



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2022 – 06:05 PM JST

PDB ID : 7X8E  
Title : Crystal structure of PfHPPD-Y13287 complex  
Authors : Dong, J.; Lin, H.-Y.; Yang, G.-F.  
Deposited on : 2022-03-12  
Resolution : 2.75 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

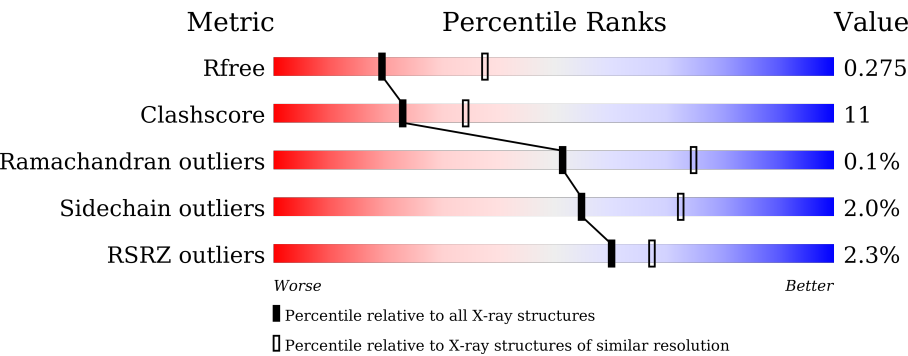
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.28.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.28.1

# 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 2.75 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	357	<div><div></div><div><div>80%</div><div>16%</div><div>.</div></div></div>
1	B	357	<div><div></div><div><div>70%</div><div>25%</div><div>.</div></div></div>
1	C	357	<div><div></div><div><div>70%</div><div>25%</div><div>.</div></div></div>
1	D	357	<div><div></div><div><div>75%</div><div>20%</div><div>5%</div></div></div>
1	E	357	<div><div></div><div><div>71%</div><div>23%</div><div>6%</div></div></div>
1	F	357	<div><div></div><div><div>70%</div><div>23%</div><div>6%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	357	<div><div></div><div>3%</div><div>70%</div><div>23%</div><div>7%</div></div>
1	H	357	<div><div></div><div>2%</div><div>68%</div><div>26%</div><div>6%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21540 atoms, of which 0 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 4-hydroxyphenylpyruvate dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2692	1724	455	499	14			
1	B	341	Total	C	N	O	S	0	1	0
			2680	1717	450	499	14			
1	C	341	Total	C	N	O	S	0	0	0
			2669	1710	450	495	14			
1	D	340	Total	C	N	O	S	0	0	0
			2672	1711	451	496	14			
1	E	335	Total	C	N	O	S	0	0	0
			2605	1672	434	485	14			
1	F	336	Total	C	N	O	S	0	0	0
			2604	1669	435	486	14			
1	G	332	Total	C	N	O	S	0	0	0
			2590	1664	434	478	14			
1	H	335	Total	C	N	O	S	0	0	0
			2598	1662	436	486	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	ASP	GLU	variant	UNP A0A0W0HIR1
A	280	ASP	ASN	variant	UNP A0A0W0HIR1
A	355	ALA	THR	variant	UNP A0A0W0HIR1
B	105	ASP	GLU	variant	UNP A0A0W0HIR1
B	280	ASP	ASN	variant	UNP A0A0W0HIR1
B	355	ALA	THR	variant	UNP A0A0W0HIR1
C	105	ASP	GLU	variant	UNP A0A0W0HIR1
C	280	ASP	ASN	variant	UNP A0A0W0HIR1
C	355	ALA	THR	variant	UNP A0A0W0HIR1
D	105	ASP	GLU	variant	UNP A0A0W0HIR1
D	280	ASP	ASN	variant	UNP A0A0W0HIR1
D	355	ALA	THR	variant	UNP A0A0W0HIR1
E	105	ASP	GLU	variant	UNP A0A0W0HIR1

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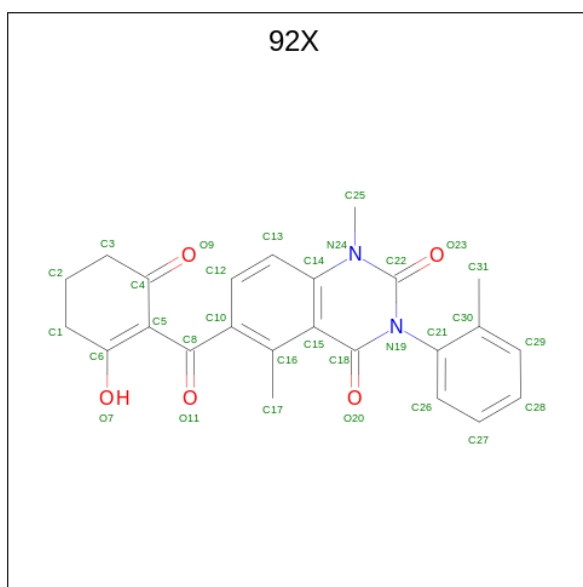
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Chain	Residue	Modelled	Actual	Comment	Reference
E	280	ASP	ASN	variant	UNP A0A0W0HIR1
E	355	ALA	THR	variant	UNP A0A0W0HIR1
F	105	ASP	GLU	variant	UNP A0A0W0HIR1
F	280	ASP	ASN	variant	UNP A0A0W0HIR1
F	355	ALA	THR	variant	UNP A0A0W0HIR1
G	105	ASP	GLU	variant	UNP A0A0W0HIR1
G	280	ASP	ASN	variant	UNP A0A0W0HIR1
G	355	ALA	THR	variant	UNP A0A0W0HIR1
H	105	ASP	GLU	variant	UNP A0A0W0HIR1
H	280	ASP	ASN	variant	UNP A0A0W0HIR1
H	355	ALA	THR	variant	UNP A0A0W0HIR1

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

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

- Molecule 3 is 1,5-dimethyl-3-(2-methylphenyl)-6-(2-oxidanyl-6-oxidanylidene-cyclohexen-1-yl)carbonyl-quinazoline-2,4-dione (three-letter code: 92X) (formula: C<sub>24</sub>H<sub>22</sub>N<sub>2</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			31	24	2	5		
3	B	1	Total	C	N	O	0	0
			31	24	2	5		
3	C	1	Total	C	N	O	0	0
			31	24	2	5		
3	D	1	Total	C	N	O	0	0
			31	24	2	5		
3	E	1	Total	C	N	O	0	0
			31	24	2	5		
3	F	1	Total	C	N	O	0	0
			31	24	2	5		
3	G	1	Total	C	N	O	0	0
			31	24	2	5		
3	H	1	Total	C	N	O	0	0
			31	24	2	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	B	25	Total	O	0	0
			25	25		
4	C	17	Total	O	0	0
			17	17		
4	D	29	Total	O	0	0
			29	29		

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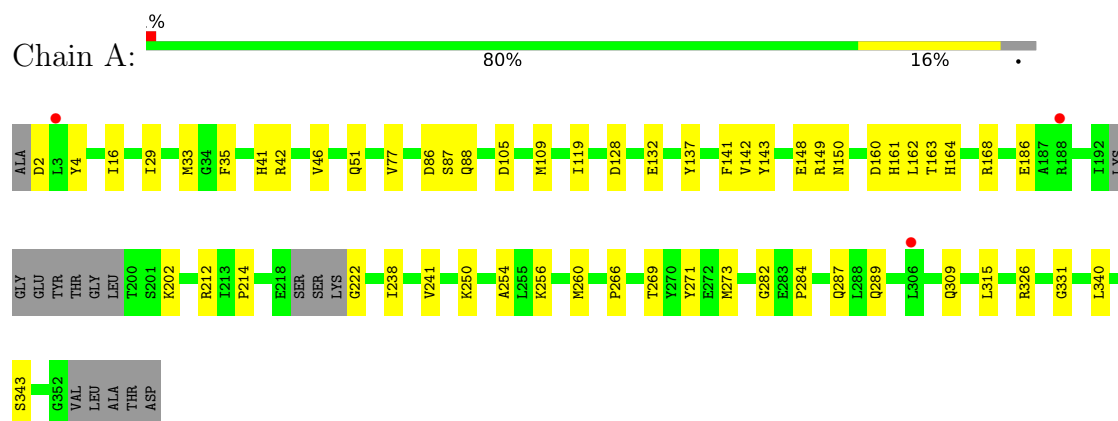
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	14	Total 14	O 14	0	0
4	F	19	Total 19	O 19	0	0
4	G	19	Total 19	O 19	0	0
4	H	27	Total 27	O 27	0	0

