3	1:F:428:ILE:HD11	1.88	0.56
1:C:240:VAL:HG11	1:G:531:PRO:HB2	1.87	0.55
1:H:66:ALA:O	1:H:72:ARG:HD2	2.06	0.55
1:A:67:SER:HA	1:A:72:ARG:HG2	1.89	0.55
1:G:60:ILE:HB	1:G:374:MET:HG3	1.88	0.55
1:A:409:PHE:HE2	1:A:413:ARG:HH12	1.55	0.54
1:C:533:SER:O	1:G:270:ALA:HB1	2.07	0.54
1:D:339:VAL:HG22	1:D:372:CYS:HB2	1.89	0.54
1:D:530:ARG:HD2	1:D:535:TYR:CD2	2.42	0.54
1:H:67:SER:HA	1:H:72:ARG:HG2	1.89	0.54
1:A:423:THR:HG22	1:A:454:LEU:HD12	1.88	0.54
1:C:60:ILE:HB	1:C:374:MET:HG3	1.88	0.53
1:B:339:VAL:HG22	1:B:372:CYS:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:PHE:HB3	1:C:387:GLU:HB2	1.90	0.53
1:D:60:ILE:HB	1:D:374:MET:HG3	1.89	0.53
1:A:339:VAL:HG22	1:A:372:CYS:HB2	1.90	0.53
1:E:384:PHE:HB3	1:E:387:GLU:HB2	1.90	0.53
1:E:423:THR:HG22	1:E:454:LEU:HD12	1.90	0.53
1:H:60:ILE:HB	1:H:374:MET:HG3	1.91	0.53
1:A:409:PHE:CE2	1:A:413:ARG:NH1	2.76	0.53
1:D:384:PHE:HB3	1:D:387:GLU:HB2	1.90	0.53
1:E:353:ARG:HH21	1:G:317:ALA:HB2	1.74	0.53
1:G:413:ARG:HG3	1:G:428:ILE:HD11	1.90	0.53
1:H:423:THR:HG22	1:H:454:LEU:HD12	1.91	0.53
1:F:16:LEU:HD23	1:F:25:PHE:HZ	1.73	0.52
1:B:384:PHE:HB3	1:B:387:GLU:HB2	1.91	0.52
1:C:540:ARG:HG3	1:D:538:ILE:HG12	1.90	0.52
1:H:68:ARG:NH2	1:H:98:GLU:HB2	2.23	0.52
1:G:342:THR:HG22	1:G:343:GLN:HG3	1.92	0.52
1:H:384:PHE:HB3	1:H:387:GLU:HB2	1.92	0.52
1:E:339:VAL:HG22	1:E:372:CYS:HB2	1.92	0.51
1:D:342:THR:HG22	1:D:343:GLN:HG3	1.93	0.51
1:E:60:ILE:HB	1:E:374:MET:HG3	1.91	0.51
1:B:409:PHE:CE2	1:B:413:ARG:NH1	2.77	0.51
1:A:488:TYR:OH	1:A:502:ARG:HG3	2.11	0.51
1:B:413:ARG:HG3	1:B:428:ILE:HD11	1.93	0.50
1:A:538:ILE:HG12	1:B:540:ARG:HG3	1.93	0.50
1:D:68:ARG:NH2	1:D:98:GLU:HB2	2.27	0.50
1:B:423:THR:HG22	1:B:454:LEU:HD12	1.94	0.50
1:G:354:PRO:HG3	1:G:391:MET:HG2	1.93	0.50
1:A:384:PHE:HB3	1:A:387:GLU:HB2	1.94	0.50
1:F:423:THR:HG22	1:F:454:LEU:HD12	1.94	0.49
1:E:342:THR:HG22	1:E:343:GLN:HG3	1.94	0.49
1:F:60:ILE:HB	1:F:374:MET:HG3	1.94	0.49
1:C:270:ALA:HB1	1:G:533:SER:O	2.12	0.49
1:D:488:TYR:CE2	1:D:490:GLU:HB2	2.48	0.48
1:H:233:PRO:O	1:H:260:ARG:NH2	2.46	0.48
1:C:410:GLU:HG2	1:C:413:ARG:HH22	1.79	0.48
1:H:413:ARG:HB2	1:H:413:ARG:HH21	1.79	0.48
1:F:409:PHE:CE2	1:F:413:ARG:NH1	2.82	0.48
1:G:488:TYR:CZ	1:G:490:GLU:HB2	2.49	0.48
1:B:60:ILE:HB	1:B:374:MET:HG3	1.96	0.48
1:C:488:TYR:CZ	1:C:490:GLU:HB2	2.49	0.48
1:A:342:THR:HG22	1:A:343:GLN:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:PHE:HE2	1:B:413:ARG:HH12	1.56	0.47
1:C:268:VAL:O	1:C:272[B]:LEU:HG	2.14	0.47
1:F:342:THR:HG22	1:F:343:GLN:HG3	1.96	0.47
1:F:384:PHE:HB3	1:F:387:GLU:HB2	1.95	0.47
1:D:488:TYR:CZ	1:D:490:GLU:HB2	2.50	0.47
1:B:488:TYR:CZ	1:B:490:GLU:HB2	2.50	0.47
1:C:253:ILE:HG12	1:C:479:LEU:HD11	1.96	0.47
1:F:488:TYR:CE2	1:F:490:GLU:HB2	2.51	0.46
1:G:345:LEU:HD23	1:G:358:GLU:HB3	1.97	0.46
1:H:342:THR:HG22	1:H:343:GLN:HG3	1.96	0.46
1:B:342:THR:HG22	1:B:343:GLN:HG3	1.96	0.46
1:G:125:ASP:HA	1:G:255:PHE:HB2	1.97	0.46
1:C:339:VAL:HG22	1:C:372:CYS:HB2	1.96	0.46
1:G:339:VAL:HG22	1:G:372:CYS:HB2	1.97	0.46
1:G:384:PHE:HB3	1:G:387:GLU:HB2	1.96	0.46
1:G:540:ARG:HG3	1:H:538:ILE:HG12	1.96	0.46
1:C:125:ASP:HA	1:C:255:PHE:HB2	1.97	0.46
1:A:522:LEU:HD12	1:B:420:ARG:HD2	1.97	0.46
1:G:269:ARG:HG2	1:G:281:ILE:CD1	2.46	0.46
1:A:353:ARG:HH21	1:C:317:ALA:HB2	1.80	0.46
1:C:488:TYR:CE2	1:C:490:GLU:HB2	2.50	0.46
1:G:253:ILE:HG12	1:G:479:LEU:HD11	1.98	0.46
1:B:269[A]:ARG:HE	1:B:281:ILE:HD12	1.82	0.46
1:G:432[A]:GLU:OE1	1:H:432[A]:GLU:OE1	2.34	0.46
1:H:539:MET:O	1:H:539:MET:HG3	2.16	0.46
1:F:345:LEU:HD23	1:F:358:GLU:HB3	1.98	0.45
1:H:488:TYR:CZ	1:H:490:GLU:HB2	2.52	0.45
1:A:345:LEU:HD23	1:A:358:GLU:HB3	1.99	0.45
1:B:55:ARG:HD2	1:B:57:THR:O	2.16	0.45
1:C:35:ALA:O	1:C:406:ARG:HD2	2.16	0.45
1:A:125:ASP:HA	1:A:255:PHE:HB2	1.99	0.45
1:F:409:PHE:HE2	1:F:413:ARG:HH12	1.60	0.45
1:F:488:TYR:CZ	1:F:490:GLU:HB2	2.51	0.45
1:E:488:TYR:CZ	1:E:490:GLU:HB2	2.52	0.45
1:B:345:LEU:HD23	1:B:358:GLU:HB3	1.99	0.45
1:D:125:ASP:HA	1:D:255:PHE:HB2	1.97	0.45
1:A:354:PRO:HG3	1:A:391:MET:HG2	1.98	0.44
1:G:437:CYS:HB3	1:H:425:VAL:HG21	1.98	0.44
1:A:255:PHE:HB3	1:A:284:LYS:HD2	1.99	0.44
1:C:354:PRO:HG3	1:C:391:MET:HG2	1.99	0.44
1:D:35:ALA:HB1	1:D:40:GLU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:525:VAL:HG21	1:G:542[A]:LEU:HD12	1.99	0.44
1:E:538:ILE:HG12	1:F:540:ARG:HG3	1.99	0.44
1:H:125:ASP:HA	1:H:255:PHE:HB2	1.99	0.44
1:H:253:ILE:HG12	1:H:479:LEU:HD11	1.99	0.44
1:E:125:ASP:HA	1:E:255:PHE:HB2	1.98	0.44
1:E:255:PHE:HB3	1:E:284:LYS:HD2	2.00	0.44
1:F:410:GLU:HG3	1:F:413:ARG:HH21	1.83	0.44
1:D:94:GLU:O	1:D:98:GLU:HG3	2.18	0.44
1:E:345:LEU:HD23	1:E:358:GLU:HB3	2.00	0.44
1:C:342:THR:HG22	1:C:343:GLN:HG3	2.00	0.44
1:C:448:THR:HG22	1:G:274:PRO:HD3	2.00	0.44
1:H:339:VAL:HG22	1:H:372:CYS:HB2	2.00	0.43
1:F:55:ARG:HD2	1:F:57:THR:O	2.19	0.43
1:H:488:TYR:CE2	1:H:490:GLU:HB2	2.52	0.43
1:G:477:VAL:CG2	1:G:483:VAL:HG11	2.48	0.43
1:B:53:ALA:O	1:B:397:ARG:NH2	2.48	0.43
1:F:443:ILE:HD12	1:F:523:VAL:HG11	2.00	0.43
1:H:341:ALA:HB1	1:H:374:MET:HE2	1.99	0.43
1:B:341:ALA:HB1	1:B:374:MET:HE2	2.00	0.43
1:G:424[A]:GLU:HG3	1:G:454:LEU:HD13	2.00	0.43
1:A:424:GLU:HG2	1:A:454:LEU:HD13	2.00	0.43
1:C:345:LEU:HD23	1:C:358:GLU:HB3	2.00	0.43
1:G:538:ILE:HG12	1:H:540[B]:ARG:HB3	2.01	0.43
1:G:454:LEU:O	1:G:457:ARG:HG2	2.19	0.43
1:B:67:SER:HB2	1:B:76[B]:MET:SD	2.59	0.43
1:E:418:LEU:HB3	1:F:16:LEU:HD22	2.00	0.42
1:E:354:PRO:HG3	1:E:391:MET:HG2	2.02	0.42
1:G:488:TYR:CE2	1:G:490:GLU:HB2	2.54	0.42
1:B:35:ALA:O	1:B:406:ARG:HD2	2.19	0.42
1:B:67:SER:HA	1:B:72:ARG:HG2	2.01	0.42
1:D:341:ALA:HB1	1:D:374:MET:HE2	2.01	0.42
1:E:540:ARG:HG3	1:F:538:ILE:HG12	2.02	0.42
1:H:94:GLU:O	1:H:98:GLU:HG3	2.18	0.42
1:B:488:TYR:CE2	1:B:490:GLU:HB2	2.54	0.42
1:G:35:ALA:O	1:G:406:ARG:HD2	2.19	0.42
1:E:286:GLU:HB3	1:E:310:ASP:HB2	2.02	0.42
1:G:529:TRP:CE2	1:G:530:ARG:HG2	2.55	0.42
1:A:446:THR:OG1	2:A:601:FBP:O4P	2.33	0.42
1:C:255:PHE:HB3	1:C:284:LYS:HD2	2.01	0.41
1:G:67:SER:HB2	1:G:76[B]:MET:SD	2.61	0.41
1:D:35:ALA:O	1:D:406:ARG:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:ARG:HH11	1:D:413:ARG:HB2	1.86	0.41
1:E:488:TYR:CE2	1:E:490:GLU:HB2	2.55	0.41
1:F:125:ASP:HA	1:F:255:PHE:HB2	2.03	0.41
1:F:244:ARG:HH22	1:F:273:GLY:HA3	1.86	0.41
1:A:35:ALA:O	1:A:406:ARG:HD2	2.21	0.41
1:B:265:VAL:HG11	1:B:300:VAL:HG23	2.02	0.41
1:C:341:ALA:HB1	1:C:374:MET:HE2	2.02	0.41
1:E:274:PRO:HA	1:E:277[A]:HIS:ND1	2.35	0.41
1:F:67:SER:HB2	1:F:76[B]:MET:SD	2.60	0.41
1:B:491:PRO:HA	1:B:492:PRO:HD3	1.96	0.41
1:H:255:PHE:HB3	1:H:284:LYS:HD2	2.03	0.41
1:A:253:ILE:HG12	1:A:479:LEU:HD11	2.03	0.41
1:B:503:ARG:NH1	2:B:601:FBP:O3P	2.44	0.41
1:C:454:LEU:O	1:C:457:ARG:HG2	2.21	0.41
1:D:283:SER:HB2	1:D:304:ILE:HD13	2.02	0.41
1:G:286:GLU:HB3	1:G:310:ASP:HB2	2.03	0.41
1:H:274:PRO:HA	1:H:277[A]:HIS:ND1	2.36	0.41
1:D:286:GLU:HB3	1:D:310:ASP:HB2	2.03	0.41
1:E:424:GLU:HG2	1:E:454:LEU:HD13	2.03	0.41
1:E:520:GLY:O	1:F:420:ARG:NH2	2.54	0.41
1:H:503:ARG:NH1	2:H:601:FBP:O1P	2.40	0.41
1:B:354:PRO:HG3	1:B:391:MET:HG2	2.03	0.40
1:D:354:PRO:HG3	1:D:391:MET:HG2	2.03	0.40
1:C:437:CYS:HB3	1:D:425:VAL:HG21	2.02	0.40
1:C:529:TRP:CE2	1:C:530:ARG:HG2	2.56	0.40
1:F:253:ILE:HG12	1:F:479:LEU:HD11	2.04	0.40
1:E:235:LEU:HD22	1:E:267:ALA:HB1	2.04	0.40
1:C:414:ARG:NH2	1:D:406:ARG:HD3	2.36	0.40
1:D:443:ILE:HD12	1:D:523:VAL:HG11	2.03	0.40
1:H:112:GLY:O	1:H:114:PRO:HD3	2.22	0.40
1:B:125:ASP:HA	1:B:255:PHE:HB2	2.02	0.40
1:E:446:THR:OG1	2:E:601:FBP:O4P	2.35	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:LEU:O	1:B:513:LEU:O[2_555]	2.19	0.01

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	426/447 (95%)	418 (98%)	6 (1%)	2 (0%)	24	40
1	B	442/447 (99%)	433 (98%)	8 (2%)	1 (0%)	43	61
1	C	429/447 (96%)	425 (99%)	3 (1%)	1 (0%)	43	61
1	D	428/447 (96%)	422 (99%)	4 (1%)	2 (0%)	24	40
1	E	428/447 (96%)	421 (98%)	5 (1%)	2 (0%)	24	40
1	F	436/447 (98%)	429 (98%)	6 (1%)	1 (0%)	43	61
1	G	428/447 (96%)	422 (99%)	5 (1%)	1 (0%)	43	61
1	H	432/447 (97%)	424 (98%)	5 (1%)	3 (1%)	18	32
All	All	3449/3576 (96%)	3394 (98%)	42 (1%)	13 (0%)	30	46