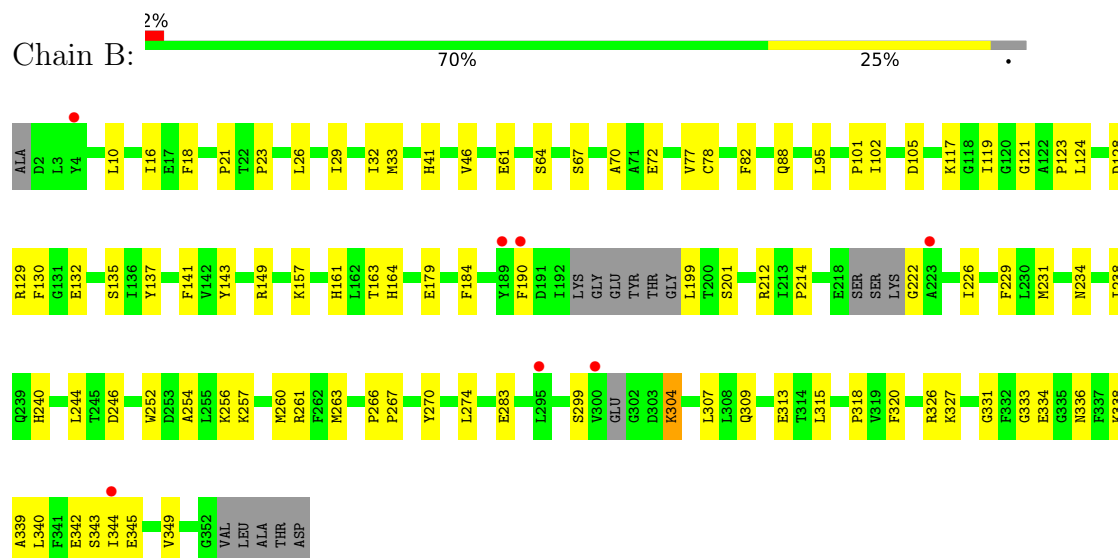
### 3 Residue-property plots [i](#)

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.

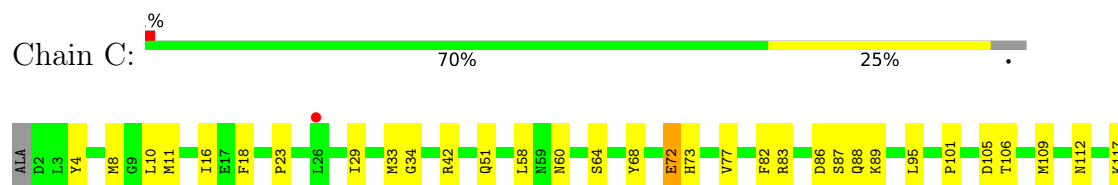
- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase



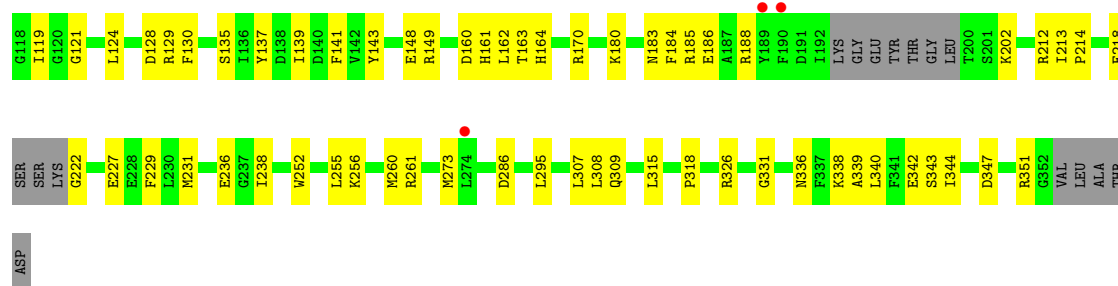
- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase



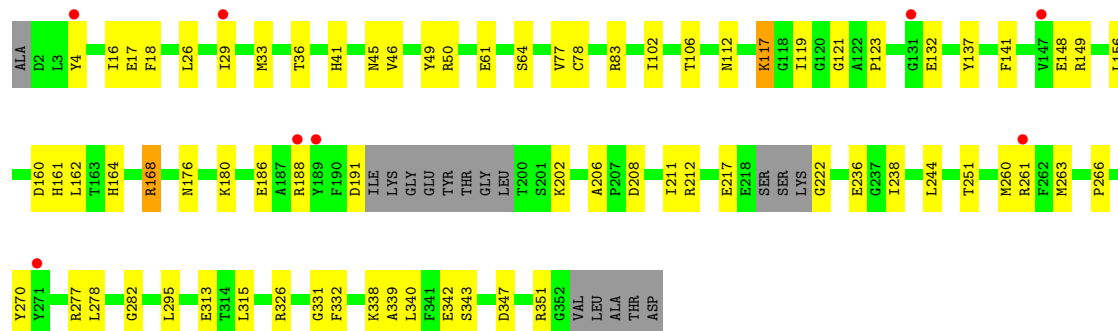
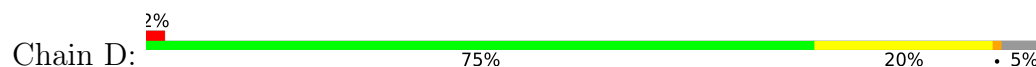
- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase



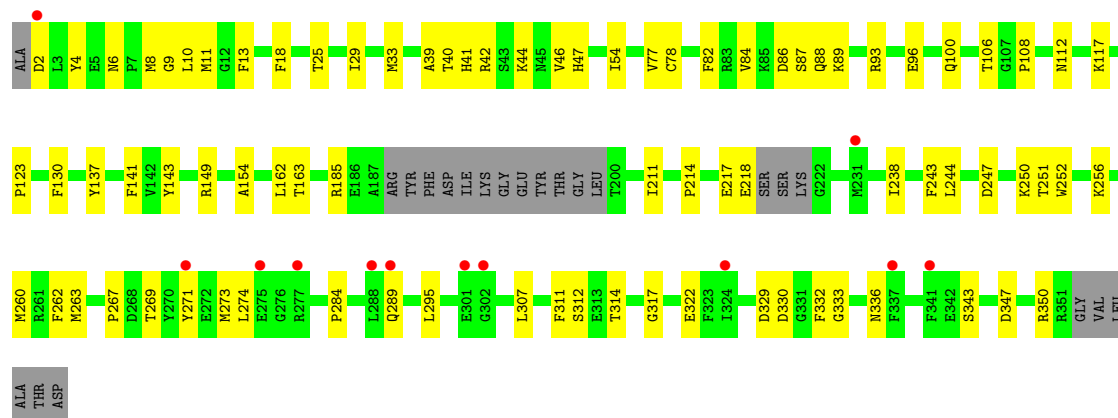




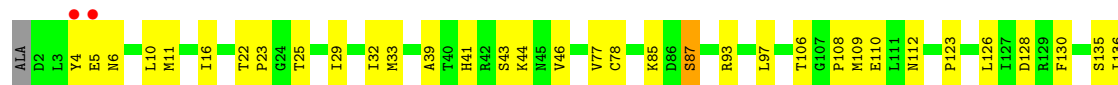
• Molecule 1: 4-hydroxyphenylpyruvate dioxygenase