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	130	GLY
1	D	131	SER
1	H	131	SER
1	A	342	THR
1	A	494	ALA
1	C	342	THR
1	D	342	THR
1	E	342	THR
1	F	342	THR
1	G	342	THR
1	H	342	THR
1	B	342	THR
1	E	129	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	344/352 (98%)	332 (96%)	12 (4%)	32	55
1	B	353/352 (100%)	336 (95%)	17 (5%)	23	43
1	C	346/352 (98%)	336 (97%)	10 (3%)	37	62
1	D	343/352 (97%)	329 (96%)	14 (4%)	27	50
1	E	345/352 (98%)	332 (96%)	13 (4%)	29	53
1	F	351/352 (100%)	337 (96%)	14 (4%)	28	51
1	G	345/352 (98%)	332 (96%)	13 (4%)	29	53
1	H	345/352 (98%)	331 (96%)	14 (4%)	27	50
All	All	2772/2816 (98%)	2665 (96%)	107 (4%)	30	52

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	261	LYS
1	A	277	HIS
1	A	360	SER
1	A	413	ARG
1	A	424	GLU
1	A	472	GLN
1	A	477	VAL
1	A	513	LEU
1	A	530	ARG
1	A	539[A]	MET
1	A	539[B]	MET
1	A	542	LEU
1	B	10	ARG
1	B	16	LEU
1	B	26	GLN
1	B	68	ARG
1	B	118	ARG
1	B	261	LYS
1	B	265	VAL

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Mol	Chain	Res	Type
1	B	351	LYS
1	B	353	ARG
1	B	360	SER
1	B	413	ARG
1	B	414	ARG
1	B	472	GLN
1	B	489	ARG
1	B	513	LEU
1	B	523	VAL
1	B	543	SER
1	C	68	ARG
1	C	115	LEU
1	C	236	SER
1	C	261	LYS
1	C	272[A]	LEU
1	C	272[B]	LEU
1	C	360	SER
1	C	472	GLN
1	C	489	ARG
1	C	513	LEU
1	D	22	THR
1	D	68	ARG
1	D	131	SER
1	D	244[A]	ARG
1	D	244[B]	ARG
1	D	261	LYS
1	D	360	SER
1	D	413	ARG
1	D	472	GLN
1	D	501	ASP
1	D	513	LEU
1	D	523	VAL
1	D	530	ARG
1	D	543	SER
1	E	68	ARG
1	E	237	GLU
1	E	261	LYS
1	E	333	LEU
1	E	360	SER
1	E	414	ARG
1	E	424	GLU
1	E	472	GLN

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Mol	Chain	Res	Type
1	E	502	ARG
1	E	513	LEU
1	E	527	THR
1	E	539[A]	MET
1	E	539[B]	MET
1	F	16	LEU
1	F	26	GLN
1	F	68	ARG
1	F	118	ARG
1	F	261	LYS
1	F	293	ARG
1	F	351	LYS
1	F	360	SER
1	F	410	GLU
1	F	413	ARG
1	F	414	ARG
1	F	472	GLN
1	F	513	LEU
1	F	523	VAL
1	G	68	ARG
1	G	113	SER
1	G	115	LEU
1	G	261	LYS
1	G	275	GLU
1	G	277[A]	HIS
1	G	277[B]	HIS
1	G	360	SER
1	G	410	GLU
1	G	472	GLN
1	G	477	VAL
1	G	489	ARG
1	G	513	LEU
1	H	22	THR
1	H	68	ARG
1	H	72	ARG
1	H	244[A]	ARG
1	H	244[B]	ARG
1	H	261	LYS
1	H	269	ARG
1	H	275	GLU
1	H	360	SER
1	H	413	ARG

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Mol	Chain	Res	Type
1	H	472	GLN
1	H	513	LEU
1	H	539	MET
1	H	543	SER

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

Mol	Chain	Res	Type
1	A	238	GLN
1	B	15	GLN
1	D	238	GLN
1	H	238	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 36 ligands modelled in this entry, 16 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	OXL	E	602	4	5,5,5	2.09	2 (40%)	6,6,6	1.66	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FBP	D	601	-	18,20,20	0.65	0	21,32,32	0.62	0
2	FBP	E	601	-	18,20,20	0.42	0	21,32,32	0.55	0
2	FBP	G	601	-	18,20,20	0.46	0	21,32,32	0.66	0
2	FBP	C	601	-	18,20,20	0.57	0	21,32,32	0.74	0
2	FBP	H	601	-	18,20,20	0.62	0	21,32,32	0.72	1 (4%)
3	OXL	H	602	4	5,5,5	2.36	3 (60%)	6,6,6	1.29	1 (16%)
2	FBP	F	601	-	18,20,20	0.26	0	21,32,32	0.64	0
3	OXL	D	602	4	5,5,5	2.13	3 (60%)	6,6,6	2.51	3 (50%)
6	WWA	F	603	-	35,35,35	1.93	8 (22%)	48,54,54	1.65	10 (20%)
2	FBP	A	601	-	18,20,20	0.41	0	21,32,32	0.53	0
6	WWA	B	603	-	35,35,35	2.14	7 (20%)	48,54,54	1.70	10 (20%)
3	OXL	C	602	4	5,5,5	2.09	2 (40%)	6,6,6	1.75	2 (33%)
3	OXL	G	602	4	5,5,5	1.87	2 (40%)	6,6,6	1.54	1 (16%)
6	WWA	C	603	-	35,35,35	2.25	6 (17%)	48,54,54	1.50	9 (18%)
2	FBP	B	601	-	18,20,20	0.37	0	21,32,32	0.64	0
6	WWA	G	603	-	35,35,35	2.28	6 (17%)	48,54,54	1.43	7 (14%)
3	OXL	B	602	4	5,5,5	2.17	2 (40%)	6,6,6	2.05	2 (33%)
3	OXL	A	602	4	5,5,5	2.02	2 (40%)	6,6,6	1.79	2 (33%)
3	OXL	F	602	4	5,5,5	2.13	2 (40%)	6,6,6	2.06	3 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OXL	E	602	4	-	4/4/4/4	-
2	FBP	D	601	-	-	3/13/32/32	0/1/1/1
2	FBP	E	601	-	-	5/13/32/32	0/1/1/1
2	FBP	G	601	-	-	5/13/32/32	0/1/1/1
2	FBP	C	601	-	-	3/13/32/32	0/1/1/1
2	FBP	H	601	-	-	4/13/32/32	0/1/1/1
3	OXL	H	602	4	-	4/4/4/4	-
2	FBP	F	601	-	-	3/13/32/32	0/1/1/1
3	OXL	D	602	4	-	4/4/4/4	-
6	WWA	F	603	-	-	0/24/24/24	0/4/4/4
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	WWA	B	603	-	-	0/24/24/24	0/4/4/4
3	OXL	C	602	4	-	4/4/4/4	-
3	OXL	G	602	4	-	4/4/4/4	-
6	WWA	C	603	-	-	0/24/24/24	0/4/4/4
2	FBP	B	601	-	-	6/13/32/32	0/1/1/1
6	WWA	G	603	-	-	0/24/24/24	0/4/4/4
3	OXL	B	602	4	-	4/4/4/4	-
3	OXL	A	602	4	-	4/4/4/4	-
3	OXL	F	602	4	-	0/4/4/4	-

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	603	WWA	C8-S1	-6.40	1.67	1.77
6	G	603	WWA	C8-S1	-6.33	1.67	1.77
6	G	603	WWA	C2-S	-5.93	1.67	1.77
6	C	603	WWA	C2-S	-5.82	1.68	1.77
6	B	603	WWA	C7-S1	-5.13	1.69	1.77
6	G	603	WWA	C7-S1	-5.10	1.69	1.77
6	B	603	WWA	C8-S1	-5.01	1.69	1.77
6	B	603	WWA	C2-S	-4.80	1.69	1.77
6	C	603	WWA	C7-S1	-4.75	1.69	1.77
6	G	603	WWA	C16-C3	4.63	1.45	1.38
6	F	603	WWA	C2-S	-4.39	1.70	1.77
6	C	603	WWA	C3-S	-4.36	1.70	1.77
6	C	603	WWA	C16-C3	4.35	1.45	1.38
6	B	603	WWA	C6-C7	4.28	1.45	1.38
6	B	603	WWA	C3-S	-4.22	1.70	1.77
6	G	603	WWA	C6-C7	4.15	1.45	1.38
6	C	603	WWA	C6-C7	4.02	1.44	1.38
6	F	603	WWA	C16-C3	3.97	1.44	1.38
3	H	602	OXL	O2-C2	3.93	1.32	1.22
6	F	603	WWA	C8-S1	-3.92	1.70	1.77
6	F	603	WWA	C7-S1	-3.91	1.71	1.77
3	F	602	OXL	O2-C2	3.77	1.31	1.22
6	G	603	WWA	C3-S	-3.73	1.71	1.77
3	A	602	OXL	O2-C2	3.67	1.31	1.22
3	C	602	OXL	O2-C2	3.67	1.31	1.22
6	B	603	WWA	C16-C3	3.66	1.44	1.38
6	F	603	WWA	C6-C7	3.61	1.44	1.38
3	B	602	OXL	O2-C2	3.56	1.31	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	OXL	O2-C2	3.43	1.31	1.22
3	D	602	OXL	O2-C2	3.35	1.30	1.22
3	G	602	OXL	O2-C2	3.23	1.30	1.22
3	E	602	OXL	O4-C2	-3.14	1.22	1.30
6	F	603	WWA	C4-C5	2.97	1.46	1.41
3	B	602	OXL	O4-C2	-2.89	1.22	1.30
6	F	603	WWA	C3-S	-2.81	1.72	1.77
3	H	602	OXL	O4-C2	-2.80	1.22	1.30
3	C	602	OXL	O4-C2	-2.78	1.23	1.30
3	D	602	OXL	O4-C2	-2.65	1.23	1.30
3	F	602	OXL	O4-C2	-2.64	1.23	1.30
3	A	602	OXL	O4-C2	-2.63	1.23	1.30
3	G	602	OXL	O4-C2	-2.59	1.23	1.30
6	B	603	WWA	C9-C8	2.53	1.43	1.39
6	F	603	WWA	C13-C12	2.31	1.42	1.39
3	H	602	OXL	C2-C1	2.07	1.58	1.54
3	D	602	OXL	C2-C1	2.05	1.58	1.54

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	603	WWA	C4-C3-S	5.67	126.67	119.14
3	D	602	OXL	O4-C2-C1	4.49	121.53	112.83
6	B	603	WWA	C4-C3-S	4.43	125.03	119.14
6	C	603	WWA	C4-C3-S	4.08	124.57	119.14
3	F	602	OXL	O4-C2-C1	3.83	120.26	112.83
6	B	603	WWA	O6-S-C3	3.76	112.58	107.96
3	B	602	OXL	O4-C2-C1	3.62	119.85	112.83
6	B	603	WWA	C14-C7-S1	3.61	123.94	119.14
6	G	603	WWA	C14-C7-S1	3.59	123.91	119.14
6	C	603	WWA	C5-C15-N1	3.46	124.13	121.00
6	F	603	WWA	C14-C7-S1	3.42	123.69	119.14
3	A	602	OXL	O4-C2-C1	3.37	119.36	112.83
3	C	602	OXL	O4-C2-C1	3.31	119.25	112.83
6	G	603	WWA	C4-C3-S	3.20	123.40	119.14
3	D	602	OXL	O3-C1-C2	3.13	118.91	112.83
3	E	602	OXL	O4-C2-C1	3.12	118.89	112.83
6	G	603	WWA	C5-C15-N1	3.06	123.77	121.00
3	G	602	OXL	O4-C2-C1	3.05	118.74	112.83
6	B	603	WWA	O6-S-C2	2.94	111.58	107.96
3	B	602	OXL	O3-C1-C2	2.91	118.47	112.83
6	C	603	WWA	C14-C7-S1	2.84	122.92	119.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	603	WWA	C3-C16-N1	2.57	126.27	123.21
6	F	603	WWA	C4-C3-C16	-2.54	116.26	119.04
6	B	603	WWA	O1-C10-C11	-2.53	113.23	119.85
3	F	602	OXL	O3-C1-C2	2.50	117.68	112.83
6	B	603	WWA	C3-S-C2	-2.49	99.80	104.37
3	H	602	OXL	O4-C2-C1	2.49	117.65	112.83
3	D	602	OXL	O2-C2-C1	-2.48	115.47	120.63
6	F	603	WWA	O6-S-C3	2.42	110.94	107.96
2	H	601	FBP	O6-P2-O4P	2.39	112.89	106.44
6	F	603	WWA	C17-C2-S	2.37	122.31	119.15
6	B	603	WWA	O-C-C19	-2.37	113.66	119.85
6	C	603	WWA	O2-C12-C13	-2.29	113.85	119.85
6	G	603	WWA	C3-C16-N1	2.23	125.86	123.21
6	F	603	WWA	C4-C5-N	2.20	120.55	118.01
6	F	603	WWA	O4-S1-C8	2.18	110.64	107.96
6	G	603	WWA	O1-C10-C11	-2.16	114.19	119.85
6	C	603	WWA	C3-C16-N1	2.15	125.78	123.21
3	C	602	OXL	O3-C1-C2	2.15	116.99	112.83
6	F	603	WWA	C5-C15-N1	2.13	122.93	121.00
6	G	603	WWA	O6-S-C2	2.12	110.57	107.96
3	E	602	OXL	O3-C1-C2	2.12	116.93	112.83
6	C	603	WWA	O3-S1-C8	2.11	110.55	107.96
6	G	603	WWA	O-C-C19	-2.08	114.40	119.85
6	B	603	WWA	C3-C16-N1	2.07	125.67	123.21
6	B	603	WWA	C5-C15-N1	2.05	122.86	121.00
6	C	603	WWA	O7-C18-C17	-2.04	114.51	119.85
6	C	603	WWA	O1-C10-C11	-2.04	114.53	119.85
3	A	602	OXL	O3-C1-C2	2.03	116.76	112.83
6	C	603	WWA	O-C-C19	-2.02	114.57	119.85
6	F	603	WWA	O-C-C19	-2.02	114.58	119.85
3	F	602	OXL	O2-C2-C1	-2.01	116.43	120.63
6	B	603	WWA	O7-C18-C17	-2.01	114.59	119.85

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	FBP	C1-O1-P1-O2P
2	E	601	FBP	C1-O1-P1-O1P
2	E	601	FBP	C1-O1-P1-O2P
2	G	601	FBP	C1-O1-P1-O1P
2	G	601	FBP	C1-O1-P1-O3P

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Mol	Chain	Res	Type	Atoms
2	H	601	FBP	C1-O1-P1-O2P
2	H	601	FBP	C1-O1-P1-O3P
2	A	601	FBP	C4-C5-C6-O6
2	B	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6
2	D	601	FBP	C4-C5-C6-O6
2	E	601	FBP	C4-C5-C6-O6
2	F	601	FBP	C4-C5-C6-O6
2	G	601	FBP	C4-C5-C6-O6
2	H	601	FBP	C4-C5-C6-O6
2	A	601	FBP	O5-C5-C6-O6
2	C	601	FBP	O5-C5-C6-O6
2	D	601	FBP	O5-C5-C6-O6
2	E	601	FBP	O5-C5-C6-O6
2	F	601	FBP	O5-C5-C6-O6
2	H	601	FBP	O5-C5-C6-O6
2	B	601	FBP	O5-C5-C6-O6
2	G	601	FBP	O5-C5-C6-O6
3	G	602	OXL	O3-C1-C2-O4
2	B	601	FBP	C1-O1-P1-O1P
3	H	602	OXL	O3-C1-C2-O4
3	C	602	OXL	O3-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O4
3	B	602	OXL	O3-C1-C2-O4
3	D	602	OXL	O3-C1-C2-O4
3	B	602	OXL	O1-C1-C2-O2
3	C	602	OXL	O1-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O2
3	E	602	OXL	O1-C1-C2-O2
2	B	601	FBP	O1-C1-C2-O5
2	C	601	FBP	O1-C1-C2-O5
3	A	602	OXL	O3-C1-C2-O4
3	A	602	OXL	O1-C1-C2-O2
3	G	602	OXL	O1-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O2
3	G	602	OXL	O1-C1-C2-O4
3	G	602	OXL	O3-C1-C2-O2
3	E	602	OXL	O3-C1-C2-O2
3	B	602	OXL	O1-C1-C2-O4
3	B	602	OXL	O3-C1-C2-O2
3	C	602	OXL	O1-C1-C2-O4
3	C	602	OXL	O3-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	D	602	OXL	O1-C1-C2-O4
3	E	602	OXL	O1-C1-C2-O4
3	D	602	OXL	O3-C1-C2-O2
3	A	602	OXL	O1-C1-C2-O4
3	A	602	OXL	O3-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O4
2	B	601	FBP	C1-O1-P1-O3P
2	D	601	FBP	C1-O1-P1-O2P
2	E	601	FBP	C1-O1-P1-O3P
2	F	601	FBP	C1-O1-P1-O2P
3	H	602	OXL	O3-C1-C2-O2
2	G	601	FBP	O1-C1-C2-O5

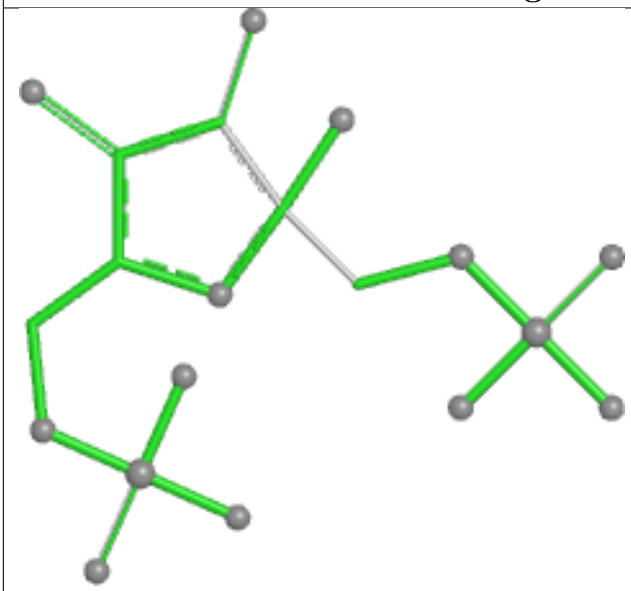
There are no ring outliers.

4 monomers are involved in 4 short contacts:

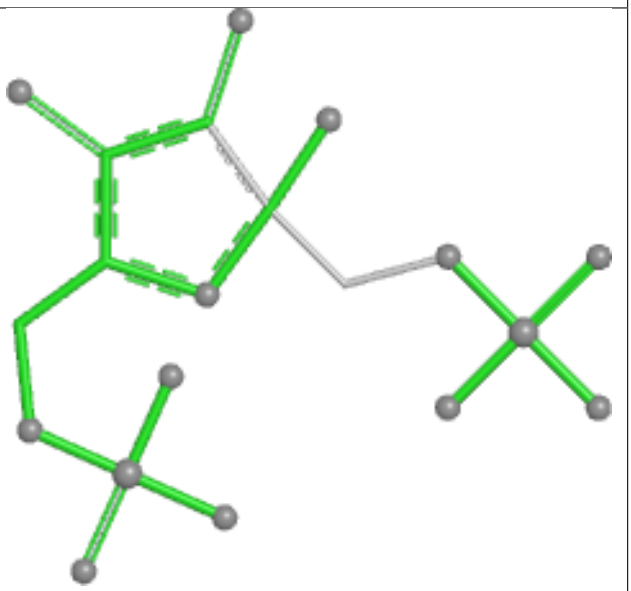
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	601	FBP	1	0
2	H	601	FBP	1	0
2	A	601	FBP	1	0
2	B	601	FBP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

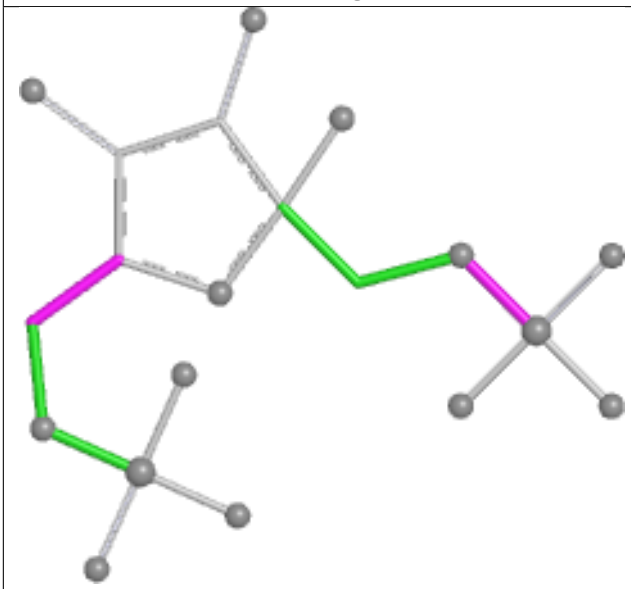
Ligand FBP D 601



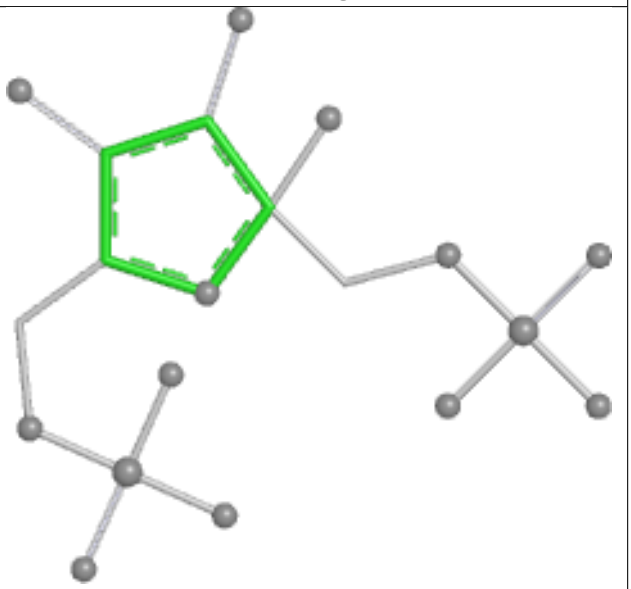
Bond lengths



Bond angles

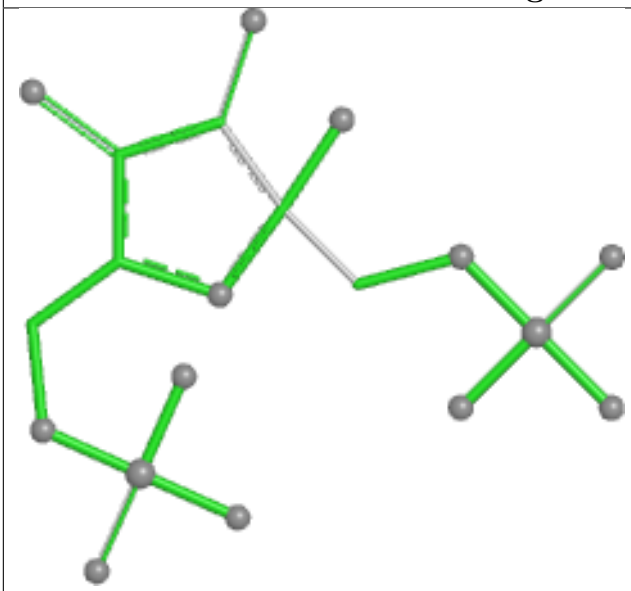


Torsions

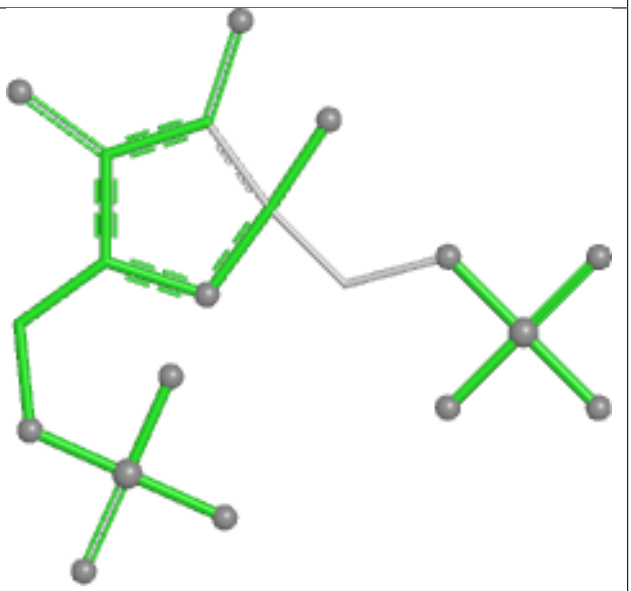


Rings

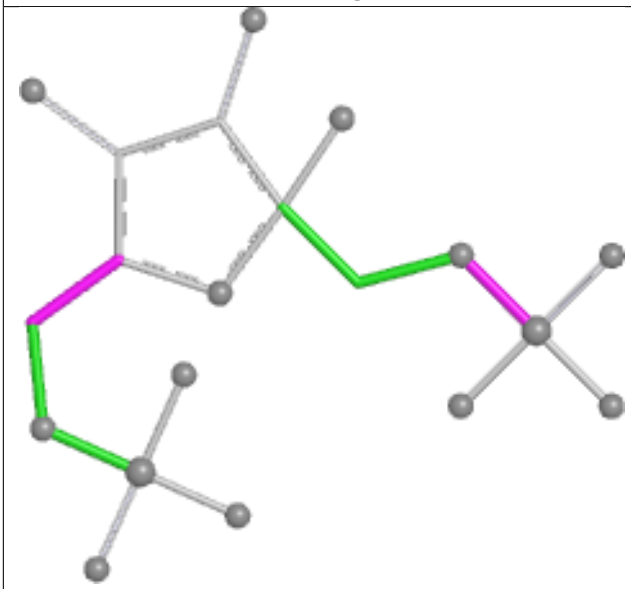
Ligand FBP E 601



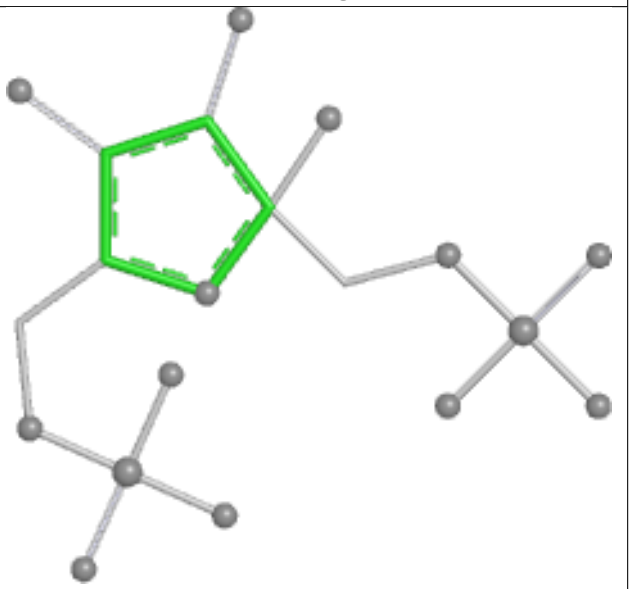
Bond lengths



Bond angles

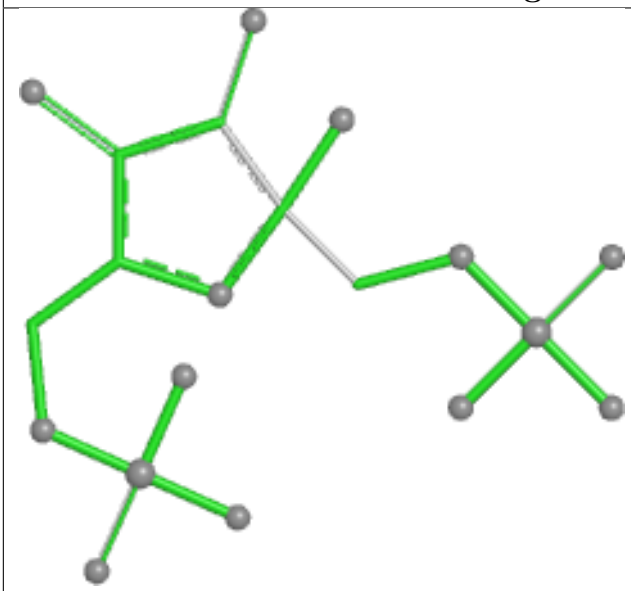


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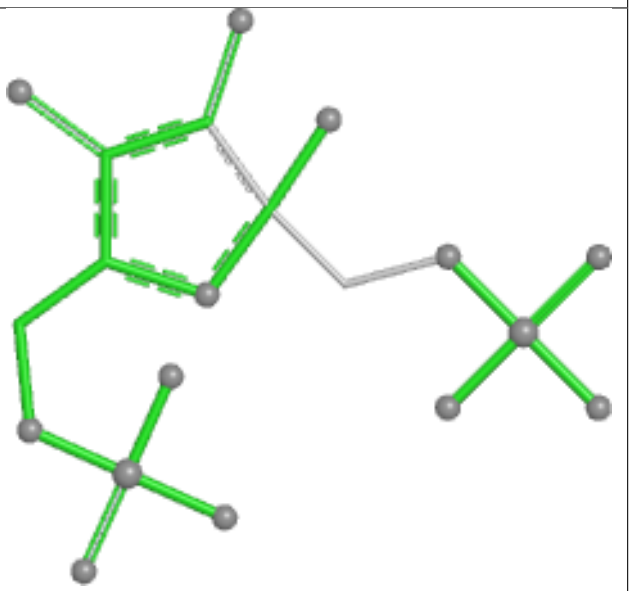