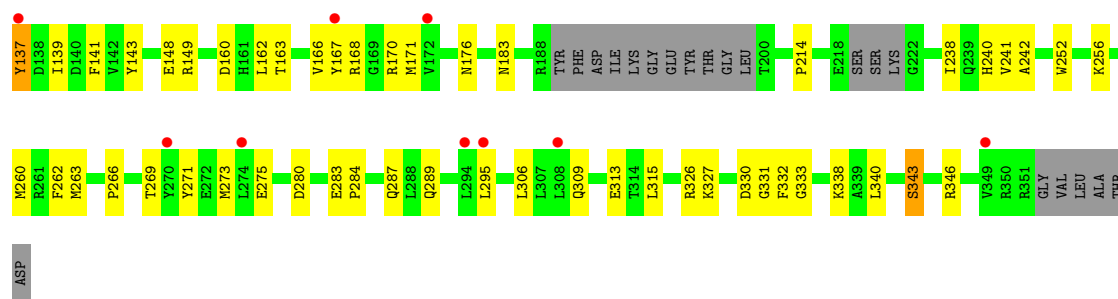


• Molecule 1: 4-hydroxyphenylpyruvate dioxygenase

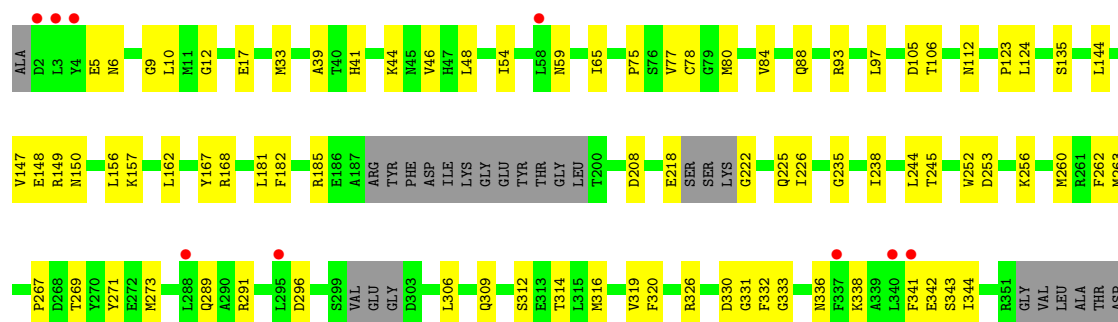


• Molecule 1: 4-hydroxyphenylpyruvate dioxygenase

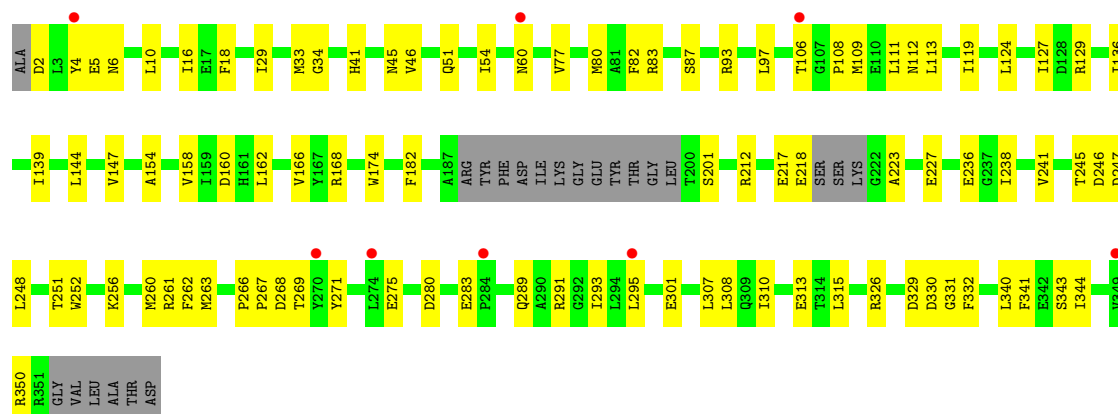




- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase



- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.70Å 161.20Å 121.98Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	38.15 – 2.75 46.92 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.2 (38.15-2.75) 98.1 (46.92-2.75)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.196 , 0.277 0.197 , 0.275	Depositor DCC
$R_{free}$ test set	3835 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.6	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 32.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.429 for k,h,-l 0.417 for -k,-h,-l 0.447 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21540	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO, 92X

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	0.46	0/2755	0.60	0/3717
1	B	0.48	0/2750	0.62	2/3712 (0.1%)
1	C	0.46	0/2732	0.62	1/3690 (0.0%)
1	D	0.47	0/2735	0.61	0/3691
1	E	0.43	0/2667	0.60	0/3605
1	F	0.43	0/2665	0.59	0/3603
1	G	0.43	0/2651	0.61	1/3581 (0.0%)
1	H	0.41	0/2658	0.57	0/3594
All	All	0.45	0/21613	0.60	4/29193 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	307	LEU	CA-CB-CG	5.94	128.97	115.30
1	C	307	LEU	CA-CB-CG	5.43	127.79	115.30
1	B	10	LEU	CA-CB-CG	5.27	127.43	115.30
1	G	306	LEU	CA-CB-CG	5.22	127.31	115.30

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	2692	0	2614	46	0
1	B	2680	0	2570	74	0
1	C	2669	0	2568	70	0
1	D	2672	0	2581	55	0
1	E	2605	0	2498	54	0
1	F	2604	0	2493	69	0
1	G	2590	0	2495	57	0
1	H	2598	0	2485	77	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	31	0	0	1	0
3	B	31	0	0	3	0
3	C	31	0	0	1	0
3	D	31	0	0	0	0
3	E	31	0	0	0	0
3	F	31	0	0	0	0
3	G	31	0	0	0	0
3	H	31	0	0	2	0
4	A	24	0	0	3	0
4	B	25	0	0	2	0
4	C	17	0	0	3	0
4	D	29	0	0	3	0
4	E	14	0	0	2	0
4	F	19	0	0	4	0
4	G	19	0	0	3	0
4	H	27	0	0	7	0
All	All	21540	0	20304	475	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 475 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:D:277:ARG:NH2	1:D:339:ALA:HB1	1.63	1.13
1:C:139:ILE:HG23	1:H:129:ARG:NH2	1.70	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:ARG:NH2	1:D:339:ALA:CB	2.22	1.03
1:D:277:ARG:HH21	1:D:339:ALA:HB1	1.14	1.03
1:C:139:ILE:CG2	1:H:129:ARG:NH2	2.24	1.01

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/357 (94%)	323 (96%)	12 (4%)	0	100	100
1	B	334/357 (94%)	316 (95%)	17 (5%)	1 (0%)	41	61
1	C	335/357 (94%)	310 (92%)	25 (8%)	0	100	100
1	D	334/357 (94%)	317 (95%)	17 (5%)	0	100	100
1	E	329/357 (92%)	313 (95%)	15 (5%)	1 (0%)	41	61
1	F	330/357 (92%)	315 (96%)	15 (4%)	0	100	100
1	G	324/357 (91%)	306 (94%)	18 (6%)	0	100	100
1	H	329/357 (92%)	309 (94%)	19 (6%)	1 (0%)	41	61
All	All	2650/2856 (93%)	2509 (95%)	138 (5%)	3 (0%)	51	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	299	SER
1	H	301	GLU
1	E	284	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/296 (95%)	275 (98%)	5 (2%)	59	75
1	B	277/296 (94%)	272 (98%)	5 (2%)	59	75
1	C	274/296 (93%)	266 (97%)	8 (3%)	42	62
1	D	276/296 (93%)	269 (98%)	7 (2%)	47	67
1	E	267/296 (90%)	261 (98%)	6 (2%)	52	71
1	F	266/296 (90%)	261 (98%)	5 (2%)	57	74
1	G	266/296 (90%)	260 (98%)	6 (2%)	50	70
1	H	265/296 (90%)	263 (99%)	2 (1%)	81	89
All	All	2171/2368 (92%)	2127 (98%)	44 (2%)	55	72

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	244	LEU
1	F	343	SER
1	E	263	MET
1	F	137	TYR
1	G	105	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	112	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	92X	C	402	2	31,34,34	1.99	9 (29%)	34,51,51	1.81	5 (14%)
3	92X	A	402	2	31,34,34	2.02	9 (29%)	34,51,51	1.79	6 (17%)
3	92X	H	402	2	31,34,34	2.16	11 (35%)	34,51,51	1.97	9 (26%)
3	92X	B	402	2	31,34,34	2.29	12 (38%)	34,51,51	2.04	12 (35%)
3	92X	F	402	2	31,34,34	1.95	9 (29%)	34,51,51	1.97	8 (23%)
3	92X	D	402	2	31,34,34	2.10	9 (29%)	34,51,51	1.89	8 (23%)
3	92X	E	402	2	31,34,34	2.05	8 (25%)	34,51,51	1.78	10 (29%)
3	92X	G	402	2	31,34,34	2.10	10 (32%)	34,51,51	2.04	8 (23%)