Rings

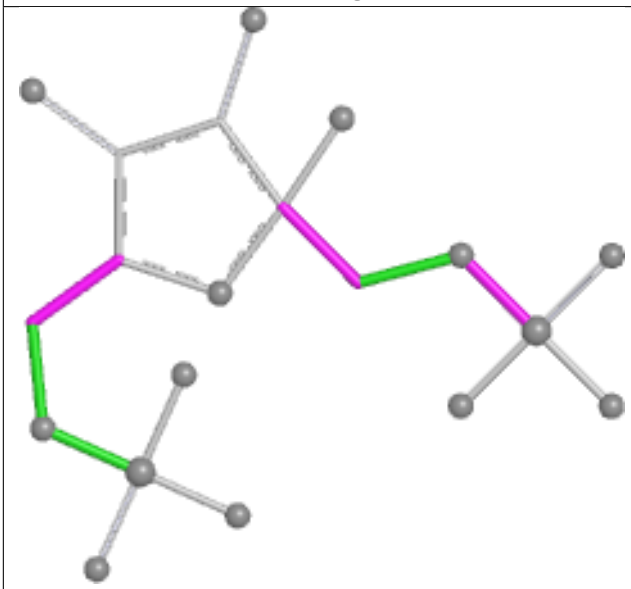
Ligand FBP G 601



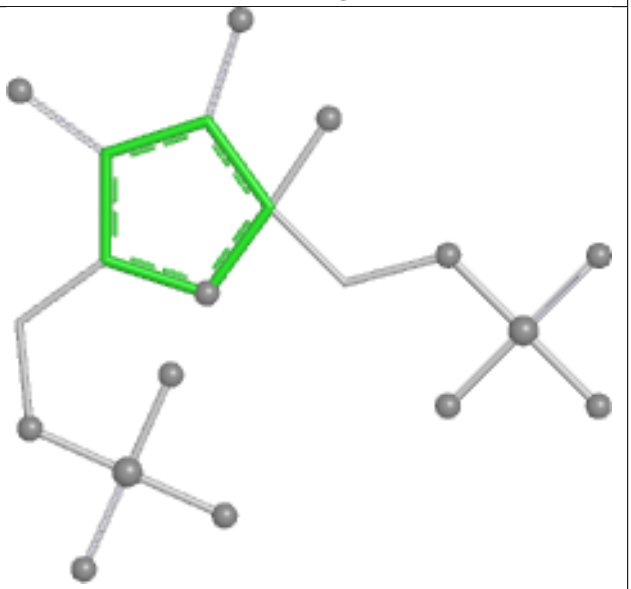
Bond lengths



Bond angles

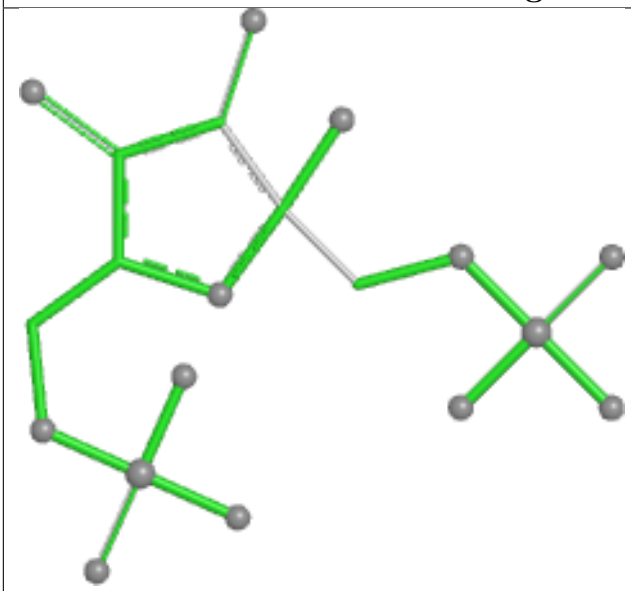


Torsions

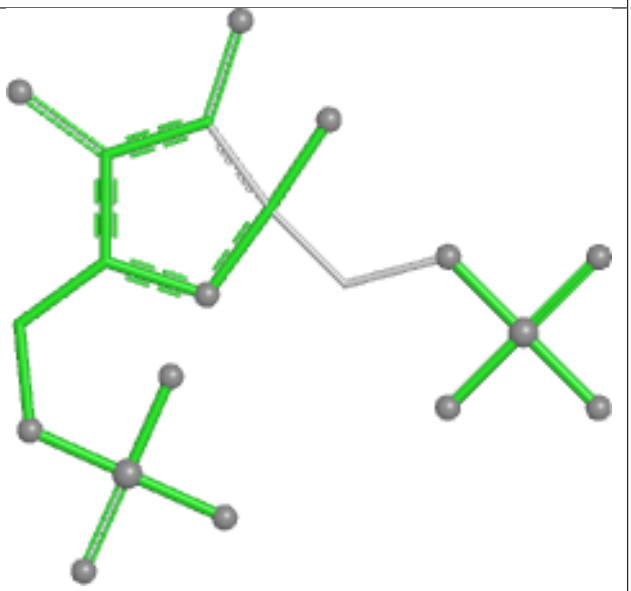


Rings

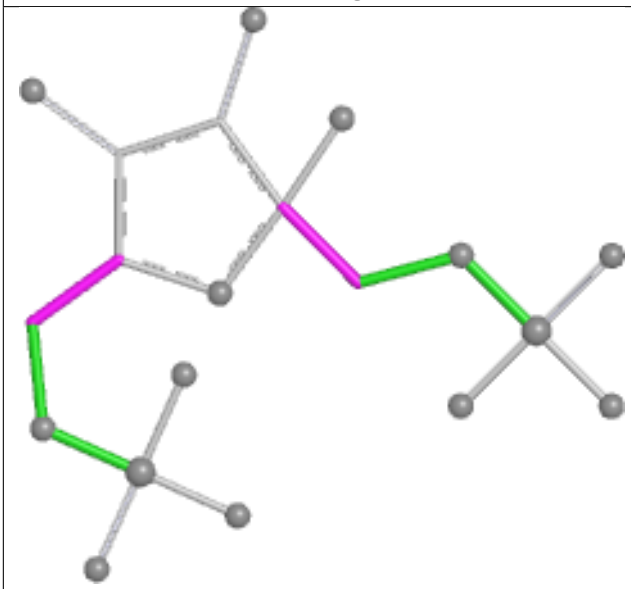
Ligand FBP C 601



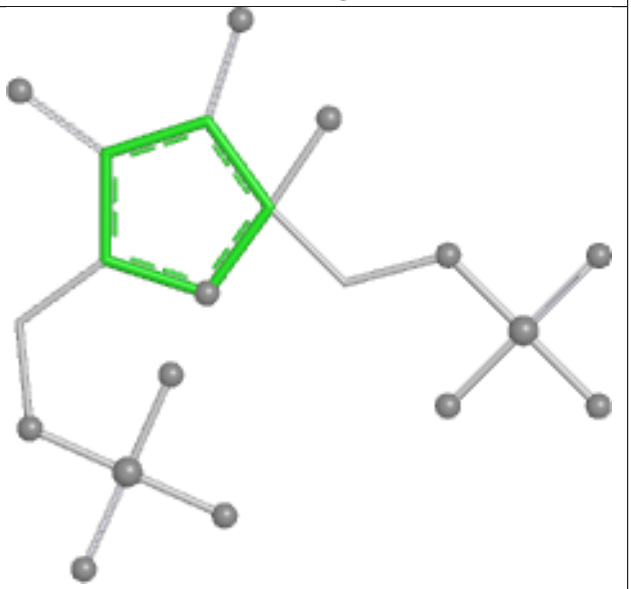
Bond lengths



Bond angles

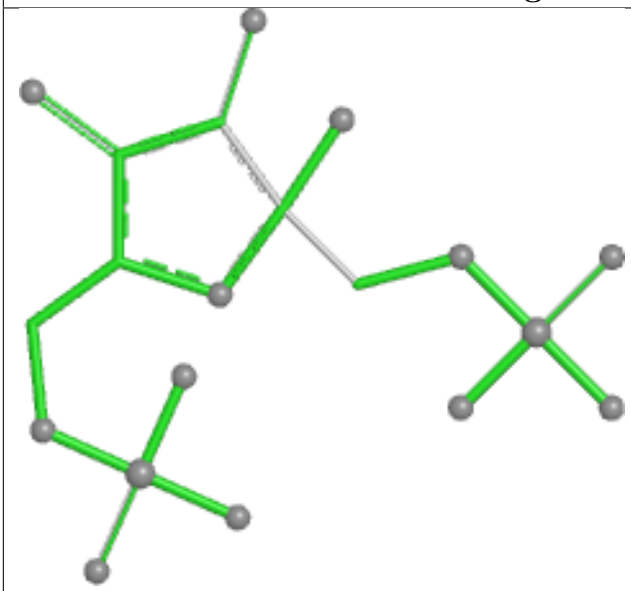


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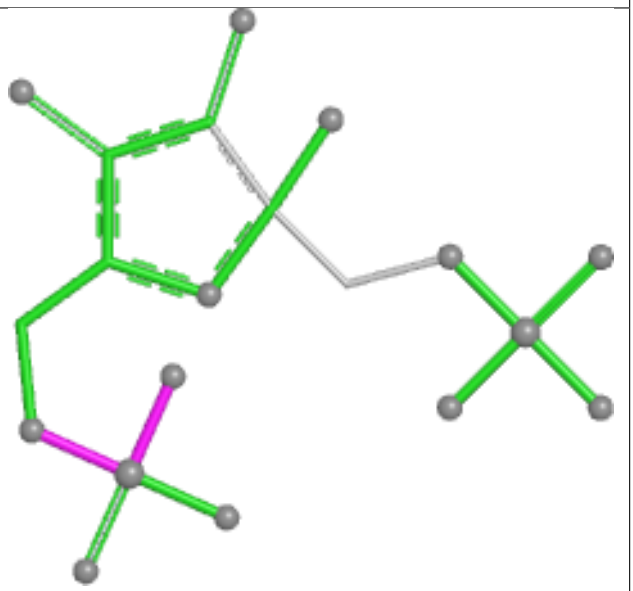


Rings

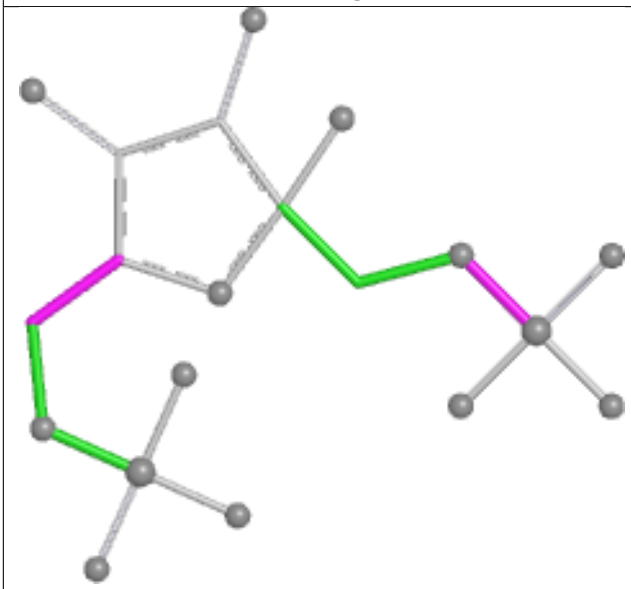
Ligand FBP H 601



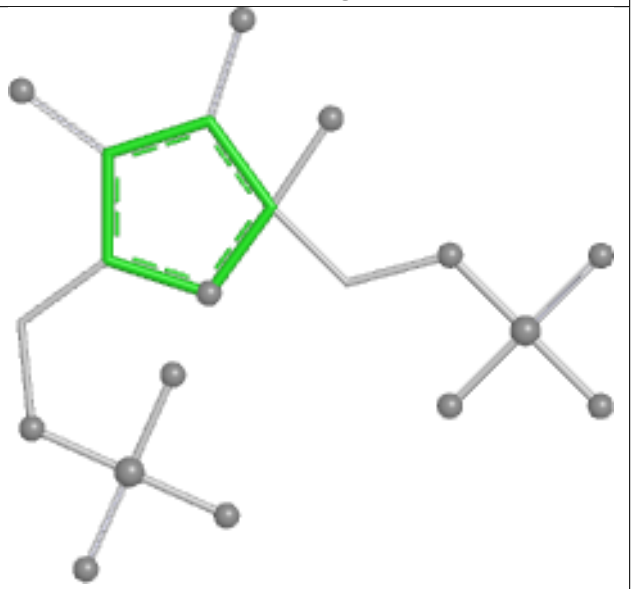
Bond lengths



Bond angles

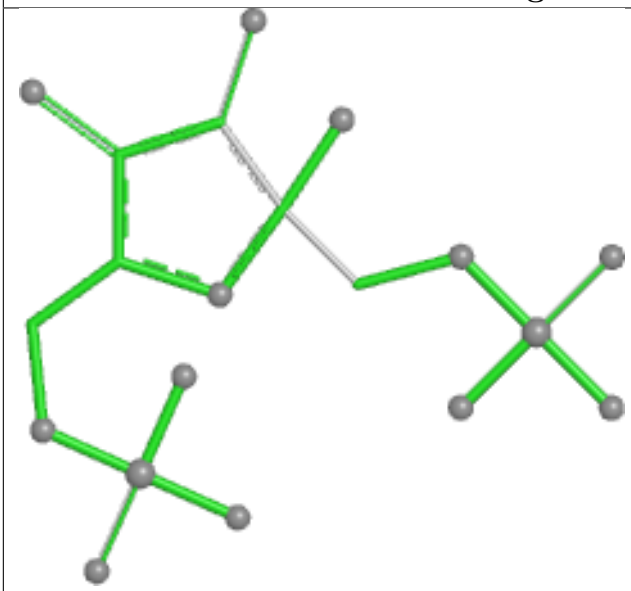


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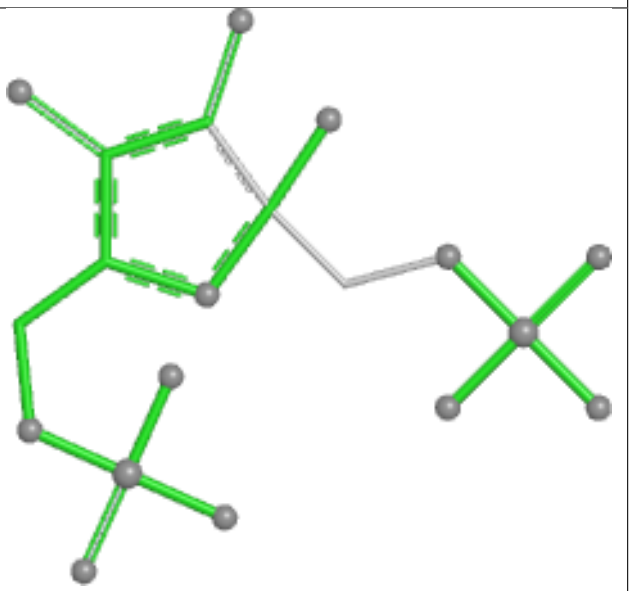


Rings

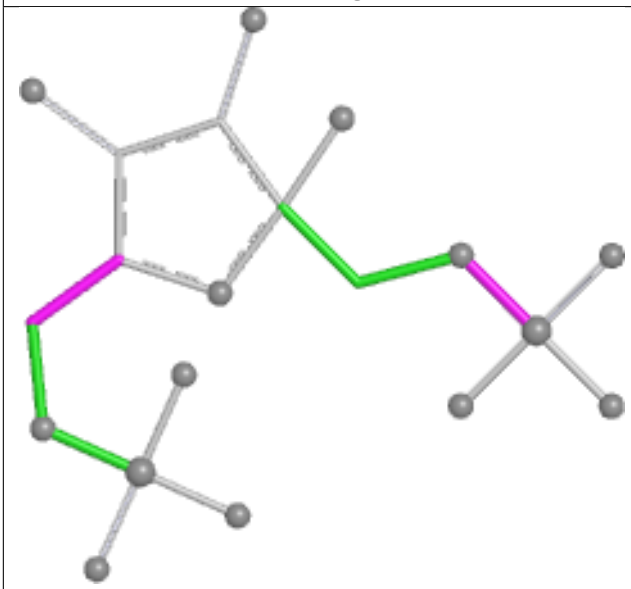
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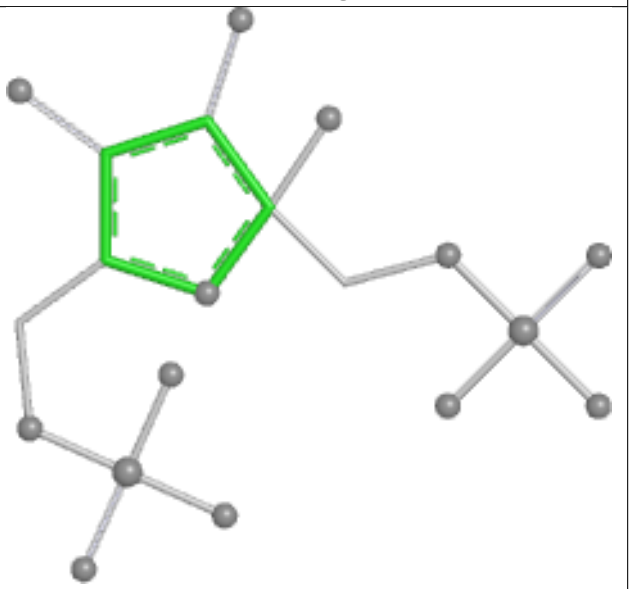
Bond lengths