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	92X	C	402	2	-	1/12/26/26	0/4/4/4
3	92X	A	402	2	-	1/12/26/26	0/4/4/4
3	92X	H	402	2	-	0/12/26/26	0/4/4/4
3	92X	B	402	2	-	1/12/26/26	0/4/4/4
3	92X	F	402	2	-	1/12/26/26	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	92X	D	402	2	-	1/12/26/26	0/4/4/4
3	92X	E	402	2	-	0/12/26/26	0/4/4/4
3	92X	G	402	2	-	0/12/26/26	0/4/4/4

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	402	92X	C14-N24	-6.51	1.32	1.40
3	G	402	92X	C14-N24	-6.36	1.33	1.40
3	E	402	92X	C14-N24	-6.25	1.33	1.40
3	A	402	92X	C14-N24	-5.97	1.33	1.40
3	F	402	92X	C14-N24	-5.82	1.33	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	402	92X	C10-C8-C5	6.47	132.00	120.77
3	D	402	92X	C10-C8-C5	5.45	130.23	120.77
3	A	402	92X	C13-C14-N24	-5.17	117.56	121.71
3	H	402	92X	C10-C8-C5	4.99	129.42	120.77
3	B	402	92X	C13-C14-C15	-4.45	115.17	119.68

There are no chirality outliers.

All (5) torsion outliers are listed below:

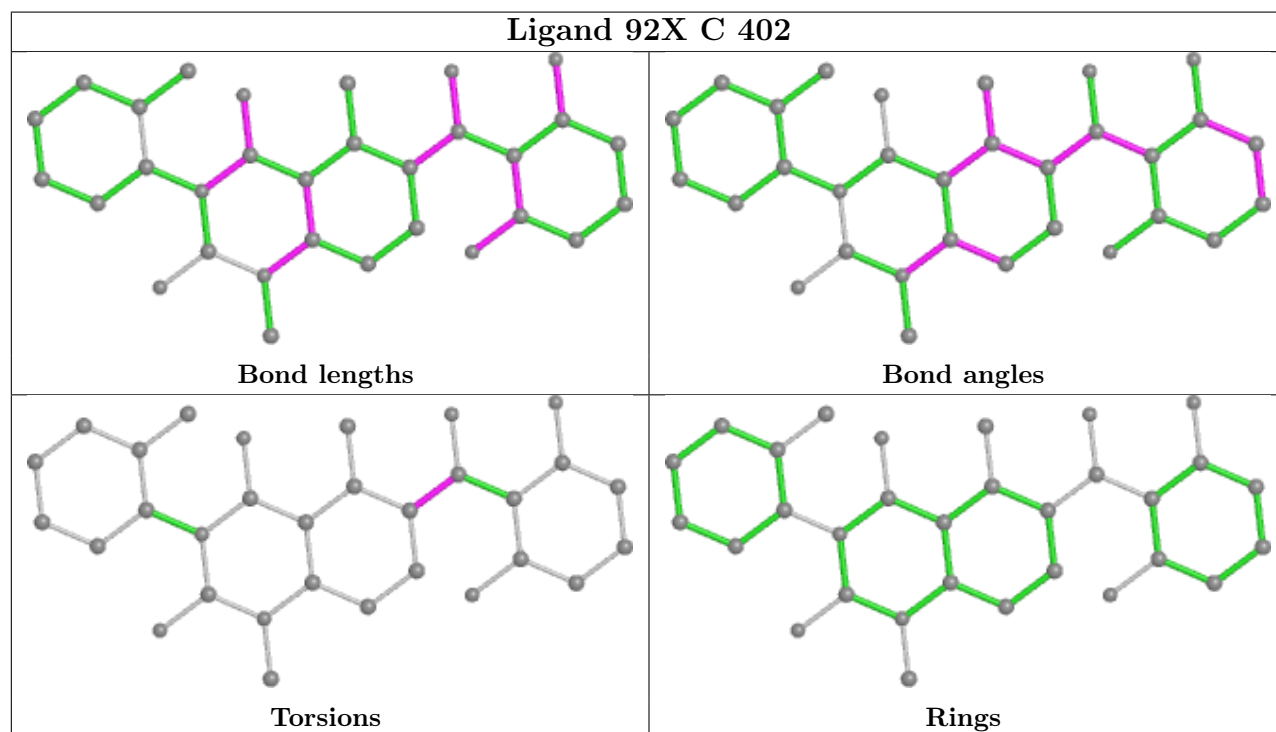
Mol	Chain	Res	Type	Atoms
3	B	402	92X	C16-C10-C8-O11
3	F	402	92X	C4-C5-C8-O11
3	A	402	92X	C16-C10-C8-O11
3	C	402	92X	C16-C10-C8-O11
3	D	402	92X	C16-C10-C8-O11

There are no ring outliers.

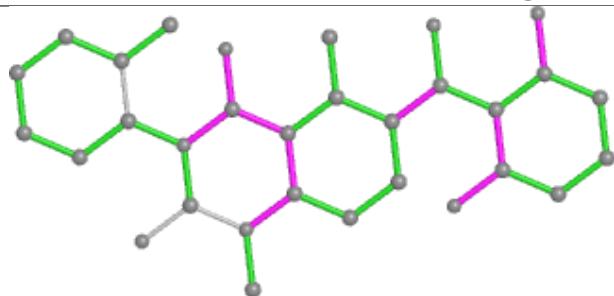
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	92X	1	0
3	A	402	92X	1	0
3	H	402	92X	2	0
3	B	402	92X	3	0

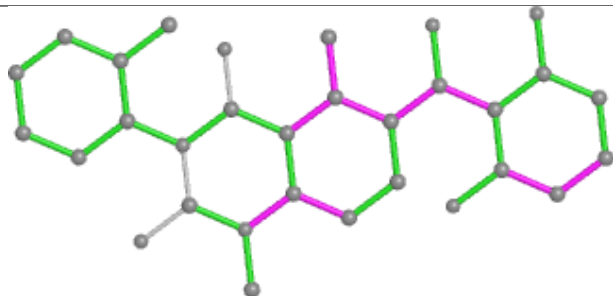
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