Bond angles

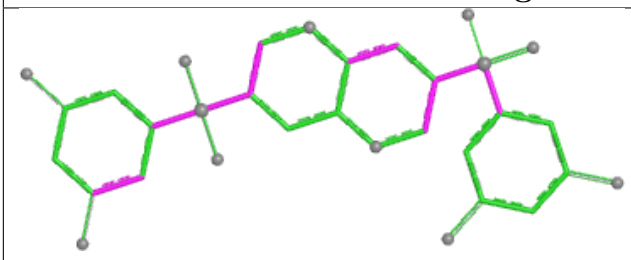


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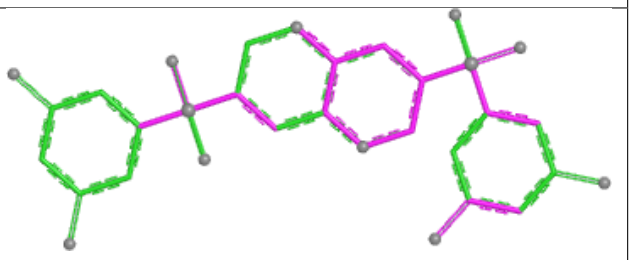


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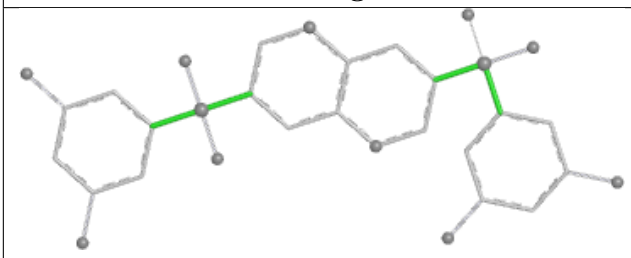
Ligand WWA F 603



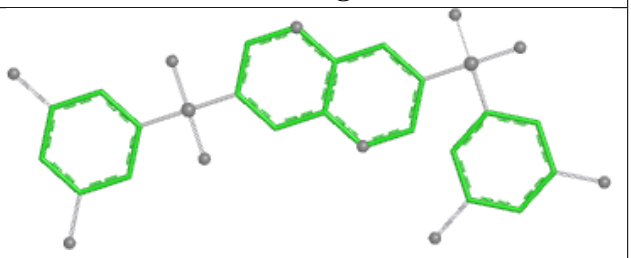
Bond lengths



Bond angles

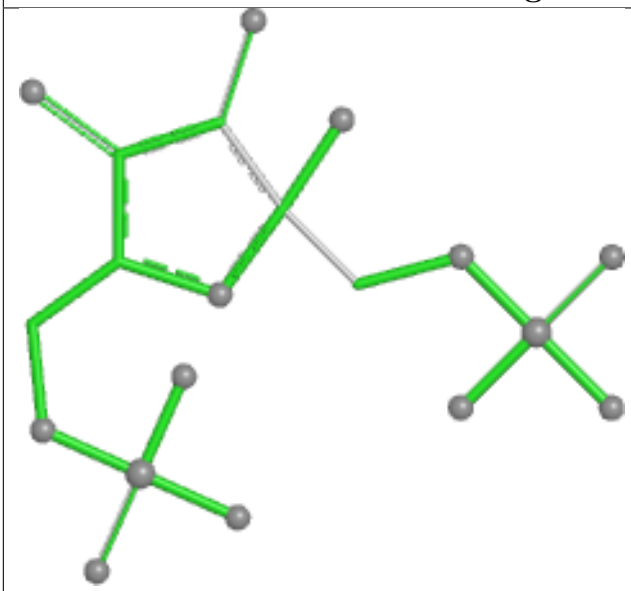


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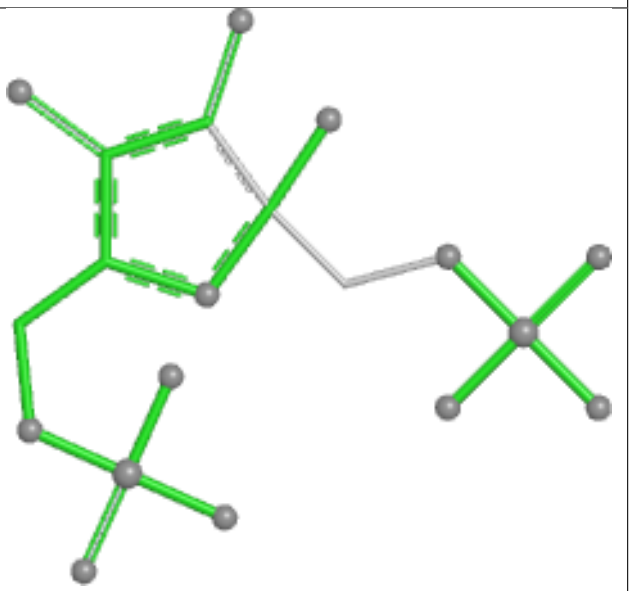


Rings

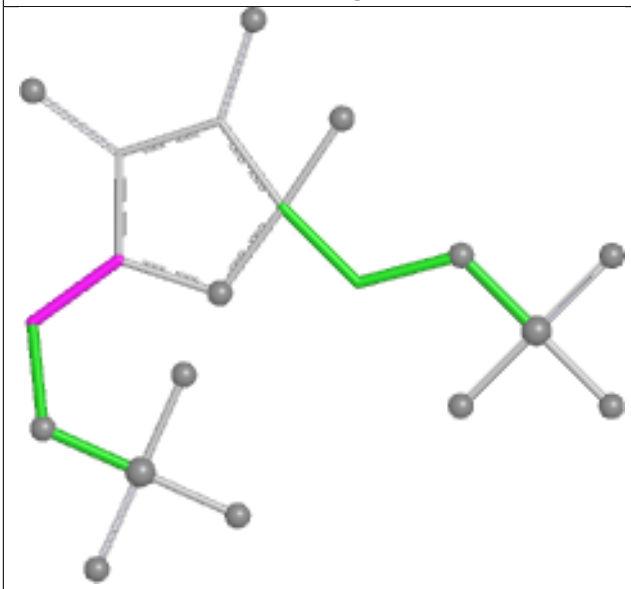
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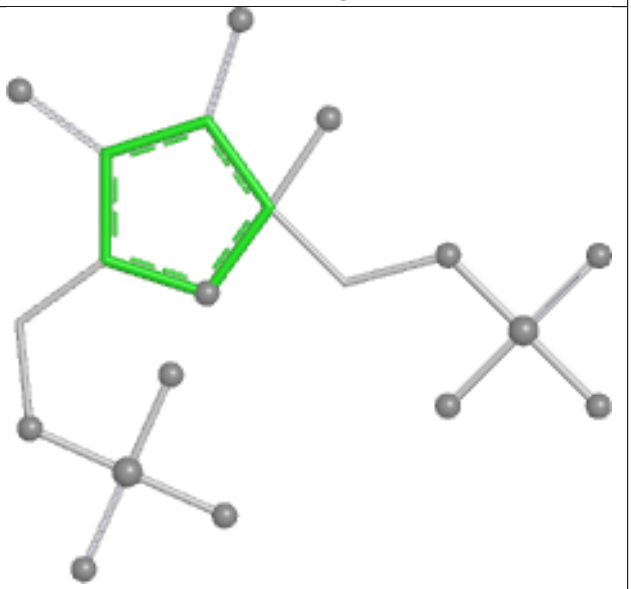
Bond lengths



Bond angles

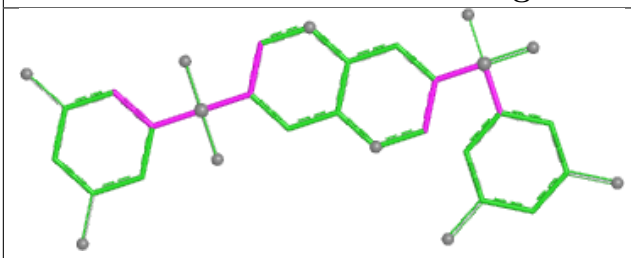


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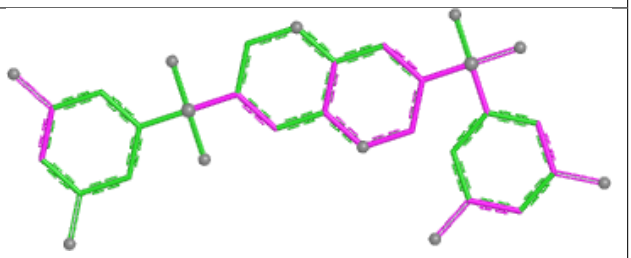


Rings

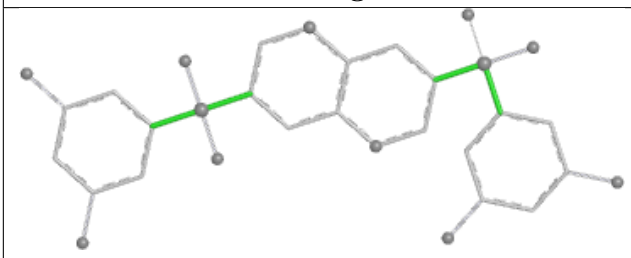
Ligand WWA B 603



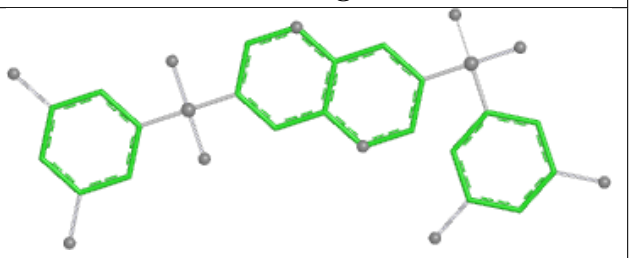
Bond lengths



Bond angles

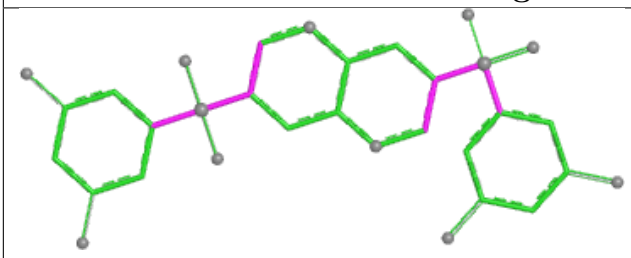


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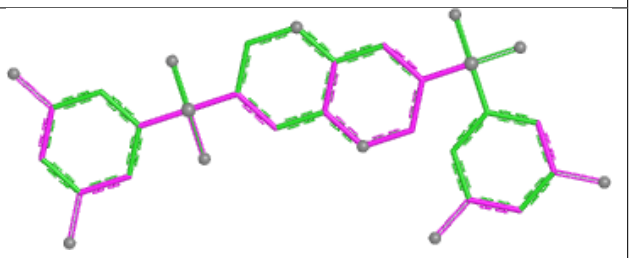


Rings

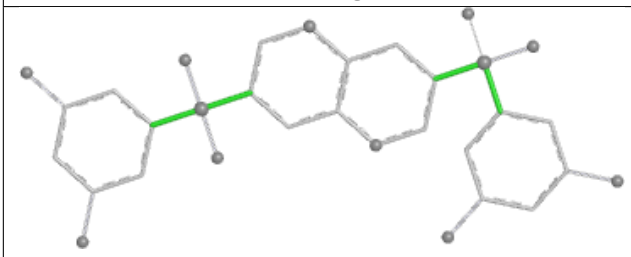
Ligand WWA C 603



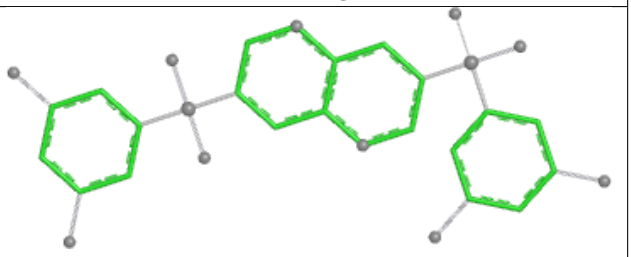
Bond lengths



Bond angles

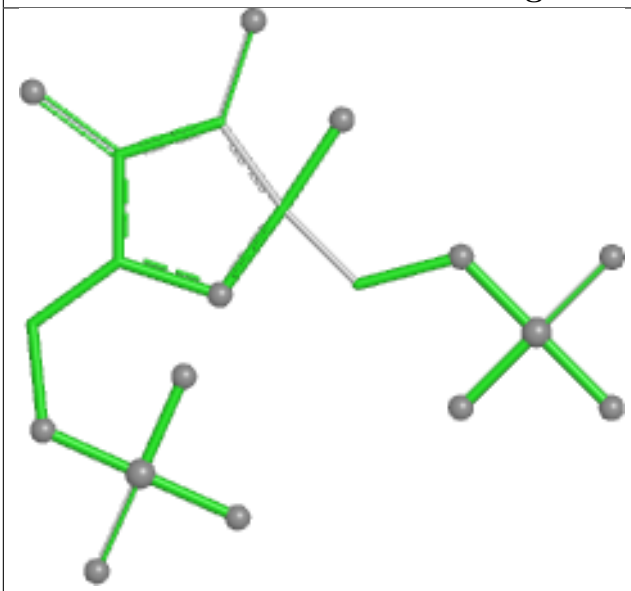


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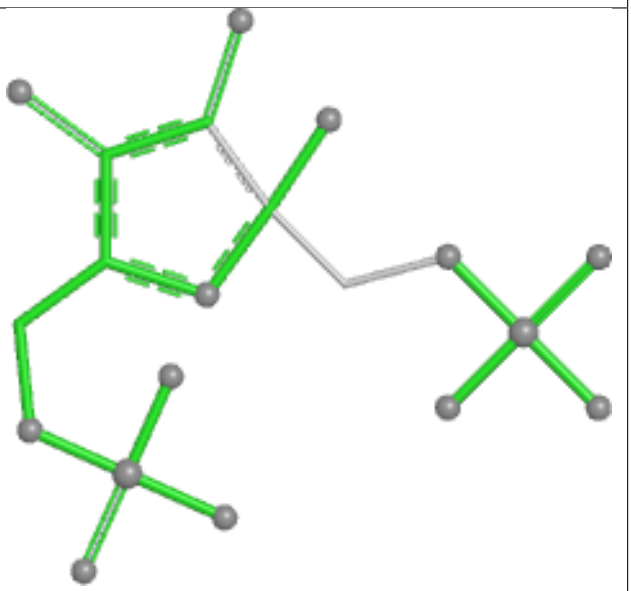