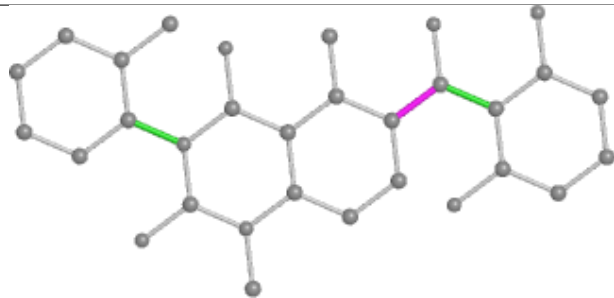
## Ligand 92X A 402



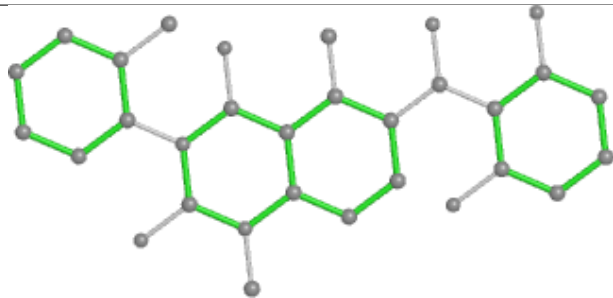
Bond lengths



Bond angles

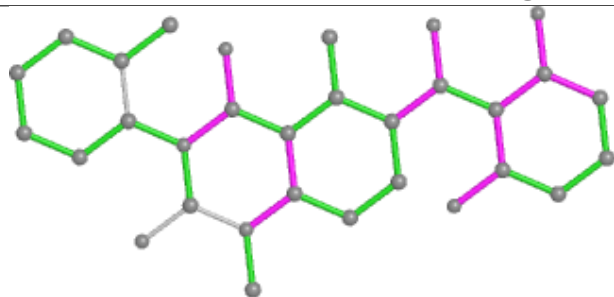


Torsions

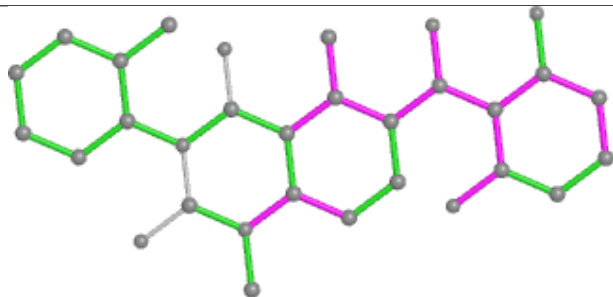


Rings

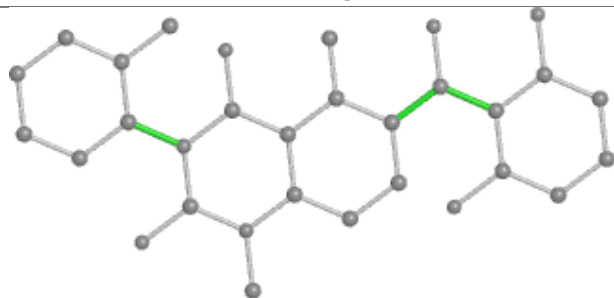
## Ligand 92X H 402



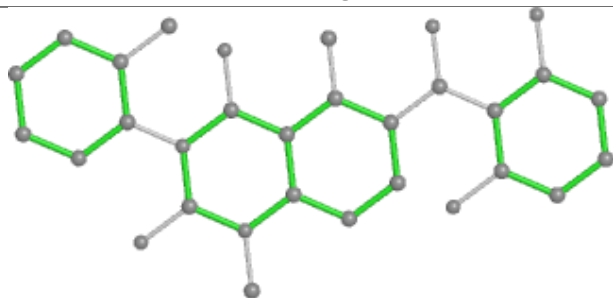
Bond lengths



Bond angles

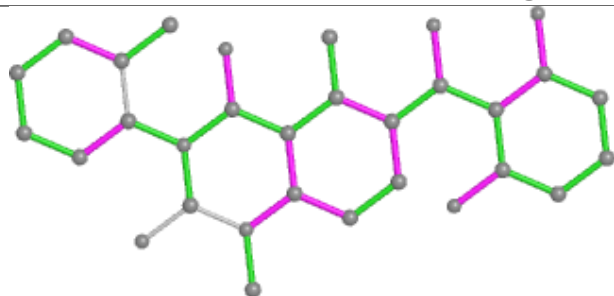


Torsions

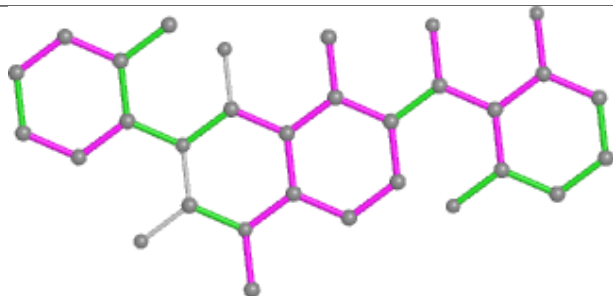


Rings

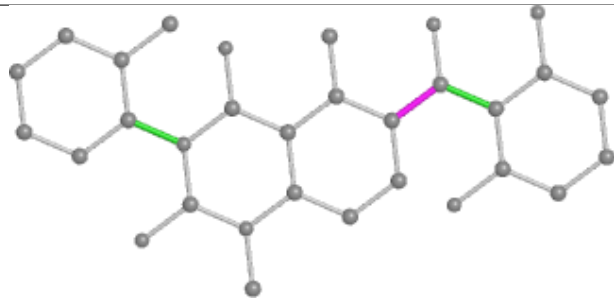
## Ligand 92X B 402



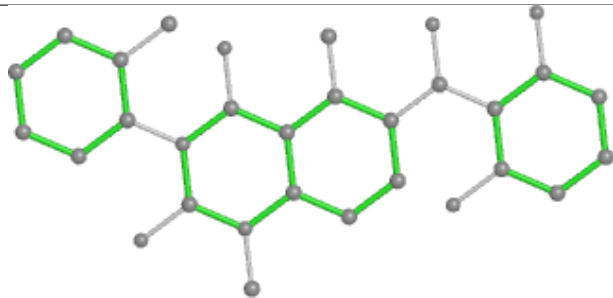
Bond lengths



Bond angles

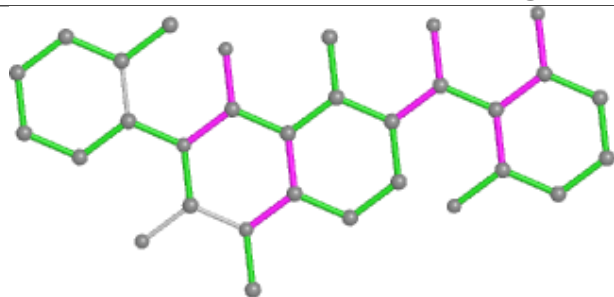


Torsions

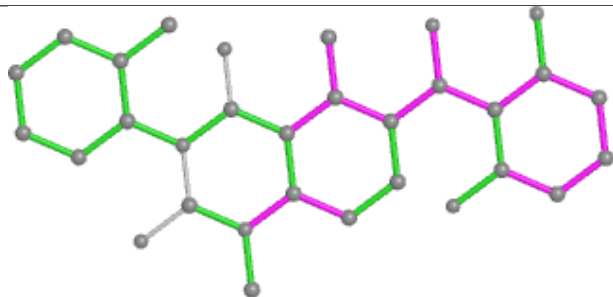


Rings

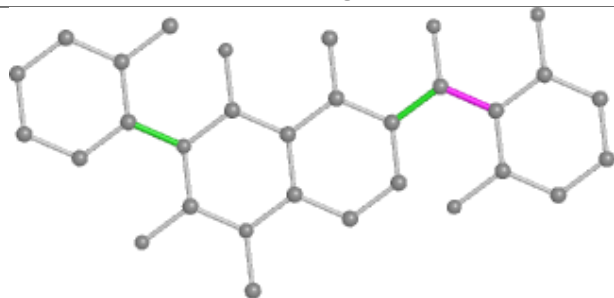
## Ligand 92X F 402



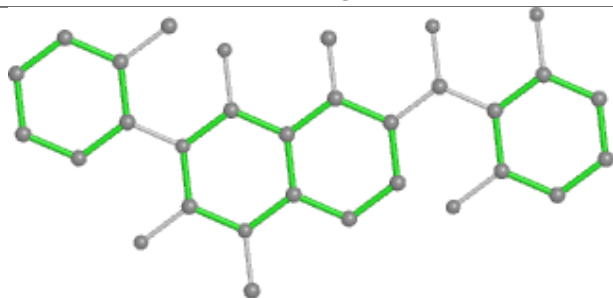
Bond lengths



Bond angles

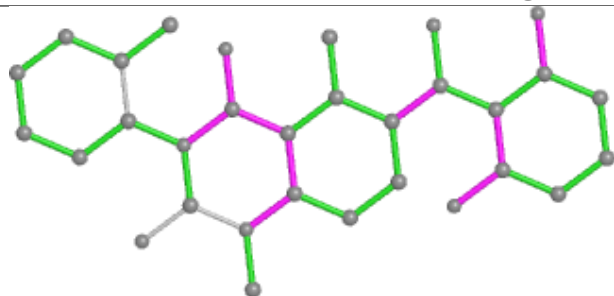


Torsions

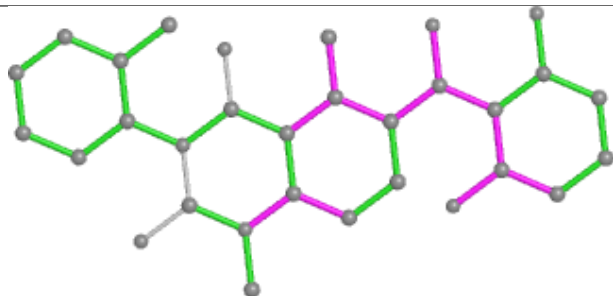


Rings

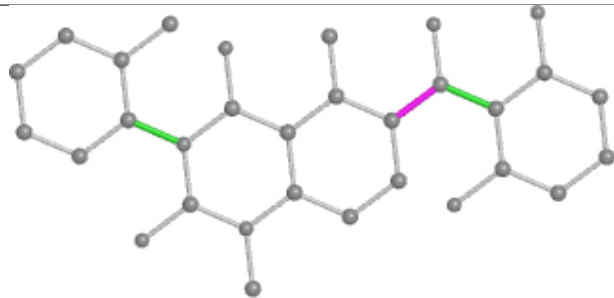
## Ligand 92X D 402



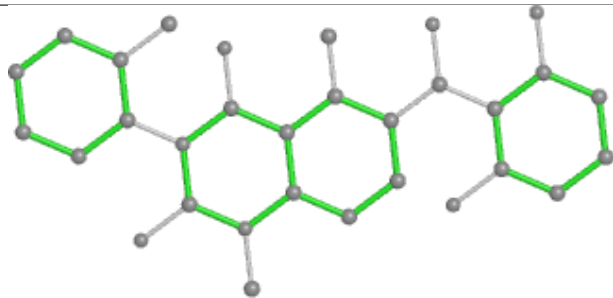
Bond lengths



Bond angles

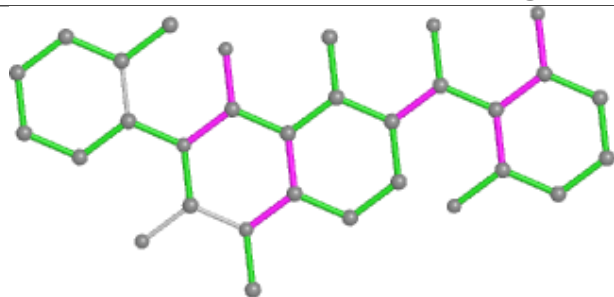


Torsions