Rings

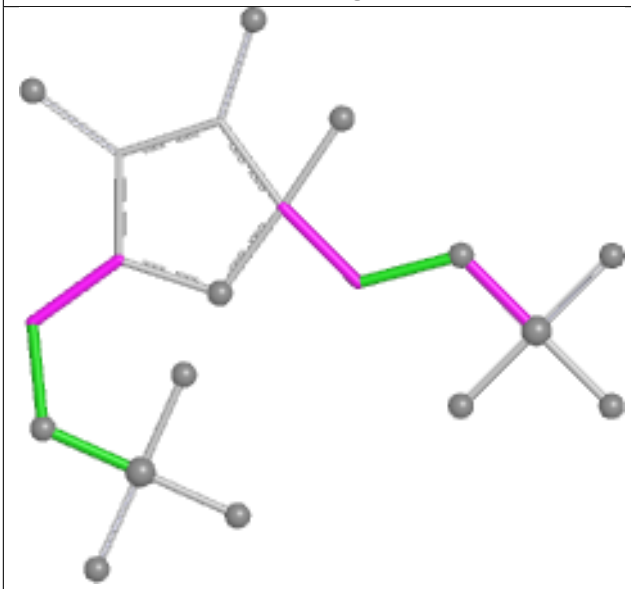
Ligand FBP B 601



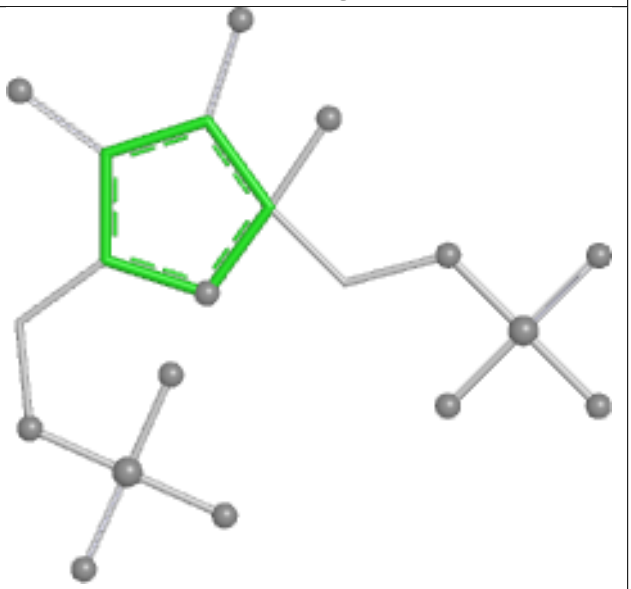
Bond lengths



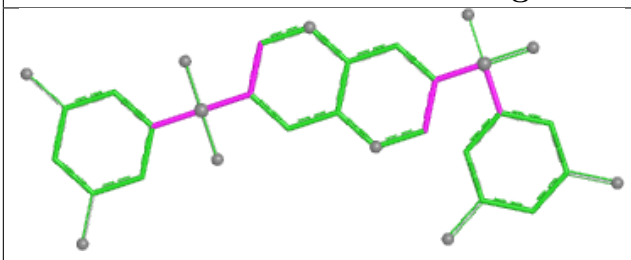
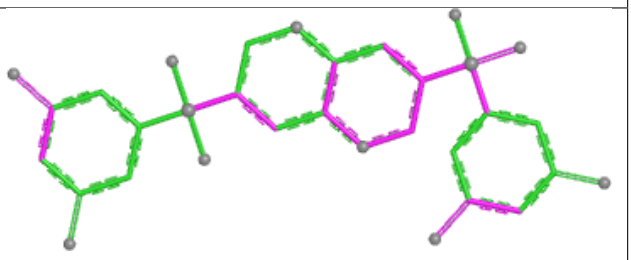
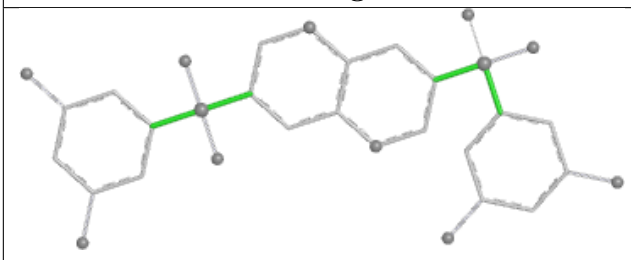
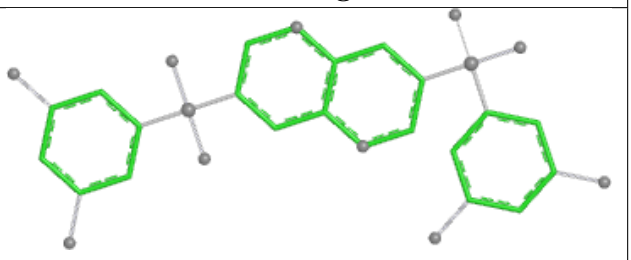
Bond angles



Torsions



Rings

Ligand WWA G 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	418/447 (93%)	1.53	117 (27%) 1 1	32, 78, 111, 121	12 (2%)
1	B	436/447 (97%)	0.55	18 (4%) 41 37	25, 53, 84, 96	8 (1%)
1	C	424/447 (94%)	0.97	56 (13%) 7 5	24, 62, 87, 106	9 (2%)
1	D	424/447 (94%)	0.13	10 (2%) 59 56	22, 41, 67, 102	8 (1%)
1	E	420/447 (93%)	1.72	149 (35%) 1 1	31, 77, 115, 126	12 (2%)
1	F	432/447 (96%)	0.88	43 (9%) 12 10	26, 57, 88, 107	8 (1%)
1	G	422/447 (94%)	1.06	61 (14%) 6 4	24, 58, 85, 97	11 (2%)
1	H	425/447 (95%)	0.16	11 (2%) 57 53	20, 41, 67, 98	9 (2%)
All	All	3401/3576 (95%)	0.87	465 (13%) 6 5	20, 58, 101, 126	77 (2%)

All (465) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	277[A]	HIS	6.5
1	E	130	GLY	6.4
1	A	545	SER	6.4
1	E	449	GLY	5.5
1	E	25	PHE	5.3
1	F	233	PRO	5.3
1	E	265	VAL	5.3
1	A	26	GLN	5.1
1	E	444	VAL	5.1
1	E	235	LEU	4.9
1	D	132	GLY	4.9
1	E	234	GLY	4.9
1	D	21	GLY	4.8
1	C	233	PRO	4.7
1	G	277[A]	HIS	4.7
1	A	243	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	23	ALA	4.6
1	A	132	GLY	4.6
1	E	103	VAL	4.6
1	E	122	ILE	4.5
1	E	495	ILE	4.4
1	G	233	PRO	4.4
1	A	61	ALA	4.4
1	A	103	VAL	4.4
1	E	250	GLY	4.3
1	E	115	LEU	4.3
1	E	497	ALA	4.2
1	H	21	GLY	4.2
1	C	103	VAL	4.2
1	A	63	ILE	4.1
1	E	516	PHE	4.1
1	G	21	GLY	4.0
1	E	269[A]	ARG	4.0
1	B	545	SER	4.0
1	A	124	LEU	4.0
1	E	487	LEU	4.0
1	G	115	LEU	4.0
1	E	120	VAL	4.0
1	F	542[A]	LEU	3.9
1	A	492	PRO	3.8
1	F	11	ALA	3.8
1	G	129	PRO	3.8
1	E	262	ALA	3.8
1	C	63	ILE	3.8
1	E	350	THR	3.8
1	E	467	VAL	3.8
1	E	494	ALA	3.8
1	E	119	PRO	3.7
1	E	545	SER	3.7
1	G	352	PRO	3.7
1	A	467	VAL	3.7
1	A	123	ALA	3.7
1	G	353	ARG	3.7
1	E	240	VAL	3.6
1	F	114	PRO	3.6
1	F	243	LEU	3.6
1	A	465	ILE	3.6
1	E	274	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	65	PRO	3.6
1	A	115	LEU	3.5
1	G	64	GLY	3.5
1	G	272	LEU	3.5
1	A	119	PRO	3.5
1	A	251	VAL	3.5
1	E	388	ALA	3.5
1	G	243	LEU	3.5
1	G	63	ILE	3.5
1	A	269[A]	ARG	3.5
1	E	500	VAL	3.5
1	F	115	LEU	3.5
1	E	465	ILE	3.5
1	E	259	VAL	3.4
1	A	122	ILE	3.4
1	F	545	SER	3.4
1	A	410[A]	GLU	3.4
1	C	115	LEU	3.4
1	C	129	PRO	3.4
1	A	413	ARG	3.4
1	A	120	VAL	3.4
1	G	103	VAL	3.4
1	E	99	SER	3.4
1	C	20	LEU	3.3
1	E	448	THR	3.3
1	E	461	ARG	3.3
1	E	486	LEU	3.3
1	A	509	GLU	3.3
1	A	495	ILE	3.3
1	A	34	MET	3.3
1	B	413	ARG	3.3
1	E	491	PRO	3.3
1	A	525	VAL	3.3
1	A	81	MET	3.3
1	E	123	ALA	3.3
1	E	251	VAL	3.3
1	E	525	VAL	3.3
1	C	273	GLY	3.3
1	G	236	SER	3.2
1	C	234	GLY	3.2
1	A	484	PHE	3.2
1	E	24	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	25	PHE	3.2
1	A	235	LEU	3.2
1	A	491	PRO	3.2
1	B	114	PRO	3.2
1	C	64	GLY	3.2
1	G	324	GLN	3.2
1	A	352	PRO	3.2
1	A	349	ILE	3.2
1	A	350	THR	3.2
1	E	527	THR	3.2
1	G	66	ALA	3.1
1	D	240	VAL	3.1
1	E	504	VAL	3.1
1	G	234	GLY	3.1
1	E	121	ALA	3.1
1	F	489	ARG	3.1
1	G	114	PRO	3.1
1	E	254	VAL	3.1
1	A	379	THR	3.1
1	E	253	ILE	3.1
1	E	272	LEU	3.1
1	F	514	ARG	3.1
1	A	359	THR	3.1
1	E	445	LEU	3.1
1	G	545	SER	3.0
1	E	538	ILE	3.0
1	E	266	ALA	3.0
1	C	375	LEU	3.0
1	E	118	ARG	3.0
1	A	56	SER	3.0
1	C	276	GLY	3.0
1	A	59	ILE	3.0
1	G	70	VAL	3.0
1	G	268	VAL	3.0
1	E	267	ALA	3.0
1	E	446	THR	3.0
1	B	542[A]	LEU	3.0
1	E	368	ASP	3.0
1	E	116	SER	3.0
1	E	543[A]	SER	3.0
1	C	395	ILE	2.9
1	A	539[A]	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	494	ALA	2.9
1	A	500	VAL	2.9
1	F	494	ALA	2.9
1	E	488	TYR	2.9
1	D	234	GLY	2.9
1	A	388	ALA	2.9
1	H	233	PRO	2.9
1	A	486	LEU	2.9
1	F	496	TRP	2.9
1	B	233	PRO	2.9
1	C	399	ALA	2.9
1	E	61	ALA	2.9
1	A	493	GLU	2.9
1	G	410	GLU	2.9
1	A	250	GLY	2.9
1	E	247	VAL	2.8
1	E	523	VAL	2.8
1	E	466	ALA	2.8
1	E	517	LEU	2.8
1	D	130	GLY	2.8
1	A	240	VAL	2.8
1	G	362	VAL	2.8
1	A	527	THR	2.8
1	E	345	LEU	2.8
1	G	345	LEU	2.8
1	D	25	PHE	2.8
1	G	461	ARG	2.8
1	C	315	ILE	2.8
1	B	492	PRO	2.8
1	C	274	PRO	2.8
1	E	342	THR	2.8
1	G	106	ALA	2.8
1	E	255	PHE	2.8
1	E	258	PHE	2.8
1	G	110	PHE	2.8
1	C	313	ILE	2.8
1	F	495	ILE	2.8
1	E	483	VAL	2.8
1	A	36	ASP	2.8
1	F	242	ASP	2.8
1	A	77	ILE	2.7
1	E	458	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	455	LEU	2.7
1	C	388	ALA	2.7
1	E	104	ARG	2.7
1	E	318	GLU	2.7
1	E	112	GLY	2.7
1	E	484	PHE	2.7
1	F	491	PRO	2.7
1	E	243	LEU	2.7
1	E	439	ALA	2.7
1	H	22	THR	2.7
1	A	353	ARG	2.7
1	E	492	PRO	2.7
1	G	386	VAL	2.7
1	C	243	LEU	2.7
1	A	355	THR	2.7
1	B	489	ARG	2.7
1	C	348	MET	2.7
1	G	235	LEU	2.7
1	A	490	GLU	2.7
1	C	509	GLU	2.7
1	G	365	ALA	2.7
1	H	23	ALA	2.7
1	E	507	GLY	2.6
1	E	395	ILE	2.6
1	G	25	PHE	2.6
1	A	502	ARG	2.6
1	G	34	MET	2.6
1	A	386	VAL	2.6
1	A	429	GLY	2.6
1	B	544	ILE	2.6
1	C	65	PRO	2.6
1	E	454	LEU	2.6
1	F	513	LEU	2.6
1	A	504	VAL	2.6
1	E	283	SER	2.6
1	E	402	ALA	2.6
1	C	382	GLY	2.6
1	F	239	ASP	2.6
1	A	259	VAL	2.6
1	F	533	SER	2.6
1	A	488	TYR	2.6
1	C	368	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	76[A]	MET	2.6
1	A	516	PHE	2.6
1	F	506	PHE	2.6
1	E	298	LEU	2.6
1	B	519	VAL	2.6
1	C	236	SER	2.6
1	E	470	SER	2.6
1	E	353	ARG	2.5
1	E	281	ILE	2.5
1	A	255	PHE	2.5
1	E	75	GLU	2.5
1	A	375	LEU	2.5
1	E	128	GLY	2.5
1	A	60	ILE	2.5
1	E	59	ILE	2.5
1	A	86	LEU	2.5
1	C	42	LEU	2.5
1	D	24	PHE	2.5
1	F	267	ALA	2.5
1	A	446	THR	2.5
1	E	113	SER	2.5
1	E	489	ARG	2.5
1	C	34	MET	2.5
1	G	276	GLY	2.5
1	C	100	ILE	2.5
1	E	279	ILE	2.5
1	E	304	ILE	2.5
1	H	24	PHE	2.5
1	E	93	HIS	2.5
1	E	256	ALA	2.5
1	E	58	SER	2.5
1	E	62	THR	2.5
1	D	501	ASP	2.5
1	B	513	LEU	2.5
1	A	96	HIS	2.5
1	D	277[A]	HIS	2.5
1	H	244[A]	ARG	2.5
1	A	84	ALA	2.5
1	C	380	ALA	2.5
1	E	101	ALA	2.5
1	G	121	ALA	2.5
1	G	116[A]	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	458	TYR	2.4
1	G	95	TYR	2.4
1	B	522	LEU	2.4
1	E	124	LEU	2.4
1	E	435	PHE	2.4
1	E	464	VAL	2.4
1	E	399	ALA	2.4
1	A	58	SER	2.4
1	E	252	ASP	2.4
1	A	272	LEU	2.4
1	F	235	LEU	2.4
1	A	254	VAL	2.4
1	A	265	VAL	2.4
1	A	496	TRP	2.4
1	E	70	VAL	2.4
1	E	268	VAL	2.4
1	F	504	VAL	2.4
1	E	34	MET	2.4
1	A	466	ALA	2.4
1	G	126	THR	2.4
1	A	398	GLU	2.4
1	A	531	PRO	2.4
1	A	542	LEU	2.4
1	F	487	LEU	2.4
1	A	32	ALA	2.4
1	G	270	ALA	2.4
1	A	65	PRO	2.4
1	E	424	GLU	2.4
1	A	130	GLY	2.4
1	F	534	GLY	2.4
1	E	100	ILE	2.4
1	A	445	LEU	2.4
1	F	129	PRO	2.3
1	E	510	SER	2.3
1	G	67	SER	2.3
1	B	130	GLY	2.3
1	E	278	GLY	2.3
1	A	73	LEU	2.3
1	E	282	ILE	2.3
1	H	34	MET	2.3
1	C	117	TYR	2.3
1	C	381	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	240	VAL	2.3
1	E	474	ALA	2.3
1	E	413	ARG	2.3
1	A	478	HIS	2.3
1	E	501[A]	ASP	2.3
1	A	88	PHE	2.3
1	C	110	PHE	2.3
1	E	299[A]	GLU	2.3
1	G	98[A]	GLU	2.3
1	E	60	ILE	2.3
1	E	83	ILE	2.3
1	E	513	LEU	2.3
1	E	81	MET	2.3
1	A	351	LYS	2.3
1	E	110	PHE	2.3
1	G	516	PHE	2.3
1	G	251	VAL	2.3
1	A	97	ALA	2.3
1	A	497	ALA	2.3
1	E	66	ALA	2.3
1	A	489	ARG	2.3
1	E	377	GLY	2.3
1	C	545	SER	2.3
1	G	113	SER	2.3
1	E	508	ILE	2.3
1	F	529	TRP	2.3
1	D	34	MET	2.3
1	F	498	ASP	2.3
1	A	483	VAL	2.3
1	A	118	ARG	2.3
1	A	274	PRO	2.3
1	C	114	PRO	2.3
1	E	480	CYS	2.3
1	E	503	ARG	2.3
1	F	485	PRO	2.3
1	G	385	PRO	2.3
1	B	440	ALA	2.2
1	C	69	SER	2.2
1	C	113	SER	2.2
1	F	428	ILE	2.2
1	G	347	SER	2.2
1	F	516	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	540	ARG	2.2
1	G	256	ALA	2.2
1	A	482	GLY	2.2
1	B	115	LEU	2.2
1	C	272[A]	LEU	2.2
1	G	375	LEU	2.2
1	A	100	ILE	2.2
1	A	533[A]	SER	2.2
1	G	253	ILE	2.2
1	C	19	GLU	2.2
1	E	410[A]	GLU	2.2
1	G	248	GLU	2.2
1	E	244	ARG	2.2
1	C	97	ALA	2.2
1	C	270	ALA	2.2
1	E	97	ALA	2.2
1	A	449	GLY	2.2
1	E	522	LEU	2.2
1	G	349	ILE	2.2
1	G	242	ASP	2.2
1	A	108	GLU	2.2
1	A	245	PHE	2.2
1	A	385	PRO	2.2
1	C	107	VAL	2.2
1	F	523	VAL	2.2
1	C	66	ALA	2.2
1	A	345	LEU	2.2
1	C	345	LEU	2.2
1	E	86	LEU	2.2
1	A	279	ILE	2.2
1	C	349	ILE	2.2
1	A	514	ARG	2.2
1	H	518	ARG	2.2
1	A	354	PRO	2.2
1	A	477	VAL	2.1
1	A	523	VAL	2.1
1	F	467	VAL	2.1
1	G	33	ALA	2.1
1	C	94	GLU	2.1
1	E	69	SER	2.1
1	F	518	ARG	2.1
1	C	352	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	506	PHE	2.1
1	G	24	PHE	2.1
1	E	476	GLN	2.1
1	E	440	ALA	2.1
1	E	462	ALA	2.1
1	C	235	LEU	2.1
1	C	379	THR	2.1
1	E	273	GLY	2.1
1	G	406	ARG	2.1
1	H	410	GLU	2.1
1	A	116	SER	2.1
1	A	347	SER	2.1
1	A	368	ASP	2.1
1	E	109	SER	2.1
1	E	239	ASP	2.1
1	F	351	LYS	2.1
1	A	348	MET	2.1
1	G	348	MET	2.1
1	B	504	VAL	2.1
1	E	541	VAL	2.1
1	F	238	GLN	2.1
1	C	121	ALA	2.1
1	E	271	ALA	2.1
1	F	112	GLY	2.1
1	G	42	LEU	2.1
1	B	269[A]	ARG	2.1
1	C	353	ARG	2.1
1	F	413	ARG	2.1
1	A	282	ILE	2.1
1	C	77	ILE	2.1
1	A	67	SER	2.1
1	A	376	SER	2.1
1	C	344	MET	2.1
1	H	277[A]	HIS	2.1
1	A	506	PHE	2.1
1	G	255	PHE	2.1
1	C	244	ARG	2.1
1	A	75[A]	GLU	2.1
1	B	108	GLU	2.1
1	A	443	ILE	2.1
1	E	95	TYR	2.1
1	E	499	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	374	MET	2.1
1	C	472	GLN	2.0
1	B	500	VAL	2.0
1	C	88	PHE	2.0
1	E	475	ARG	2.0
1	G	271	ALA	2.0
1	E	496	TRP	2.0
1	G	382	GLY	2.0
1	F	508	ILE	2.0
1	E	257	SER	2.0
1	F	492	PRO	2.0
1	E	249	HIS	2.0
1	G	96	HIS	2.0
1	E	343	GLN	2.0
1	C	25	PHE	2.0
1	E	321	PHE	2.0
1	A	111	ALA	2.0
1	E	441	ALA	2.0
1	E	473	ALA	2.0
1	F	497	ALA	2.0
1	E	383	ASN	2.0
1	A	62	THR	2.0
1	A	315	ILE	2.0
1	F	281	ILE	2.0
1	G	122	ILE	2.0
1	A	129	PRO	2.0
1	C	119	PRO	2.0
1	A	510	SER	2.0
1	F	451	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