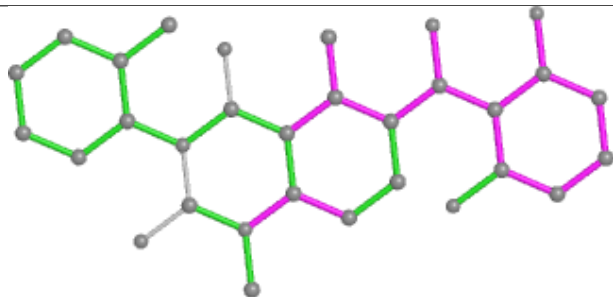


Rings

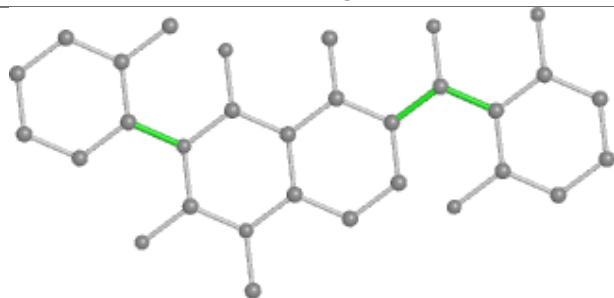
## Ligand 92X E 402



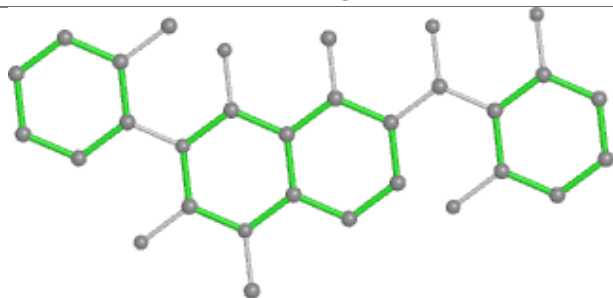
Bond lengths



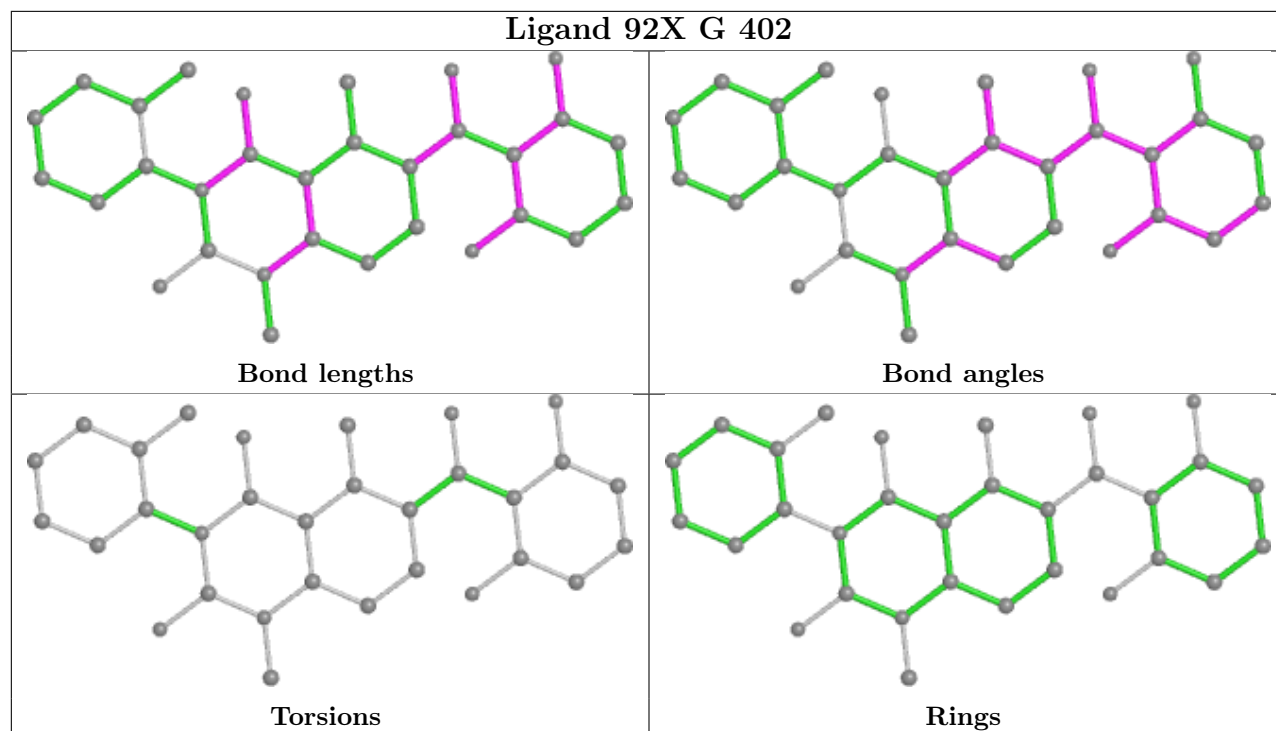
Bond angles



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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	341/357 (95%)	0.02	3 (0%) 84 88	32, 47, 77, 108	0
1	B	341/357 (95%)	0.02	7 (2%) 63 70	33, 47, 73, 100	0
1	C	341/357 (95%)	-0.00	4 (1%) 79 83	34, 47, 73, 100	0
1	D	340/357 (95%)	0.10	8 (2%) 59 66	32, 48, 74, 111	0
1	E	335/357 (93%)	0.17	12 (3%) 42 47	37, 53, 87, 134	0
1	F	336/357 (94%)	0.14	11 (3%) 46 52	36, 53, 84, 122	0
1	G	332/357 (92%)	0.18	9 (2%) 54 61	37, 54, 84, 98	0
1	H	335/357 (93%)	0.11	8 (2%) 59 66	38, 54, 86, 125	0
All	All	2701/2856 (94%)	0.09	62 (2%) 60 67	32, 51, 79, 134	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	4	TYR	4.5
1	E	301	GLU	4.2
1	H	295	LEU	4.0
1	G	288	LEU	3.9
1	H	349	VAL	3.9

### 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

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<sup>th</sup> 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.

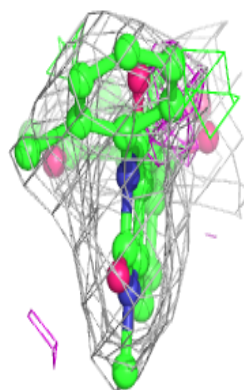
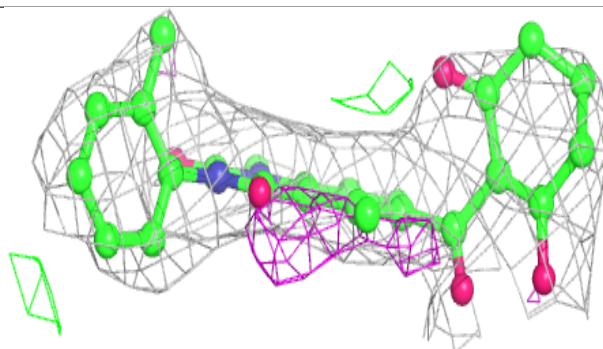
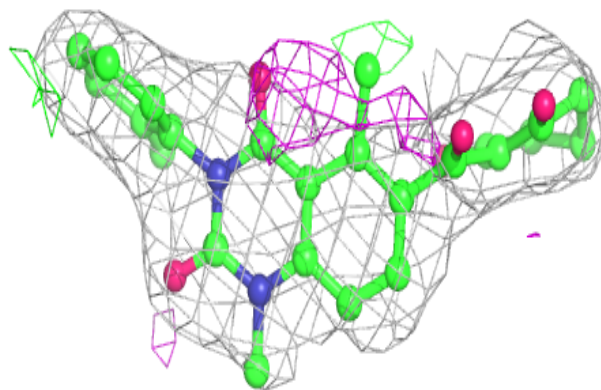
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	92X	E	402	31/31	0.91	0.23	50,63,70,70	0
3	92X	C	402	31/31	0.93	0.19	35,50,55,58	0
3	92X	D	402	31/31	0.93	0.20	38,47,54,59	0
2	CO	F	401	1/1	0.93	0.12	47,47,47,47	0
3	92X	A	402	31/31	0.94	0.21	36,48,56,59	0
2	CO	H	401	1/1	0.94	0.14	51,51,51,51	0
3	92X	H	402	31/31	0.94	0.19	46,57,63,64	0
3	92X	G	402	31/31	0.95	0.19	46,57,63,65	0
3	92X	F	402	31/31	0.95	0.17	41,57,65,67	0
2	CO	E	401	1/1	0.96	0.10	77,77,77,77	0
3	92X	B	402	31/31	0.96	0.18	39,48,57,57	0
2	CO	B	401	1/1	0.97	0.18	42,42,42,42	0
2	CO	G	401	1/1	0.98	0.15	45,45,45,45	0
2	CO	C	401	1/1	0.98	0.18	37,37,37,37	0
2	CO	D	401	1/1	0.99	0.16	39,39,39,39	0
2	CO	A	401	1/1	1.00	0.17	36,36,36,36	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.

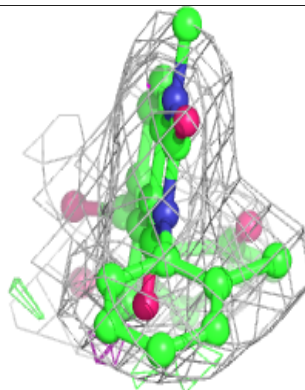
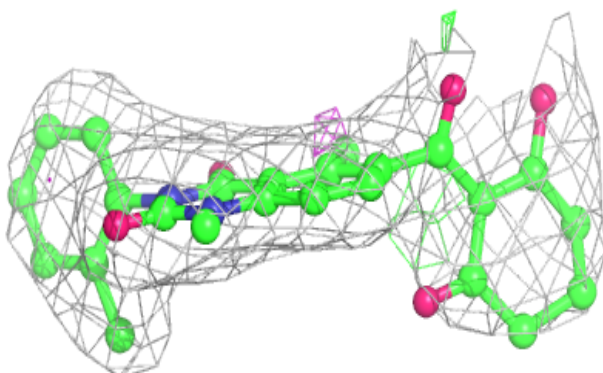
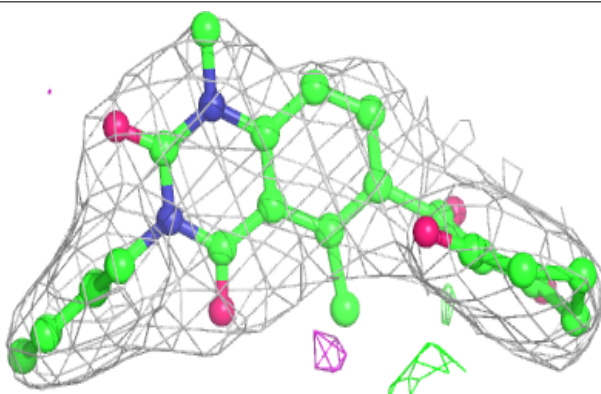


**Electron density around 92X E 402:**

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

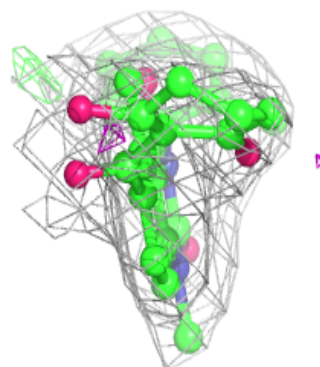
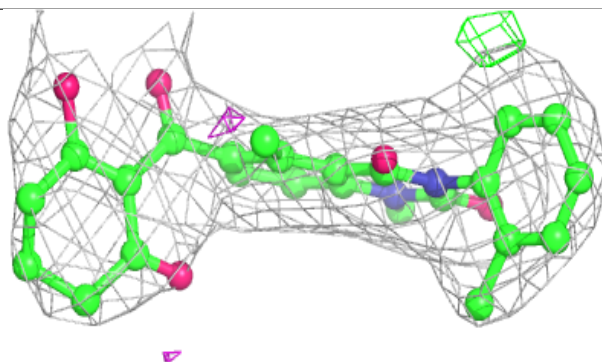
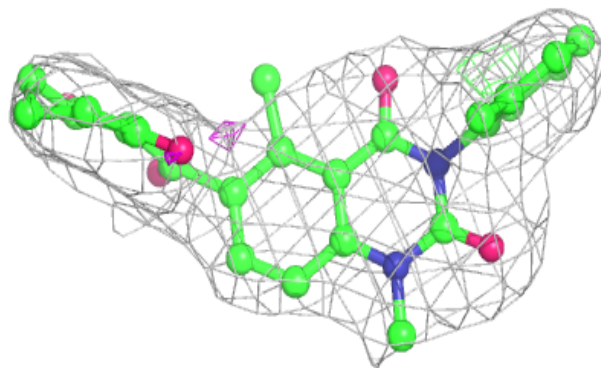
**Electron density around 92X C 402:**

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

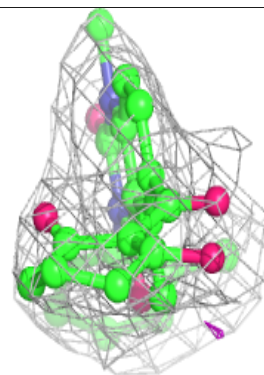
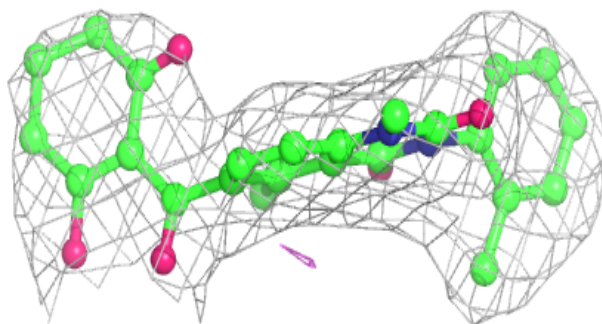
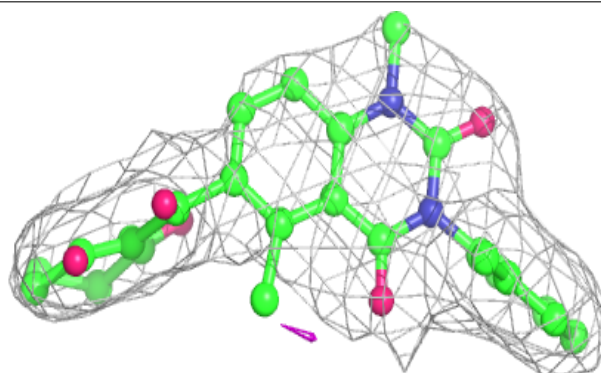