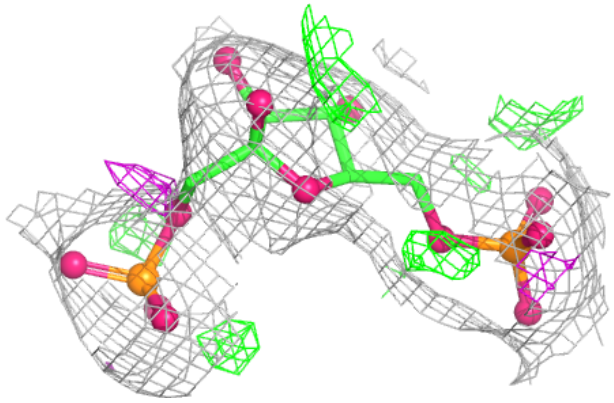
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

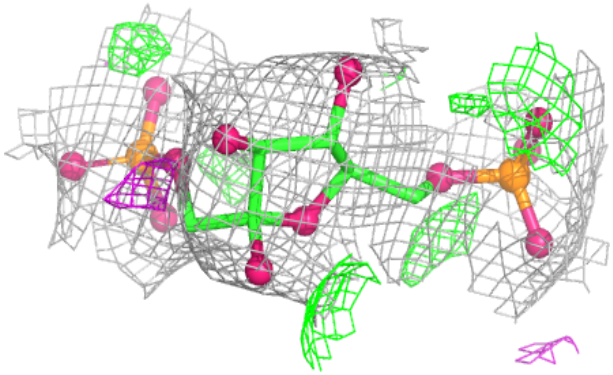
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	K	E	604	1/1	0.73	0.12	117,117,117,117	0
2	FBP	A	601	20/20	0.79	0.15	94,95,97,97	0
3	OXL	A	602	6/6	0.82	0.11	88,88,88,88	0
2	FBP	E	601	20/20	0.82	0.13	95,96,96,96	0
4	MG	A	603	1/1	0.84	0.22	84,84,84,84	0
3	OXL	G	602	6/6	0.85	0.13	79,79,79,79	0
4	MG	F	604	1/1	0.86	0.12	59,59,59,59	0
4	MG	G	604	1/1	0.86	0.20	83,83,83,83	0
3	OXL	C	602	6/6	0.86	0.12	80,80,81,81	0
3	OXL	D	602	6/6	0.87	0.12	58,59,59,60	0
5	K	C	605	1/1	0.88	0.09	98,98,98,98	0
5	K	B	605	1/1	0.89	0.08	80,80,80,80	0
3	OXL	H	602	6/6	0.89	0.12	55,55,56,56	0
3	OXL	E	602	6/6	0.89	0.10	93,93,93,93	0
2	FBP	F	601	20/20	0.90	0.10	65,70,72,72	0
5	K	F	605	1/1	0.90	0.07	90,90,90,90	0
3	OXL	F	602	6/6	0.91	0.09	68,68,68,69	0
5	K	A	604	1/1	0.91	0.06	106,106,106,106	0
2	FBP	B	601	20/20	0.92	0.09	58,61,63,64	0
2	FBP	G	601	20/20	0.93	0.09	54,57,59,60	0
6	WWA	G	603	32/32	0.93	0.09	55,58,59,59	14
4	MG	D	603	1/1	0.94	0.11	56,56,56,56	0
3	OXL	B	602	6/6	0.94	0.07	66,67,67,67	0
6	WWA	C	603	32/32	0.94	0.10	56,58,59,60	14
4	MG	C	604	1/1	0.94	0.06	48,48,48,48	0
5	K	G	605	1/1	0.95	0.06	76,76,76,76	0
6	WWA	B	603	32/32	0.95	0.08	42,43,45,45	14
4	MG	E	603	1/1	0.95	0.12	79,79,79,79	0
6	WWA	F	603	32/32	0.95	0.09	45,48,49,50	14
2	FBP	C	601	20/20	0.95	0.08	52,55,59,59	0
5	K	H	604	1/1	0.96	0.05	63,63,63,63	0
2	FBP	H	601	20/20	0.97	0.06	31,34,35,35	0
2	FBP	D	601	20/20	0.98	0.06	33,37,40,40	0
4	MG	B	604	1/1	0.98	0.04	44,44,44,44	0
4	MG	H	603	1/1	0.99	0.04	38,38,38,38	0
5	K	D	604	1/1	0.99	0.09	49,49,49,49	0

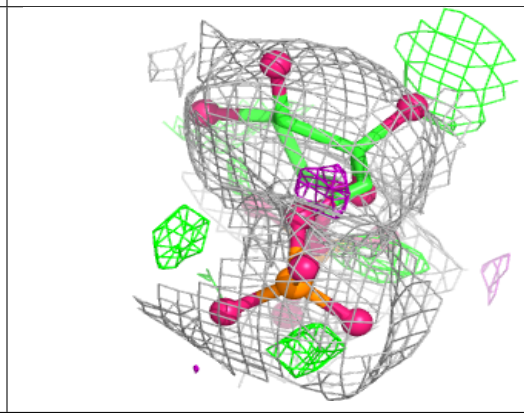
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FBP A 601:

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

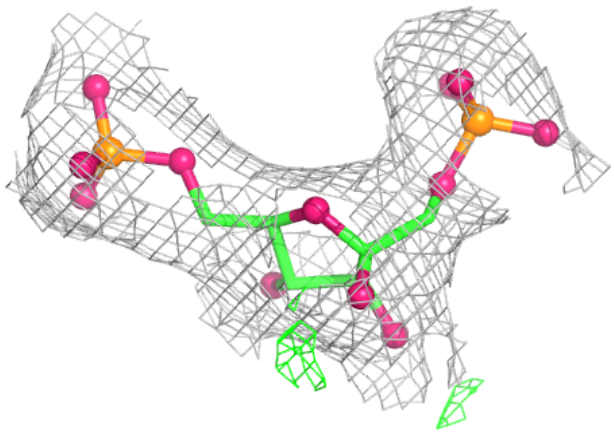


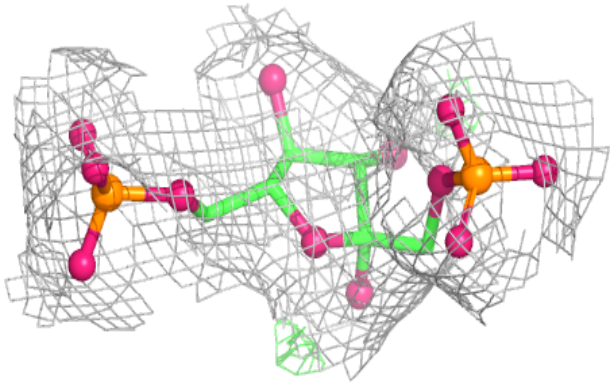


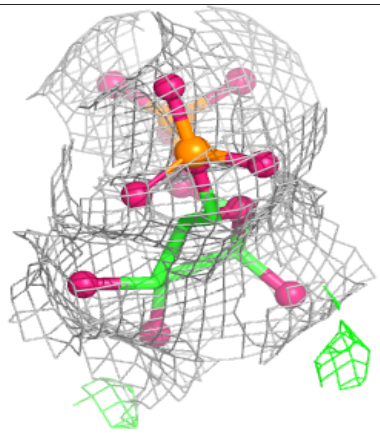


Electron density around FBP E 601:

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

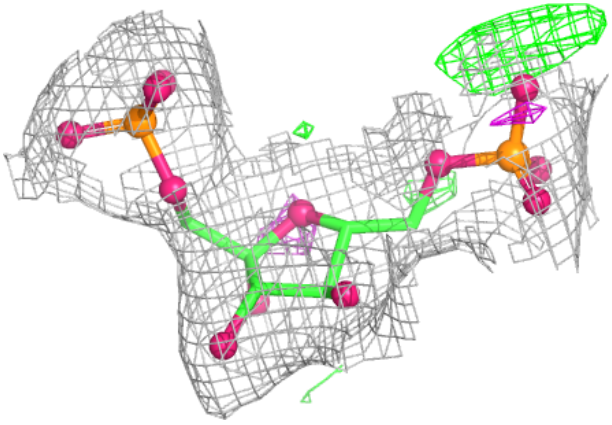


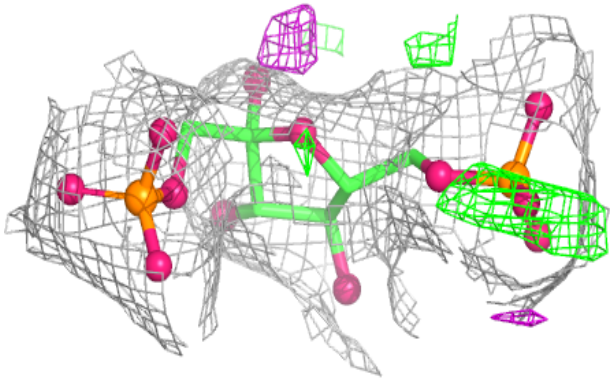


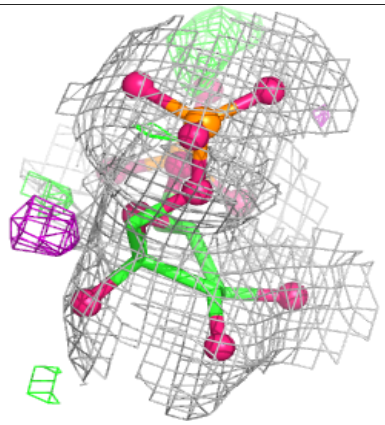


Electron density around FBP F 601:

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



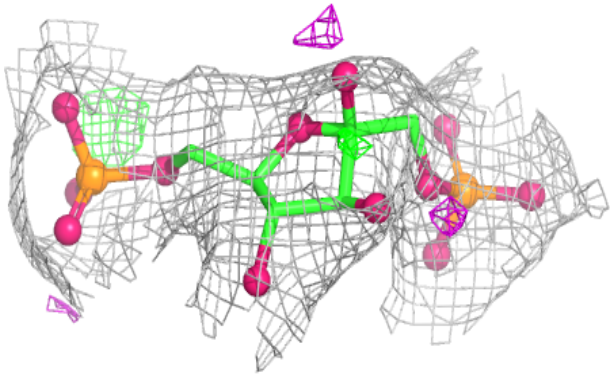


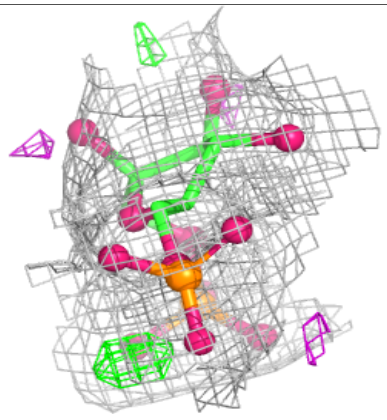


Electron density around FBP B 601:

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

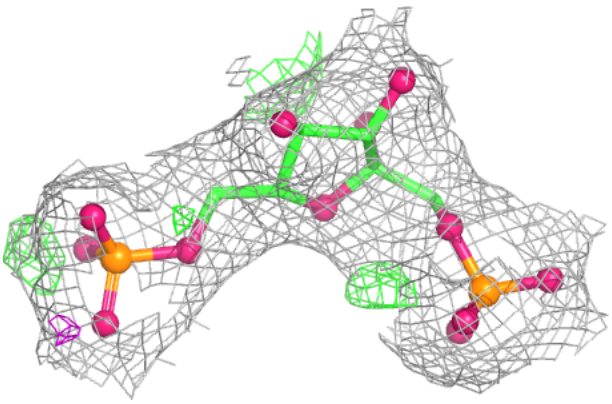


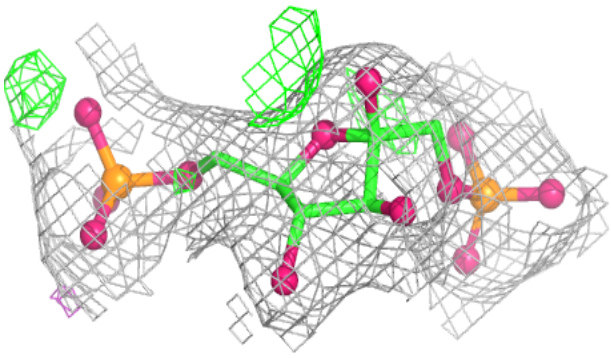


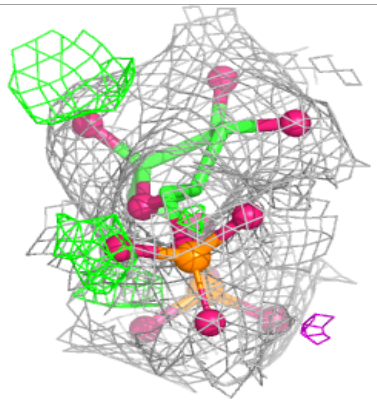


Electron density around FBP G 601:

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

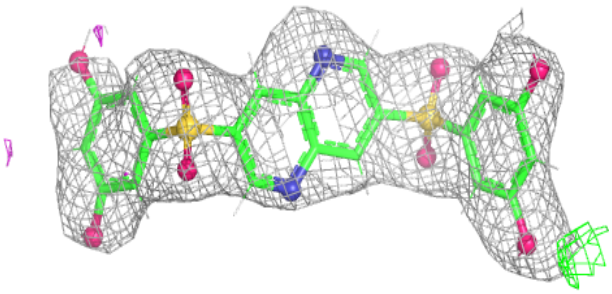


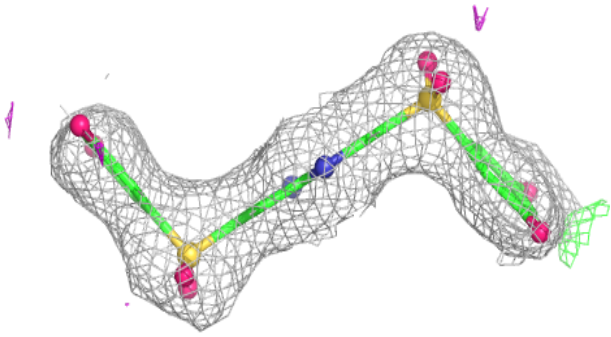


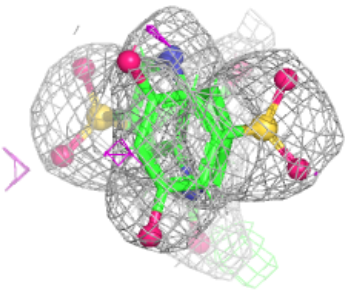


Electron density around WWA G 603:

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

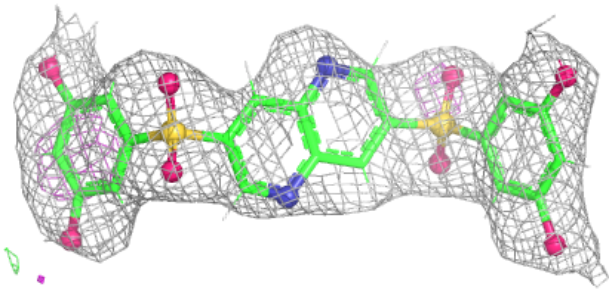


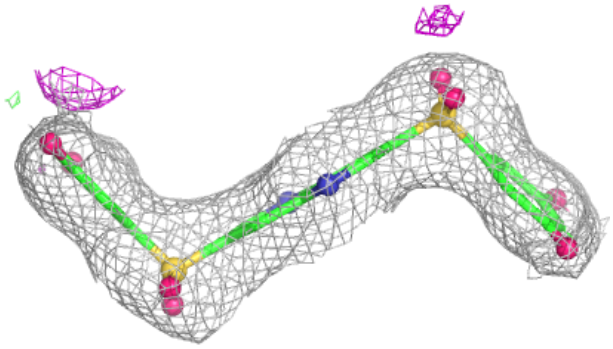


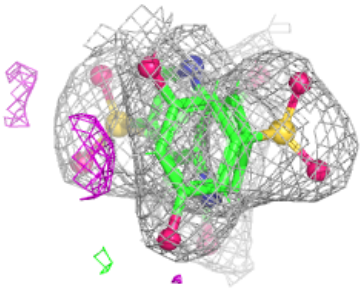


Electron density around WWA C 603:

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

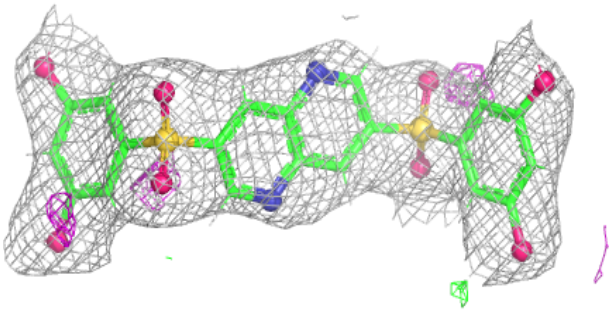


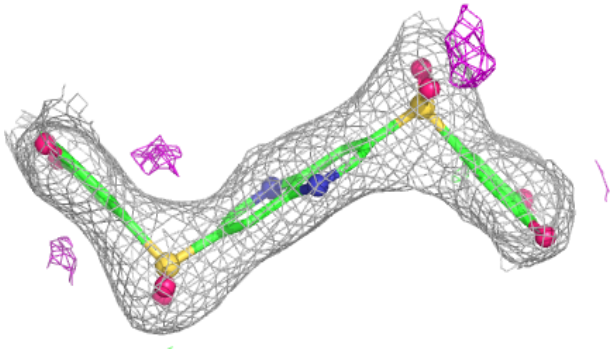


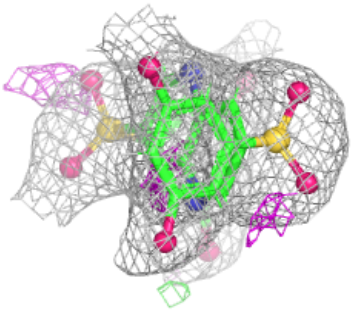


Electron density around WWA B 603:

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

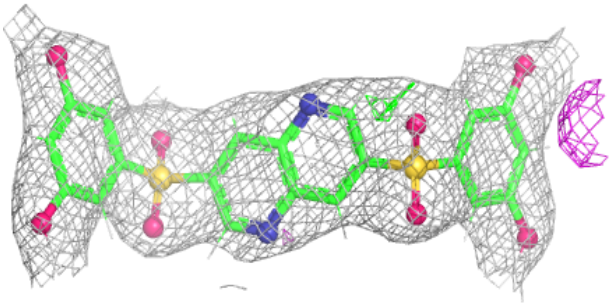


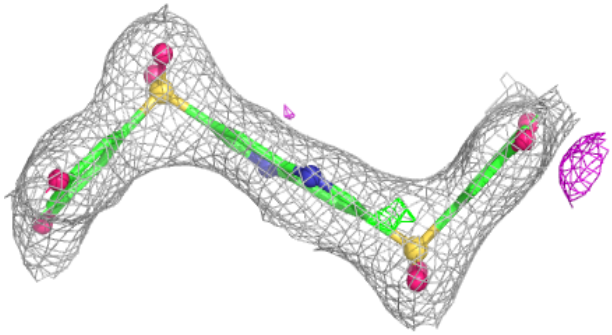


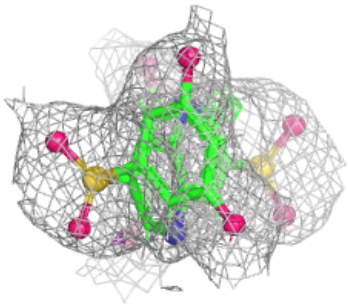


Electron density around WWA F 603:

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

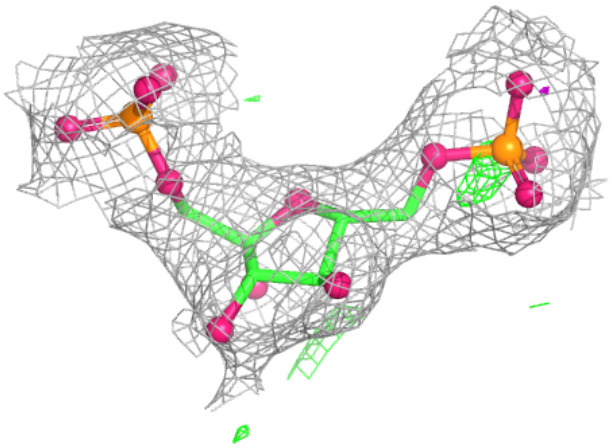


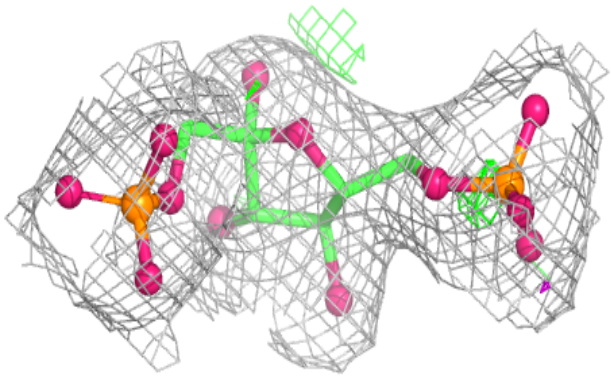


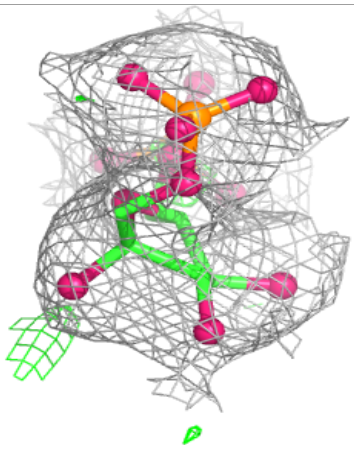


Electron density around FBP C 601:

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

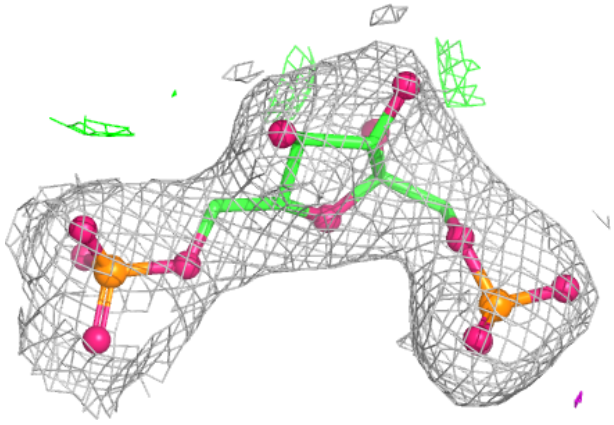


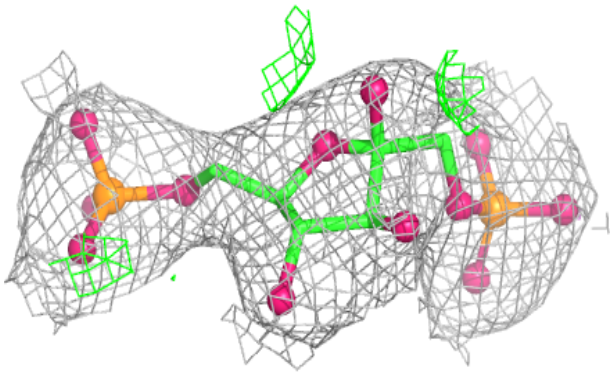


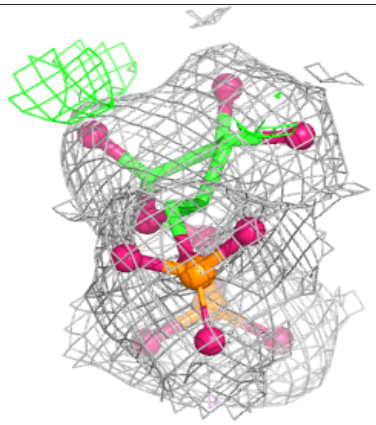


Electron density around FBP H 601:

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

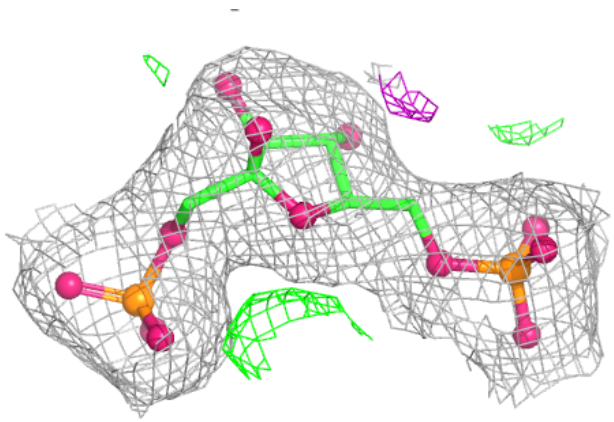


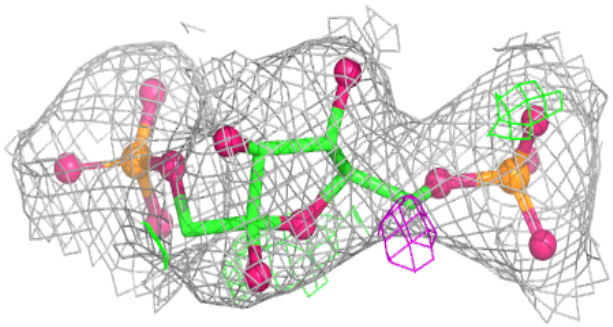


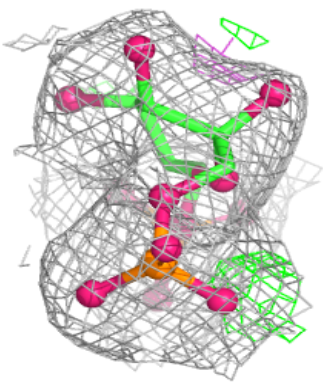


Electron density around FBP D 601:

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







6.5 Other polymers (i)

There are no such residues in this entry.