**Electron density around 92X D 402:**

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

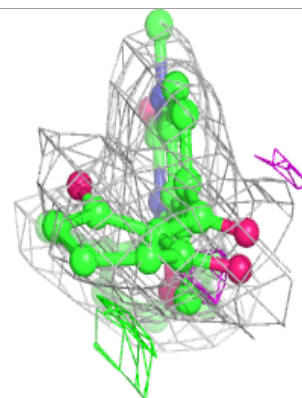
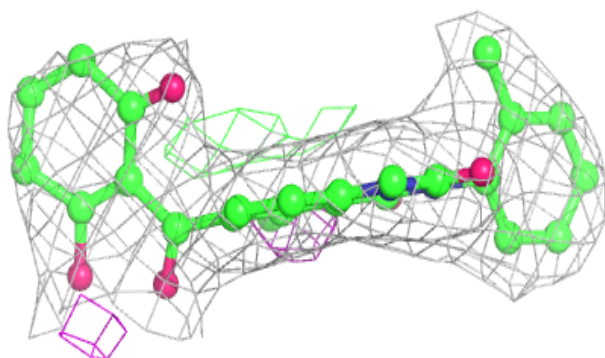
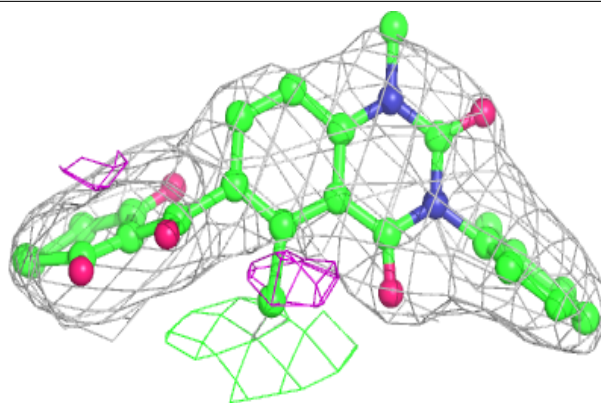
**Electron density around 92X A 402:**

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

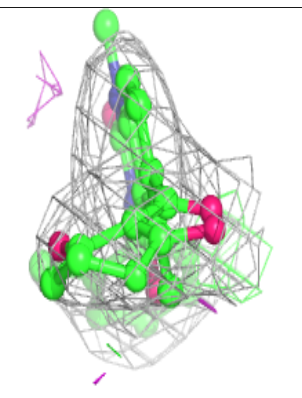
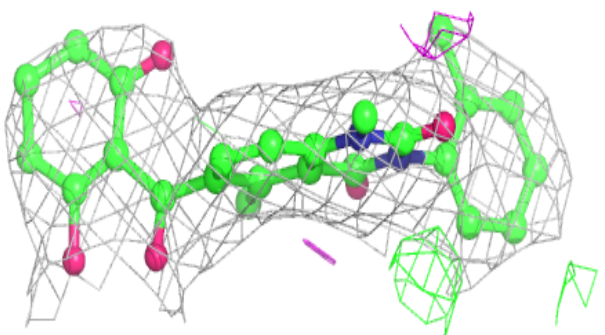
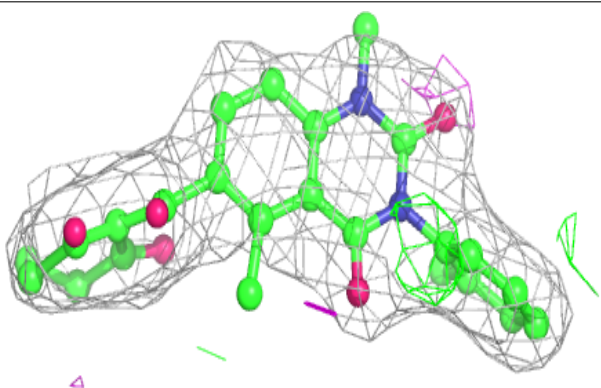


**Electron density around 92X H 402:**

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

**Electron density around 92X G 402:**

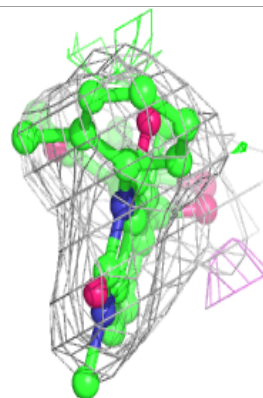
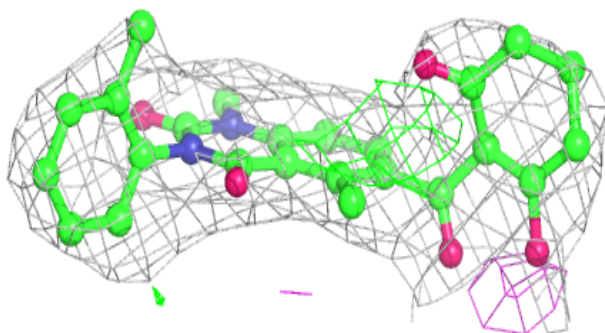
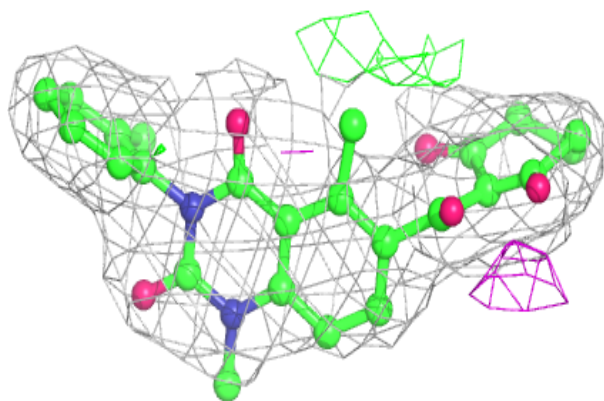
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



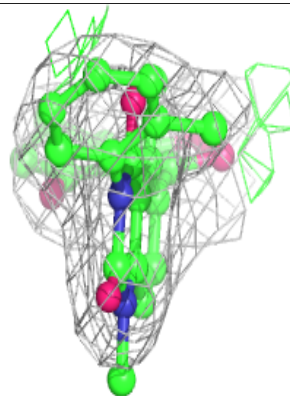
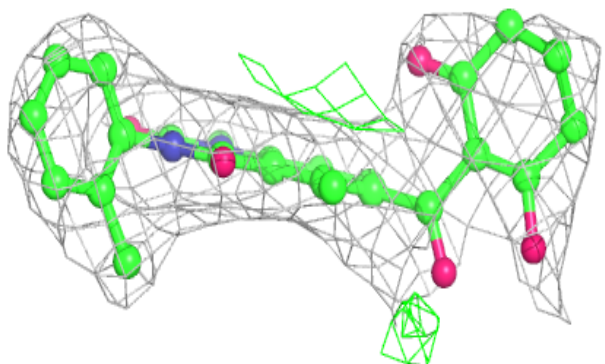
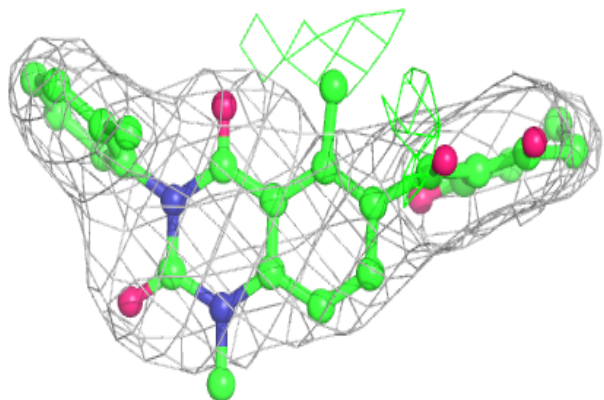


**Electron density around 92X F 402:**

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

**Electron density around 92X B 402:**

$2mF_o-DF_c$  (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.